



RESEARCH ARTICLE

Scattering and pairing by exchange interactions

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Abstract

Quantum interactions exchanging different types of particles play a pivotal rôle in quantum many-body theory, but they are not sufficiently investigated from a mathematical perspective. Here, we consider a system made of two fermions and one boson, in order to study the effect of such an off-diagonal interaction term, having in mind the physics of cuprate superconductors. Additionally, our model also includes a generalized Hubbard interaction (i.e., a general local repulsion term for the fermions). Regarding pairing, exponentially localized dressed bound fermion pairs are shown to exist, and their effective dispersion relation is studied in detail. Scattering properties of the system are derived for two channels: the unbound and bound pair channels. We give particular attention to the regime of very large on-site (Hubbard) repulsions because this situation is relevant for cuprate superconductors.

Contents

1	Introduction	2
1.1	Exchange interactions and high- T_c superconductivity	2
1.2	Mathematical results	5
1.3	Concluding remarks and structure of the paper	7
2	Setup of the problem	8
2.1	Background Lattice	8
2.2	Composite of two fermions and one boson	8
2.3	The model in spaces of quasi-momenta	12
2.4	Fiber decomposition of the Hamiltonian	14
3	Main results	16
3.1	Spectral properties	16
3.2	Dispersion relation of dressed bound fermion pairs	20
3.3	Quantum scattering	22
3.3.1	Unbound pair scattering channel	23
3.3.2	Bound pair scattering channel	27

4	Technical results	30
4.1	Notation	30
4.2	Computation of the fiber decomposition of the Hamiltonian	30
4.3	Spectrum of the fiber Hamiltonians	34
4.3.1	Essential spectrum	35
4.3.2	Discrete spectrum	36
4.3.3	Bottom of the spectrum	40
4.4	Spectral properties in the hard-core limit	44
4.4.1	The characteristic equation in the hard-core limit	44
4.4.2	Hard-core dispersion relation of bound pairs of lowest energy	47
4.5	Spectral gap and Anderson localization	52
4.6	Scattering channels	56
4.6.1	Unbound pair scattering channel	56
4.6.2	Bound pair scattering channel	60
A	Appendix	61
A.1	Toward a microscopic theory for cuprate superconductivity	61
A.2	The Fock-space formalism	68
A.3	Non-autonomous evolution equations and scattering theory	70
A.4	Constant fiber direct integrals	71
A.5	The Birman-Schwinger principle	76
A.6	Combes-Thomas estimates	77
A.7	Elementary observations	80
	References	81

1. Introduction

1.1. Exchange interactions and high- T_c superconductivity

Exchange interactions in Mathematical Physics. Off-diagonal interaction terms of the form

$$B^*A + A^*B, \quad (1)$$

with A, B being two monomials of annihilation operators of two species (a) and (b) of quantum particles, play a pivotal rôle in the rigorous understanding of quantum many-body systems at low temperatures. Such terms are also named ‘exchange’ terms because they encode (quantum) processes destroying a set of particles of one specie to create another kind of particles.

For instance, for the Bogoliubov model, an off-diagonal term of the form

$$\sum_k f_1(k) \left(b_k^* b_{-k}^* a^2 + (a^*)^2 b_k b_{-k} \right), \quad f_1(k) \geq 0, \quad (2)$$

exchanging two bosons ($a = b_0$) having zero momentum ($k = 0$) with a pair of boson having nonzero momentum of opposite sign ($b_{k \neq 0}$), is shown in [1] to imply a nonconventional Bose condensation. Made of dressed bound pairs of (zero-momentum) bosons, the nonconventional condensate is structurally different from the Bose-Einstein condensate of the ideal Bose gas. In particular, it must be depleted to take advantage of the effective attraction induced by the exchange interaction (2). See [2]. This is reminiscent of liquid helium physics, where 100% superfluid helium occurs at zero temperature with only 9% Bose condensate [3, 4, 5, 6, 7]. Off-diagonal interaction terms (2) are conjectured in [8] to be relevant to explain the macroscopic behavior of weakly interacting Bose gases.

Another example from quantum statistical mechanics is given by the spin-boson model within the so-called ‘rotating wave approximation’. In this approximation, the model has terms of the form

$$\sum_k f_2(k)(b_k^* \sigma_- + \sigma_+ b_k), \quad f_2(k) \geq 0,$$

with $\sigma_{\pm} = \sigma_x \pm \sigma_y$ (σ_x, σ_y being Pauli matrices) and b_k being the annihilation operator of a boson. Note that σ_- (σ_+) can be related to the annihilation (creation) operator a (a^*) of a fermion, via a so-called Jordan-Wigner transformation. Such off-diagonal terms make impossible the diagonalization of the quantum Hamiltonian with usual methods. In particular, the impact of these interaction terms on the properties of the model is expected to be major. For a general presentation of spin-boson models, see, for example, [9, Introduction and Section 2.3].

More recently, using the Hubbard model with nearest neighbor interaction near its Hartree-Fock ground state, Bach and Rauch demonstrate [10] that interaction terms of the form

$$\sum_{x,y} \sum_{s,t \in \{\uparrow, \downarrow\}} f_3(x-y) \left(b_{x,s}^* b_{y,t}^* a_{y,t} a_{x,s} + a_{x,s}^* a_{y,t}^* b_{y,t} b_{x,s} \right), \quad f_2(x-y) \geq 0, \quad (3)$$

exchanging fermions inside (a) and outside (b) of the Fermi surface are the only ones that can prevent from getting *uniform*¹ relative bounds of the effective interaction with respect to the effective kinetic energy. See [10, Theorems III.1, III.2 and III.3] for more details. In other words, (3) should again have a drastic impact on the corresponding quantum many-body system.

Three-body fermion-boson exchange interactions. In the present paper, for a fairly general function $v : \mathbb{Z}^2 \rightarrow \mathbb{R}$, we study the effect of the off-diagonal interaction term

$$\sum_{x,y} v(x-y) \left(c_y^* b_x + b_x^* c_y \right), \quad (4)$$

where b_x is the annihilation operator of a spinless boson on the site x of the two-dimensional (square) lattice \mathbb{Z}^2 , while c_y represents the annihilation of a fermion pair of zero total spin, the two components of which are spread around the lattice position $y \in \mathbb{Z}^2$. See Figure 1.

Note that the opposite combination can also be made: a boson b is destroyed to create two fermions f , which annihilate to recreate a boson b . This does not really create an interaction as such, but a kinetic term, or seen another way, a self-interaction. The combination of two diagrams refers to a perturbative approach of second order, but we can also combine several of the same diagrams (perturbative approach of order n).

The purely fermionic part of the considered model corresponds to the *extended* Hubbard Hamiltonian, as used in the context of ultracold atoms, ions and molecules [11], while the purely bosonic component refers to an ideal gas; that is, it has only a kinetic part (or ‘hopping term’), without interbosonic interactions. Because of the fermionic part, which is not exactly diagonalizable, the behavior of the full quantum many-body system, outside perturbative regimes, is almost inaccessible with the mathematical tools at our disposal.

We thus consider only a three-body problem, by restricting the model to the sector of one boson and two fermions of opposite spins. In fact, the system restricted to this particular sector is very interesting, both mathematically and physically. Note that such sector restrictions in Fock spaces are also performed for the study of the Pauli-Fierz and Nelson models [26, 28, 27] in nonrelativistic Quantum Field Theory (QFT).

Physical context: High- T_c superconductivity of cuprates. Physically, the model is related to cuprate superconductors,² like, for instance, $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ (LaSr 214 or LSCO) and $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$. It is

¹We mean a relative bound that is uniform with respect to the length of the discrete d -dimensional torus where the Hubbard model is defined.

²You can take, for instance, the cuprate La_2CuO_4 , which is a Mott insulator with an antiferromagnetic phase at low temperature. As with semiconductors, it is doped with atoms like Sr or Ba, which add a few charge carriers (in this case, holes). Then, with moderate doping x , the material becomes superconducting at low temperatures. This is the meaning of the chemical formulae $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ and $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$, x being a small number characterizing the cuprate doping. See also Section A.1.

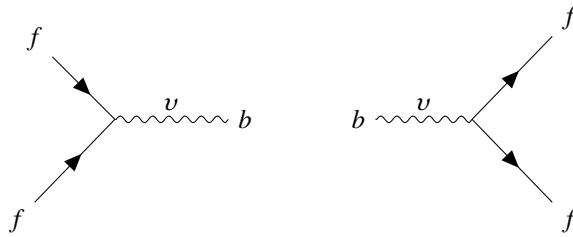


Figure 1. Illustration of fermion-boson exchange interactions in the form of two Feynman diagrams. In theoretical physics, a Feynman diagram visually represents the mathematical expressions that describe the behavior and interactions of quantum particles. In the example on the left, the two arrows indicate that two fermions, named (f), ‘collide’ to create a new particle, the boson (b). The oscillating line is generally used to describe an interaction with a mediator, which can be seen by combining the two diagrams: two fermions (f) interact to produce a boson, which annihilates again to produce two fermions (f). This can lead to an effective interaction between fermions. In particular, this process could produce a pair of fermions ($f - f$) bonded by the exchange of a bosonic field (b), according to the coupling function v . This is typically what we are going to show. Note that the opposite combination can also be made: a boson (b) is destroyed to create two fermions (f), which annihilate to recreate a boson (b). This does not really create an interaction as such, but a kinetic term, or seen another way, a self-interaction on the boson (b). The combination of two diagrams refers to a perturbative approach of second order, but we can also combine several of the same diagrams (perturbative approach of order n). Note, however, that no such perturbative argument is used here.

known [12, 13, 14] that in such crystals, charge transport occurs within two-dimensional isotropic layers of copper oxides. This is why we consider here quantum particles on 2-dimensional lattices \mathbb{Z}^2 .

A convincing microscopic mechanism behind superconductivity at high critical temperature is still lacking even after almost four decades of intensive theoretical and experimental studies. See Section A.1 for more details. Many physicists believe that the celebrated Hubbard model could be pivotal, one way or another, in order to get a microscopic theory of high-temperature superconductivity, but many alternative explanations or research directions have also been considered in theoretical physics. For some of the more popular models for cuprate superconductors, see, for example, [13, Chap. 7].

In many theoretical approaches to this problem, the existence of polaronic quasiparticles in relation with the very strong Jahn-Teller (JT) effect associated with copper ions is neglected, as stressed in (15, Part VII). The role of polarons is, however, highlighted in [16], since the JT effect actually led to the discovery of superconductivity in cuprates in 1986. See [17, p. 2] or [18, 19].

Our theoretical approach differs from most popular ones, being based on the existence of JT bipolarons in copper oxides, as is discussed in the literature [20] at least as early as 1990. The physics behind this approach is explained in detail in [21], where a simplified version of the model studied here is considered. In our microscopic model for cuprate superconductors, as presented in [22, 21], the bosonic operator b_x (b_x^*) in (4) refers to the annihilation (creation) of a JT bipolaron, whereas the fermionic one c_y (c_y^*) annihilates (creates) a fermion pair, which is reminiscent of Cooper pairs in conventional superconductivity.

Bipolaronic pairing mechanisms and cuprate superconductivity. As in the present paper, no ad hoc assumptions, in particular concerning anisotropy, are made in [21]. In fact, [21] proves that unconventional pairing may occur, breaking spontaneously discrete symmetries of the model, like the d -wave pairing, whose wave function is antisymmetric with respect to 90° -rotations. It turns out that electrostatic (screened Coulomb) repulsion is crucial for such unconventional pairings, which are meanwhile shown to be concomitant with a strong depletion of superconducting pairs.

Notice that the results of [21] are coherent with experimental observations on the cuprate LaSr 214: The coherence length at optimal doping and the d -wave pair formation in the pseudogap regime

(i.e., at temperatures much higher than the superconducting transition temperature) are predicted in good accordance with experimental data. In addition to the d -wave pairing and the high-temperature pseudogap regime, the model considered here also captures another very special feature of high- T_c cuprate superconductors – namely, the density waves [23]. For more details, see also Section A.1.

In fact, it is shown in [22, Section 4.1] that three-body fermion-boson exchange interactions, like the one studied in this paper, imply an effective fermion-fermion interaction. Then, by considering the mean-field limit of it, which corresponds to taking couplings (4) that are very localized in momentum space (22, Section 4.2), it was rigorously proven [24] that, below the critical temperature, the equilibrium states of the (purely fermionic) associated *many*-body Hamiltonian exhibit periodic modulation in space of the charge density, even incommensurate with respect to the lattice spacing.

1.2. Mathematical results

Previous results. To our knowledge, the model considered here has not been studied mathematically, apart from our own articles [21, 22] published in recent years. See also the Ph.D. thesis [24]. Mathematical studies for explicit exchange interaction terms are mainly those presented above. As far as we know, concerning its physical interpretation regarding cuprate superconductivity, our approach has also never been considered by other physicists, and we therefore doubt that any theoretical results in this direction exist in the literature. For more details, see the introductory discussions in [21], which give a concise overview of theories of high-temperature superconductivity.

Mathematically, the present paper improves [21, 22] to get more complete and general rigorous results, including, among other things, extended Hubbard interactions and scattering properties. While [21, 22] focus only on the ground state energy and the unconventional pairings in the limit of large Hubbard interactions, here we provide the full spectral properties of the corresponding Hamiltonian. In particular, we study in depth the effective dispersion relation associated with *dressed* bound fermion pairs. It confirms that off-diagonal interactions of the form (1) produce bounded states by reducing the energy of the system, similar to [2], possibly with a spectral gap.

This was already done in [21, 22], but only for usual (*non*-extended) Hubbard interactions and *one-range* creation / annihilation operators of fermion pairs. Even in this specific case, the dispersion relation of dressed bound fermion pairs was analyzed only to a level of detail enough to deduce unconventional pairings near the ground state. By contrast, in the present paper, other important properties of the dispersion relation, like its regularity, are studied for the first time and in a more general framework.

Last but not least, the localization of dressed bound fermion pairs or the scattering properties of the model have not been studied before.

Localized dressed bound fermion pairs. Using Combes-Thomas estimates, we show, among other things, that the dressed bound fermion pairs are localized, in the sense that the fermion-fermion correlation decays very fast in space. Group velocities and tensor masses of dressed bound fermion pairs are also shown to exist under very natural conditions on the (absolutely summable function) $\nu : \mathbb{Z}^2 \rightarrow \mathbb{R}$ appearing in (4).

In fact, our analysis allows one to accurately understand which features of the exchange strength function ν can strengthen the stability of the dressed bound fermion pairs. For instance, ν has to be sufficiently strong and localized in Fourier space in order to get a sufficiently strong ‘gluing effect’. Additionally, the boson should be heavier than two fermions.

Notice that this second condition is consistent with the physical interpretation that the boson is a bipolaron, which is known to be (effectively) much heavier than the fermions (electrons or holes), in superconducting cuprates. Observe additionally that the very large mass of bipolarons (and polarons, in general) is one of the main arguments used to discredit theoretical approaches based on bipolarons because it is known from experiments that the charge carriers in superconducting cuprates have an effective mass comparable to that of electrons and holes.

In fact, we prove that the effective mass of bound pairs mainly depends on the properties of the function ν , that encodes the fermion-boson exchange processes, but not much on the mass of the boson

itself. This issue is discussed in [21], in detail. See also the discussion at the end of Section 3.2. That is why we are interested in results concerning the mass tensor for bound pairs and we think we provide here a convincing solution for the ‘mass paradox’ related to bipolaronic pairing mechanisms in the microscopic theory of cuprate superconductors.

Relationship with the enhanced binding of QFT. The formation of dressed bonded fermion pairs as described above is reminiscent of what is known as *enhanced binding* in Quantum Field Theory (QFT). For more details on this phenomenon, we recommend the lecture notes [25], where it is well explained in the context of nonrelativistic QFT. See also the references therein.

For example, the Pauli-Fierz model, which refers to nonrelativistic quantum charge particles interacting with a massless quantized radiation field (photons), can have at low energies a dressed particle with an effective mass bigger than the noninteracting one, leading to the existence of a ground state for the model. A similar fact occurs in the Nelson model, in which N quantum particles interact linearly with a field of photons (or mesons). The formation of such dressed particles is a direct consequence of the bosonic field acting as mediator of a force.

Indeed, in both cases, the model involves a sum of interaction terms of the form $\psi_k \otimes b_k + \bar{\psi}_k \otimes b_k^*$, coupling the N -body quantum system with a spinless boson field of momentum k via annihilation/creation operators b_k, b_k^* . Note that in this case, there is no transformation of particles of one type into another, as in the exchange interactions described above, but both cases are still similar, especially as we are carrying out our analysis in the sector with only two fermions and one boson. This makes the comparison quite relevant, even if the model and mathematical methods considered here have essential differences as compared to the previous ones.

Scattering properties of the model. We also study here scattering properties of the three-body model in two channels, the *unbound* and *bound* pair channels:

- The unbound pair (scattering) channel corresponds to the wave and scattering operators with respect to fermionic part, respectively defined via the strong limits

$$W^\pm \doteq s - \lim_{t \rightarrow \pm\infty} e^{itH} e^{-itH_f} P_{ac}(H_f) \quad \text{and} \quad S \doteq (W^+)^* W^-,$$

where H_f is a generic, purely fermionic Hamiltonian representing free fermions that do not interact with any bosonic field, H is the Hamiltonian of the full model and $P_{ac}(H_f)$ is the orthogonal projection onto the absolutely continuous space of H_f . It refers to the case in which two fermions start far apart from each other and only experience a very weak repulsion force due to the extended Hubbard interaction, while the probability that they bind together to form a boson is very small. In this situation, we show that two (almost) freely propagating fermions in the distant past can come together and interact with one another, either via the repulsive electrostatic force or by exchanging a boson, and then propagate away, again freely in the distant future. In this channel, the scattering matrix can be explicitly computed via convergent (Dyson) series, making in particular the study of the scattering effect of the fermion-boson-exchange interaction (1) technically uncomplicated.

- The bound pair (scattering) channel corresponds to the time evolution $e^{itH}\mathfrak{P}$, $t \in \mathbb{R}$, where H is again the Hamiltonian of the full model and \mathfrak{P} is an isometry from the L^2 -functions on the Brillouin zone to the subspace associated with the fiber bound states of H . We show in particular that

$$e^{itH}\mathfrak{P} = \mathfrak{P}e^{itM_{E(\cdot)}}, \quad t \in \mathbb{R},$$

with $M_{E(\cdot)}$ being some multiplication operator given by the dispersion relation $k \mapsto E(k)$ characterizing the (fiber) bound states at fixed quasi-momentum in the normalized Brillouin zone $\mathbb{T}^2 \doteq [-\pi, \pi)^2$. In terms of wave operators, it follows that

$$W^\pm \doteq s - \lim_{t \rightarrow \pm\infty} e^{itH}\mathfrak{P}e^{-itM_{E(\cdot)}} P_{ac}(M_{E(\cdot)}) = \mathfrak{P}P_{ac}(M_{E(\cdot)}),$$

which gives a scattering operator equal to

$$S \doteq (W^+)^* W^- = P_{\text{ac}}(M_{\text{E}(\cdot)}).$$

It refers to the case in which dressed bound fermion pairs are formed. In contrast with the first channel, now there is a non-negligible bosonic component related with the exchanged boson that ‘glues’ the two fermions together. We prove that those (spatially localized) dressed bound fermion pairs effectively move like a free (quantum spinless) particle. In this case, strictly speaking in the physical sense, there is no scattering, and the pairs evolve freely in space, governed by an effective dispersion relation, the Fourier transform of which is the effective hopping strength for the (spatially localized) dressed bound pairs.

Composite system at strong on-site Hubbard repulsions. We additionally prove that all these properties hold also true in the limit of large on-site fermionic repulsions, provided that two fermions on two different lattice sites can interact via the fermion-boson exchange interaction. It refers to a hard core limit, preventing two fermions from occupying the same lattice site.

For cuprate superconductors, it is an important issue addressed and answered here, because of the undeniable experimental evidence of very strong on-site Coulomb repulsions in cuprates, leading to the universally observed Mott transition at zero doping [29, 30].

1.3. Concluding remarks and structure of the paper

To conclude, the mathematical properties of the model studied in the present work are well understood, and as a consequence, the model can serve as a prototypical example of a quantum system including exchange interaction terms of the form (1). From a physics viewpoint, it is also interesting, since dressed bound fermion pairs are good candidates for superconducting charge carriers in cuprate superconductors, as advocated in [21].

More specifically, our main results are Theorems 3.1, 3.5, 3.6, 3.9, 3.11 and 3.14. The paper is organized as follows: Section 2 explains in detail the model, while Section 3 gives the main results. Technical outcomes, along with all their proofs, are gathered in Section 4. Section A is an appendix that gathers important standard mathematical results used here, an overview of cuprate physics for non-physicists, as well as the Fock-space formalism, in order to make the article self-contained and accessible to a wide audience.

Remark 1.1 (d -dimensional lattices). Our study focuses on two-dimensional lattice systems because of their application to the superconductivity of cuprates and, in particular, their d -wave symmetry. However, it can also be done at arbitrary dimension $d \geq 1$ provided the coupling functions used (i.e., $u, \mathfrak{p}_1, \mathfrak{p}_2, v : \mathbb{Z}^d \rightarrow \mathbb{R}_0^+$ below) stays absolutely summable. It is also important that the Fourier transforms $\hat{v}, \hat{\mathfrak{p}}_1$ and $\hat{\mathfrak{p}}_2$ of the functions v, \mathfrak{p}_1 and \mathfrak{p}_2 remain real-valued³ continuous functions on the d -dimensional torus \mathbb{T}^d .

Remark 1.2 (Notation). For any normed vector space \mathcal{X} over \mathbb{C} , we omit the subscript \mathcal{X} to denote its norm $\|\cdot\| \equiv \|\cdot\|_{\mathcal{X}}$, unless there is any risk of confusion. Mutatis mutandis for the scalar product $\langle \cdot, \cdot \rangle \equiv \langle \cdot, \cdot \rangle_{\mathcal{X}}$ in Hilbert spaces. As is usual, $\mathcal{B}(\mathcal{X}, \mathcal{Y})$ denotes the set of bounded (linear) operators $\mathcal{X} \rightarrow \mathcal{Y}$ between two normed spaces \mathcal{X} to \mathcal{Y} . If $\mathcal{X} = \mathcal{Y}$, $\mathcal{B}(\mathcal{X}) \equiv \mathcal{B}(\mathcal{X}, \mathcal{X})$ and its (operator) norm and its identity are respectively denoted by $\|\cdot\|_{\text{op}} \equiv \|\cdot\|_{\mathcal{B}(\mathcal{X})}$ and $\mathbf{1}_{\mathcal{X}} \equiv \mathbf{1}$. \mathbb{R}_0^+ denotes the set of positive real numbers including zero, whereas $\mathbb{R}^+ \doteq \mathbb{R}_0^+ \setminus \{0\}$ is the set of strictly positive real numbers.

³A real-valued absolutely summable function f on \mathbb{Z}^d has a real-valued Fourier transform iff $f(-z) = f(z)$. Considering two-dimensional systems that are invariant under 90° -degree rotations (like we did, because of cuprates), this property is always true and has not to be additionally imposed.

2. Setup of the problem

2.1. Background Lattice

Copper oxide superconductors have a relatively complex three-dimensional lattice structure. However, they always contain parallel two-dimensional layers of copper (Cu^{++}) and oxygen (O^{--}) ions. These CuO_2 layers are essential to understanding low-temperature superconducting properties because the (superconducting) charge transport takes place within the layers. This is explained in [12, 13, 14]. Considering a weak inter-layer interaction might also help to increase prediction accuracy, but charge transport between each CuO_2 layer or, more generally, in the direction orthogonal to each layer remains negligible.⁴ Each CuO_2 layer generally has the symmetries of the square. In other words, it is invariant under the group $\{0, \pi/2, \pi, 3\pi/2\}$ generated by 90° -degree rotations. See, for example, (31, Section 9.1.2), [12, Section 2.3] and (14, Section 6.3.1). This is an important symmetry property that we keep in mind throughout our study.

Having in mind these physical observations on cuprates, we consider here quantum particles on lattices \mathbb{Z}^2 . It means in particular that (disregarding internal degrees of freedom of the quantum particles, like their spin) the (separable) Hilbert space $\ell^2(\mathbb{Z}^2)$ is the ‘one-particle space’ associated with the physical system we are interested in. Its canonical orthonormal basis is $\{\mathbf{e}_x\}_{x \in \mathbb{Z}^2}$:

$$\mathbf{e}_x(y) \doteq \delta_{x,y}, \quad x, y \in \mathbb{Z}^2, \quad (5)$$

where $\delta_{i,j}$ is the Kronecker delta.

2.2. Composite of two fermions and one boson

We consider a system of two fermions (electrons or holes in cuprates) with opposite spins interacting via the exchange of one boson in a two-dimensional square lattice. Physically, the boson that we have in mind in cuprate superconductors is a spinless bipolaron, since the very strong Jahn-Teller (JT) effect associated with copper ions is an important property of such cuprates [16, 15]. See Section A.1 for more details. However, the exchanged spinless boson could be of any type, like a phonon or a spin wave, depending on the physical system and mechanism one has in mind.

Hilbert Spaces. All quantum particles possess an intrinsic form of angular momentum known as spin, which is characterized by a quantum number $s \in \mathbb{N}/2$ and a finite spin set⁵ $S \doteq \{-s, -s+1, \dots, s-1, s\} \subseteq \mathbb{N}$. If $s \notin \mathbb{N}$ is half-integer, then the corresponding particles are named *fermions* while $s \in \mathbb{N}$ means by definition that we have *bosons*. For example, photons or spinless bipolarons ($s = 0$) are bosons, while electrons ($s = 1/2$) are fermions. In the latter case, $S \doteq \{-1/2, 1/2\}$, and in physics, the spin set is always written as $S \equiv \{\uparrow, \downarrow\}$, and we thus use this completely standard notation. By the celebrated spin-statistics theorem, fermionic wave functions are antisymmetric with respect to permutations of particles, whereas the bosonic ones are symmetric.

Therefore, the one-particle Hilbert space for the fermions is $\ell^2(\mathbb{Z}^2 \times \{\uparrow, \downarrow\})$, $\{\uparrow, \downarrow\}$ being the usual spin set for electrons or holes, and for two fermions, we hence use the Hilbert space

$$\mathfrak{h}_f \doteq \bigwedge^2 \ell^2(\mathbb{Z}^2 \times \{\uparrow, \downarrow\}) \subseteq \mathfrak{F}_- \equiv \mathfrak{F}(\ell^2(\mathbb{Z}^2 \times \{\uparrow, \downarrow\}))$$

of antisymmetric functions,⁶ which is a subspace of the fermionic (–) Fock space⁷ \mathfrak{F}_- associated with the one-particle Hilbert space $\ell^2(\mathbb{Z}^2 \times \{\uparrow, \downarrow\})$. See Equation (A.4) below for the precise definition of

⁴The superconducting coherence length is much smaller in this orthogonal direction than in the parallel planes made of copper and oxygen ions.

⁵ S represents the spectrum of the spin observable.

⁶ $\bigwedge^2 \ell^2(\mathbb{Z}^2 \times \{\uparrow, \downarrow\})$ denotes the 2-fold antisymmetric tensor product of $\ell^2(\mathbb{Z}^2 \times \{\uparrow, \downarrow\})$.

⁷I.e., $\mathfrak{F}_- \doteq \bigoplus_{n=0}^{\infty} \bigwedge^n \ell^2(\mathbb{Z}^2 \times \{\uparrow, \downarrow\})$.

\mathfrak{F}_- . The one-particle Hilbert space of the spinless boson is $\ell^2(\mathbb{Z}^2)$, which can also be seen as a subspace of the bosonic (+) Fock space

$$\mathfrak{F}_+ \equiv \mathfrak{F}(\ell^2(\mathbb{Z}^2))$$

associated with $\ell^2(\mathbb{Z}^2)$. See Equation (A.5) below for the precise definition of \mathfrak{F}_+ . For a concise review of bosonic and fermionic Fock spaces, as well as the corresponding annihilation and creation operators, see Section A.2.

We study here the effect of processes of annihilation of two fermions of opposite spins to create a boson, which can conversely be annihilated to create two new fermions. The Hilbert space associated with this composite system, made of two fermions and one boson, is the direct sum $\mathfrak{h}_f \oplus \ell^2(\mathbb{Z}^2)$, and not the tensor product $\mathfrak{h}_f \otimes \ell^2(\mathbb{Z}^2)$. Note indeed that $\mathfrak{h}_f \oplus \ell^2(\mathbb{Z}^2)$ can naturally be identified⁸ with a subspace of $\mathfrak{F}_- \otimes \mathfrak{F}_+$. This fact already unveils the strong interdependence of the bosonic and fermionic parts. For this reason, from now on, we rather use the term ‘composite of two fermions and one boson instead of ‘three-body system’, in order to avoid any misinterpretation.

Fermionic Hamiltonian. The fermionic part of the (infinite volume) Hamiltonian of the composite is defined to be the restriction $H_f \in \mathcal{B}(\mathfrak{h}_f)$ of the formal expression

$$-\frac{\epsilon}{2} \sum_{s \in \{\uparrow, \downarrow\}, x, y \in \mathbb{Z}^2: |x-y|=1} a_{x,s}^* a_{y,s} + 2\epsilon \sum_{s \in \{\uparrow, \downarrow\}, x \in \mathbb{Z}^2} a_{x,s}^* a_{x,s} + U \sum_{x \in \mathbb{Z}^2} n_{x,\uparrow} n_{x,\downarrow} + \sum_{x,z \in \mathbb{Z}^2} u(z) n_{x,\uparrow} n_{x+z,\downarrow} \quad (6)$$

to the Hilbert space \mathfrak{h}_f . Here, $a_{x,s}$ ($a_{x,s}^*$) denotes the annihilation (creation) operator acting on the fermionic Fock space \mathfrak{F}_- of a fermion at lattice position $x \in \mathbb{Z}^2$, the spin of which is $s \in \{\uparrow, \downarrow\}$. As is usual, $n_{x,s} \doteq a_{x,s}^* a_{x,s}$ stands for the number operator of fermions at lattice position $x \in \mathbb{Z}^2$ and spin $s \in \{\uparrow, \downarrow\}$.

The parameter $\epsilon \in \mathbb{R}_0^+$ quantifies the hopping amplitude of fermions. In high- T_c superconductors [29, 30], ϵ is expected to be much smaller than the fermion-fermion interaction energy – more precisely the on-site repulsion strength $U \in \mathbb{R}_0^+$. The function $u : \mathbb{Z}^2 \rightarrow \mathbb{R}_0^+$, which represents the fermion-fermion repulsion at all distances, is absolutely summable and invariant with respect to 90° -rotations, that is,

$$\sum_{z \in \mathbb{Z}^2} |u(z)| < \infty \quad \text{and} \quad u(x, y) = u(-y, x), \quad x, y \in \mathbb{Z}. \quad (7)$$

Clearly, one could set $U = 0$, by redefining the coupling function $u : \mathbb{Z}^2 \rightarrow \mathbb{R}_0^+$. It is, however, convenient to have a separate parameter $U \in \mathbb{R}_0^+$ for the on-site repulsion because we shall later on consider the ‘hard-core limit’ $U \rightarrow \infty$ for some fixed coupling function u .

Extended Hubbard interactions. The above fermion-fermion interactions have been extensively studied in condensed matter physics during the last decade, in particular for two-dimensional systems. For nonzero functions u , they are named *extended* Hubbard interactions and they can drastically change the behavior of the system, as compared to the zero-range case (usual Hubbard interaction, $u = 0$). As one example, they are used in the context of ultracold atoms, ions and molecules [11]. Its bosonic version is also experimentally investigated. See, for example, [32] published in 2022.

In theoretical studies, frequently, only nearest-neighbor interactions added to the on-site (zero-range) Hubbard interactions are considered. Here, we do not need the restriction to one-range (nearest-neighbor) interactions. We only assume that u is absolutely summable (see (7)), which is physically a very mild restriction, since the effective two-particle repulsive electrostatic potential in crystals is expected to decay exponentially fast in space, because of screening effects.

⁸Denote the vacuum of the Fock space \mathfrak{F}_\pm by Ω_\pm and define the mapping ς from $\mathfrak{h}_f \oplus \ell^2(\mathbb{Z}^2)$ to $\mathfrak{F}_- \otimes \mathfrak{F}_+$ by $\varsigma(\varphi \oplus \psi) = \varphi \otimes \Omega_- + \Omega_+ \otimes \psi$. Then, observe that ς is an isometric linear transformation from $\mathfrak{h}_f \oplus \ell^2(\mathbb{Z}^2)$ to $\mathfrak{F}_- \otimes \mathfrak{F}_+$.

The rotation invariance in Equation (7) refers to the isotropy of the system under consideration. However, as shown in [22, 21], the system has low energy states that spontaneously break the isotropy. This refers to unconventional pairings, typically of d -wave type, of electrons one experimentally observes in many high- T_c superconductors [33, 30, 13]. In fact, to derive the existence of d - and p -wave pairings starting from a physically sound microscopic model was the aim of [22, 21]. Here, instead, we keep a broader perspective and do not study this particular question.

Bosonic Hamiltonian. Similar to the fermionic part, the bosonic part of the (infinite volume) Hamiltonian of the system is defined to be the restriction $H_b \in \mathcal{B}(\ell^2(\mathbb{Z}^2))$ to the one-boson Hilbert space $\ell^2(\mathbb{Z}^2)$ of the formal expression

$$\epsilon \left(-\frac{h_b}{2} \sum_{x,y \in \mathbb{Z}^2 : |x-y|=1} b_x^* b_y + 2h_b \sum_{x \in \mathbb{Z}^2} b_x^* b_x \right). \quad (8)$$

Here, b_x (b_x^*) denotes the annihilation (creation) operator acting on the bosonic Fock space \mathfrak{F}_+ of a boson at lattice position $x \in \mathbb{Z}^2$. Observe that the bosonic part only contains a kinetic term. The parameter $h_b \in \mathbb{R}_0^+$ quantifies the ratio of the effective masses of fermions and bosons: Taking h_b smaller than one physically means that the bosons are heavier than the fermions. As experimentally found [34, 35, 36, 37] for cuprate superconductors, bipolarons should be much more massive than electrons or holes, and, thus, in the physically relevant regime, h_b is to be taken very small (or even zero, in an idealized situation). See (21, Section 3.1). In the sequel, we take $h_b \in [0, 1/2]$, meaning that the boson mass is at least as big as the mass of two fermions, as discussed in Section 3.

Exchange interactions. The term of the Hamiltonian that encodes the decay of a boson into two fermions (i.e., one of the two-electron(hole)-bipolaron-exchange interaction of the Hamiltonian) refers to the bounded operator

$$W_{b \rightarrow f} : \ell^2(\mathbb{Z}^2) \rightarrow \mathfrak{h}_f, \quad (9)$$

which is defined to be the restriction of the formal expression

$$2^{-1/2} \sum_{x,y \in \mathbb{Z}^2} v(x-y) c_y^* b_x \quad (10)$$

to $\ell^2(\mathbb{Z}^2)$, where

$$c_y^* \doteq \sum_{z \in \mathbb{Z}^2} \left(p_1(z) a_{y+z, \uparrow}^* a_{y, \downarrow}^* + p_2(2z) a_{y+z, \uparrow}^* a_{y-z, \downarrow}^* \right) \quad (11)$$

for some fixed functions $p_1, p_2 : \mathbb{Z}^2 \rightarrow \mathbb{R}$ that are invariant under 90° -rotations and exponentially decay in space, that is,

$$\sum_{z \in \mathbb{Z}^2} e^{\alpha_0 |z|} |p_\#(z)| < \infty \quad \text{and} \quad p_\#(x, y) = p_\#(-y, x), \quad x, y \in \mathbb{Z}, \# \in \{1, 2\}, \quad (12)$$

for some $\alpha_0 > 0$. In particular, the functions p_1, p_2 are absolutely summable in space.

By definition, we take $p_2(z) \doteq 0$ if $z \in \mathbb{Z}^2 \setminus (2\mathbb{Z})^2$ and we also assume that

$$p_1 + p_2 \neq 0 \quad \text{and} \quad p_2(x) \neq -e^{i\frac{k}{2} \cdot x} p_1(x), \quad x \in \mathbb{Z}, k \in [-\pi, \pi)^2. \quad (13)$$

The condition $p_1 + p_2 \neq 0$ only ensures the nontriviality of the exchange interaction, while the second condition avoids the singular case of a quasi-momentum $k_0 \in [-\pi, \pi)^2$ at which the exchange interaction

trivially vanishes; see below (36). This case can easily be analyzed, but it makes the argumentation cumbersome. So, we omit it here, as it is a highly unusual and irrelevant situation. For example, (13) is already satisfied as soon as $p_1(z) \neq 0$ for some $z \in \mathbb{Z}^2 \setminus (2\mathbb{Z})^2$, since $p_2(z) \doteq 0$ for any $z \notin (2\mathbb{Z})^2$. In (22, Eq. (6)), $p_2 = 0$ and, given $\kappa > 0$, $p_1(z) = e^{-\kappa|z|}$ for $|z| \leq 1$ and $p_1(z) = 0$ otherwise, while in [21, Eq. (4)], $p_2(2z) = p_1(z) = 1$ when $|z| \leq 1$ and $p_1(z) = p_2(z) = 0$ otherwise. This are the typical examples we have in mind, the point here being the fact two fermions on *different* lattice sites can interact by exchanging a boson. See also Section A.1.

Physically, c_y^* represents the creation of a fermion pair of zero total spin, the two components of which are slightly spread around the lattice position $y \in \mathbb{Z}^2$. Such pairs have finite size, because of (12). In fact,

$$r_p \doteq \frac{1}{2}(r_{p_1} + r_{p_2}), \quad (14)$$

where, for any $\sharp \in \{1, 2\}$, $r_{p_\sharp} \doteq 0$ if $p_\sharp = 0$, otherwise it is equal to

$$r_{p_\sharp} \doteq \frac{\sum_{z \in \mathbb{Z}^2} |z| |p_\sharp(z)|}{\sum_{z \in \mathbb{Z}^2} |p_\sharp(z)|} \leq \inf_{\alpha_0 > 0} \alpha_0^{-1} \sqrt{\frac{\sum_{z \in \mathbb{Z}^2} e^{\alpha_0|z|} |p_\sharp(z)|}{\sum_{z \in \mathbb{Z}^2} |p_\sharp(z)|}} < \infty, \quad (15)$$

is naturally seen as being the actual size of such pairs. Note that the last inequality is a consequence of the Cauchy-Schwarz inequality, along with the bound

$$|z|^2 e^{-\alpha_0|z|} \leq \alpha_0^{-2}, \quad \alpha_0 > 0.$$

Allowing two fermions in different lattice site to interact by exchanging a boson simply means that $r_p > 0$. For the physical significance of this property for cuprates, see [22, 21].

Recall that the exchange strength function $\nu : \mathbb{Z}^2 \rightarrow \mathbb{R}$ is only absolutely summable, not necessarily exponentially decaying as p_1 and p_2 , and invariant under 90° -rotations, that is,

$$\sum_{z \in \mathbb{Z}^2} |\nu(z)| < \infty \quad \text{and} \quad \nu(x, y) = \nu(-y, x), \quad x, y \in \mathbb{Z}. \quad (16)$$

Note that the Fourier transforms $\hat{\nu}, \hat{p}_1$ and \hat{p}_2 of ν, p_1 and p_2 are real-valued continuous functions (on the two-dimensional torus \mathbb{T}^2) that are again invariant under 90° -rotations. Additionally, \hat{p}_1 and \hat{p}_2 are real analytic, for p_1 and p_2 are exponentially decaying. The reverse process – that is, the annihilation of two unbound fermions to form a boson – is represented by the adjoint operator

$$W_{f \rightarrow b} \doteq W_{b \rightarrow f}^* : \mathfrak{h}_f \rightarrow \ell^2(\mathbb{Z}^2). \quad (17)$$

Mathematical remarks. The infinite sums (6), (8) and (10) defining formally $H_f \in \mathcal{B}(\mathfrak{h}_f)$, $H_b \in \mathcal{B}(\ell^2(\mathbb{Z}^2))$ and $W_{b \rightarrow f} \in \mathcal{B}(\ell^2(\mathbb{Z}^2), \mathfrak{h}_f)$ (9) are to be understood as follows: If $\psi \in \mathfrak{h}_f$ or $\psi \in \ell^2(\mathbb{Z}^2)$ is a finitely supported function, then the sum corresponding to $H_f \psi$, $H_b \psi$ or $W_{b \rightarrow f} \psi$ is absolutely convergent. Thus, H_f , H_b and $W_{b \rightarrow f}$ are well-defined linear operators acting on the dense subspace of such functions. One checks that H_f , H_b and $W_{b \rightarrow f}$ are all bounded on this subspace, and they thus have a unique bounded linear extension to the whole Hilbert space where they are defined – namely, \mathfrak{h}_f for H_f , and $\ell^2(\mathbb{Z}^2)$ for H_b and $W_{b \rightarrow f}$. We denote the extensions again by H_f , H_b and $W_{b \rightarrow f}$. Note that, being a bounded operator, $W_{b \rightarrow f}$ has an adjoint (17), while H_f and H_b are clearly symmetric and so, self-adjoint, for they are also bounded.

Full model. Finally, the full Hamiltonian for the fermion-boson composite is defined, in matrix notation for the direct sum $\mathfrak{h}_f \oplus \ell^2(\mathbb{Z}^2)$, as follows:

$$\begin{pmatrix} H_f & W_{b \rightarrow f} \\ W_{f \rightarrow b} & H_b \end{pmatrix} \in \mathcal{B}(\mathfrak{h}_f \oplus \ell^2(\mathbb{Z}^2)). \quad (18)$$

Observe that this Hamiltonian is invariant under translations, as well as 90° -rotations.

Using the canonical orthonormal basis⁹

$$\{e_{(x,s)} : x \in \mathbb{Z}^2, s \in \{\uparrow, \downarrow\}\} \subseteq \ell^2(\mathbb{Z}^2 \times \{\uparrow, \downarrow\})$$

to define the closed subspace

$$\mathfrak{h}_0 \doteq \overline{\text{span}}\{e_{(x,\uparrow)} \wedge e_{(y,\downarrow)} : x, y \in \mathbb{Z}^2\} \subseteq \mathfrak{h}_f, \quad (19)$$

we remark that the zero-spin subspace

$$\mathfrak{H} \doteq \mathfrak{h}_0 \oplus \ell^2(\mathbb{Z}^2) \subseteq \mathfrak{h}_f \oplus \ell^2(\mathbb{Z}^2) \quad (20)$$

is invariant under the action of the (full) Hamiltonian (18). We can thus consider its restriction

$$H \doteq \left(\begin{pmatrix} H_f & W_{b \rightarrow f} \\ W_{f \rightarrow b} & H_b \end{pmatrix} \right) \Big|_{\mathfrak{H}} \in \mathcal{B}(\mathfrak{H}) \quad (21)$$

to this particular subspace $\mathfrak{H} \subseteq \mathfrak{h}_f \oplus \ell^2(\mathbb{Z}^2)$.

In fact, as the boson is assumed to be spinless, by the conservation of angular momentum, we have that the total spin of the fermion pair resulting from a bosonic decay must be zero. In other words, the physically relevant (vector) states of the fermion-boson compound system always lie in \mathfrak{H} . Note finally that H inherits the symmetries of the Hamiltonian (18) (i.e., H is invariant under translations and 90° -rotations). Note that this last symmetry (i.e., the rotation invariance) is mainly relevant for the study of unconventional pairings, which is not done here.

2.3. The model in spaces of quasi-momenta

We have a composite of two fermions and one boson whose Hamiltonian is translation invariant. In this case, it is a standard procedure (see, for example, [38, Chapter XIII.16]) to use the direct integral decomposition of the Hamiltonian in Fourier space in order to study its spectral properties.

For the two-dimensional lattice \mathbb{Z}^2 , the (Fourier) space of quasi-momenta is nothing else than the torus

$$\mathbb{T}^2 \doteq [-\pi, \pi)^2 \subseteq \mathbb{R}^2.$$

This set is endowed with the metric $d_{\mathbb{T}^2}$ defined by

$$d_{\mathbb{T}^2}(k, p) \doteq \min\{|k - p - q| : q \in 2\pi\mathbb{Z}^2\}, \quad (22)$$

where $|k - p - q|$ is the Euclidean distance between k and $p + q$ in \mathbb{R}^2 . This defines a compact metric space $(\mathbb{T}^2, d_{\mathbb{T}^2})$. Observe also that the usual group operation in \mathbb{T}^2 (i.e., the sum in \mathbb{R}^2 modulo $(2\pi, 2\pi)$) is a continuous operation, while any Borel set in \mathbb{T}^2 is also a Borel set in \mathbb{R}^2 (endowed with the Euclidean metric).

We also need the normalized Haar measure ν on \mathbb{T}^2 defined for any Borel set $B \subseteq \mathbb{T}^2$ by

$$\nu(B) = (2\pi)^{-2} \lambda(B), \quad (23)$$

⁹I.e., for any $x, y \in \mathbb{Z}^2$ and $s, t \in \{\uparrow, \downarrow\}$, $e_{(x,s)}(y, s) = \delta_{s,t} \delta_{x,y}$, where $\delta_{x,y}$ is the Kronecker delta.

where λ is the Lebesgue measure in \mathbb{R}^2 . This measure appears in relation with direct integrals of constant Hilbert spaces on the two-dimensional torus \mathbb{T}^2 , like the Hilbert space

$$L^2(\mathbb{T}^2) \equiv L^2(\mathbb{T}^2, \mathbb{C}) \equiv L^2(\mathbb{T}^2, \mathbb{C}, \nu) \doteq \int_{\mathbb{T}^2}^{\oplus} \mathbb{C} \nu(dk)$$

of square-integrable, complex-valued functions on \mathbb{T}^2 . Since the Haar measure ν is used in all our direct integrals on \mathbb{T}^2 , for simplicity, we often remove the symbol ν from the notation of L^2 -spaces, unless this information is important to recall.

The Fourier transform can be applied in the fermionic and bosonic sectors. In the fermionic one, there is more than one natural way of implementing the transform, as the corresponding functions have two arguments in \mathbb{Z}^2 . It turns out that to be very useful to extract the total quasi-momentum of fermionic pairs. In fact, we consider the direct integral

$$L^2(\mathbb{T}^2, \mathcal{H}) \equiv L^2(\mathbb{T}^2, \mathcal{H}, \nu) \doteq \int_{\mathbb{T}^2}^{\oplus} L^2(\mathbb{T}^2, \mathbb{C}, \nu) \oplus \mathbb{C} \nu(dk) \quad (24)$$

of the (constant fiber) Hilbert space

$$\mathcal{H} \doteq L^2(\mathbb{T}^2) \oplus \mathbb{C} \equiv L^2(\mathbb{T}^2, \mathbb{C}, \nu) \oplus \mathbb{C} \quad (25)$$

over the torus \mathbb{T}^2 , and choose a unitary transformation

$$\mathbb{U} : \mathfrak{H} \longrightarrow L^2(\mathbb{T}^2, \mathcal{H})$$

in such a way that $k \in \mathbb{T}^2$, the fiber quasi-momentum, is exactly the total quasi-momentum of the fermion pair.

Recall that \mathfrak{H} defined in (20) is the Hilbert space on which H is originally defined. More precisely,

$$\mathbb{U} \doteq U_f \oplus \mathcal{F}, \quad (26)$$

where

$$\mathcal{F} : \ell^2(\mathbb{Z}^2) \rightarrow L^2(\mathbb{T}^2) \quad (27)$$

is the Fourier transform on $\ell^2(\mathbb{Z}^2)$, while the fermionic part

$$U_f \doteq U_2 U_1 : \mathfrak{h}_0 \rightarrow \int_{\mathbb{T}^2}^{\oplus} L^2(\mathbb{T}^2) \nu(dk) \quad (28)$$

is the composition of two unitary (linear) transformations U_1 and U_2 , whose exact definitions are given as follows:

$$\begin{aligned} U_1 : \quad \mathfrak{h}_0 &\rightarrow \ell^2(\mathbb{Z}^2 \times \mathbb{Z}^2) \rightarrow \ell^2(\mathbb{Z}^2 \times \mathbb{Z}^2) \rightarrow \ell^2(\mathbb{Z}^2) \otimes \ell^2(\mathbb{Z}^2) \\ \mathbf{e}_{(x, \uparrow)} \wedge \mathbf{e}_{(y, \downarrow)} &\mapsto \mathbf{e}_{(x, y)} \mapsto \mathbf{e}_{(x, x-y)} \mapsto \mathbf{e}_x \otimes \mathbf{e}_{x-y} \end{aligned} \quad (29)$$

and

$$\begin{aligned} U_2 : \ell^2(\mathbb{Z}^2) \otimes \ell^2(\mathbb{Z}^2) &\rightarrow L^2(\mathbb{T}^2) \otimes L^2(\mathbb{T}^2) \rightarrow \int_{\mathbb{T}^2}^{\oplus} L^2(\mathbb{T}^2) \nu(dk) \\ \mathbf{e}_x \otimes \mathbf{e}_{x-y} &\mapsto \hat{\mathbf{e}}_x \otimes \hat{\mathbf{e}}_{x-y} \mapsto \hat{\mathbf{e}}_x(\cdot) \hat{\mathbf{e}}_{x-y} \end{aligned} \quad (30)$$

Because $\{\mathbf{e}_{(x, \uparrow)} \wedge \mathbf{e}_{(y, \downarrow)}\}_{x, y \in \mathbb{Z}^2}$, $\{\mathbf{e}_{(x, y)}\}_{x, y \in \mathbb{Z}^2}$ and $\{\mathbf{e}_x \otimes \mathbf{e}_y\}_{x, y \in \mathbb{Z}^2}$ are orthonormal bases and $(x, y) \mapsto (x, x - y)$ is a bijection on $\mathbb{Z}^2 \times \mathbb{Z}^2$, U_1 is well-defined as a composition of three unitary linear

transformations. Note also that the last unitary linear transformation defining U_2 is defined as in Proposition A.8, while the first one defining U_2 is the tensor product $\mathcal{F} \otimes \mathcal{F}$ of the Fourier transform \mathcal{F} on $\ell^2(\mathbb{Z}^2)$, defined for any $f \in \ell^1(\mathbb{Z}^2) \subseteq \ell^2(\mathbb{Z}^2)$ by

$$\hat{f}(k) \equiv \mathcal{F}f(k) = \sum_{x \in \mathbb{Z}^2} e^{ik \cdot x} f(x), \quad k \in \mathbb{T}^2, \quad (31)$$

$k \cdot x$ being the usual scalar product of $k \in \mathbb{T}^2$ and $x \in \mathbb{Z}^2$, seen as vectors of \mathbb{R}^2 . Here, we use the symbol $\widehat{(\cdot)}$ to shorten the notation of the Fourier transform. For instance, for any $x \in \mathbb{Z}^2$, we write above \hat{e}_x to denote the function $e^{i(\cdot) \cdot x}$ on the torus \mathbb{T}^2 . That is, $\{\hat{e}_x\}_{x \in \mathbb{Z}^2}$ is the image under the Fourier transform of the canonical orthonormal basis $\{e_x\}_{x \in \mathbb{Z}^2}$ (5) of $\ell^2(\mathbb{Z}^2)$.

For the reader's convenience and completeness, in Section A.4, we gather key results from the theory of direct integrals with constant fiber Hilbert spaces. In the next subsection, we explain how the properties of the Hamiltonian $H \in \mathcal{B}(\mathfrak{H})$ defined by (21) can be studied on the direct integral (24) over total quasi-momenta.

2.4. Fiber decomposition of the Hamiltonian

By explicit computations, exactly like in [22, 21], we show that the conjugation of the Hamiltonian $H \in \mathcal{B}(\mathfrak{H})$ with the unitary transformation \mathbb{U} of Equation (26) is a decomposable operator on the direct integral $L^2(\mathbb{T}^2, \mathcal{H})$. To state this result precisely, we need preliminary definitions allowing to define the so-called ‘fiber Hamiltonians’, or ‘fibers’ for short, $A(k) \in \mathcal{B}(\mathcal{H})$ of $\mathbb{U}H\mathbb{U}^*$ at total quasi-momenta $k \in \mathbb{T}^2$. In fact, the mapping $k \mapsto A(k)$ defines an element of the von Neumann algebra¹⁰

$$L^\infty(\mathbb{T}^2, \mathcal{B}(\mathcal{H})) \equiv L^\infty(\mathbb{T}^2, \mathcal{B}(\mathcal{H}), \nu)$$

of (equivalence classes of) strongly measurable functions $\mathbb{T}^2 \rightarrow \mathcal{B}(\mathcal{H})$. See Section A.4 for more details.

Given a total quasi-momentum $k \in \mathbb{T}^2$ and the parameters $\epsilon, h_b \in \mathbb{R}_0^+$ tuning the strengths of the two (fermionic and bosonic) kinetic parts of the model, we define continuous, real-valued functions $\mathfrak{f}(k), \mathfrak{d}(k), \mathfrak{b} \in C(\mathbb{T}^2)$ on the torus \mathbb{T}^2 by

$$\mathfrak{b}(p) \doteq h_b \epsilon (2 - \cos(p)), \quad (32)$$

$$\mathfrak{f}(k)(p) \doteq \epsilon \{4 - \cos(p+k) - \cos(p)\}, \quad (33)$$

$$\mathfrak{d}(k)(p) \doteq \hat{\mathfrak{p}}_1(k+p) + \hat{\mathfrak{p}}_2(k/2+p), \quad (34)$$

for all $p = (p_1, p_2) \in \mathbb{T}^2$, where

$$\cos(q) \doteq \cos(q_1) + \cos(q_2), \quad q = (q_1, q_2) \in \mathbb{R}^2. \quad (35)$$

Recall that (the $(2\pi, 2\pi)$ -periodic function) $\hat{\mathfrak{p}}_1$ and $\hat{\mathfrak{p}}_2$ are the Fourier transform of \mathfrak{p}_1 and \mathfrak{p}_2 , which are the functions defining the operator c_y^* in (11), representing the creation of fermion pairs in the model. Note also from (13) that $\mathfrak{d}(k) \neq 0$ for all $k \in \mathbb{T}^2$. Indeed, using $\mathfrak{p}_2(z) \doteq 0$ for $z \notin 2\mathbb{Z}$ as well as (31) and (34),

$$\mathfrak{d}(k) = \mathcal{F} \left[e^{ik \cdot x} \mathfrak{p}_1(x) + e^{i\frac{k}{2} \cdot x} \mathfrak{p}_2(x) \right], \quad (36)$$

where $e^{ik \cdot x} \mathfrak{p}_\#(x)$ stands for the function $x \mapsto e^{ik \cdot x} \mathfrak{p}_\#(x)$ with $\# \in \{1, 2\}$.

¹⁰The (unique) norm of this C^* -algebra is the essential supremum with respect to the measure ν on the torus; see (A.14).

Then, at any quasi-momentum $k \in \mathbb{T}^2$ and on-site repulsion strength $U \in \mathbb{R}_0^+$, we define the bounded operators $B_{1,1}(k)$ and $A_{1,1}(U, k)$ acting on the Hilbert space $L^2(\mathbb{T}^2)$ by

$$B_{1,1}(k) \doteq M_{\mathfrak{f}(k)} + \sum_{x \in \mathbb{Z}^2} u(x) P_x, \quad (37)$$

$$A_{1,1}(U, k) \doteq B_{1,1}(k) + UP_0, \quad (38)$$

where $M_{\mathfrak{f}(k)}$ stands for the multiplication operator by $\mathfrak{f}(k) \in C(\mathbb{T}^2)$ and P_x is the orthogonal projection onto the one-dimensional subspace $\mathbb{C}\hat{e}_x \subseteq L^2(\mathbb{T}^2)$. Note that the infinite sum defining the bounded operator $B_{1,1}(k)$ is absolutely convergent, for the function $u : \mathbb{Z}^2 \rightarrow \mathbb{R}$ is, by assumption, absolutely summable. See (7).

We define next

$$\begin{aligned} A_{2,1}(k) : L^2(\mathbb{T}^2) &\rightarrow \mathbb{C} \\ \varphi &\mapsto \hat{v}(k) \langle \mathfrak{d}(k), \varphi \rangle, \end{aligned} \quad (39)$$

$$\begin{aligned} A_{1,2}(k) : \mathbb{C} &\rightarrow L^2(\mathbb{T}^2) \\ z &\mapsto \hat{v}(k) \mathfrak{d}(k) z \end{aligned} \quad (40)$$

as well as

$$\begin{aligned} A_{2,2}(k) : \mathbb{C} &\rightarrow \mathbb{C} \\ z &\mapsto \mathfrak{b}(k) z \end{aligned} \quad (41)$$

for any fixed $k \in \mathbb{T}^2$. By compactness of \mathbb{T}^2 and continuity (in operator norm) of the mappings $k \mapsto A_{i,j}(k)$ for all $i, j \in \{1, 2\}$, we have

$$A(\cdot) \equiv A(U, \cdot) \doteq \begin{pmatrix} A_{1,1}(U, \cdot) & A_{1,2}(\cdot) \\ A_{2,1}(\cdot) & A_{2,2}(\cdot) \end{pmatrix} \in L^\infty(\mathbb{T}^2, \mathcal{B}(\mathcal{H})) \quad (42)$$

(see Lemma 4.1), which is meanwhile the fiber decomposition of the operator $\mathbb{U}H\mathbb{U}^*$:

Proposition 2.1 (Fiber decomposition of the quantum model). *The conjugation of H by \mathbb{U} (26) is decomposable and has $A(\cdot)$ as its fibers; that is,*

$$\mathbb{U}H\mathbb{U}^* = \int_{\mathbb{T}^2}^\oplus A(k) \nu(dk).$$

Proof. This is proven from explicit computations which are almost the same as those done in [22, 21]. We postpone the details of this calculation to Section 4.2. \square

The fiber decomposition given by Proposition 2.1 is useful because it gives access to spectral properties of H . In fact, for an operator that is decomposable on $L^2(\mathbb{T}^2, \mathcal{H})$, that is, an operator unitarily equivalent to an element of the von Neumann algebra $L^2(\mathbb{T}^2, \mathcal{B}(\mathcal{H}))$, like the Hamiltonian H , the fibers $A(k)$ of which are all self-adjoint, it is known that $\lambda \in \sigma(H)$ if, and only if, for all $\varepsilon > 0$,

$$\nu\left(\left\{k \in \mathbb{T}^2 : \sigma(A(k)) \cap (\lambda - \varepsilon, \lambda + \varepsilon) \neq \emptyset\right\}\right) > 0.$$

See Theorem A.3. As is usual, here, $\sigma(X)$ denotes the spectrum of any operator X acting on some Hilbert space.

3. Main results

In this section, we state our main results, starting with general spectral properties of the Hamiltonian H to finish with results related with scattering.

Recall that the model has parameters $\epsilon, U, h_b \in \mathbb{R}_0^+$ and $\alpha_0 \in \mathbb{R}^+$, and it depends on the choice of functions

$$u : \mathbb{Z}^2 \rightarrow \mathbb{R}_0^+, \quad p_1 : \mathbb{Z}^2 \rightarrow \mathbb{R}, \quad p_2 : \mathbb{Z}^2 \rightarrow \mathbb{R} \quad \text{and} \quad v : \mathbb{Z}^2 \rightarrow \mathbb{R}$$

(with $p_2(z) \doteq 0$ for $z \notin 2\mathbb{Z}$) that are absolutely summable and invariant with respect to 90° -rotations. Observe additionally that the functions p_1 and p_2 are required to be exponentially decaying; that is, $e^{\alpha_0|\cdot|}p_1$ and $e^{\alpha_0|\cdot|}p_2$ are absolutely summable for some $\alpha_0 > 0$. See Equations (7), (12) and (16). All details of the Hamiltonian, like the precise choice of its parameters and functions, are not explicitly mentioned in our discussions or statements below, unless it is important for clearness. There is however one important condition to clarify:

While some of our results can be obtained without any other restriction, frequently we fix the parameter h_b in the interval $[0, 1/2]$. This choice physically means that the boson is heavier than two fermions. As already discussed above, the assumption is perfectly justified when one views the two fermions and the boson of the model as being electrons or holes and a bipolaron, respectively, in a cuprate. In fact, polarons (and thus bipolarons) are charge carriers that are self-trapped inside a strong and local lattice deformation that surrounds them, caused by electrostatic interactions between the carriers and the lattice. A priori, such (strong and local) lattice deformations can barely move; that is, their effective mass is huge. See, for example, [34, 35, 36]. This is coherent with the assumption of a large mass of JT bipolarons in copper oxides [37], similar to JT polarons [39]. See also Section A.1 for more details.

We show that the condition $h_b \in [0, 1/2]$ is crucial to obtain dressed bound fermion pairs, which are expected to represent the charge carriers below the pseudogap temperature [21].

3.1. Spectral properties

Having in mind Proposition 2.1 and Theorem A.3, we start with the spectral properties of fiber Hamiltonians (42) at any quasi-momentum $k \in \mathbb{T}^2$. This refers to the following theorem:

Theorem 3.1 (Spectral properties of fiber Hamiltonians). *Fix $\epsilon, U \in \mathbb{R}_0^+$, $h_b \in [0, 1/2]$ and $k \in \mathbb{T}^2$.*

i.) *Essential spectrum $\sigma_{\text{ess}}(\cdot)$ of the fiber Hamiltonian:*

$$\sigma_{\text{ess}}(A(U, k)) = \mathbf{f}(k)\left(\mathbb{T}^2\right) = 2\epsilon \cos(k/2)[-1, 1] + 4\epsilon.$$

ii.) *Ground state energy: There is a unique nondegenerate eigenvalue $E(U, k) \leq \mathbf{b}(k)$ of $A(U, k)$ below the essential spectrum, with associated eigenvector*

$$\Psi(U, k) \doteq (\hat{\psi}_k(U), -1), \quad \text{where} \quad \hat{\psi}_{U,k} \doteq \hat{v}(k)(A_{1,1}(U, k) - E(U, k)\mathbf{1})^{-1}\mathbf{d}(k) \in L^2\left(\mathbb{T}^2\right).$$

In addition, $E(U, k) = \mathbf{b}(k)$ iff $\hat{v}(k) = 0$. Recall that $\mathbf{b}(k)$ is defined by Equation (32).

iii.) *Spectral gap and Anderson localization: If $\hat{v}(0) \neq 0$ and $r_p > 0$, then*

$$\inf_{U \in \mathbb{R}_0^+} \min_{k \in \mathbb{T}^2} \{\min \sigma_{\text{ess}}(A(U, k)) - E(U, k)\} > 0$$

and there are $C, \alpha \in \mathbb{R}^+$ such that, for all $k \in \mathbb{T}^2$ and $U \in \mathbb{R}_0^+$,

$$|\mathcal{F}^{-1}[\hat{\psi}_{U,k}](x)| \leq Ce^{-\alpha|x|}, \quad x \in \mathbb{Z}^2.$$

iv.) $E(U, \cdot) : \mathbb{T}^2 \rightarrow \mathbb{R}$ is a continuous function, and if \hat{v} is of class¹¹ C^d on $(-\pi, \pi)^2 \setminus \{0\} \subseteq \mathbb{R}^2$ with $d \in \mathbb{N} \cup \{\omega, a\}$, then so does $E(U, \cdot)$ on $(-\pi, \pi)^2 \setminus \{0\}$.

Proof. The theorem is a combination of Theorems 4.8, 4.9, 4.18 and 4.20 together with Propositions 4.2, 4.19 and Corollary 4.6 (see (130)). \square

Remark 3.2. Recall that if, for some natural number $d \geq 1$,

$$\sum_{x \in \mathbb{Z}^2} |x|^d |v(x)| < \infty,$$

then the Fourier transform \hat{v} of the function $v : \mathbb{Z}^2 \rightarrow \mathbb{R}$, as defined by (31), is of class C^d on the whole torus \mathbb{T}^2 .

Remark 3.3. If $p_1 = p_2 \in \mathbb{C}e_0$, i.e., $r_p = 0$, then Theorem 3.1 (iii) remains true, but not uniformly in $U \in \mathbb{R}_0^+$. That is, in this case, one only has

$$\min_{k \in \mathbb{T}^2} \{\min \sigma_{\text{ess}}(A(U, k)) - E(U, k)\} > 0,$$

and there are $C_U, \alpha_U \in \mathbb{R}^+$ such that, for all $k \in \mathbb{T}^2$,

$$|\mathcal{F}^{-1}[\hat{\psi}_{U,k}](x)| \leq C_U e^{-\alpha_U |x|}, \quad x \in \mathbb{Z}^2.$$

Assertion (i) of Theorem 3.1 holds true for all $h_b \in \mathbb{R}_0^+$, but the other assertions need the restriction $h_b \in [0, 1/2]$ to ensure that the eigenvalues are below the essential spectrum, as stated in Assertion (ii). In fact, $h_b \in [0, 1/2]$ iff

$$b(k) \leq \mathfrak{z}(k) \doteq 4\epsilon - 2\epsilon \cos(k/2) = \min \sigma_{\text{ess}}(A(U, k)) \quad (43)$$

for all $k \in \mathbb{T}^2$, with equality *only* at $k = 0$. See Equation (32). Therefore, by Assertion (ii), $E(U, k)$ belongs to the essential spectrum iff $k = 0$ and $\hat{v}(0) = 0$. Otherwise, we have a uniform spectral gap, as stated in Assertion (iii).

As is explained in [22, 21], the eigenvalue $E(U, k)$ given by Theorem 3.1 is associated with the formation of *dressed bound fermion pairs* with total quasi-momentum $k \in \mathbb{T}^2$. These pairs are generally exponentially localized, thanks to Theorem 3.1 (iii), which basically implies that the two fermions move together confined within some small ball; that is, they are tightly bound in space, provided $\hat{v}(0) \neq 0$. When $p_1(z) \neq 0$ or $p_2(z) \neq 0$ for some $z \neq 0$, or, equivalently, $r_p > 0$, the size of the small does not depend upon the Hubbard coupling constant U and a very large $U \gg 1$ only prevents two fermions from occupying the same lattice site. The condition $p_1(z) \neq 0$ or $p_2(z) \neq 0$ for some $z \neq 0$, or equivalently, $r_p > 0$, is therefore **pivotal** to get (Cooper) fermion pairs, the natural candidates for superconducting charge carriers, in presence of strong on-site Coulomb repulsions, like in cuprates [29, 30].

For the usual (i.e., nonextended) Hubbard interaction ($u = 0$) and one-range¹² creation operators c_y^* of fermion pairs (in this case (12) holds true for all $\alpha_0 \in \mathbb{R}_0^+$), note that a weak form of pair localization was previously shown in the ground state. See, for instance, [22, Theorem 3 and Proposition 13]. In this particular case, estimates of $E(U, k)$ and $\Psi(U, k)$ are known for large $U \gg 1$. See, for example, [22, Theorem 4, Corollary 5, Theorem 16]. Recall that the aim in [22, 21] was to show the existence of d - and p -wave pairings in the ground state for some physically sound model, and not the systematic study of a general class of models. In [21], we conjecture that such dressed bound fermion pairs represent the charge carriers below the pseudogap temperature in cuprates.

¹¹Given $n, d \in \mathbb{N}$ and an open set $\Omega \subseteq \mathbb{R}^n$, $C^d(\Omega)$ denotes the set of d times continuously differentiable, complex-valued functions on Ω , while $C^\omega(\Omega)$ and $C^a(\Omega)$ refer to the space of smooth and real analytic functions on Ω , respectively.

¹²It means here that $c_y^* \doteq \sum_{|z| \leq 1} (p_1(z) a_{y+z, \uparrow}^* a_{y, \downarrow}^* + p_2(2z) a_{y+z, \uparrow}^* a_{y-z, \downarrow}^*)$.

Theorem 3.1 combined with Proposition 2.1 and the theory of direct integrals (cf. Theorem A.3) has direct consequences for the spectrum of the full Hamiltonian $H \in \mathcal{B}(\mathfrak{H})$, which is defined by Equation (21). Among other things, we obtain the following corollary:

Corollary 3.4 (Spectral properties of H). *Fix $\epsilon, U \in \mathbb{R}_0^+$ and $h_b \in [0, 1/2]$. Then,*

$$\sigma(H) \cap (-\infty, 8\epsilon] = \{E(U, k) : k \in \mathbb{T}^2\} \cup (0, 8\epsilon),$$

where $\sigma(H)$ denotes, as is usual, the spectrum of H , and

$$\min \sigma(H) = E(U) \doteq \min_{k \in \mathbb{T}^2} E(U, k) \leq 0.$$

If additionally $\hat{v}(0) \neq 0$ and $r_p > 0$, then

$$\sup_{U \in \mathbb{R}_0^+} E(U) < 0.$$

Proof. To prove the first assertion, it suffices to combine Proposition 2.1 and Theorem 3.1 with Theorem A.3. The second one can be proven like in [22] by using Kato's perturbation theory [40]. In Proposition 4.11, we give an alternative and more direct proof of it. Finally, the last assertion is a consequence of the inequalities

$$\min_{k \in \mathbb{T}^2} E(U, k) \leq E(U, 0) = E(U, 0) - \min \sigma_{\text{ess}}(A(U, 0))$$

and Theorem 3.1 (iii). □

Physically speaking, the spectral values of H represent the energy levels that are available to the composite of two fermions and one boson – in particular, for a fermion pair exchanging a boson. As expected, the minimum energy E , also well-known as the ground state energy, is given by minimizing the eigenvalues $E(U, k)$ over the torus \mathbb{T}^2 .

We now study the model at very large on-site repulsion $U \gg 1$. In fact, quoting [21], ‘in all cuprates, there is undeniable experimental evidence of strong on-site Coulomb repulsions, leading to the universally observed Mott transition at zero doping [29, 30]. This phase is characterized by a periodic distribution of fermions (electrons or holes) with exactly one particle per lattice site. Doping copper oxides with holes or electrons can prevent this situation. Instead, at sufficiently small temperatures a superconducting phase is achieved, as first discovered in 1986 for the copper oxide perovskite $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$ [16]’. However, instead of the usual s -wave superconductivity, one experimentally observes d -wave superconductivity [33, 30, 13]. The fact that *only* the s -wave pairing is suppressed also advocates for a very local (i.e., on-site) and strong effective repulsion of fermions. For this reason, we consider the limit $U \rightarrow \infty$ in our model. It corresponds to a hard core limit because it prevents two fermions from being on the same lattice site.

In the limit $U \rightarrow \infty$, it is easy to see that the ground state energy $E(U)$ of Corollary 3.4 defines an increasing function of $U \in \mathbb{R}_0^+$, which is bounded from above by 0. Hence,

$$E(\infty) \doteq \lim_{U \rightarrow \infty} E(U) = \sup_{U \in \mathbb{R}_0^+} E(U) \leq 0. \quad (44)$$

For more details, see Lemma 4.14. The limit $U \rightarrow \infty$ of the eigenvalue and eigenvector of each fiber, given by Theorem 3.1, is less trivial to obtain and is the object of the next theorem:

Theorem 3.5 (Spectral properties of fiber Hamiltonians – Hard-core limit). *Fix $\epsilon, U \in \mathbb{R}_0^+$ and $h_b \in [0, 1/2]$. The following limits exist:*

$$E(\infty, k) \doteq \lim_{U \rightarrow \infty} E(U, k) = \sup_{U \in \mathbb{R}_0^+} E(U, k) \leq \mathfrak{b}(k), \quad k \in \mathbb{T}^2.$$

$$\Psi(\infty, k) \doteq \lim_{U \rightarrow \infty} \Psi(U, k) \in \mathcal{H} \setminus \{0\}, \quad k \in \mathbb{T}^2 \setminus \{0\}.$$

Assertion (iv) of Theorem 3.1 also holds true for $U = \infty$. In addition, when $r_p > 0$, $E(\infty, k) = \mathfrak{b}(k)$ iff $\hat{v}(k) = 0$. If $r_p > 0$ and $\hat{v}(0) \neq 0$, then $\Psi(\infty, 0)$ exists.

Proof. See Theorems 4.15 and 4.18. □

Note that the eigenvalues given by Theorem 3.1 are not explicitly known. The same is of course true in the hard-core limit $U \rightarrow \infty$. For applications, it is important to have a sufficiently good control on these objects to be able to compute them, either analytically or numerically. This is done in [22, 21] for the special case of the usual Hubbard interaction ($u = 0$) and one-range creation operators c_y^* of fermion pairs, by providing estimates for $E(U, k)$ and $\Psi(U, k)$ at large U . See [22, Theorem 4, Corollary 5, Theorem 16].

Recall that \hat{v} is the Fourier transform of v , which is the function appearing in Equation (10), encoding the (exchange) interaction between fermion pairs and bosons. By Theorem 3.1, if $\hat{v}(k) = 0$, then $E(U, k)$ is nothing else than the explicit function $\mathfrak{b}(k)$ (32). Hence, we focus on the physically more relevant case $\hat{v}(k) \neq 0$. Using the Birman-Schwinger principle (Theorem A.10), we show in this case that the eigenvalue $E(U, k)$ is the unique solution to a relatively simple equation for real numbers, similar to the characteristic equation used to compute eigenvalues of matrices.

To this end, we define a function $\mathfrak{T} : \mathcal{D} \rightarrow \mathbb{R}$ on the set

$$\mathcal{D} \doteq \{(U, k, x) \in [0, \infty] \times \mathbb{T}^2 \times \mathbb{R} : x < \mathfrak{z}(k)\} \subseteq \mathbb{R}^3$$

by

$$\mathfrak{T}(U, k, x) \doteq \left\langle \mathfrak{d}(k), (A_{1,1}(U, k) - x\mathbf{1})^{-1} \mathfrak{d}(k) \right\rangle \quad (45)$$

for any finite $U \in \mathbb{R}_0^+$, $k \in \mathbb{T}^2$ and $x \in (0, \mathfrak{z}(k))$, while for the infinite on-site repulsion, $k \in \mathbb{T}^2$ and $x \in (0, \mathfrak{z}(k))$,

$$\mathfrak{T}(\infty, k, x) \doteq \lim_{U \rightarrow \infty} \mathfrak{T}(U, k, x),$$

the above limit existing by virtue of Corollary 4.13. Recall that $\mathfrak{z}(k)$ is defined by Equation (75). In fact, for any $k \in \mathbb{T}^2$ and $x \in (0, \mathfrak{z}(k))$,

$$\mathfrak{T}(\infty, k, x) = R_{\mathfrak{s}, \mathfrak{s}}^{-1} \left(R_{\mathfrak{d}, \mathfrak{d}} R_{\mathfrak{s}, \mathfrak{s}} - |R_{\mathfrak{s}, \mathfrak{d}}|^2 \right) > 0,$$

where $R_{\mathfrak{s}, \mathfrak{s}}$, $R_{\mathfrak{s}, \mathfrak{d}}$, $R_{\mathfrak{d}, \mathfrak{s}}$ and $R_{\mathfrak{d}, \mathfrak{d}}$ are four constants defined by Equations (99)–(102) with $\lambda = x$. When $u = 0$, these constants are given by explicit integrals on the torus \mathbb{T}^2 [22, 21]. Then, the eigenvalues, the existence of which is stated in Theorem 3.1, as well as their limits (Theorem 3.5), can be studied via the following characteristic equation:

Theorem 3.6 (Characteristic equation for the fiber ground states). *Fix $\epsilon \in \mathbb{R}_0^+$, $h_b \in [0, 1/2]$ and $k \in \mathbb{T}^2$ such that $\hat{v}(k) \neq 0$. Then, for any $U \in [0, \infty]$, $E(U, k)$ is the unique solution to the equation*

$$\hat{v}(k)^2 \mathfrak{T}(U, k, x) + x - \mathfrak{b}(k) = 0, \quad x < \mathfrak{z}(k).$$

Proof. For $U \in \mathbb{R}_0^+$, combine Theorem 4.5 with Theorem 4.8, while for $U = \infty$, use Theorem 4.15. □

Notice that, more generally, for any fixed $U \in \mathbb{R}_0^+$, the same characteristic equation determines all eigenvalues of the fiber lying in the resolvent set $\rho(A_{1,1}(U, k))$ of the operator $A_{1,1}(U, k)$. See Theorem 4.5. Also the associated eigenspaces can be explicitly characterized, thanks to Corollary 4.6. In this context, Corollary 4.7 shows that, for any $h_b \in [0, 1/2]$ and total quasi-momentum $k \in \mathbb{T}^2$, there is at most one eigenvalue of $A(U, k)$ in each connected component of $\rho(A_{1,1}(U, k)) \cap \mathbb{R}$.

3.2. Dispersion relation of dressed bound fermion pairs

By Theorem 3.1, $E : \mathbb{T}^2 \rightarrow \mathbb{R}$ is a continuous family of nondegenerate eigenvalues, generally (at least for $k \neq 0$) associated with exponentially localized eigenvectors. Note that the case $k = 0$ is particular when $\hat{v}(0) = 0$, since $E(0)$ is not an isolated eigenvalue of $A(U, 0)$. However, the family $(E(k))_{k \in \mathbb{T}^2}$ is still continuous. The peculiar behavior at $k = 0$ leads us to only consider total quasi-momenta in the subset

$$\mathbb{S}^2 \doteq (-\pi, \pi)^2 \setminus \{0\} \subseteq \mathbb{T}^2, \quad (46)$$

as, for instance, in Theorem 3.1 (iv).

Because of Proposition 2.1, the family $(E(k))_{k \in \mathbb{T}^2}$ can thus be seen as the effective dispersion relation of dressed bound fermion pairs. It is expected to determine transport properties of the quantum system at low temperatures. We now define in mathematical terms what a dispersion relation is.

First, a dispersion relation $\varkappa : \mathbb{T}^2 \rightarrow \mathbb{R}$ should be a functions mapping quasi-momenta $k \in \mathbb{T}^2$ on the torus to spectral values of the corresponding fibers. More precisely, $\varkappa(k)$ should be an isolated eigenvalue of the fiber associated with the total quasi-momentum k . Recall that the dispersion relation of a (nonrelativistic) particle in the d -dimensional continuum (that is, the particle moves in the continuum d -dimensional space \mathbb{R}^d), whose (isotropic) mass is m , is $k^2/2m$ and velocity $v(k) = k/m$, $k \in \mathbb{R}^d$. Having this standard example in mind, we would like also to derive from a dispersion relation a group velocity and a mass tensor, at any fixed quasi-momentum $k \in \mathbb{T}^2$, as is usual. These are key objects, for instance, in the study of transport properties. Notice that they require sufficient regularity of the dispersion relation to be defined.

Keeping in mind that all our quantities are parametrized by the on-site repulsion $U \in [0, \infty]$, we define a family of dispersion relations associated with the fiber Hamiltonians $A(U, k)$ as follows:

Definition 3.7 (Family of dispersion relations). A function $\varkappa : [0, \infty] \times \mathbb{T}^2 \rightarrow \mathbb{R}$ is said to be a family of dispersion relations $\varkappa(U, \cdot)$ if the following properties are satisfied for all $U \in [0, \infty]$:

- i.) For any $k \in \mathbb{T}^2$ and $U \in \mathbb{R}_0^+$, $\varkappa(U, k)$ is an eigenvalue of $A(U, k)$ and

$$\varkappa(\infty, k) = \lim_{U \rightarrow \infty} \varkappa(U, k).$$

- ii.) For all $U \in [0, \infty]$, $\varkappa(U, \cdot) \in C(\mathbb{T}^2)$ and is of class C^2 on the open set $\mathbb{S}^2 \subseteq \mathbb{R}^2$.

The first property is a very natural property, having in mind Proposition 2.1 and the theory of direct integrals (Theorem A.3). The second property of Definition 3.7 is needed to define *group velocities* and *mass tensors*.

To explain these two concepts, we need the Hessian of functions $f \in C^2(\mathbb{S}^2)$ at fixed k , which is denoted by

$$\text{Hess}(f)(k) \doteq \begin{pmatrix} \partial_{k_1}^2 f & \partial_{k_1} \partial_{k_2} f \\ \partial_{k_2} \partial_{k_1} f & \partial_{k_2}^2 f \end{pmatrix}(k) \in M_2(\mathbb{R}), \quad k \in \mathbb{S}^2, \quad (47)$$

where $M_2(\mathbb{R})$ is the set of 2×2 matrices with real coefficients. It is a straightforward consequence of the regularity of $f \in C^2(\mathbb{S}^2)$ that

$$\text{Hess}(f) : \mathbb{S}^2 \longrightarrow M_2(\mathbb{R})$$

is continuous. For any $f \in C^2(\mathbb{S}^2)$, we consider the set

$$\mathfrak{M}_f \doteq \{k \in \mathbb{S}^2 : \text{Hess}(f)(k) \in \text{GL}_2(\mathbb{R})\} \subseteq \mathbb{S}^2 \quad (48)$$

with $\text{GL}_2(\mathbb{R}) \subseteq \text{M}_2(\mathbb{R})$ being the set of invertible 2×2 matrices with real coefficients. As $\text{GL}_2(\mathbb{R}) \subseteq \text{M}_2(\mathbb{R})$ is an open set (see [50, Theorem 1.4]), it then follows that

$$\mathfrak{M}_f = \text{Hess}(f)^{-1}(\text{GL}_2(\mathbb{R}))$$

is also an open set.

We are now in a position to define group velocities and mass tensors of a family of dispersion relations.

Definition 3.8 (Group velocities and mass tensors). At any $U \in [0, \infty]$, the group velocity $\mathbf{v}_{\kappa, U} : \mathbb{S}^2 \rightarrow \mathbb{R}$ and the mass tensor $\mathbf{m}_{\kappa, U} : \mathfrak{M}_{\kappa(U, \cdot)} \rightarrow \text{M}_2(\mathbb{R})$ associated with a family $\kappa : [0, \infty] \times \mathbb{T}^2 \rightarrow \mathbb{R}$ of dispersion relations are respectively defined by

$$\mathbf{v}_{\kappa, U}(k) \doteq \vec{\nabla}_k \kappa(U, k) \quad \text{and} \quad \mathbf{m}_{\kappa, U}(k) \doteq \text{Hess}(\kappa(U, \cdot))(k)^{-1}.$$

We deduce from Theorem 4.9 that E is a dispersion relation when the function $v : \mathbb{Z}^2 \rightarrow \mathbb{R}$ is at least 2 times continuously differentiable and, in this case, we can even compute the group velocity via the characteristic equation (Theorem 3.6).

Theorem 3.9 (Dispersion relations of dressed bound fermion pairs). Fix $\epsilon \in \mathbb{R}_0^+$ and $h_b \in [0, 1/2]$. Assume that $\hat{v} \in C^2(\mathbb{S}^2)$.

- i.) Then, $E : [0, \infty] \times \mathbb{T}^2 \rightarrow \mathbb{R}$ given by Theorems 3.1 and 3.5 is a family of dispersion relations.
- ii.) The associated group velocities are equal to

$$\mathbf{v}_{E, U}(k) = \left(\hat{v}(k)^2 \partial_x \mathfrak{T}(U, k, x) + 1 \right)^{-1} \vec{\nabla} \left(\hat{v}(k)^2 \mathfrak{T}(U, k, x) - \mathfrak{b}(k) \right) \Big|_{x=E(U, k)}$$

for any $U \in [0, \infty]$ and $k \in \mathbb{S}^2$, with

$$\mathbf{v}_{E, \infty}(k) = \lim_{U \rightarrow \infty} \mathbf{v}_{E, U}(k), \quad k \in \mathbb{S}^2.$$

- iii.) If \hat{v} is real analytic on \mathbb{S}^2 , then, for any $U \in [0, \infty]$, either $\mathfrak{M}_{E(U, \cdot)}$ has full measure or $\mathfrak{M}_E = \emptyset$. In particular, the tensor masses $\mathbf{m}_{E, U}$ are either defined almost everywhere in \mathbb{S}^2 or not defined at all.

Proof. Use Corollaries 4.10 and 4.17. □

Similar to Remark 3.2, if for some strictly positive constant $\gamma > 0$,

$$\sum_{x \in \mathbb{Z}^2} e^{\gamma|x|} |\nu(x)| < \infty,$$

then the Fourier transform \hat{v} of the function $v : \mathbb{Z}^2 \rightarrow \mathbb{R}$, as defined via (31), is real analytic on the whole torus \mathbb{T}^2 . It is very natural to expect a local interaction between fermion pairs and bosons in (10), meaning here that the function v should even have finite support. In particular, all conditions of Theorem 3.9, including the ones of the third assertion, should hold true in the application to superconducting cuprates.

In fact, as shown in [21], the dispersion relation of Theorem 3.9 yields the formation of d -wave pairs when one adjusts the parameters of the model (with $u = 0$) to fit those of cuprate superconductors – in particular, the ones of the cuprate $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ (LaSr 214) near optimal doping. When considering the usual Hubbard model – that is, the case where there is no other fermionic repulsion than the on-site

one (i.e., $u = 0$) and no fermion-boson exchange (i.e., $v = 0$) – E turns out to be the function $\mathfrak{b} : \mathbb{T}^2 \rightarrow \mathbb{R}$, defined by (32), which is nothing else than the dispersion relation

$$\mathfrak{b}(k) \doteq h_b \epsilon(2 - \cos(k)), \quad k \in \mathbb{T}^2,$$

of free bosons (bipolarons for cuprates).

By turning on the fermion-boson-exchange interaction, the dispersion relation of dressed bound fermion pairs with lowest energy can strongly deviate from \mathfrak{b} , the unperturbed one. Recall, for instance, that \mathfrak{b} describes bosons with a very large mass as compared to the effective mass of electrons or holes in cuprates. However, as shown in [21], for typical parameters of the cuprate LaSr 214, the effective mass of the bound pair (with dispersion relation E) is comparable to the mass of electrons or holes. This is a consequence of the mass of charge carriers calculated in [52], and the fact that a large effective mass of dressed bound fermion pairs and a high fermion-pair depletion,¹³ close to 90% as measured in [53], is not compatible with our model. This solves the so-called ‘large mass paradox’ of the microscopic theory of cuprate superconductors, based on some kind mechanism involving bipolarons. For more details, see [21] and references therein.

In fact, the effective mass of dressed bound fermion pairs, or more generally its (effective) mass tensor, depends strongly on the coupling function \hat{v} near its maximum. Bearing in mind Definitions 3.7 and 3.8, one can therefore provide via Theorems 3.6 and 3.8 not only qualitative but also quantitative information, which is important for describing the physical behavior of fermionic pairs formed in this way by means of a bosonic field. A natural question is then to study its scattering properties and this is precisely what we propose to do in the next section.

3.3. Quantum scattering

Scattering in quantum mechanics constitutes a well-established mathematical theory aiming at analyzing the behavior of quantum systems at large times. To this end, a reference (or free) Hamiltonian Y is chosen and the dynamics $(e^{itX})_{t \in \mathbb{R}}$ of the quantum system driven by the (full) Hamiltonian X is compared at large (negative and positive) times to $(e^{itY})_{t \in \mathbb{R}}$. In fact, scattering theory can be viewed as a kind of perturbation theory for the absolutely continuous spectrum of X . See, for example, [40, Chapter X]. For standard textbooks explaining in detail the scattering theory, we recommend [41, 42, 43]. Below, for the reader’s convenience, we shortly recall definitions that are relevant here.

Take two bounded self-adjoint operators X and Y acting on two Hilbert spaces \mathcal{X} and \mathcal{Y} , respectively. Let $P_{\text{ac}}(Y)$ be the orthogonal projection onto the absolutely continuous space of Y , which is defined as follows:

$$\begin{aligned} \text{ran}(P_{\text{ac}}(Y)) \doteq \{ \psi \in \mathcal{Y} : \langle \psi, \chi_{(\cdot)}(Y) \psi \rangle_{\mathcal{Y}} \text{ is absolutely continuous} \\ \text{with respect to the Lebesgue measure} \}, \end{aligned} \quad (49)$$

where χ_{Ω} is its characteristic function¹⁴ of any Borel set $\Omega \subseteq \mathbb{R}$. The so-called *wave operators* for the pair (X, Y) with *identification operator* $J \in \mathcal{B}(\mathcal{Y}, \mathcal{X})$ is, by definition, the strong limit

$$W^{\pm}(X, Y; J) \doteq s - \lim_{t \rightarrow \pm\infty} e^{itX} J e^{-itY} P_{\text{ac}}(Y), \quad (50)$$

when it exists. See, for instance, [43, Definition 1.3]. When $\mathcal{Y} = \mathcal{X}$ and $J = \mathbf{1}$, like in (43, Definition 1.1), we use the shorter notation

$$W^{\pm}(X, Y) \equiv W^{\pm}(X, Y; \mathbf{1}) \doteq s - \lim_{t \rightarrow \pm\infty} e^{itX} e^{-itY} P_{\text{ac}}(Y). \quad (51)$$

¹³I.e., the fermionic component of the dressed bound fermion pairs is very small in comparison with the bipolaronic component.

¹⁴ $\chi_{\Omega}(x) = 1$ for $x \in \Omega$ and $\chi_{\Omega}(x) = 0$ otherwise.

In case the above wave operators exist, they are partial isometries [41, Proposition 1, Sect. XI.3]. They are said to be *complete* when

$$\operatorname{ran}(W^+(X, Y)) = \operatorname{ran}(W^-(X, Y)) = \operatorname{ran}(P_{\text{ac}}(X)).$$

See [41, p. 19, Sect. XI.3].

Similarly, in the general case, $W^\pm(X, Y; J)$ are said to be complete whenever

$$\overline{\operatorname{ran}(W^+(X, Y; J))} = \overline{\operatorname{ran}(W^-(X, Y; J))} = \operatorname{ran}(P_{\text{ac}}(X)).$$

See [41, p. 35, Sect. XI.3]. The corresponding scattering operator is equal to

$$S(X, Y; J) \doteq W^+(X, Y; J)^* W^-(X, Y; J) \in \mathcal{B}(\mathcal{Y}). \quad (52)$$

It leads to the scattering matrix (or simply S -matrix) in a representation where Y is diagonal, because the scattering operator commutes with Y . See [43, Equation (1.12)].

Remark 3.10. For two bounded self-adjoint operators X and Y acting on two Hilbert spaces \mathcal{X} and \mathcal{Y} , note¹⁵ that

$$\operatorname{ran}(P_{\text{ac}}(X \oplus Y)) = \operatorname{ran}(P_{\text{ac}}(X)) \oplus \operatorname{ran}(P_{\text{ac}}(Y)).$$

This is an elementary observation used to study the scattering channels in Section 4.6.

In our framework, the Hamiltonian X is the bounded self-adjoint operator

$$\mathbb{U}H\mathbb{U}^* = \int_{\mathbb{T}^2}^{\oplus} A(k) \nu(dk)$$

of Proposition 2.1, which acts on the Hilbert space $L^2(\mathbb{T}^2, \mathcal{H})$. Below, two different (reference) Hamiltonians Y are taken into account, corresponding to two scattering channels: the *unbound* and *bound* pair channels. For cuprates, the first channel should be associated with the high temperature regime, while the second one is related to sufficiently low temperatures.

3.3.1. Unbound pair scattering channel

Far apart from each other, two fermions only experience a very weak repulsion force due to the extended Hubbard interaction while the probability that they bind together to form a boson is also very small. Thus, in this situation, one expects that the dynamics of such a pair is governed by the fermionic part, and even by the hopping term alone. During intermediate times, they could of course interact, as they may get close to each other, and they could even be bound together via the effective attraction caused by fermion-boson exchange processes. The lifetime of bound fermions should, however, be finite in this situation, and they are expected to be released at some point and behave again as two free fermions that go far apart from each other for large times. See Figure 2. We show below that this heuristics can be put in precise mathematical terms.

To this end, define the Hilbert space

$$\mathfrak{H}_f \doteq L^2\left(\mathbb{T}^2, L^2\left(\mathbb{T}^2\right), \nu\right) \doteq \int_{\mathbb{T}^2}^{\oplus} L^2\left(\mathbb{T}^2, \mathbb{C}, \nu\right) \nu(dk) \quad (53)$$

¹⁵To show this property, take any Borel set $\Omega \subseteq \mathbb{R}$ and observe that $\langle (\varphi, \psi), \chi_\Omega(X \oplus Y)(\varphi, \psi) \rangle_{\mathcal{X} \oplus \mathcal{Y}} = \langle \varphi, \chi_\Omega(X)\varphi \rangle_{\mathcal{X}} + \langle \psi, \chi_\Omega(Y)\psi \rangle_{\mathcal{Y}}$. Since $\chi_\Omega(X)$ and $\chi_\Omega(Y)$ are positive operators, the left-hand side of the last expression is zero iff each term in the right-hand side is zero.

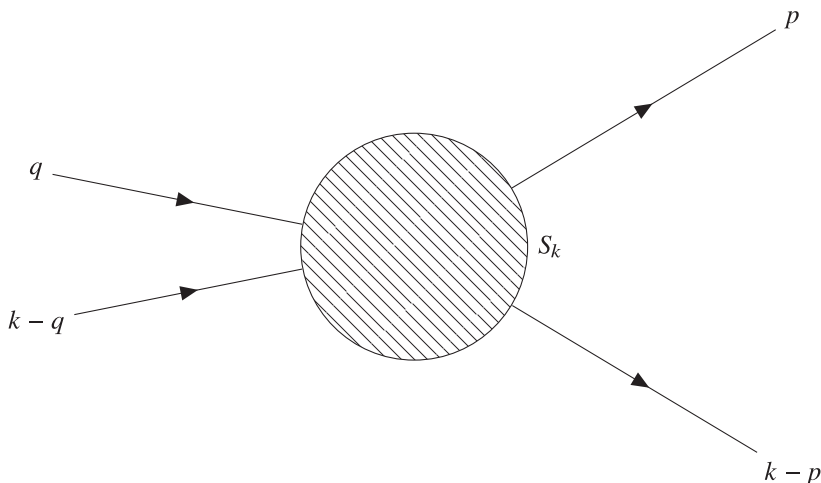


Figure 2. Illustration of the unbound pair scattering channel: Two free fermions of (quasi-) momentum $k - p$ and q respectively (i.e., the full momentum of the fermionic pair is k) at time $t = -\infty$ interact in finite time with the composite system – in particular with the bosonic field – to be asymptotically free again at time $t = +\infty$, thanks to Theorem 3.11. Here, $S_k = S(A(k), (M_{\mathfrak{f}(k)} + R(V, v)) \oplus A_{2,2}(k))$ is the scattering operator of this process in each fiber k , which depends explicitly on $\hat{v}(k)$. See Theorem 3.13 and the example given by Equations (63)–(64).

as well as the Hamiltonian

$$H_f \equiv H_f(V, v) \doteq \int_{\mathbb{T}^2}^{\oplus} (M_{\mathfrak{f}(k)} + R(V, v)) v(dk) \in \mathcal{B}(\mathfrak{H}_f) \quad (54)$$

for any $V \in \mathbb{R}_0^+$ and absolutely summable function $v : \mathbb{Z}^2 \rightarrow \mathbb{R}_0^+$, where

$$R(V, v) \doteq \sum_{x \in \mathbb{Z}^2} v(x) P_x + VP_0 \in \mathcal{B}(L^2(\mathbb{T}^2)), \quad (55)$$

$M_{\mathfrak{f}(k)}$ being the fiber Hamiltonian defined as the multiplication operator by $\mathfrak{f}(k) \in C(\mathbb{T}^2)$ (see (33)) while P_x is the orthogonal projection onto the one-dimensional subspace $\mathbb{C}\hat{e}_x \subseteq L^2(\mathbb{T}^2)$. Observe then that

$$\mathbb{U}H\mathbb{U}^* - \begin{pmatrix} H_f & 0 \\ 0 & 0 \end{pmatrix} = \int_{\mathbb{T}^2}^{\oplus} \begin{pmatrix} \sum_{x \in \mathbb{Z}^2} (u(x) - v(x)) P_x + (U - V)P_0 & A_{1,2}(k) \\ A_{2,1}(k) & A_{2,2}(k) \end{pmatrix} v(dk).$$

Compare indeed (54) with Equations 42–37 and Proposition 2.1. By Lemma 4.21, note that $P_{\text{ac}}(H_f) = \mathbf{1}$.

Let us consider the identification operator $\mathfrak{U} : \mathfrak{H}_f \rightarrow L^2(\mathbb{T}^2, \mathcal{H})$ defined for any purely fermionic state $\psi \in \mathfrak{H}_f$ by

$$\begin{aligned} \mathfrak{U}\psi : \mathbb{T}^2 &\rightarrow \mathcal{H} \doteq L^2(\mathbb{T}^2) \oplus \mathbb{C} \\ k &\mapsto (\psi(k), 0) \end{aligned} \quad (56)$$

See Equation (25). Note that \mathfrak{U} is an isometry (i.e., a norm preserving linear transformation). In fact, it is the canonical fiberwise inclusion of \mathfrak{H}_f into $L^2(\mathbb{T}^2, \mathcal{H})$. Recall from Proposition 2.1 that $A(U, \cdot)$, defined by (37)–(42), is the fiber decomposition of the operator $\mathbb{U}H\mathbb{U}^*$. Then, we obtain wave and scattering operators with respect to fermionic parts:

Theorem 3.11 (Unbound pair (scattering) channel). *Let $V \in \mathbb{R}_0^+$ and $v : \mathbb{Z}^2 \rightarrow \mathbb{R}_0^+$ be any absolutely summable function.*

i.) *The wave operators, as defined by (50) for $X = \mathbb{U}H\mathbb{U}^*$, $Y = H_f$ and $J = \mathfrak{U}$, satisfy*

$$W^\pm(\mathbb{U}H\mathbb{U}^*, H_f; \mathfrak{U}) = \left(\int_{\mathbb{T}^2}^\oplus W^\pm(A(k), (M_{\mathfrak{f}(k)} + R(V, v)) \oplus A_{2,2}(k)) v(dk) \right) \mathfrak{U} \quad (57)$$

with range equal to

$$\text{ran}(W^\pm(\mathbb{U}H\mathbb{U}^*, H_f; \mathfrak{U})) = \int_{\mathbb{T}^2}^\oplus L^2(\mathbb{T}^2) \oplus \{0\} v(dk). \quad (58)$$

ii.) *The scattering operator, as defined by (52) for $X = \mathbb{U}H\mathbb{U}^*$, $Y = H_f$ and $J = \mathfrak{U}$, equals*

$$S(\mathbb{U}H\mathbb{U}^*, H_f; \mathfrak{U}) = \mathfrak{U}^* \left(\int_{\mathbb{T}^2}^\oplus S(A(k), (M_{\mathfrak{f}(k)} + R(V, v)) \oplus A_{2,2}(k)) v(dk) \right) \mathfrak{U}.$$

Proof. Observe that the operator difference $(\mathbb{U}H\mathbb{U}^* - H_f)$ is not trace-class (it is not even compact) and, thus, the existence of this scattering channel is not a direct consequence of the well-known Kato-Rosenblum theorem [41, Theorem XI.8]. In fact, one of the main steps of the proof is to show that this difference is the direct integral of a strongly measurable family of trace-class operators. By this means, we are then able to apply the Kato-Rosenblum theorem ‘fiberwise’ to deduce the first assertion. See Section 4.6.1 for more details – in particular, Theorem 4.23. Assertion (ii) is a direct consequence of Assertion (i) together with the theory of direct integrals. \square

Remark 3.12. If one would like to go back to the original Hilbert space \mathfrak{h}_0 (19) for fermion pairs with opposite spins – that is, if one wishes to use space coordinates, instead of the quasi-momenta – then one employs Theorem 3.11, along with the observation that

$$W^\pm(H, U_f^* H_f U_f; \mathbb{U}^* \mathfrak{U} U_f) = U^* W^\pm(\mathbb{U}H\mathbb{U}^*, H_f; \mathfrak{U}) U_f,$$

where U_f is defined by (28). See also Equation (26) and Proposition 2.1.

Theorem 3.11 refers to the unbound pair (scattering) channel. The subspace $\mathfrak{H}_f \subseteq \mathfrak{H}$ corresponds to the ‘incoming’ (+) and ‘outcoming’ (−) scattering states of the quantum system, in this particular scattering channel. Physically, this theorem shows, among other things, that the bosonic component of e^{itH} vanishes on this channel, as $t \rightarrow \pm\infty$. This is a direct consequence of Equation (58).

In addition, Equation (57) gives an explicit fiber decomposition of wave operators with respect to the purely fermionic Hamiltonian in terms of k -dependent wave operators defined naturally from the fiber decomposition of the operator $\mathbb{U}H\mathbb{U}^*$. Mutatis mutandis for the scattering operator, thanks to Theorem 3.11 (ii). In other words, the knowledge of scattering properties of each fiber, almost everywhere, entirely determines the scattering properties of the composite system, made of two fermions and one boson. We can now use this property (i.e., Theorem 3.11) to obtain a more computable expression for the wave and scattering operators in each given fiber. This can be done via infinite series (perturbative expansions), thanks to Corollary A.2.

Below, we give an example of such a computation by taking $U = V \in \mathbb{R}_0^+$ and $v = u : \mathbb{Z}^2 \rightarrow \mathbb{R}_0^+$ in Theorem 3.11. With this particular choice, the unbound pair channel allows one to isolate the fermion-boson exchange mechanism, which in terms of Hamiltonians refers to the use of off-diagonal operators

$$B^{(t)}(k) \doteq \begin{pmatrix} 0 & B_{1,2}^{(t)}(k) \\ B_{2,1}^{(t)}(k) & 0 \end{pmatrix} \in \mathcal{B}(\mathcal{H}), \quad t \in \mathbb{R}, k \in \mathbb{T}^2, \quad (59)$$

in the fibers, where, for any $t \in \mathbb{R}$ and $k \in \mathbb{T}^2$,

$$B_{1,2}^{(t)}(k) \doteq e^{itA_{1,1}(\mathbf{U},k)} A_{1,2}(k) e^{-itA_{2,2}(k)} \quad \text{and} \quad B_{2,1}^{(t)}(k) \doteq e^{itA_{2,2}(k)} A_{2,1}(k) e^{-itA_{1,1}(\mathbf{U},k)}. \quad (60)$$

Recall that, for $m, n \in \{1, 2\}$, $A_{m,n}(k)$ is defined by (37)–(41). Below, $B_{m,n}(k)$, $m \neq n$, stands for the norm-continuous family of operators $(B_{m,n}^{(t)}(k))_{t \in \mathbb{R}}$.

To shorten the notation, for any $s, t \in \mathbb{R}$, as well as two norm-continuous families $X \equiv (X_t)_{t \in \mathbb{R}}$ and $Y \equiv (Y_t)_{t \in \mathbb{R}}$ of bounded operators $X_t : \mathcal{X} \rightarrow \mathcal{Y}$ and $Y_t : \mathcal{Y} \rightarrow \mathcal{X}$ on two Hilbert spaces \mathcal{X} and \mathcal{Y} , respectively, we define the bounded operators:

$$\cos_{>}(XY; s, t) \doteq \mathbf{1} + \sum_{p=1}^{\infty} (-1)^p \int_s^t d\tau_1 \cdots \int_s^{\tau_{2p-1}} d\tau_{2p} (X_{\tau_1} Y_{\tau_2}) \cdots (X_{\tau_{2p-1}} Y_{\tau_{2p}}), \quad (61)$$

$$\sin_{>}(XY; s, t) \doteq \int_s^t d\tau X_{\tau} + \sum_{p=1}^{\infty} (-1)^p \int_s^t d\tau_1 \cdots \int_s^{\tau_{2p}} d\tau_{2p+1} X_{\tau_1} \left((Y_{\tau_2} X_{\tau_3}) \cdots (Y_{\tau_{2p}} X_{\tau_{2p+1}}) \right). \quad (62)$$

The integrals above are Riemann ones, noting that $(X_t)_{t \in \mathbb{R}}$ and $(Y_t)_{t \in \mathbb{R}}$ are continuous families in Banach spaces – namely, $\mathcal{B}(\mathcal{X}; \mathcal{Y})$ and $\mathcal{B}(\mathcal{Y}; \mathcal{X})$, respectively. Note that $\cos_{>}(XY; s, t) \in \mathcal{B}(\mathcal{Y})$ and $\sin_{>}(XY; s, t) \in \mathcal{B}(\mathcal{X}; \mathcal{Y})$ are always absolutely summable series in the operator norm. Then, we obtain the following results:

Theorem 3.13 (Scattering operators as perturbative series). *Let $\varepsilon \in \mathbb{R}^+$ and $H_f \equiv H_f(\mathbf{U}, \mathbf{u})$. Then, for any $\varphi \in \mathfrak{H}_f$, there is $T > 0$ such that*

$$\begin{aligned} T < t &\implies \|(W^+(\mathbf{U}H\mathbf{U}^*, H_f; \mathbf{U}) - V_{0,t}\mathbf{U})\varphi\|_{\mathcal{X}} \leq \varepsilon, \\ t < -T &\implies \|(W^-(\mathbf{U}H\mathbf{U}^*, H_f; \mathbf{U}) - V_{0,t}\mathbf{U})\varphi\|_{\mathcal{X}} \leq \varepsilon, \end{aligned}$$

Moreover, for any $\varphi, \psi \in \mathfrak{H}_f$, there is $T > 0$ such that

$$s < -T < T < t \implies \langle \psi, S(\mathbf{U}H\mathbf{U}^*, H_f; \mathbf{U})\varphi \rangle_{\mathcal{X}} = \langle \mathbf{U}\psi, V_{t,s}\mathbf{U}\varphi \rangle_{\mathcal{X}} + \mathcal{O}(\varepsilon),$$

where, for all $s, t \in \mathbb{R}$,

$$V_{t,s} \doteq \int_{\mathbb{T}^2}^{\oplus} \begin{pmatrix} \cos_{>}(B_{1,2}(k)B_{2,1}(k); s, t) & -i \sin_{>}(B_{1,2}(k)B_{2,1}(k); s, t) \\ -i \sin_{>}(B_{2,1}(k)B_{1,2}(k); s, t) & \cos_{>}(B_{2,1}(k)B_{1,2}(k); s, t) \end{pmatrix} \nu(dk).$$

Proof. It suffices to combine Lemma 4.24 with Equation (141) and Theorem 3.11, similar to Corollary A.2. \square

Theorem 3.13 provides a way to approximate the scattering matrix associated with the fermion-boson-exchange interaction. Note for instance from (37)–(41) that the operator $B_{1,2}^{(t)}(k)B_{2,1}^{(s)}(k)$ and $B_{2,1}^{(t)}(k)B_{1,2}^{(s)}(k)$ have a relatively simple form for any $s, t \in \mathbb{R}$ and $k \in \mathbb{T}^2$:

$$B_{1,2}^{(t)}(k)B_{2,1}^{(s)}(k) = \left(\hat{v}(k)^2 e^{i(s-t)\mathbf{b}(k)} \right) e^{itA_{1,1}(\mathbf{U},k)} P_{\mathbf{d}(k)} e^{-isa:1,1(\mathbf{U},k)}, \quad (63)$$

$$B_{2,1}^{(t)}(k)B_{1,2}^{(s)}(k) = \left(\hat{v}(k)^2 e^{i(t-s)\mathbf{b}(k)} \right) \left\langle \mathbf{d}(k), e^{i(s-t)A_{1,1}(\mathbf{U},k)} \mathbf{d}(k) \right\rangle, \quad (64)$$

where $P_{\mathbf{d}(k)}$ is the orthogonal projection onto the one-dimensional subspace $\mathbb{C}\mathbf{d}(k) \subseteq L^2(\mathbb{T}^2)$. Similar computations can be done for other choices of $\mathbf{V} \in \mathbb{R}_0^+$ and $\mathbf{v} : \mathbb{Z}^2 \rightarrow \mathbb{R}_0^+$ in Theorem 3.11, like $\mathbf{V} = 0 = \mathbf{v}$ (noninteracting fermion systems). See again Corollary A.2.

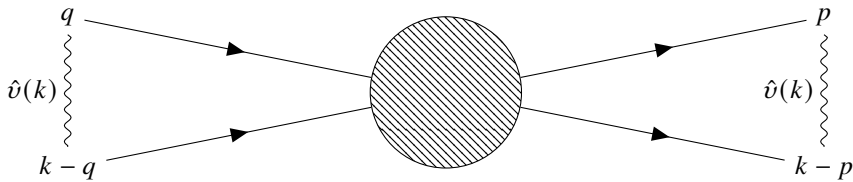


Figure 3. Illustration of the bound pair scattering channel. Here, k is the full (quasi-)momentum of the (exponentially localized) dressed bound fermion pairs. The oscillating vertical lines between the two fermions (e.g., electrons) before the scattering process and afterwards characterize their bound via a bosonic (e.g., bipolaronic) particle transfer with coupling function $\hat{v}(k)$; see Figure 1. It illustrates the stability of these pairs of fermions in time, as expressed by Theorem 3.14, that is, the pairs cannot decay into an (even only asymptotically) unbound pair of fermions.

The understanding of this kind of scattering, regarding free fermion (electron) collisions, is relevant in physics, because it can allow the exchange function v of a real system to be studied. It is therefore important to have a model from which not only qualitative, but also quantitative, information can be obtained. This is the purpose of this section, in particular of Theorem 3.11, which gives the explicit dependency of scattering in terms of v .

3.3.2. Bound pair scattering channel

Similarly, we also prove the existence of a scattering channel for dressed bound pairs. As dressed bound pairs are space-localized objects (see, for example, Theorem 3.1 (iii)), the fermions forming the pair efficiently exchange a boson, at a non-negligible rate, via the terms $W_{b \rightarrow f}$ (9) and $W_{f \rightarrow b}$ (17) in the Hamiltonian H . In particular, such quantum states must have some non-negligible bosonic component representing the exchanged boson that ‘glues’ the two fermions together. This dressed bound pair is however expected to move like a free (quantum spinless) particle in the real space. See Figure 3. We translate this physical heuristics in precise mathematical terms by considering the effective dispersion relations

$$E : [0, \infty] \times \mathbb{T}^2 \rightarrow \mathbb{R}$$

given by Theorems 3.1, 3.5 and 3.9.

For any $U \in \mathbb{R}_0^+ \cup \{\infty\}$, we consider the identification operator

$$\mathfrak{P}_U : L^2(\mathbb{T}^2) \rightarrow L^2(\mathbb{T}^2, \mathcal{H})$$

defined for any $\varphi \in L^2(\mathbb{T}^2)$ by¹⁶

$$\begin{aligned} \mathfrak{P}_U \varphi : \mathbb{T}^2 \setminus \{0\} &\rightarrow \mathcal{H} \doteq L^2(\mathbb{T}^2) \oplus \mathbb{C} \\ k &\mapsto \varphi(k) \|\Psi(U, k)\|^{-1} \Psi(U, k), \end{aligned} \quad (65)$$

where $\Psi(U, k)$ is the eigenvector associated with the (nondegenerate) eigenvalue $E(U, k)$, as given by Theorems 3.1, 3.5 and 3.9. Note from Theorem 3.1 that the mapping

$$k \mapsto \|\Psi(U, k)\|^{-1} \Psi(U, k)$$

¹⁶Despite the fact that $E(0)$ might not be in the resolvent set of $A_{1,1}(U, 0)$, we can simply ignore it for $\{k = 0\}$ has null Lebesgue measure.

is continuous on \mathbb{T}^2 for any $U \in \mathbb{R}_0^+$, and its pointwise limit

$$k \mapsto \|\Psi(\infty, k)\|^{-1} \Psi(\infty, k)$$

(cf. Theorem 3.5) is therefore measurable. In particular, the linear transformation \mathfrak{P}_U is well-defined for any $U \in \mathbb{R}_0^+ \cup \{\infty\}$. Moreover, one checks that it is norm-preserving.

Since $E(U, \cdot) \in C(\mathbb{T}^2; \mathbb{R}) \subseteq L^\infty(\mathbb{T}^2, \nu)$ (see Theorems 3.1 (iv) and 3.5), we can consider the multiplication operator by $E(U, \cdot)$ on $L^2(\mathbb{T}^2)$, which is denoted by

$$M_{E(U, \cdot)} \doteq \int_{\mathbb{T}^2}^{\oplus} E(U, k) \nu(dk), \quad U \in \mathbb{R}_0^+ \cup \{\infty\}. \quad (66)$$

Remark also from Theorems 3.1 (iv) and 3.5 together with Corollary A.5 that $P_{ac}(M_{E(U, \cdot)}) = \mathbf{1}$ whenever \hat{v} is real analytic on \mathbb{S}^2 . We then study now the (dressed) bound pair scattering channel, which is much simpler than in the unbound pair channel:

Theorem 3.14 (Bound pair (scattering) channel). *Let $h_b \in [0, 1/2]$. Then the following assertions hold true:*

i.) *Dynamics and wave operators at finite $U \in \mathbb{R}_0^+$:*

$$e^{itUH U^*} \mathfrak{P}_U = \mathfrak{P}_U e^{itM_{E(U, \cdot)}}, \quad t \in \mathbb{R}.$$

ii.) *Dynamics in the hard-core limit $U \rightarrow \infty$:*

$$s - \lim_{U \rightarrow \infty} \mathfrak{P}_U = \mathfrak{P}_\infty \quad \text{and} \quad s - \lim_{U \rightarrow \infty} e^{itUH U^*} \mathfrak{P}_U = \mathfrak{P}_\infty e^{itM_{E(\infty, \cdot)}}, \quad t \in \mathbb{R}.$$

Proof. Assertion (i) is Proposition 4.25. Assertion (ii) results from Proposition 4.26. \square

From Theorem 3.14, (i) the scattering channel is time independent. For instance, for any $U \in \mathbb{R}_0^+$, one trivially checks that

$$W^\pm(UH U^*, M_{E(U, \cdot)}; \mathfrak{P}_U) = \mathfrak{P}_U P_{ac}(M_{E(U, \cdot)}),$$

and since $\mathfrak{P}_U^* \mathfrak{P}_U = \mathbf{1}$ and P_{ac} is a projection, its scattering operator is equal to

$$S(UH U^*, M_{E(U, \cdot)}; \mathfrak{P}_U) = P_{ac}(M_{E(U, \cdot)}).$$

If \hat{v} is additionally real analytic on \mathbb{S}^2 , then $P_{ac}(M_{E(U, \cdot)}) = \mathbf{1}$, thanks to Theorem 3.1 and Corollary A.5. In this case, the wave and scattering operators are given by

$$W^\pm(UH U^*, M_{E(U, \cdot)}; \mathfrak{P}_U) = \mathfrak{P}_U \quad \text{and} \quad S(UH U^*, M_{E(U, \cdot)}; \mathfrak{P}_U) = \mathbf{1}$$

for any $U \in \mathbb{R}_0^+$. Their hard-core limit are then also trivial, thanks to Theorem 3.14 (ii).

This scattering channel is therefore easy to study. In particular, similar to Remark 3.12, we can easily go back to the original Hilbert space \mathfrak{h}_0 (19), referring to space coordinates instead of the quasi-momenta. With this aim, we first observe that, for any $U \in \mathbb{R}_0^+$,

$$e^{itH} \mathcal{P}_U = \mathcal{P}_U e^{itU_f^* M_{E(U, \cdot)} U_f}, \quad t \in \mathbb{R}, \quad (67)$$

where $\mathcal{P}_U \in \mathcal{B}(\mathfrak{h}_0, \mathfrak{H})$ is the new identification operator

$$\mathcal{P}_U \doteq U^* \mathfrak{P}_U U_f, \quad U \in \mathbb{R}_0^+,$$

and $U_f \doteq U_2 U_1$. See Equations (26)–(28) and Proposition 2.1.

On the one hand, Equation (67) together with Theorem 3.9 shows that $E(U, \cdot)$ defines (a family of) dispersion relations, in the sense of Definition 3.7. The Fourier transform of $E(U, \cdot)$ is the (effective) hopping strength for the (spatially localized) dressed bound pairs. On the other hand, the new identification operator \mathcal{P}_U is translation invariant, that is,

$$\mathcal{P}_U \theta_x = \Theta_x \mathcal{P}_U, \quad x \in \mathbb{Z}^2,$$

where, for any fixed $x \in \mathbb{Z}^2$, $\theta_x \in \mathcal{B}(\mathfrak{h}_0)$ and $\Theta_x \in \mathcal{B}(\mathfrak{H})$ are the unique unitary operators respectively satisfying

$$\theta_x(\mathbf{e}_{(y,\uparrow)} \wedge \mathbf{e}_{(z,\downarrow)}) = \mathbf{e}_{(y+x,\uparrow)} \wedge \mathbf{e}_{(z+x,\downarrow)}, \quad y, z \in \mathbb{Z}^2,$$

(see Equations (19)) and

$$\Theta_x(\psi \oplus \varphi) = (\theta_x \psi) \oplus \varphi(x + \cdot), \quad \psi \in \mathfrak{h}_0, \varphi \in \ell^2(\mathbb{Z}^2).$$

See Equations (20). In addition, when $\hat{v}(0) \neq 0$, Theorem 3.1 (iii) shows that the (dressed) fermion pair in the bound pair channel is exponentially localized in space; that is, the associate fermion-fermion correlation function decays exponentially fast with respect to the distance between the fermions, uniformly in time. Note that it is not required that the range of \mathcal{P}_U has a vanishing bosonic component, because of the expected presence of ‘gluing bosons’ in the *dressed* bound fermionic pair.

As a consequence, the bound channel describes an effective system of free localized, spinless quasi-particles which minimize the energy at any fixed total quasi-momentum. In particular, such quasi-particles of lowest energy, or dressed fermion pairs, are stable in time; that is, they cannot decay into an (even only asymptotically) unbound pair of fermions. Conversely, we also show in Section 3.3.1 that a pair of fermions that is asymptotically unbound far in the past is not able to bind together to form a stable bound pair in the distant future.

Nevertheless, these quasi-particles should only be stable with respect to *external* perturbations as soon as their states are related to quasi-momenta k such that $E(U, k) < 0$. If the (dressed) quasi-particle is in a state whose support contains fibers k such that $E(U, k) \geq 0$, it is not in the most energetically favorable state, since

$$\min \sigma_{\text{ess}}(A(U, 0)) = 0$$

(see Theorem 3.1). In fact, if the component corresponding to quasi-momenta k such that $E(U, k) \geq 0$ has nonvanishing Lebesgue measure, then the quasi-particle should be instable with respect to *external* perturbations, by possibly creating unbounded fermions with small quasi-momenta to decrease its total energy. This situation clearly appears for quasi-momenta $k \in \mathbb{T}^2$ such that $\hat{v}(k) = 0$ or sufficiently small $|\hat{v}(k)| \ll 1$ when $k \neq 0$, since in these two cases, either $E(U, k) = \mathfrak{b}(k)$ ($\hat{v}(k) = 0$) or $E(U, k) \simeq \mathfrak{b}(k)$ ($|\hat{v}(k)| \ll 1$) with $\mathfrak{b}(k) \doteq h_b \epsilon(2 - \cos(k))$ (see (32)). If such a decay process really occurs, one should see critical quasi-momenta, like in physical superconductors.

To prevent from this situation, one needs sufficiently strong $|\hat{v}(k)| \gg 1$ to have $E(U, k) < 0$ for all $k \in \mathbb{T}^2$. In the position space, this means that the exchange strength between the two fermions and the boson, represented by the function $v : \mathbb{Z}^2 \rightarrow \mathbb{R}$ appearing in (9)–(17), has to be sufficiently strong and localized, like in Remark 3.2, in order to get a sufficiently strong ‘gluing effect’ for dressed pairs, at all quasi-momenta. Recall also that the boson should be heavier than the two fermions (i.e., $h_b \in [0, 1/2]$).

Last but not least, all this discussion can be extended to the hard-core limit $U \rightarrow \infty$, in view of Theorems 3.9 and 3.14 (ii).

4. Technical results

4.1. Notation

The purpose of this section is to fix (or recall) the notation and terminology that is used throughout the rest of the article. Let \mathcal{X} be any complex Hilbert space. We denote its scalar product by $\langle \cdot, \cdot \rangle_{\mathcal{X}}$, with the convention that it is antilinear in the first argument and linear in the second one. The norm of \mathcal{X} is thus

$$\|\varphi\|_{\mathcal{X}} \doteq \sqrt{\langle \varphi, \varphi \rangle_{\mathcal{X}}}, \quad \varphi \in \mathcal{X}.$$

When there is no danger of confusion, as already said in Remark 1.2, we usually omit the subscript referring to the Hilbert space and write $\|\cdot\|$ for $\|\cdot\|_{\mathcal{X}}$ and $\langle \cdot, \cdot \rangle$ for $\langle \cdot, \cdot \rangle_{\mathcal{X}}$.

Recall that $\mathcal{B}(\mathcal{X})$ denotes the set of bounded (linear) operators on \mathcal{X} . $\mathbf{1} \equiv \mathbf{1}_{\mathcal{X}} \in \mathcal{B}(\mathcal{X})$ is the identity operator. Given $T \in \mathcal{B}(\mathcal{X})$, T^* denotes its adjoint operator. The (full) spectrum, essential spectrum and resolvent set of any $T \in \mathcal{B}(\mathcal{X})$ are denoted by $\sigma(T)$, $\sigma_{\text{ess}}(T)$ and $\rho(T)$, respectively. The operator norm of $\mathcal{B}(\mathcal{X})$ is

$$\|T\|_{\text{op}} \doteq \sup\{\|T\varphi\|_{\mathcal{X}} : \varphi \in \mathcal{X} \text{ with } \|\varphi\|_{\mathcal{X}} = 1\}.$$

Given $T \in \mathcal{B}(\mathcal{X})$, $\mathcal{E}_T(\lambda)$ stands for the eigenspace associated with an eigenvalue $\lambda \in \sigma(T)$ of T .

In all the Section 4, we study properties of the Hamiltonian $H \in \mathcal{B}(\mathfrak{H})$ defined by (21). As one can see from (18)–(21) combined with (6), (8)–(11) and (17), it depends on several parameters. More precisely, $\epsilon, U, h_b \in \mathbb{R}_0^+$ and $\alpha_0 \in \mathbb{R}^+$, while

$$u : \mathbb{Z}^2 \rightarrow \mathbb{R}_0^+, \quad e^{\alpha_0|\cdot|} \mathbf{p}_1 : \mathbb{Z}^2 \rightarrow \mathbb{R}, \quad e^{\alpha_0|\cdot|} \mathbf{p}_2 : \mathbb{Z}^2 \rightarrow \mathbb{R} \quad \text{and} \quad v : \mathbb{Z}^2 \rightarrow \mathbb{R}$$

(with $\mathbf{p}_2(z) \doteq 0$ for $z \notin 2\mathbb{Z}$) are all absolutely summable functions that are invariant with respect to 90° -rotations. See Equations (7), (12) and (16). The parameters of the operator H are always fixed and arbitrary, unless we need to specify them to clarify some particular statement. Recall that the invariance under 90° -rotation is not that important here. In fact, here, the only important point concerning this symmetry is that it implies that the Fourier transforms \hat{v} , $\hat{\mathbf{p}}_1$ and $\hat{\mathbf{p}}_2$ are real-valued, because

$$v(-x) = v(x) = \overline{v(x)}, \quad \mathbf{p}_1(-x) = \mathbf{p}_1(x) = \overline{\mathbf{p}_1(x)} \quad \text{and} \quad \mathbf{p}_2(-x) = \mathbf{p}_2(x) = \overline{\mathbf{p}_2(x)},$$

that is, the real valued functions v , \mathbf{p}_1 and \mathbf{p}_2 are reflection invariant, as a consequence of their 90° -rotation invariance. Apart of this technical point, it is mainly relevant for the study of unconventional pairings, which is not done in the present work.

Note additionally that the on-site repulsion $U \in \mathbb{R}_0^+$ appears explicitly in all the quantities defined in Sections 2–3. However, in Section 4, this parameter is only important for the Subsections 4.4 and 4.6. Therefore, unless the parameter U is important for our discussions or statements, we omit it in order to shorten the notation, by writing

$$f(k) \equiv f(U, k)$$

for any function $f(U, k)$ of the parameters U and k .

4.2. Computation of the fiber decomposition of the Hamiltonian

For completeness, we first proof in a simple lemma that the fiber Hamiltonians defined by (42) yield an element of $L^\infty(\mathbb{T}^2, \mathcal{B}(\mathcal{H}))$. Then, we prove Proposition 2.1.

Lemma 4.1 (Elementary properties of fiber Hamiltonians). *Fix $h_b, \epsilon, U \in \mathbb{R}_0^+$. Then, $A : \mathbb{T}^2 \rightarrow \mathcal{B}(\mathcal{H})$, as defined by (42), is continuous and, in particular, $A(\cdot) \in L^\infty(\mathbb{T}^2, \mathcal{B}(\mathcal{H}))$.*

Proof. Since $\cos : \mathbb{R}^2 \rightarrow \mathbb{R}$, as defined by (35), is a nonexpansive mapping with period 2π , given $k, k', p \in \mathbb{T}^2$, the quantity

$$\mathfrak{f}(k')(p) - \mathfrak{f}(k)(p) = \epsilon \{\cos(p+k) - \cos(p+k')\} = \epsilon \{\cos(p+k) - \cos(p+k' + 2\pi q)\}$$

(see (33)) is bounded for any $q \in \mathbb{Z}^2$ by

$$|\mathfrak{f}(k')(p) - \mathfrak{f}(k)(p)| \leq \epsilon |(p+k) - (p+k' + 2\pi q)| = \epsilon |k - k' + 2\pi q|.$$

Hence, taking the minimum over all $q \in \mathbb{Z}^2$ and the supremum over all $p \in \mathbb{T}^2$, we obtain from (22) and (38) that

$$\begin{aligned} \|A_{1,1}(k') - A_{1,1}(k)\|_{\text{op}} &= \|M_{\mathfrak{f}(k')} - M_{\mathfrak{f}(k)}\|_{\text{op}} = \sup_{p \in \mathbb{T}^2} |\mathfrak{f}(k')(p) - \mathfrak{f}(k)(p)| \\ &\leq \epsilon \min_{q \in \mathbb{Z}^2} |k - k' + 2\pi q| = \epsilon d_{\mathbb{T}^2}(k, k') \end{aligned}$$

for all $k, k' \in \mathbb{T}^2$. In other words, the mapping

$$A_{1,1}(\cdot) : \mathbb{T}^2 \rightarrow \mathcal{B}(L^2(\mathbb{T}^2))$$

is (ϵ -Lipschitz) continuous with respect to the metric $d_{\mathbb{T}^2}$. Similarly, we see that $\mathfrak{b} : \mathbb{T}^2 \rightarrow \mathbb{R}$, defined by (32), is continuous with respect to $d_{\mathbb{T}^2}$, and hence, so is $A_{2,2} : \mathbb{T}^2 \rightarrow \mathcal{L}(\mathbb{C})$ (see (41)). In addition, by the triangle and Cauchy-Schwarz inequalities, for any $k, k' \in \mathbb{T}^2$ and $\varphi \in L^2(\mathbb{T}^2)$,

$$|\hat{v}(k')\langle \mathfrak{d}(k'), \varphi \rangle - \hat{v}(k)\langle \mathfrak{d}(k), \varphi \rangle| \leq |\hat{v}(k') - \hat{v}(k)| \|\mathfrak{d}(k')\| \|\varphi\| + |\hat{v}(k)| \|\mathfrak{d}(k') - \mathfrak{d}(k)\| \|\varphi\|.$$

Because of (12) and (16), $\mathfrak{d}(k), \hat{v} \in C(\mathbb{T}^2)$. So, since \mathbb{T}^2 is ($d_{\mathbb{T}^2}$ -)compact and

$$\|A_{2,1}(k') - A_{2,1}(k)\|_{\text{op}} = \sup_{\varphi \in L^2(\mathbb{T}^2), \|\varphi\|_2=1} |\hat{v}(k')\langle \mathfrak{d}(k'), \varphi \rangle - \hat{v}(k)\langle \mathfrak{d}(k), \varphi \rangle|,$$

we deduce from the last inequality and (39) that $A_{2,1} : \mathbb{T}^2 \rightarrow L^2(\mathbb{T}^2)^*$ is continuous. As $A_{1,2}(k) = A_{2,1}(k)^*$ for all $k \in \mathbb{T}^2$, we conclude that the mapping $A : \mathbb{T}^2 \rightarrow \mathcal{B}(\mathcal{H})$ is continuous, and hence bounded on the $d_{\mathbb{T}^2}$ -compact set \mathbb{T}^2 . \square

We now compute the following unitary transformation of the Hamiltonian H (see (18)):

$$\mathbb{U}H\mathbb{U}^* = \begin{pmatrix} U_f & 0 \\ 0 & \mathcal{F} \end{pmatrix} \begin{pmatrix} H_f & W_{b \rightarrow f} \\ W_{f \rightarrow b} & H_b \end{pmatrix} \begin{pmatrix} U_f^* & 0 \\ 0 & \mathcal{F}^* \end{pmatrix} = \begin{pmatrix} U_f H_f U_f^* & U_f W_{b \rightarrow f} \mathcal{F}^* \\ \mathcal{F} W_{f \rightarrow b} U_f^* & \mathcal{F} H_b \mathcal{F}^* \end{pmatrix} \quad (68)$$

with \mathbb{U} defined by (26)–(31). In fact, the remaining part of this section is devoted to the computations leading to Proposition 2.1.

To begin with, we observe that, for any lattice site $x \in \mathbb{Z}^2$ and spin $s \in \{\uparrow, \downarrow\}$, $b_x \doteq b(\mathbf{e}_x)$ and $a_{x,s} \doteq a(\mathbf{e}_{(x,s)})$, where $\{\mathbf{e}_x \doteq \delta_{x,\cdot}\}_{x \in \mathbb{Z}^2}$ is the canonical orthonormal basis (5) of $\ell^2(\mathbb{Z}^2)$ and $a_{x,s}$ (b_x^*) denotes the annihilation operator acting on the fermionic (bosonic) Fock space \mathfrak{F}_- (\mathfrak{F}_+) of a fermion (boson). In both cases, Ω denotes the vacuum state. We compute each term of the the right-hand side (68) separately:

Computation of $U_f H_f U_f^*$ in relation to $A_{1,1}$. We first note from (A.6) that, for any $x, y, u \in \mathbb{Z}^2$ and $s \in \{\uparrow, \downarrow\}$,

$$a_{x,s}(\mathbf{e}_{(y,\uparrow)} \wedge \mathbf{e}_{(u,\downarrow)}) = \frac{1}{\sqrt{2}} (\langle \mathbf{e}_{(x,s)}, \mathbf{e}_{(y,\uparrow)} \rangle \mathbf{e}_{(u,\downarrow)} - \langle \mathbf{e}_{(x,s)}, \mathbf{e}_{(u,\downarrow)} \rangle \mathbf{e}_{(y,\uparrow)})$$

vanishes whenever $(x, s) \notin \{(y, \uparrow), (u, \downarrow)\}$. Using this observation and (A.7), one concludes that, for any $y, u \in \mathbb{Z}^2$,

$$\begin{aligned}
 & \sum_{s \in \{\uparrow, \downarrow\}, x, z \in \mathbb{Z}^2 : |z|=1} a_{x,s}^* a_{x+z,s} (\mathbf{e}_{(y,\uparrow)} \wedge \mathbf{e}_{(u,\downarrow)}) \\
 &= \sum_{z \in \mathbb{Z}^2 : |z|=1} \left(a_{y+z,\uparrow}^* a_{y,\uparrow} (\mathbf{e}_{(y,\uparrow)} \wedge \mathbf{e}_{(u,\downarrow)}) + a_{u+z,\downarrow}^* a_{u,\downarrow} (\mathbf{e}_{(y,\uparrow)} \wedge \mathbf{e}_{(u,\downarrow)}) \right) \\
 &= \frac{1}{\sqrt{2}} \sum_{z \in \mathbb{Z}^2 : |z|=1} \left(a_{y+z,\uparrow}^* (\mathbf{e}_{(u,\downarrow)}) - a_{u+z,\downarrow}^* (\mathbf{e}_{(y,\uparrow)}) \right) \\
 &= \sum_{z \in \mathbb{Z}^2 : |z|=1} (\mathbf{e}_{(y+z,\uparrow)} \wedge \mathbf{e}_{(u,\downarrow)} + \mathbf{e}_{(y,\uparrow)} \wedge \mathbf{e}_{(u+z,\downarrow)}). \tag{69}
 \end{aligned}$$

Likewise, we see that, for any $y, u \in \mathbb{Z}^2$,

$$\sum_{s \in \{\uparrow, \downarrow\}, x \in \mathbb{Z}^2} a_{x,s}^* a_{x,s} (\mathbf{e}_{(y,\uparrow)} \wedge \mathbf{e}_{(u,\downarrow)}) = 2\mathbf{e}_{(y,\uparrow)} \wedge \mathbf{e}_{(u,\downarrow)}. \tag{70}$$

Moreover, as $u : \mathbb{Z}^2 \rightarrow \mathbb{R}$ is absolutely summable and invariant with respect to 180° -rotations (cf. (7)), we also get that

$$\begin{aligned}
 \sum_{x,z \in \mathbb{Z}^2} u(z) n_{x,\uparrow} n_{x+z,\downarrow} (\mathbf{e}_{(y,\uparrow)} \wedge \mathbf{e}_{(u,\downarrow)}) &= \sum_{z \in \mathbb{Z}^2} u(z) n_{u-z,\uparrow} (\mathbf{e}_{(y,\uparrow)} \wedge \mathbf{e}_{(u,\downarrow)}) = u(u-y) (\mathbf{e}_{(y,\uparrow)} \wedge \mathbf{e}_{(u,\downarrow)}) \\
 &= u(y-u) (\mathbf{e}_{(y,\uparrow)} \wedge \mathbf{e}_{(u,\downarrow)}), \tag{71}
 \end{aligned}$$

for any $y, u \in \mathbb{Z}^2$, which, for $u(z) = \delta_{z,0}$, is equal to

$$\sum_{x \in \mathbb{Z}^2} n_{x,\uparrow} n_{x,\downarrow} (\mathbf{e}_{(y,\uparrow)} \wedge \mathbf{e}_{(u,\downarrow)}) = \delta_{y,u} (\mathbf{e}_{(y,\uparrow)} \wedge \mathbf{e}_{(u,\downarrow)}). \tag{72}$$

We thus infer from (6) combined with (69)–(72) that

$$\begin{aligned}
 H_f (\mathbf{e}_{(y,\uparrow)} \wedge \mathbf{e}_{(u,\downarrow)}) &= -\frac{\epsilon}{2} \sum_{z \in \mathbb{Z}^2 : |z|=1} (\mathbf{e}_{(y+z,\uparrow)} \wedge \mathbf{e}_{(u,\downarrow)} + \mathbf{e}_{(y,\uparrow)} \wedge \mathbf{e}_{(u+z,\downarrow)}) \\
 &\quad + (4\epsilon + U\delta_{y,u} + u(y-u)) (\mathbf{e}_{(y,\uparrow)} \wedge \mathbf{e}_{(u,\downarrow)}),
 \end{aligned}$$

for any $y, u \in \mathbb{Z}^2$. Then, conjugating H_f by the unitary operator U_f (28)–(31) gives the equality

$$\begin{aligned}
 U_f H_f U_f^* (\hat{\mathbf{e}}_y(\cdot) \hat{\mathbf{e}}_{y-u}) &= U_f H_f (\mathbf{e}_{(y,\uparrow)} \wedge \mathbf{e}_{(u,\downarrow)}) \\
 &= -\frac{\epsilon}{2} \sum_{z \in \mathbb{Z}^2 : |z|=1} (\hat{\mathbf{e}}_{y+z}(\cdot) \hat{\mathbf{e}}_{y+z-u} + \hat{\mathbf{e}}_y(\cdot) \hat{\mathbf{e}}_{y-(u+z)}) \\
 &\quad + (4\epsilon + U\delta_{y,u} + u(y-u)) \hat{\mathbf{e}}_y(\cdot) \hat{\mathbf{e}}_{y-u}
 \end{aligned}$$

for any $y, u \in \mathbb{Z}^2$. By first evaluating the above expression at $k \in \mathbb{T}^2$, and then at $p \in \mathbb{T}^2$, and using (33) and (35), we obtain that

$$\begin{aligned}
 \left(U_f H_f U_f^* (\hat{\mathbf{e}}_y(\cdot) \hat{\mathbf{e}}_{y-u})(k) \right)(p) &= \hat{\mathbf{e}}_y(k) \hat{\mathbf{e}}_{y-u}(p) (U \delta_{y,u} + u(y-u)) \\
 &\quad + \hat{\mathbf{e}}_y(k) \hat{\mathbf{e}}_{y-u}(p) \epsilon \left(4 - \frac{1}{2} \sum_{z \in \mathbb{Z}^2 : |z|=1} \left(e^{i(k+p) \cdot z} + e^{ip \cdot z} \right) \right) \\
 &= \hat{\mathbf{e}}_y(k) \hat{\mathbf{e}}_{y-u}(p) (U \delta_{y,u} + u(y-u) + \mathfrak{f}(k)(p)) \\
 &= \hat{\mathbf{e}}_y(k) \left(U P_0 + \sum_{x \in \mathbb{Z}^2} u(x) P_x + M_{\mathfrak{f}(k)}(p) \right) (\hat{\mathbf{e}}_{y-u})(p),
 \end{aligned}$$

for any $y, u \in \mathbb{Z}^2$. By (37)–(38), it follows that

$$U_f H_f U_f^* (\hat{\mathbf{e}}_y(\cdot) \hat{\mathbf{e}}_{y-u}) = \left(\int_{\mathbb{T}^2}^{\oplus} A_{1,1}(p) \nu(dp) \right) \hat{\mathbf{e}}_y(\cdot) \hat{\mathbf{e}}_{y-u}. \quad (73)$$

As $\{\hat{\mathbf{e}}_y(\cdot) \hat{\mathbf{e}}_{y-u}\}_{y,u \in \mathbb{Z}^2}$ is an orthonormal basis for the Hilbert space

$$\int_{\mathbb{T}^2}^{\oplus} L^2(\mathbb{T}^2) \nu(dk),$$

we deduce from (73) that

$$U_f H_f U_f^* = \int_{\mathbb{T}^2}^{\oplus} A_{1,1}(k) \nu(dk).$$

Computation of $\mathcal{F}H_b\mathcal{F}^*$ in relation to $A_{2,2}$. Using (A.8) and (A.9), we conclude that, for any $y \in \mathbb{Z}^2$,

$$H_b(\mathbf{e}_y) = \epsilon h_b \left(2 \sum_{x \in \mathbb{Z}^2} \langle \mathbf{e}_x, \mathbf{e}_y \rangle b_x^* \Omega - \frac{1}{2} \sum_{z \in \mathbb{Z}^2 : |z|=1} \langle \mathbf{e}_{x+z}, \mathbf{e}_y \rangle b_x^* \Omega \right) = \epsilon h_b \left(2\mathbf{e}_y - \frac{1}{2} \sum_{z \in \mathbb{Z}^2 : |z|=1} \mathbf{e}_{y+z} \right)$$

so that

$$\mathcal{F}H_b(\mathbf{e}_y) = \epsilon h_b \left(2\hat{\mathbf{e}}_y - \frac{1}{2} \sum_{z \in \mathbb{Z}^2 : |z|=1} \hat{\mathbf{e}}_{y+z} \right), \quad y \in \mathbb{Z}^2.$$

Therefore, using that $\hat{\mathbf{e}}_y \equiv \mathcal{F}(\mathbf{e}_y) = e^{ik \cdot y}$ (see (31)) as well as (32), (35) and (41), we arrive at the result

$$\begin{aligned}
 \mathcal{F}H_b\mathcal{F}^*(\hat{\mathbf{e}}_y)(k) &= \epsilon h_b e^{ik \cdot y} \left(2 - \frac{1}{2} \sum_{z \in \mathbb{Z}^2 : |z|=1} e^{ik \cdot z} \right) = \epsilon h_b (2 - \cos(k)) e^{ik \cdot y} \\
 &= \mathfrak{b}(k) e^{ik \cdot y} = A_{2,2}(k) \hat{\mathbf{e}}_y(k)
 \end{aligned}$$

for all $y \in \mathbb{Z}^2$ and $k \in \mathbb{T}^2$. As $\{\hat{\mathbf{e}}_y\}_{y \in \mathbb{Z}^2}$ is an orthonormal basis for $L^2(\mathbb{T}^2)$, it follows that

$$\mathcal{F}H_b\mathcal{F}^* = \int_{\mathbb{T}^2}^{\oplus} A_{2,2}(k) \nu(dk).$$

Computation of $\mathcal{F}W_{\mathfrak{f} \rightarrow \mathfrak{b}}U_f^*$ and $U_f W_{\mathfrak{b} \rightarrow \mathfrak{f}}\mathcal{F}^*$ in relation to $A_{2,1}$ and $A_{1,2}$. Observe from (11) and (A.7) that, for all $y \in \mathbb{Z}^2$,

$$c_y^* \Omega = \sqrt{2} \sum_{z \in \mathbb{Z}^2} (\mathfrak{p}_1(z) \mathbf{e}_{(y+z, \uparrow)} \wedge \mathbf{e}_{(y, \downarrow)} + \mathfrak{p}_2(2z) \mathbf{e}_{(y+z, \uparrow)} \wedge \mathbf{e}_{(y-z, \downarrow)}),$$

and as a consequence, using (9)–(10) as well as (A.8), we get that, for any $u \in \mathbb{Z}^2$,

$$W_{b \rightarrow f}(\mathbf{e}_u) = \sum_{y \in \mathbb{Z}^2} v(u-y) \sum_{z \in \mathbb{Z}^2} (\mathfrak{p}_1(z) \mathbf{e}_{(y+z, \uparrow)} \wedge \mathbf{e}_{(y, \downarrow)} + \mathfrak{p}_2(2z) \mathbf{e}_{(y+z, \uparrow)} \wedge \mathbf{e}_{(y-z, \downarrow)}).$$

Therefore, by (28)–(31), for any $u \in \mathbb{Z}^2$,

$$U_f W_{b \rightarrow f} \mathcal{F}^*(\hat{\mathbf{e}}_u) = \sum_{y \in \mathbb{Z}^2} v(u-y) \sum_{z \in \mathbb{Z}^2} (\mathfrak{p}_1(z) \hat{\mathbf{e}}_{y+z}(\cdot) \hat{\mathbf{e}}_z + \mathfrak{p}_2(2z) \hat{\mathbf{e}}_{y+z}(\cdot) \hat{\mathbf{e}}_{2z}).$$

In particular, as $v, \mathfrak{p}_1, \mathfrak{p}_2 : \mathbb{Z}^2 \rightarrow \mathbb{R}$ are absolutely summable and invariant with respect to 180° -rotations (cf. (12) and (16)), we deduce from the last equality that, for any $u \in \mathbb{Z}^2$ and $k, p \in \mathbb{T}^2$,

$$\begin{aligned} (U_f W_{b \rightarrow f} \mathcal{F}^*(\hat{\mathbf{e}}_u)(k))(p) &= \sum_{y \in \mathbb{Z}^2} v(u-y) \sum_{z \in \mathbb{Z}^2} (\mathfrak{p}_1(z) e^{ik \cdot (y+z)} e^{ip \cdot z} + \mathfrak{p}_2(2z) e^{ik \cdot (y+z)} e^{i2p \cdot z}) \\ &= \sum_{z \in \mathbb{Z}^2} (\mathfrak{p}_1(z) e^{i(k+p) \cdot z} + \mathfrak{p}_2(2z) e^{i(k+2p) \cdot z}) e^{ik \cdot u} \sum_{y \in \mathbb{Z}^2} v(y-u) e^{ik \cdot (y-u)}. \end{aligned}$$

Using now that

$$\sum_{z \in \mathbb{Z}^2} \mathfrak{p}_1(z) e^{i(k+p) \cdot z} = \hat{\mathfrak{p}}_1(k+p) \quad \text{and} \quad \sum_{z \in \mathbb{Z}^2} \mathfrak{p}_2(2z) e^{i(k+2p) \cdot z} = \hat{\mathfrak{p}}_2(k/2+p)$$

($\mathfrak{p}_2(z) \doteq 0$ for $z \notin (2\mathbb{Z})^2$), we arrive at the equalities

$$\begin{aligned} (U_f W_{b \rightarrow f} \mathcal{F}^*(\hat{\mathbf{e}}_u)(k))(p) &= (\hat{\mathfrak{p}}_1(k+p) + \hat{\mathfrak{p}}_2(k/2+p)) e^{ik \cdot u} \sum_{z \in \mathbb{Z}^2} v(z) e^{ik \cdot z} \\ &= \hat{v}(k) \mathfrak{d}(k)(p) \hat{\mathbf{e}}_u(k) = [A_{1,2}(k) \hat{\mathbf{e}}_u(k)](p), \end{aligned}$$

with $\mathfrak{d}(k)(p)$ and $A_{1,2}(k)$ defined by (34) and (40), respectively. As $u \in \mathbb{Z}^2$ and $k, p \in \mathbb{T}^2$ are arbitrary in the above equations, this shows that $U_f W_{b \rightarrow f} \mathcal{F}^*$ coincides with the bounded linear transformation

$$\begin{aligned} J : L^2(\mathbb{T}^2) &\rightarrow \int_{\mathbb{T}^2}^{\oplus} L^2(\mathbb{T}^2) \nu(dk) \\ \varphi &\mapsto A_{1,2}(\cdot) \hat{\mathbf{e}}_u(\cdot) \end{aligned}$$

on the orthonormal basis $\{\hat{\mathbf{e}}_u\}_{u \in \mathbb{Z}^2}$ and, therefore, $U_f W_{b \rightarrow f} \mathcal{F}^* = J$. By taking adjoints on both sides, we also obtain $\mathcal{F} W_{f \rightarrow b} U_f^* = J^*$. Finally, one can easily check from (39) that

$$(J^* \psi)(k) = A_{2,1}(k) \psi(k), \quad k \in \mathbb{T}^2, \quad \psi \in \int_{\mathbb{T}^2}^{\oplus} L^2(\mathbb{T}^2) \nu(dk).$$

This completes the proof of Proposition 2.1.

4.3. Spectrum of the fiber Hamiltonians

We start with the study of the essential spectrum of fiber Hamiltonians (42) at any total quasi-momentum $k \in \mathbb{T}^2$, before considering afterwards the discrete one in Section 4.3.2. Then, in Section 4.3.3, we study

the bottom of the spectrum ($k \in \mathbb{T}^2$ being fixed). The whole study leads to important spectral properties of H , as previously explained, via Proposition 2.1 combined with Theorem A.3.

4.3.1. Essential spectrum

The essential spectrum $\sigma_{\text{ess}}(A(k))$ of the fiber Hamiltonian

$$A(k) \equiv A(U, k),$$

defined by (42) at fixed $U \in \mathbb{R}_0^+$ and total quasi-momentum $k \in \mathbb{T}^2$, is completely determined by the following proposition:

Proposition 4.2 (Essential spectrum of fiber Hamiltonians). *For any $k \in \mathbb{T}^2$ and $h_b, \epsilon, U \in \mathbb{R}_0^+$, one has*

$$\sigma_{\text{ess}}(A(k)) = \sigma_{\text{ess}}(A_{1,1}(k)) = \sigma_{\text{ess}}(B_{1,1}(k)) = \sigma(M_{\mathfrak{f}(k)}) = 2\epsilon \cos(k/2)[-1, 1] + 4\epsilon,$$

where $M_{\mathfrak{f}(k)}$ stands for the multiplication operator associated with the function $\mathfrak{f}(k)$ (33), while $B_{1,1}(k)$ and $A_{1,1}(k) \equiv A_{1,1}(U, k)$ are defined by (37) and (38), respectively.

Proof. Recall that ν is the normalized Haar measure defined by (23) on \mathbb{T}^2 . Fix $k \in \mathbb{T}^2$. If λ is an eigenvalue of $M_{\mathfrak{f}(k)}$ with associated eigenvector $\varphi \in L^2(\mathbb{T}^2)$, then

$$M_{\mathfrak{f}(k)}\varphi(p) \doteq \mathfrak{f}(k)(p)\varphi(p) = \lambda\varphi(p)$$

for almost every $p \in \mathbb{T}^2$. As $\varphi \neq 0$, there exists $\Omega \subseteq \mathbb{T}^2$ with strictly positive measure $\nu(\Omega) > 0$ such that the above equality holds true with $\varphi(p) \neq 0$ for every $p \in \Omega$. Thus, $\mathfrak{f}(k)(p) = \lambda$ for all $p \in \Omega$. Because

$$\nu([- \pi, \pi)^2 \setminus (-\pi, \pi)^2) = 0,$$

we can assume without loss of generality that $\Omega \subseteq (-\pi, \pi)^2$. Since $\mathfrak{f}(k) - \lambda$ is real analytic on the open domain $(-\pi, \pi)^2$ in \mathbb{R}^2 and the zeros of any nonconstant real analytic function have null Lebesgue measure [49], we would have $\nu(\Omega) = 0$, which contradicts our choice of the set Ω . Recall indeed that ν is the Lebesgue measure, up to a normalization constant (see (23)). Hence, $M_{\mathfrak{f}(k)}$ has no eigenvalues and, thus,

$$\sigma_{\text{ess}}(M_{\mathfrak{f}(k)}) = \sigma(M_{\mathfrak{f}(k)}) = \mathfrak{f}(k)(\mathbb{T}^2).$$

The last equality holds true, for \mathfrak{f} is a continuous function on a compact domain – namely, the torus \mathbb{T}^2 . Clearly,

$$\mathfrak{f}(k)(\mathbb{T}^2) = 2\epsilon \cos(k/2)[-1, 1] + 4\epsilon.$$

Observing that $A_{1,2}(k)$, $A_{2,1}(k)$, $A_{2,2}(k)$ and P_x are all rank-one linear transformations, we can apply the stability of the essential spectrum under compact perturbations (see [95, Corollary 8.16]) to conclude that

$$\sigma_{\text{ess}}(A(k)) = \sigma_{\text{ess}}(M_{\mathfrak{f}(k)}) = \mathfrak{f}(k)(\mathbb{T}^2). \quad (74)$$

In fact, from the absolute summability of the function $u : \mathbb{Z}^2 \rightarrow \mathbb{R}_0^+$ (see (7)), along with the closedness of the subspace of compact operators in the Banach space of all bounded operators, the operator defined by the infinite sum

$$\sum_{x \in \mathbb{Z}^2} u(x)P_x$$

is not only bounded, but even compact on the Hilbert space $L^2(\mathbb{T}^2)$. Recall that P_x denotes the orthogonal projection onto the one-dimensional subspace $\mathbb{C}\hat{e}_x \subseteq L^2(\mathbb{T}^2)$ for any $x \in \mathbb{Z}^2$. For the same reasons,

$$\sigma_{\text{ess}}(A_{1,1}(k)) = \sigma_{\text{ess}}(B_{1,1}(k)) = \sigma_{\text{ess}}(M_{\mathfrak{f}(k)} + UP_0) = \sigma_{\text{ess}}(M_{\mathfrak{f}(k)}). \quad \square$$

Corollary 4.3 (Bottom of the spectrum of $A_{1,1}(k)$ and $B_{1,1}(k)$). *For any $k \in \mathbb{T}^2$, one has that*

$$\min \sigma(A_{1,1}(k)) = \min \sigma(B_{1,1}(k)) = \min \sigma(M_{\mathfrak{f}(k)}) = 4\epsilon - 2\epsilon \cos(k/2) \doteq \mathfrak{z}(k).$$

Proof. Fix $k \in \mathbb{T}^2$. Since $U \in \mathbb{R}_0^+$, one has the operator inequalities

$$M_{\mathfrak{f}(k)} \leq M_{\mathfrak{f}(k)} + \sum_{x \in \mathbb{Z}^2} u(x)P_x \doteq B_{1,1}(k) \leq B_{1,1}(k) + UP_0 \doteq A_{1,1}(k),$$

for the set of positive operators on a Hilbert space forms a norm-closed convex cone. By combining the last inequalities with Proposition 4.2, one arrives at the assertion. \square

4.3.2. Discrete spectrum

In the following, it is technically convenient to assume that $\mathfrak{b}(k)$, which is the kinetic energy of a boson with quasi-momentum k , is below the bottom of the spectrum of $A_{1,1}(k)$ – that is, the minimum energy of the fermion pair for the same total quasi-momentum. In other words, we assume from now on that

$$\mathfrak{b}(k) \doteq h_b \epsilon(2 - \cos(k)) \leq \mathfrak{z}(k) \doteq 4\epsilon - 2\epsilon \cos(k/2) \quad (75)$$

for all $k \in \mathbb{T}^2$, with equality *only* at $k = 0$. See Equation (32) and Corollary 4.3. By direct computations,¹⁷ one verifies that this amounts to take h_b in the interval $[0, 1/2]$. This means that we consider a regime where the boson mass is at least the mass of the two fermions, as physically expected for cuprate superconductors; see [21, Section 3.1].

Proposition 4.4 (Eigenvalues of fiber Hamiltonians – I). *Take any $k \in \mathbb{T}^2$ and $h_b \in [0, 1/2]$.*

i.) $\lambda \neq \mathfrak{b}(k)$ is an eigenvalue of $A(k)$ iff there is a nonzero vector $\varphi \in L^2(\mathbb{T}^2)$ in the kernel of the bounded operator

$$A_{1,1}(k) - \lambda \mathbf{1} - (\mathfrak{b}(k) - \lambda)^{-1} A_{1,2}(k) A_{2,1}(k) \in \mathcal{B}(L^2(\mathbb{T}^2)).$$

In this case, λ is an eigenvalue of $A(k)$ with associated eigenvector

$$\left(\varphi, -(\mathfrak{b}(k) - \lambda)^{-1} A_{2,1}(k) \varphi \right) \in \mathcal{H} \doteq L^2(\mathbb{T}^2) \oplus \mathbb{C}.$$

ii.) $\mathfrak{b}(k)$ is an eigenvalue of $A(k)$ iff $\hat{v}(k) = 0$.

Proof. Fix $k \in \mathbb{T}^2$ and $h_b \in [0, 1/2]$. We start with the proof of Assertion (i): If $\lambda \neq \mathfrak{b}(k)$ is an eigenvalue of $A(k)$ with associated eigenvector $(\varphi, z) \in \mathcal{H} \setminus \{0\}$, then we directly deduce from (42) that

$$(A_{1,1}(k) - \lambda \mathbf{1})\varphi + A_{1,2}(k)z = 0, \quad (76)$$

$$A_{2,1}(k)\varphi + (\mathfrak{b}(k) - \lambda)z = 0. \quad (77)$$

¹⁷(75) is clearly true for $h_b = 0$. Take $h_b > 0$. Using $\cos(\theta) = 2\cos^2(\theta/2) - 1$ and (35), one verifies that (75) is equivalent to $h_b(4 - 2x^2 - 2y^2) \leq 4 - 2(x + y)$ for $x, y \in [0, 1]$. Since $\inf_{x \in [0, 1]} \{h_b x^2 - x\} = -1/(4h_b)$ for $h_b \geq 1/2$ and $\inf_{x \in [0, 1]} \{h_b x^2 - x\} = h_b - 1$ for $h_b \in (0, 1/2]$, we deduce that (75) holds true iff $h_b \in [0, 1/2]$.

By combining these two equations, we obtain

$$z = -(\mathfrak{b}(k) - \lambda)^{-1} A_{2,1}(k)\varphi, \quad (78)$$

and thus,

$$\left[A_{1,1}(k) - \lambda \mathbf{1} - (\mathfrak{b}(k) - \lambda)^{-1} A_{1,2}(k) A_{2,1}(k) \right] \varphi = 0.$$

We have that $\varphi \neq 0$, for otherwise z would also be zero, by (78), and this would contradict the fact that (φ, z) is a nonzero vector. The converse is obvious and Assertion (i) holds true.

We now prove Assertion (ii): It is easy to check from (42) that $\hat{v}(k) = 0$ implies that

$$A(k)(0, 1) = \mathfrak{b}(k)(0, 1). \quad (79)$$

Conversely, suppose that $\mathfrak{b}(k)$ is an eigenvalue of $A(k)$ with associated eigenvector $(\varphi, z) \in \mathcal{H} \setminus \{0\}$, but $\hat{v}(k) \neq 0$. Then, by (39) and (42),

$$(A_{1,1}(k) - \mathfrak{b}(k)\mathbf{1})\varphi + A_{1,2}(k)z = 0 \quad \text{and} \quad A_{2,1}(k)\varphi \doteq \hat{v}(k)\langle \mathfrak{d}(k), \varphi \rangle = 0. \quad (80)$$

Remark that the second equality says that $\varphi \perp \mathfrak{d}(k)$, since we assume $\hat{v}(k) \neq 0$. Considering the scalar product of φ with both sides of the first equation, we then get that

$$\langle \varphi, (A_{1,1}(k) - \mathfrak{b}(k)\mathbf{1})\varphi \rangle + z\hat{v}(k)\langle \varphi, \mathfrak{d}(k) \rangle = \langle \varphi, (A_{1,1}(k) - \mathfrak{b}(k)\mathbf{1})\varphi \rangle = 0; \quad (81)$$

see (40). Because $h_b \in [0, 1/2]$, if $k \neq 0$, then (75) holds true with a strict inequality, and therefore,

$$\mathfrak{b}(k) < 4\epsilon - 2\epsilon \cos(k/2) = \min \sigma(A_{1,1}(k)),$$

thanks to Corollary 4.3. Hence,

$$A_{1,1}(k) - \mathfrak{b}(k)\mathbf{1} \geq c\mathbf{1},$$

for some constant $c > 0$, which, combined with (81), in turn implies that $\varphi = 0$. If now $k = 0$, then $\mathfrak{b}(0) = 0$ (see (32)) and we obtain from (81) that

$$\int_{\mathbb{T}^2} |\varphi(p)|^2 \mathfrak{f}(0)(p) \nu(dp) = \langle \varphi, M_{\mathfrak{f}(0)} \varphi \rangle \leq \langle \varphi, A_{1,1}(0)\varphi \rangle = 0, \quad (82)$$

since $M_{\mathfrak{f}(0)} \leq A_{1,1}(U, 0)$ (see (37)–(38)). As

$$\mathfrak{f}(0)(p) \doteq \epsilon\{4 - 2\cos(p)\}, \quad p \in \mathbb{T}^2,$$

(see (33) and (35)) defines a positive and continuous function that vanishes at $p = 0$ only, one deduces from (82) that $\varphi = 0$ also when $k = 0$. In any case, $\varphi = 0$ and so, (80) combined with (40) yields

$$A_{1,2}(k)z \doteq \hat{v}(k)\mathfrak{d}(k)z = 0.$$

Since $\mathfrak{d}(k) \neq 0$ and $\hat{v}(k) \neq 0$, we must have that $z = 0$. Thus, we arrive at $(\varphi, z) = (0, 0)$, which contradicts the fact that (φ, z) is a nonzero vector. Therefore, if $\mathfrak{b}(k)$ is an eigenvalue of $A(k)$, then we must have $\hat{v}(k) = 0$. \square

The Birman-Schwinger principle (Theorem A.10) allows us to transform the eigenvalue problem for the fiber Hamiltonian $A(k)$ into a nonlinear equation on the resolvent set $\rho(A_{1,1}(U, k))$ of the operator $A_{1,1}(U, k)$, which is the resolvent set for a fermion pair with total quasi-momentum $k \in \mathbb{T}^2$:

Theorem 4.5 (Characteristic equation for eigenvalues). Fix $h_b \in [0, 1/2]$ and $k \in \mathbb{T}^2$. Then, $\lambda \in \rho(A_{1,1}(k))$ is an eigenvalue of $A(k)$ iff it is a solution to the equation

$$\hat{v}(k)^2 \mathfrak{T}(k, z) + z - \mathfrak{b}(k) = 0, \quad z \in \rho(A_{1,1}(k)), \quad (83)$$

where \mathfrak{T} is the function defined by (45); that is,

$$\mathfrak{T}(k, z) \equiv \mathfrak{T}(U, k, z) \doteq \left\langle \mathfrak{d}(k), (A_{1,1}(k) - z\mathbf{1})^{-1} \mathfrak{d}(k) \right\rangle, \quad (84)$$

Proof. Fix $h_b \in [0, 1/2]$ and $k \in \mathbb{T}^2$. We divide the proof in several cases:

Case 1: We first consider the case $\hat{v}(k) = 0$ and $k \neq 0$. In that situation, $\mathfrak{b}(k)$ is trivially the only solution to (83). However, we already know from Proposition 4.4 (ii) that $\mathfrak{b}(k)$ is an eigenvalue of $A(k)$. We must therefore prove that there is no other eigenvalue λ of $A(k)$ in $\rho(A_{1,1}(k))$ but $\mathfrak{b}(k)$. In fact, if such a $\lambda \in \rho(A_{1,1}(k))$ exists, then, by Proposition 4.4 (i) with $\hat{v}(k) = 0$, $A_{1,1}(k) - \lambda\mathbf{1}$ would have a nontrivial kernel, which is not possible, for λ is in the resolvent set of $A_{1,1}(k)$.

Case 2: Suppose that $k = 0$ and $\hat{v}(0) = 0$. We observe that (83) has no solution because

$$0 \in [0, 8\epsilon] = \sigma_{\text{ess}}(A_{1,1}(0)),$$

thanks to Proposition 4.2. In addition, by applying Proposition 4.4 (i) and noting that $\mathfrak{b}(0) = 0$, we see that $A(0)$ has no eigenvalues in $\rho(A_{1,1}(0))$.

Case 3: Finally, assume that $\hat{v}(k) \neq 0$ and take $\lambda \in \rho(A_{1,1}(k))$. Observe from Proposition 4.4 (ii) that $\mathfrak{b}(k)$ cannot be an eigenvalue of $A(k)$. Additionally, $\mathfrak{b}(k)$ cannot be a solution to Equation (83). This last observation is proven as follows: When $k = 0$, this is clear because $\mathfrak{b}(0) = 0$ is not even in the domain of the equation to be solved in (83). For $k \neq 0$, if $\mathfrak{b}(k)$ is a solution to (83), then $\mathfrak{T}(k, \mathfrak{b}(k)) = 0$, but we know from Corollary 4.3 and $h_b \in [0, 1/2]$ that

$$A_{1,1}(k) - \mathfrak{b}(k)\mathbf{1} \geq c\mathbf{1}$$

for some constant $c > 0$. Therefore, $\mathfrak{T}(k, \mathfrak{b}(k)) = 0$ would yield $\mathfrak{d}(k) = 0$, which is obviously wrong, by (34). Therefore, in all cases, $\mathfrak{b}(k)$ cannot be a solution to Equation (83), and we can assume that $\lambda \neq \mathfrak{b}(k)$. Now, the remaining part of the proof is essentially the same as the one of [22, Proposition 10], but we reproduce it for completeness. By (39)–(40), the orthogonal projection S onto the subspace $\mathbb{C}\mathfrak{d}(k) \subseteq L^2(\mathbb{T}^2)$ can be written as

$$S\varphi = \|\mathfrak{d}(k)\|^{-2} \langle \mathfrak{d}(k), \varphi \rangle \mathfrak{d}(k) = \hat{v}(k)^{-2} \|\mathfrak{d}(k)\|^2 A_{1,2}(k) A_{2,1}(k) \varphi, \quad \varphi \in L^2(\mathbb{T}^2).$$

Then, observe from Proposition 4.4 (i) that λ is an eigenvalue of $A(k)$ iff λ is an eigenvalue of $T - V^2$ with

$$V \doteq \hat{v}(k)(\mathfrak{b}(k) - \lambda)^{-1/2} \|\mathfrak{d}(k)\| S, \quad (85)$$

$$T \doteq A_{1,1}(k). \quad (86)$$

Thus, by applying Theorem A.10, we deduce that λ is an eigenvalue of $A(k)$ iff 1 is an eigenvalue of the corresponding Birman-Schwinger operator, which, with the above operators T and V , is equal to

$$B(\lambda) = \hat{v}(k)^2 (\mathfrak{b}(k) - \lambda)^{-1} \|\mathfrak{d}(k)\|^2 S (A_{1,1}(k) - \lambda\mathbf{1})^{-1} S.$$

Remark in this case that

$$\mathcal{E}_{B(\lambda)}(1) = \mathbb{C}\mathfrak{d}(k) \quad \text{and} \quad \dim \mathcal{E}_{T-V^2}(\lambda) = \dim \mathcal{E}_{B(\lambda)}(1) = 1, \quad (87)$$

since, obviously,

$$\mathbf{B}(\lambda)L^2(\mathbb{T}^2) \subseteq SL^2(\mathbb{T}^2) = \mathbb{C}\mathbf{d}(k).$$

We thus conclude that λ is an eigenvalue of $A(k)$ iff

$$\begin{aligned} \mathbf{B}(\lambda)\mathbf{d}(k) = \mathbf{d}(k) &\Leftrightarrow \langle \mathbf{d}(k), \mathbf{B}(\lambda)\mathbf{d}(k) - \mathbf{d}(k) \rangle = 0 \\ &\Leftrightarrow \langle \mathbf{d}(k), \mathbf{B}(\lambda)\mathbf{d}(k) \rangle = \|\mathbf{d}(k)\|^2 \\ &\Leftrightarrow \hat{v}(k)^2(\mathbf{b}(k) - \lambda)^{-1}\|\mathbf{d}(k)\|^2\langle \mathbf{d}(k), S(A_{1,1}(k) - \lambda\mathbf{1})^{-1}S\mathbf{d}(k) \rangle = \|\mathbf{d}(k)\|^2 \\ &\Leftrightarrow \hat{v}(k)^2\mathfrak{T}(k, \lambda) = \mathbf{b}(k) - \lambda. \end{aligned}$$

This completes the proof. □

Corollary 4.6 (Eigenspaces of fiber Hamiltonians). *Fix $h_b \in [0, 1/2]$ and $k \in \mathbb{T}^2$. If $\lambda \in \rho(A_{1,1}(k))$ is an eigenvalue of the fiber Hamiltonian $A(k)$, then the associated eigenspace is*

$$\mathcal{E}_{A(k)}(\lambda) = \mathbb{C}g(k, \lambda),$$

where

$$g(k, \lambda) \doteq \left(\hat{v}(k)(A_{1,1}(k) - \lambda\mathbf{1})^{-1}\mathbf{d}(k), -1 \right) \in \mathcal{H}.$$

In particular, λ is a nondegenerated eigenvalue of $A(k)$.

Proof. Assume that $\hat{v}(k) \neq 0$. Recall from the proof of Theorem 4.5 that in this case, $\mathbf{b}(k)$ is not an eigenvalue of $A(k)$, and so we assume without loss of generality that $\lambda \neq \mathbf{b}(k)$. In this case, observe that we have (87) and a close look at the proof of Theorem A.10, in particular Lemma A.9, leads us to

$$\mathcal{E}_{T-V^2}(\lambda) \doteq \ker(T - V^2 - \lambda\mathbf{1}) = \mathbb{C}\varphi_0,$$

where

$$\varphi_0 \doteq (T - \lambda\mathbf{1})^{-1}V\mathbf{d}(k) = \hat{v}(k)(\mathbf{b}(k) - \lambda)^{-1/2}\|\mathbf{d}(k)\|(A_{1,1}(k) - \lambda\mathbf{1})^{-1}\mathbf{d}(k), \quad (88)$$

by (85) and (86). From Proposition 4.4 (i) ($\hat{v}(k) \neq 0$), one then obtains that

$$\begin{aligned} \mathcal{E}_{A(k)}(\lambda) &= \{(\varphi, -(\mathbf{b}(k) - \lambda)^{-1}A_{2,1}(k)\varphi) \in \mathcal{H} : \varphi \in \ker(T - V^2 - \lambda\mathbf{1})\} \\ &= \mathbb{C}(\varphi_0, -(\mathbf{b}(k) - \lambda)^{-1}A_{2,1}(k)\varphi_0). \end{aligned}$$

In view of Equation (39), (88) and Theorem 4.5, the last vector can be rewritten as follows:

$$\begin{aligned} (\varphi_0, -(\mathbf{b}(k) - \lambda)^{-1}A_{2,1}(k)\varphi_0) &= (\varphi_0, -(\mathbf{b}(k) - \lambda)^{-1}\hat{v}(k)\langle \mathbf{d}(k), \varphi_0 \rangle) \\ &= (\varphi_0, -(\mathbf{b}(k) - \lambda)^{-3/2}\hat{v}(k)^2\|\mathbf{d}(k)\|\mathfrak{T}(k, \lambda)) \\ &= (\varphi_0, -(\mathbf{b}(k) - \lambda)^{-1/2}\|\mathbf{d}(k)\|) \\ &= (\mathbf{b}(k) - \lambda)^{-1/2}\|\mathbf{d}(k)\|g(k, \lambda), \end{aligned}$$

whenever $\hat{v}(k) \neq 0$. Finally, if $\hat{v}(k) = 0$ and $\lambda \in \rho(A_{1,1}(k))$ is an eigenvalue of $A(k)$, then it is straightforward to check that $\lambda = \mathfrak{b}(k)$ with eigenspace generated by the vector $(0, 1) \in \mathcal{H}$; see, for instance, (76)–(77) and (79). \square

Corollary 4.7 (Eigenvalues of fiber Hamiltonians – II). *Fix $h_b \in [0, 1/2]$ and $k \in \mathbb{T}^2$. There is at most one eigenvalue of $A(k)$ in each connected component of $\rho(A_{1,1}(k)) \cap \mathbb{R}$.*

Proof. In view of Theorem 4.5, it suffices to show that the derivative of the mapping

$$\rho(A_{1,1}(k)) \cap \mathbb{R} \ni x \mapsto \hat{v}(k)^2 \mathfrak{T}(k, x) + x - \mathfrak{b}(k) \in \mathbb{R}$$

is strictly positive. For any $x_0 \in \rho(A_{1,1}(k)) \cap \mathbb{R}$, we have that

$$\partial_x \{ \hat{v}(k)^2 \mathfrak{T}(k, x) + x - \mathfrak{b}(k) \} \Big|_{x=x_0} = \hat{v}(k)^2 \| (A_{1,1}(k) - x_0 \mathbf{1})^{-1} \mathfrak{b}(k) \|^2 + 1 > 1. \quad (89)$$

\square

4.3.3. Bottom of the spectrum

As is well-known, physical properties of quantum systems at very low temperatures are essentially determined by the bottom of the spectrum of the corresponding Hamiltonian. In our case, having in mind the application to superconductivity in cuprates, we would like to study the bottom of the spectrum of the Hamiltonian $H \in \mathcal{B}(\mathfrak{H})$ defined by (21). By Proposition 2.1 and Theorem A.3, we thus study the bottom of the spectrum of the fiber Hamiltonian $A(k)$ (42) at fixed total quasi-momentum $k \in \mathbb{T}^2$, similar to [22, 21].

Theorem 4.8 (Bottom of the spectrum of $A(k)$). *Fix $h_b \in [0, 1/2]$. If $k \neq 0$, then there is exactly one eigenvalue $E(k) \equiv E(U, k)$ of the Hamiltonian $A(k)$ strictly below $\sigma_{\text{ess}}(A(k))$. In this case, the eigenvalue is nondegenerated and $E(k) < \mathfrak{b}(k)$ when $\hat{v}(k) \neq 0$, whereas $E(k) = \mathfrak{b}(k)$ if $\hat{v}(k) = 0$. This statement remains valid for $k = 0$ provided $\hat{v}(0) \neq 0$.*

Proof. Assume that $k \neq 0$. Recall that $\mathfrak{z}(k)$ is defined in Corollary 4.3. From Corollaries 4.3 and 4.7, the interval $(-\infty, \mathfrak{z}(k))$ contains at most one eigenvalue of $A(k)$. By Corollary 4.6, the eigenvalue is nondegenerate, if it exists. If $\hat{v}(k) = 0$, we know from Proposition 4.4 (ii) that $\mathfrak{b}(k)$ is such an eigenvalue. Recall that for $k \neq 0$, one has that $\mathfrak{b}(k) < \mathfrak{z}(k)$, because $h_b \in [0, 1/2]$. Now, suppose that $\hat{v}(k) \neq 0$. When $\mathfrak{b}(k) \leq x < \mathfrak{z}(k)$, we have

$$(A_{1,1}(k) - x\mathbf{1})^{-1} \geq c\mathbf{1}$$

for some constant $c > 0$, and hence, $\mathfrak{T}(k, x) > 0$; see (84). Consequently,

$$\hat{v}(k)^2 \mathfrak{T}(k, x) + x - \mathfrak{b}(k) > 0,$$

which means that $A(k)$ has no eigenvalues in the interval $[\mathfrak{b}(k), \mathfrak{z}(k))$, by Theorem 4.5. We shall now look for an eigenvalue in the interval $(-\infty, \mathfrak{b}(k))$. On the one hand, using Corollary 4.3, observe that

$$\|\mathfrak{b}(k)\|^{-2} |\mathfrak{T}(k, x)| \leq \|(A_{1,1}(k) - x\mathbf{1})^{-1}\|_{\text{op}} = (\mathfrak{z}(k) - x)^{-1} \leq (\mathfrak{b}(k) - x)^{-1},$$

whenever $x < \mathfrak{b}(k)$. Taking $x \rightarrow -\infty$, $\mathfrak{T}(k, x)$ tends to zero, and hence,

$$\lim_{x \rightarrow -\infty} \{ \hat{v}(k)^2 \mathfrak{T}(k, x) + x - \mathfrak{b}(k) \} = -\infty.$$

On the other hand, the continuity of the mapping

$$\mathfrak{T}(k, \cdot) : \rho(A_{1,1}(k)) \rightarrow \mathbb{R}$$

on $(-\infty, \mathfrak{b}(k)]$ gives us

$$\lim_{x \rightarrow \mathfrak{b}(k)} \{ \hat{v}(k)^2 \mathfrak{T}(k, x) + x - \mathfrak{b}(k) \} = \hat{v}(k)^2 \mathfrak{T}(k, \mathfrak{b}(k)) > 0.$$

By the intermediate value theorem, there is $E(k) \in (-\infty, \mathfrak{b}(k))$ such that

$$\hat{v}(k)^2 \mathfrak{T}(k, E(k)) + E(k) - \mathfrak{b}(k) = 0.$$

By Theorem 4.5, $E(k)$ must be an eigenvalue of $A(k)$.

The proof for $k = 0$ is done in a similar way. Basically, the only difference is that, in this case, $\mathfrak{b}(0) = \mathfrak{z}(0) = 0$ and

$$\lim_{x \rightarrow 0^-} \{ \hat{v}(0)^2 \mathfrak{T}(0, x) + x \} \in (0, \infty]$$

occurs due to other reasons. Indeed, from Corollary 4.3, we deduce that $\mathfrak{T}(0, \cdot)$ is strictly positive on the interval $(-\infty, 0)$. Because of (89), we also have that $\partial_x \mathfrak{T}(0, x)|_{x=x_0} \geq 0$ whenever $x_0 < 0$. Thus, the limit of $\mathfrak{T}(0, x)$ as $x \rightarrow 0^-$ exists, being possibly infinite. \square

If $\hat{v}(0) = 0$, then, by Theorem 4.5, the fiber Hamiltonian $A(0)$ has no negative eigenvalues. In this case, we set $E(0) = 0$, which is obviously an eigenvalue of $A(0)$ with associated eigenvector $(0, 1)$. (Note that $\sigma_{\text{ess}}(A(0)) = [0, 8\epsilon]$, by Proposition 4.2.) With this definition, observe that, for all $k \in \mathbb{T}^2$, $E(k)$ is the minimum spectral value of $A(k)$:

$$E(k) = \min \sigma(A(k)) \leq \mathfrak{z}(k) = \min \sigma_{\text{ess}}(A(k)). \quad (90)$$

The lowest eigenvalue $E(k)$ of $A(k)$, when $E(k) < 0$, is related to the formation of dressed bound fermion pairs of fermions with total quasi-momentum $k \in \mathbb{T}^2$. In Theorem 4.20, we make this claim more precise and prove the spatial localization of such bounded pairs. Before doing that, we study the regularity of the real-valued function

$$E \equiv E(\mathbf{U}, \cdot) : \mathbb{T}^2 \rightarrow \mathbb{R}$$

on the two-dimensional torus.

To this end, we rewrite the characteristic equation given by Theorem 4.5 via the function $\Phi : \mathcal{O} \rightarrow \mathbb{R}$ defined by

$$\Phi(k, x) \equiv \Phi(\mathbf{U}, k, x) \doteq \hat{v}(k)^2 \mathfrak{T}(k, x) + x - \mathfrak{b}(k), \quad (91)$$

where \mathcal{O} is the open set

$$\mathcal{O} \doteq \{ (k, x) \in \mathbb{S}^2 \times \mathbb{R} : x < \mathfrak{z}(k) \} \subseteq \mathbb{R}^3. \quad (92)$$

Observe from Equation (89) that $\partial_x \Phi > 0$ over the whole domain of Φ .

We now study the continuity of the function $E : \mathbb{T}^2 \rightarrow \mathbb{R}$ and give a sufficient condition for E to be of class C^d on \mathbb{S}^2 for every $d \in \mathbb{N} \cup \{\omega, a\}$, where $C^d(\Omega)$, $d \in \mathbb{N}$, stands for the space of d times continuously differentiable functions on Ω , while $C^\omega(\Omega)$ and $C^a(\Omega)$ refer to the space of smooth and real analytic functions on Ω , respectively.

Theorem 4.9 (Regularity of the function E). *Let $h_b \in [0, 1/2]$.*

- i.) *The family $\{E(\mathbf{U}, \cdot)\}_{\mathbf{U} \in \mathbb{R}_0^+}$ of real-valued functions on \mathbb{T}^2 is equicontinuous with respect to the metric¹⁸ $d_{\mathbb{T}^2}$.*

¹⁸Note that as $d_{\mathbb{T}^2}$ is smaller than the Euclidean metric for \mathbb{T}^2 as a subset of \mathbb{R}^2 , the equicontinuity also holds true for the Euclidean metric.

ii.) If $\hat{v} \in C^d(\mathbb{S}^2)$ ($\mathbb{S}^2 \subseteq \mathbb{R}^2$) for some $d \in \mathbb{N} \cup \{\omega, a\}$, then $E \equiv E(U, \cdot) \in C^d(\mathbb{S}^2)$ for all $U \in \mathbb{R}_0^+$. In this case,

$$\partial_{k_j} E(k) = -(\partial_x \Phi(k, E(k)))^{-1} \partial_{k_j} \Phi(k, E(k)), \quad k \in \mathbb{S}^2, \quad j \in \{1, 2\}. \quad (93)$$

Proof. By the spectral theorem, we deduce from (90) that, for any $U \in \mathbb{R}_0^+$,

$$E(U, k) = \min \sigma(A(U, k)) = \inf_{\psi \in \mathcal{H}, \|\psi\|=1} \langle \psi, A(U, k) \psi \rangle, \quad k \in \mathbb{T}^2. \quad (94)$$

Given any $\varepsilon > 0$ and $k_0 \in \mathbb{T}^2$, by the (operator norm) continuity of the mapping $A(0, \cdot) : \mathbb{T}^2 \rightarrow \mathcal{B}(\mathcal{H})$ at the point k_0 , we can find $\delta > 0$ such that

$$\begin{aligned} \sup_{U \in \mathbb{R}_0^+} \sup_{\psi \in \mathcal{H}, \|\psi\|=1} |\langle \psi, A(U, k) \psi \rangle - \langle \psi, A(U, k_0) \psi \rangle| &\leq \sup_{U \in \mathbb{R}_0^+} \|A(U, k) - A(U, k_0)\|_{\text{op}} \\ &= \sup_{U \in \mathbb{R}_0^+} \|A(0, k) - A(0, k_0)\|_{\text{op}} < \varepsilon \end{aligned}$$

for every $k \in \mathbb{T}^2$ with $d_{\mathbb{T}^2}(k, k_0) < \delta$. Recall that \mathcal{H} stands for the (fiber) Hilbert space $L^2(\mathbb{T}^2) \oplus \mathbb{C}$ (see (25)), while $d_{\mathbb{T}^2}$ is the metric (22) on the torus \mathbb{T}^2 . Therefore, $E : \mathbb{T}^2 \rightarrow \mathbb{R}$ can be expressed as the infimum over the equicontinuous family $\{\langle \psi, A(U, \cdot) \psi \rangle\}_{U \in \mathbb{R}_0^+, \psi \in \mathcal{H}, \|\psi\|=1}$ of (continuous) functions and Assertion (i) follows.

Take again some $k_0 \in \mathbb{S}^2$. Assume that \hat{v} is of class C^d on $\mathbb{S}^2 \subseteq \mathbb{R}^2$ with $d \in \mathbb{N} \cup \{\omega, a\}$. Let $\vartheta = (k_0, E(k_0)) \in \mathcal{O}$. Using Theorems 4.5 and 4.8 as well as Equation (89) and the (operator norm) continuity of the mapping

$$A_{1,1}(\cdot) : \mathbb{T}^2 \rightarrow \mathcal{B}(L^2(\mathbb{T}^2)), \quad (95)$$

one checks that $\Phi \in C^d(\mathcal{O})$ with $d \geq 1$, $\Phi(\vartheta) = 0$ and $\partial_x \Phi(\vartheta) \neq 0$. See, for instance, (89). We can thus apply the implicit function theorem (see, for example, [91] for an ordinary version and [92] for an analytic version) to obtain open subsets $U \subseteq \mathbb{R}^2$ and $J \subseteq \mathbb{R}$ such that $\vartheta \in U \times J \subseteq \mathcal{O}$ and, for each $k \in U$, there is a unique real number $\xi(k) \in J$ satisfying $\Phi(k, \xi(k)) = 0$. Moreover, the mapping $\xi : U \rightarrow J$ defined in this way is of class C^d and its partial derivatives are given by

$$\partial_{k_j} \xi(k) = -(\partial_x \Phi(k, \xi(k)))^{-1} \partial_{k_j} \Phi(k, \xi(k)), \quad k \in U, \quad j \in \{1, 2\}. \quad (96)$$

As $\xi(k_0) = E(k_0) < \mathfrak{z}(k_0)$ (see (90)), by continuity, there exists a neighborhood $V \subseteq U$ of k_0 such that $\xi(k) < \mathfrak{z}(k)$ for every $k \in V$. It follows that, for all $k \in V$, $\xi(k)$ and $E(k)$ are in the same connected component $(-\infty, \mathfrak{z}(k))$, and from $\partial_x \Phi > 0$, we conclude that $E \upharpoonright V = \xi \upharpoonright V$. So, E is of class C^d near k_0 and (96) yields (93) for any $k \in V$ – in particular, for $k = k_0$. As k_0 is arbitrary, Assertion (ii) follows. \square

We can now deduce from Theorem 4.9 that E is a dispersion relation (see Definition 3.7) when the function $\hat{v} : \mathbb{S}^2 \rightarrow \mathbb{R}$ is at least 2 times continuously differentiable, and in this case, we can even compute the group velocity. To see this, recall that, for any $f \in C^2(\mathbb{S}^2)$, we define in (48) the subset

$$\mathfrak{M}_f \doteq \{k \in \mathbb{S}^2 : \text{Hess}(f)(k) \in \text{GL}_2(\mathbb{R})\} \subseteq \mathbb{S}^2$$

with $\text{GL}_2(\mathbb{R})$ being the set of invertible 2×2 matrices with real coefficients.

Corollary 4.10 (E as a dispersion relation and group velocity). *Let $h_b \in [0, 1/2]$ and $U \in \mathbb{R}_0^+$. Then, $E \equiv E(U, \cdot) \in C(\mathbb{T}^2)$ and is of class C^2 on the open set $\mathbb{S}^2 \subseteq \mathbb{R}^2$ whenever \hat{v} is of class C^2 on \mathbb{S}^2 . In this case, the corresponding group velocity is*

$$\mathbf{v}_E(k) \doteq \vec{\nabla}_k E(k) = -(\partial_x \Phi(k, E(k)))^{-1} \vec{\nabla}_k \Phi(k, E(k)), \quad k \in \mathbb{S}^2.$$

Moreover, if \hat{v} is real analytic (i.e., of class C^a in the above terminology) on \mathbb{S}^2 , then either \mathfrak{M}_E has full measure or is empty.

Proof. The first part of the assertion is a direct application of Theorem 4.9. It remains to study the set \mathfrak{M}_E . If \hat{v} is real analytic then, from Equation (47) and Theorem 4.9, the function $f : \mathbb{S}^2 \rightarrow \mathbb{R}$ defined by

$$f(k) \doteq \det(\text{Hess}(E)(k)), \quad k \in \mathbb{S}^2,$$

is real analytic and satisfies $f^{-1}(\{0\}) = \mathbb{S}^2 \setminus \mathfrak{M}_E$. Since the zeros of any nonconstant real analytic function have null Lebesgue measure (see, for example, [49]), either \mathfrak{M}_E has full measure or is empty. \square

It is natural to derive now the ground state energy of the Hamiltonian $H \in \mathcal{B}(\mathfrak{H})$ defined by (21), which is related to the ground state energy of fiber Hamiltonians, thanks to Proposition 2.1 and Theorem A.3. As expected, one has the following equality for the ground state energy

$$E(U) \doteq \min \sigma(H) = \min E(\mathbb{T}^2).$$

A proof can be done like [22, Lemma 8] by using Kato's perturbation theory. In the sequel, we provide an alternative way of proving the equality, which is much more direct.

Proposition 4.11 (Bottom of the spectrum of H). *We have that*

$$E(U) = \min_{k \in \mathbb{T}^2} \min \sigma(A(k)) = \min E(\mathbb{T}^2) \leq 0.$$

Proof. We first remark that the union

$$\mathcal{K} \doteq \bigcup \{ \sigma(A(k)) : k \in \mathbb{T}^2 \} \subseteq \mathbb{R}$$

of the spectra of all fiber Hamiltonians is closed. To see this, let $(\lambda_n)_{n \in \mathbb{N}}$ be a sequence of real numbers converging to $\lambda \in \mathbb{R}$ with $\lambda_n \in \sigma(A(k_n))$ for some $k_n \in \mathbb{T}^2$ at $n \in \mathbb{N}$. By compactness of \mathbb{T}^2 , we can assume without loss of generality that $(k_n)_{n \in \mathbb{N}}$ converges to some point $k_0 \in \mathbb{T}^2$. By the (operator norm) continuity of the mapping $A : \mathbb{T}^2 \rightarrow \mathcal{B}(\mathcal{H})$, it follows that

$$\lim_{n \rightarrow \infty} (A(k_n) - \lambda_n \mathbf{1}) = A(k_0) - \lambda \mathbf{1}$$

(in operator norm). Hence, $\lambda \in \sigma(A(k_0))$, for otherwise $A(k_n) - \lambda_n \mathbf{1}$ would be invertible¹⁹ for sufficiently large n . Thus, \mathcal{K} is a closed set, and as a consequence, for any $s \notin \mathcal{K}$, there is $\varepsilon > 0$ such that

$$(s - \varepsilon, s + \varepsilon) \cap \sigma(A(k)) = \emptyset, \quad k \in \mathbb{T}^2.$$

With this property, we infer from Proposition 2.1 and Theorem A.3 that $\sigma(H) \subseteq \mathcal{K}$, which yields the inequality

$$E(U) \geq \min_{k \in \mathbb{T}^2} \min \sigma(A(k)) = \min E(\mathbb{T}^2). \quad (97)$$

Note that the last equality results from (90). By Theorem 4.9 (i), $E : \mathbb{T}^2 \rightarrow \mathbb{R}$ is continuous. From the compactness of the torus \mathbb{T}^2 and the Weierstrass extreme value theorem, E has a minimizer in \mathbb{T}^2 , say $k_0 \in \mathbb{T}^2$. The continuity of E at k_0 implies that, for every $\varepsilon > 0$, there is $\delta > 0$ such that, for all $k \in \mathbb{T}^2$ satisfying $d_{\mathbb{T}^2}(k, k_0) < \delta$,

$$E(k) \in (E(k_0) - \varepsilon, E(k_0) + \varepsilon),$$

¹⁹Recall that the set of invertible operators on a Banach space X is an open subset of $\mathcal{B}(X)$, with respect to the operator norm. See, for example, [50, Theorem 1.4].

and as a consequence,

$$\nu\left(\{k \in \mathbb{T}^2 : \sigma(A(k)) \cap (E(k_0) - \varepsilon, E(k_0) + \varepsilon) \neq \emptyset\}\right) \geq \nu\left(\mathbb{T}^2 \cap B_\delta(k_0)\right) > 0,$$

where $B_\delta(k_0)$ is the open ball (for the metric $d_{\mathbb{T}^2}$) centered at $k_0 \in \mathbb{T}^2$ of radius $\delta \in \mathbb{R}^+$. By Theorem A.3, this implies that $E(k_0) \in \sigma(H)$, which, combined with (97), yields the equalities

$$E(U) = \min_{k \in \mathbb{T}^2} \min \sigma(A(k)) = \min E\left(\mathbb{T}^2\right).$$

Using Equations (75) and (90), we note that

$$E(U) = \min E\left(\mathbb{T}^2\right) \leq \min_{k \in \mathbb{T}^2} \mathfrak{z}(k) = 4\epsilon - 2\epsilon \max_{k \in \mathbb{T}^2} \cos(k/2) = \mathfrak{z}(0) = 0. \quad \square$$

4.4. Spectral properties in the hard-core limit

We now study the spectral properties of fiber Hamiltonians $A(k)$ (42) in the hard-core limit. It refers to the limit $U \rightarrow \infty$. In fact, a very strong on-site repulsion U (see Equation (6)) prevents two fermions of opposite spins from occupying the same lattice site. We study in particular the continuous function $E : \mathbb{T}^2 \rightarrow \mathbb{R}$ defined by Theorem 4.8, which corresponds to the continuous family of nondegenerate eigenvalues at lowest energies in each fiber, in this limit.

An important result in this context is the characterization of such eigenvalues via the Birman-Schwinger principle, given by Theorem 4.5. In particular, we need first to study the hard-core limit of the characteristic equation, which amounts to determine the limit $U \rightarrow \infty$ of the quantity (84); that is,

$$\mathfrak{I}(U, k, \lambda) \equiv \mathfrak{I}(k, \lambda) \doteq \left\langle \mathfrak{d}(k), (A_{1,1}(U, k) - \lambda \mathbf{1})^{-1} \mathfrak{d}(k) \right\rangle, \quad \lambda \in \rho(A_{1,1}(U, k)), \quad (98)$$

for $h_b \in [0, 1/2]$ and $k \in \mathbb{T}^2$. We start with this point, which allows us to study afterwards the limit of the lowest eigenvalues and all the derived quantities, like, for instance, the group velocity.

4.4.1. The characteristic equation in the hard-core limit

Let $\mathfrak{s} = \hat{\mathbf{e}}_0 \in L^2(\mathbb{T}^2)$ denote the constant function 1 on the torus \mathbb{T}^2 . For any fixed $k \in \mathbb{T}^2$ and $\lambda \in \rho(B_{1,1}(k))$, define the following four constants:

$$R_{\mathfrak{s}, \mathfrak{s}} \equiv R_{\mathfrak{s}, \mathfrak{s}}(k, \lambda) \doteq \left\langle \mathfrak{s}, (B_{1,1}(k) - \lambda \mathbf{1})^{-1} \mathfrak{s} \right\rangle, \quad (99)$$

$$R_{\mathfrak{s}, \mathfrak{d}} \equiv R_{\mathfrak{s}, \mathfrak{d}}(k, \lambda) \doteq \left\langle \mathfrak{s}, (B_{1,1}(k) - \lambda \mathbf{1})^{-1} \mathfrak{d}(k) \right\rangle, \quad (100)$$

$$R_{\mathfrak{d}, \mathfrak{s}} \equiv R_{\mathfrak{d}, \mathfrak{s}}(k, \lambda) \doteq \left\langle \mathfrak{d}(k), (B_{1,1}(k) - \lambda \mathbf{1})^{-1} \mathfrak{s} \right\rangle, \quad (101)$$

$$R_{\mathfrak{d}, \mathfrak{d}} \equiv R_{\mathfrak{d}, \mathfrak{d}}(k, \lambda) \doteq \left\langle \mathfrak{d}(k), (B_{1,1}(k) - \lambda \mathbf{1})^{-1} \mathfrak{d}(k) \right\rangle, \quad (102)$$

where we recall that $B_{1,1}(k)$ is defined by (37). In the following lemma, we write $\mathfrak{I}(U, k, \lambda)$, which is defined by (98), in terms of these four quantities.

In the following, it is technically convenient to assume that $\mathfrak{d}(k) \notin \mathbb{C}\mathfrak{s}$ for all $k \in \mathbb{T}^2$. Notice that this holds true iff $\mathfrak{p}_1 \notin \mathbb{C}\mathbf{e}_0$ or $\mathfrak{p}_2 \notin \mathbb{C}\mathbf{e}_0$ (i.e., $r_{\mathfrak{p}} > 0$). Indeed, recall (36); that is,

$$\mathfrak{d}(k) = \mathcal{F}\left[e^{ik \cdot x} \mathfrak{p}_1(x) + e^{i\frac{k}{2} \cdot x} \mathfrak{p}_2(x)\right],$$

where $e^{ik \cdot x} \mathfrak{p}_{\sharp}(x)$ stands for the function $x \mapsto e^{ik \cdot x} \mathfrak{p}_{\sharp}(x)$ with $\sharp \in \{1, 2\}$. See also discussions around Equations 13–14.

Lemma 4.12. Let $k \in \mathbb{T}^2$, $U \in \mathbb{R}_0^+$ and $\lambda < \mathfrak{z}(k)$, with $\mathfrak{z}(k) \in \mathbb{R}$ defined in Corollary 4.3. Then,

$$\mathfrak{T}(U, k, \lambda) = \frac{R_{\mathfrak{d}, \mathfrak{d}}}{UR_{\mathfrak{s}, \mathfrak{s}} + 1} + U \frac{R_{\mathfrak{d}, \mathfrak{d}}R_{\mathfrak{s}, \mathfrak{s}} - |R_{\mathfrak{s}, \mathfrak{d}}|^2}{UR_{\mathfrak{s}, \mathfrak{s}} + 1},$$

with $R_{\mathfrak{d}, \mathfrak{d}}R_{\mathfrak{s}, \mathfrak{s}} - |R_{\mathfrak{s}, \mathfrak{d}}|^2 \geq 0$. Moreover, if $r_p > 0$ (see (14)–(15)), then the inequality is strict.

Proof. The proof of the first part is a slightly more complicated version of the one of [22, Lemma 14]. Fix $k \in \mathbb{T}^2$, $U \in \mathbb{R}_0^+$ and $\lambda < \mathfrak{z}(k)$. Define the complex numbers

$$\begin{aligned} Q_{\mathfrak{s}, \mathfrak{s}} &\doteq \left\langle \mathfrak{s}, (A_{1,1}(U, k) - \lambda \mathbf{1})^{-1} \mathfrak{s} \right\rangle, \\ Q_{\mathfrak{s}, \mathfrak{d}} &\doteq \left\langle \mathfrak{s}, (A_{1,1}(U, k) - \lambda \mathbf{1})^{-1} \mathfrak{d}(k) \right\rangle, \\ Q_{\mathfrak{d}, \mathfrak{s}} &\doteq \left\langle \mathfrak{d}(k), (A_{1,1}(U, k) - \lambda \mathbf{1})^{-1} \mathfrak{s} \right\rangle, \\ Q_{\mathfrak{d}, \mathfrak{d}} &\doteq \left\langle \mathfrak{d}(k), (A_{1,1}(U, k) - \lambda \mathbf{1})^{-1} \mathfrak{d}(k) \right\rangle = \mathfrak{T}(U, k, \lambda), \end{aligned}$$

where we recall that

$$A_{1,1}(U, k) \doteq B_{1,1}(k) + UP_0 \geq B_{1,1}(k), \quad (103)$$

by Equation (38). Using Corollary 4.3, note at this point that

$$\mathfrak{z}(k) = \min \sigma(A_{1,1}(U, k)) = \min \sigma(B_{1,1}(k)) \geq 0. \quad (104)$$

In particular,

$$\lambda \in (-\infty, \mathfrak{z}(k)) \subseteq \rho(A_{1,1}(U, k)) \cap \rho(B_{1,1}(k)), \quad (105)$$

and the resolvent operators $(A_{1,1}(U, k) - \lambda \mathbf{1})^{-1}$ and $(B_{1,1}(k) - \lambda \mathbf{1})^{-1}$ are strictly positive. By using the second resolvent identity together with Equation (103), we compute that

$$(A_{1,1}(U, k) - \lambda \mathbf{1})^{-1} = (B_{1,1}(k) - \lambda \mathbf{1})^{-1} - U(A_{1,1}(U, k) - \lambda \mathbf{1})^{-1}P_0(B_{1,1}(k) - \lambda \mathbf{1})^{-1}.$$

Recalling that P_0 is the orthogonal projection onto $\mathbb{C}\mathfrak{s} = \mathbb{C}\hat{\mathfrak{e}}_0$, we have that

$$\begin{aligned} Q_{\mathfrak{s}, \mathfrak{s}} &= R_{\mathfrak{s}, \mathfrak{s}} - U \left\langle \mathfrak{s}, (A_{1,1}(U, k) - \lambda \mathbf{1})^{-1} P_0 (B_{1,1}(k) - \lambda \mathbf{1})^{-1} \mathfrak{s} \right\rangle \\ &= R_{\mathfrak{s}, \mathfrak{s}} - U Q_{\mathfrak{s}, \mathfrak{s}} R_{\mathfrak{s}, \mathfrak{s}}, \\ Q_{\mathfrak{d}, \mathfrak{d}} &= R_{\mathfrak{d}, \mathfrak{d}} - U \left\langle \mathfrak{d}(k), (A_{1,1}(U, k) - \lambda \mathbf{1})^{-1} P_0 (B_{1,1}(k) - \lambda \mathbf{1})^{-1} \mathfrak{d}(k) \right\rangle \\ &= R_{\mathfrak{d}, \mathfrak{d}} - U Q_{\mathfrak{d}, \mathfrak{s}} R_{\mathfrak{s}, \mathfrak{d}}, \\ Q_{\mathfrak{s}, \mathfrak{d}} &= R_{\mathfrak{s}, \mathfrak{d}} - U \left\langle \mathfrak{s}, (A_{1,1}(U, k) - \lambda \mathbf{1})^{-1} P_0 (B_{1,1}(k) - \lambda \mathbf{1})^{-1} \mathfrak{d}(k) \right\rangle \\ &= R_{\mathfrak{s}, \mathfrak{d}} - U Q_{\mathfrak{s}, \mathfrak{s}} R_{\mathfrak{s}, \mathfrak{d}}, \\ Q_{\mathfrak{d}, \mathfrak{s}} &= R_{\mathfrak{d}, \mathfrak{s}} - U \left\langle \mathfrak{d}(k), (A_{1,1}(U, k) - \lambda \mathbf{1})^{-1} P_0 (B_{1,1}(k) - \lambda \mathbf{1})^{-1} \mathfrak{s} \right\rangle \\ &= R_{\mathfrak{d}, \mathfrak{s}} - U Q_{\mathfrak{d}, \mathfrak{s}} R_{\mathfrak{s}, \mathfrak{s}}. \end{aligned}$$

In matrix notation, the above equations can be rewritten as

$$\begin{pmatrix} R_{s,s} & R_{d,s} \\ R_{s,d} & R_{d,d} \end{pmatrix} = U \begin{pmatrix} Q_{s,s} R_{s,s} & Q_{d,s} R_{s,s} \\ Q_{s,s} R_{s,d} & Q_{d,s} R_{s,d} \end{pmatrix} + \begin{pmatrix} Q_{s,s} & Q_{d,s} \\ Q_{s,d} & Q_{d,d} \end{pmatrix} = \begin{pmatrix} UR_{s,s} + 1 & 0 \\ UR_{s,d} & 1 \end{pmatrix} \begin{pmatrix} Q_{s,s} & Q_{d,s} \\ Q_{s,d} & Q_{d,d} \end{pmatrix}.$$

As $(B_{1,1}(k) - \lambda \mathbf{1})^{-1} \geq 0$ (because of (105)) and $UR_{s,s} \geq 0$,

$$\det \begin{pmatrix} UR_{s,s} + 1 & 0 \\ UR_{s,d} & 1 \end{pmatrix} = UR_{s,s} + 1 > 0,$$

which means that the matrix appearing in the above determinant is invertible. From this, we conclude that

$$\begin{pmatrix} Q_{s,s} & Q_{d,s} \\ Q_{s,d} & Q_{d,d} \end{pmatrix} = \frac{1}{UR_{s,s} + 1} \begin{pmatrix} 1 & 0 \\ -UR_{s,d} & UR_{s,s} + 1 \end{pmatrix} \begin{pmatrix} R_{s,s} & R_{d,s} \\ R_{s,d} & R_{d,d} \end{pmatrix}.$$

In particular, since $R_{s,d} = \overline{R_{d,s}}$,

$$\mathfrak{T}(U, k, \lambda) = Q_{d,d} = R_{d,d} - \frac{U}{UR_{s,s} + 1} |R_{s,d}|^2 = \frac{R_{d,d}}{UR_{s,s} + 1} + U \frac{R_{d,d}R_{s,s} - |R_{s,d}|^2}{UR_{s,s} + 1}.$$

Because $\lambda < \mathfrak{z}(k) \leq 0$ and $(B_{1,1}(k) - \lambda \mathbf{6})^{-1} \geq |\mathfrak{z}(k) - \lambda|^{-1} \mathbf{1}$ (see (105)), the sesquilinear form

$$(\varphi, \psi) \mapsto \langle \varphi, (B_{1,1}(k) - \lambda \mathbf{1})^{-1} \psi \rangle$$

is a scalar product, and using the Cauchy-Schwarz inequality,²⁰ we deduce that

$$R_{d,d}R_{s,s} - |R_{s,d}|^2 \geq 0.$$

When $r_p > 0$, the set $\{\mathfrak{d}(k), s\}$ is linearly independent for every $k \in \mathbb{T}^2$. □

The last lemma is useful to deduce the behavior of the quantity $\mathfrak{T}(U, k, \lambda)$ at large Hubbard coupling constant $U \gg 1$:

Corollary 4.13 ($\mathfrak{T}(U_0, k, \lambda)$ at large on-site repulsions). *Let $k \in \mathbb{T}^2$ and $\lambda < \mathfrak{z}(k)$, with $\mathfrak{z}(k) \in \mathbb{R}$ defined in Corollary 4.3. Then, for all $U \in \mathbb{R}_0^+$,*

$$0 \leq \mathfrak{T}(U, k, \lambda) - \mathfrak{T}(\infty, k, \lambda) \leq \frac{R_{d,d}}{1 + UR_{s,s}},$$

where

$$\mathfrak{T}(\infty, k, \lambda) \doteq R_{s,s}^{-1} \left(R_{d,d}R_{s,s} - |R_{s,d}|^2 \right) \geq 0. \quad (106)$$

Proof. By Lemma 4.12, we have $R_{s,s} > 0$ and $R_{d,d}R_{s,s} \geq |R_{s,d}|^2$ while

$$\mathfrak{T}(U, k, \lambda) - \frac{R_{d,d}R_{s,s} - |R_{s,d}|^2}{R_{s,s}} = \frac{|R_{s,d}|^2}{(1 + UR_{s,s})R_{s,s}} \leq \frac{R_{d,d}}{1 + UR_{s,s}}. \quad \square$$

²⁰Recall that the Cauchy-Schwarz inequality applied to a scalar product is an equality iff the vectors are linearly dependent.

4.4.2. Hard-core dispersion relation of bound pairs of lowest energy

We are now in a position to study the spectral properties of the model $H \in \mathcal{B}(\mathfrak{H})$ defined by (21) in the hard-core limit. We study in particular its ground state energy $E(U)$ (see Corollary 3.4) and the limit of the continuous function $E : \mathbb{T}^2 \rightarrow \mathbb{R}$ defined by Theorem 4.8, which corresponds to the continuous family of nondegenerate eigenvalues at lowest energies in the fibers.

We start with the hard-core ground state energy, which is a well-defined quantity that even stays negative:

Lemma 4.14 (Existence of the hard-core ground state energy). *In the hard-core limit $U \rightarrow \infty$, the hard-core ground state energy (44) is well-defined and is equal to*

$$E(\infty) = \sup_{U \in \mathbb{R}_0^+} E(U) \leq 0.$$

Proof. When $0 \leq U \leq V$, one obviously has

$$A(V, k) - A(U, k) = (V - U) \begin{pmatrix} P_0 & 0 \\ 0 & 0 \end{pmatrix} \geq 0$$

see Equation (42). In other words, $A(U, k)$, $U \in \mathbb{R}_0^+$, defines an increasing family of bounded operators and by Proposition 4.2 and Equation (75),

$$\min \sigma(A(U, k)) \leq \min \sigma(A(V, k)) \leq \mathfrak{z}(k) \quad (107)$$

whenever $0 \leq U \leq V$. In particular, by taking the minimum over $k \in \mathbb{T}^2$, if $0 \leq U \leq V$ then

$$E(U) \leq E(V) \leq 0.$$

See Proposition 4.11. This shows that E is an increasing function of $U \in \mathbb{R}_0^+$, which is bounded from above by 0. This yields the assertion, thanks to the monotone convergence theorem. \square

We give in the next theorem a hard-core limit version of Theorems 4.5, 4.8 and 4.9. To this end, recall that $E(k), k \in \mathbb{T}^2$, are given by Theorem 4.8 as a family of nondegenerate eigenvalues. This family depends upon the parameter $U \in \mathbb{R}_0^+$, and we thus use here the notation $E(U, k) \equiv E(k)$. This defines a function $E : \mathbb{R}_0^+ \times \mathbb{T}^2 \rightarrow \mathbb{R}$.

Theorem 4.15 (Dispersion relation in the hard-core limit). *Let $h_b \in [0, 1/2]$. Recall that $\mathfrak{T}(\infty, k, \lambda) \geq 0$ is defined by (106).*

i.) *For every $k \in \mathbb{T}^2$, the following limit exists:*

$$E(\infty, k) = \lim_{U \rightarrow \infty} E(U, k) = \sup_{U \in \mathbb{R}_0^+} E(U, k)$$

ii.) $E(\infty, \cdot) : \mathbb{T}^2 \rightarrow \mathbb{R}$ *is a continuous function;*

iii.) *For $k \neq 0$, $E(\infty, k)$ is the unique solution to the equation*

$$\hat{v}(k)^2 \mathfrak{T}(\infty, k, z) + z - \mathfrak{b}(k) = 0, \quad z < \mathfrak{z}(k). \quad (108)$$

iv.) *If \hat{v} is of class C^d on $\mathbb{S}^2 \subseteq \mathbb{R}^2$ with $d \in \mathbb{N} \cup \{\omega, a\}$, then so does $E(\infty, \cdot)$.*

If, in addition, $r_p > 0$, then

v.) *For every $k \in \mathbb{T}^2$, $E(\infty, k) \leq \mathfrak{b}(k)$ with equality iff $\hat{v}(k) = 0$.*

Proof. Fix $h_b \in [0, 1/2]$. By (90) and (107) together with Corollary 4.3 and Theorem 4.8,

$$E(U, k) \leq E(V, k) \leq \mathfrak{b}(k) \leq \mathfrak{z}(k) = \min \sigma(B_{1,1}(k)), \quad k \in \mathbb{T}^2, \quad (109)$$

whenever $0 \leq U \leq V$. This shows that, at any fixed $k \in \mathbb{T}^2$, the function $U \mapsto E(U, k)$ from \mathbb{R}_0^+ to \mathbb{R} is increasing and bounded. Therefore, for any $k \in \mathbb{T}^2$,

$$E(\infty, k) = \lim_{U \rightarrow \infty} E(U, k) = \sup_{U \in \mathbb{R}_0^+} E(U, k) \leq \mathfrak{b}(k), \quad (110)$$

thanks to the monotone convergence theorem. In particular, Assertion (i) holds true.

By Combining Equation (110) with (94), note that

$$E(\infty, k) = \sup_{U \in \mathbb{R}_0^+} \inf_{\psi \in \mathcal{H}, \|\psi\|=1} \langle \psi, A(U, k)\psi \rangle, \quad k \in \mathbb{T}^2.$$

Meanwhile, for any $\varepsilon > 0$ and $k_0 \in \mathbb{T}^2$, there is $\delta > 0$ such that

$$\|A(U, k) - A(U, k_0)\|_{\text{op}} = \|A(0, k) - A(0, k_0)\|_{\text{op}} \leq \delta.$$

As a consequence, similar to what is done after (94), the set

$$\{\langle \psi, A(U, \cdot)\psi \rangle : U \in \mathbb{R}_0^+, \psi \in \mathcal{H} \text{ with } \|\psi\| = 1\}$$

is a family of equicontinuous functions on \mathbb{T}^2 . Therefore, $E(\infty, \cdot)$ is continuous and Assertion (ii) holds true.

Fix $k \neq 0$. If $\hat{v}(k) \neq 0$ and $U \in \mathbb{R}^+$, then we deduce from Corollary 4.3, Theorem 4.5 and Equations (109)–(110) that

$$\{E(U, k) : U \in \mathbb{R}_0^+ \cup \{\infty\}\} \subseteq \rho(B_{1,1}(k))$$

and

$$\hat{v}(k)^{-2}(\mathfrak{b}(k) - E(U, k)) - \mathfrak{I}(\infty, k, E(U, k)) = \mathfrak{I}(k, E(U, k)) - \mathfrak{I}(\infty, k, E(U, k)).$$

Invoking next Corollary 4.13, we obtain the inequality

$$|\mathfrak{b}(k) - E(U, k) - \hat{v}(k)^2 \mathfrak{I}(\infty, k, E(U, k))| < \frac{\hat{v}(k)^2 R_{\mathfrak{b}, \mathfrak{b}}}{UR_{\mathfrak{s}, \mathfrak{s}}}.$$

We can take the limit $U \rightarrow \infty$ in this last inequality by using (110) and the continuity of the mapping

$$\mathfrak{I}(\infty, k, \cdot) : \rho(B_{1,1}(k)) \rightarrow \mathbb{R}^+$$

at the point $E(\infty, k)$, to arrive at the equality

$$\hat{v}(k)^2 \mathfrak{I}(\infty, k, E(\infty, k)) + E(\infty, k) - \mathfrak{b}(k) = 0. \quad (111)$$

This proves that $E(\infty, k)$ is a solution to (108). There is no other solution below $\mathfrak{z}(k)$ because of the following arguments: Given any $U \in [0, \infty]$, let

$$f_U(x) \doteq \hat{v}(k)^2 \mathfrak{I}(U, k, x) + x, \quad x \in (-\infty, \mathfrak{z}(k)).$$

By Corollary 4.13, $(f_U)_{U \in \mathbb{R}_0^+}$ converges pointwise to f_∞ , as $U \rightarrow \infty$. Since the pointwise limit of monotonically increasing function is again monotonically increasing, it follows that f_∞ is monotonically

increasing. Given any $x < y < \mathfrak{z}(k)$, take any $r > 0$ with $r \geq f_\infty(y) - f_\infty(x) \geq 0$. Then, for some $U_0 \in \mathbb{R}_0^+$ sufficiently large, one has

$$-r < f_{U_0}(y) - f_\infty(y) < r \quad \text{and} \quad -r < f_{U_0}(x) - f_\infty(x) < r,$$

so that

$$\begin{aligned} 2r &> (f_{U_0}(y) - f_\infty(y)) - (f_{U_0}(x) - f_\infty(x)) \\ &= (f_{U_0}(y) - f_{U_0}(x)) - (f_\infty(y) - f_\infty(x)) \\ &\geq f_{U_0}(y) - f_{U_0}(x) - r. \end{aligned}$$

Then, the mean value theorem combined with (89) implies that

$$3r \geq f_{U_0}(y) - f_{U_0}(x) = f'_{U_0}(c)(y - x) \geq y - x > 0 \quad (112)$$

for some $c \in (x, y)$. This implies that the function f_∞ is strictly increasing on $(-\infty, \mathfrak{z}(k))$, and hence, there is a unique solution, $E(\infty, k)$, to (108). Meanwhile, if $\hat{v}(k) = 0$, then Theorem 4.8 implies that $E(U, k) = \mathfrak{b}(k)$ for all $U \in \mathbb{R}_0^+$, and obviously, $E(\infty, k) = \mathfrak{b}(k)$ is the unique solution to (108).

Consider now the open set \mathcal{O} defined by (92). Let $\Phi(\infty, \cdot) : \mathcal{O} \rightarrow \mathbb{R}$ be defined by

$$\Phi(\infty, k, x) \doteq \hat{v}(k)^2 \mathfrak{T}(\infty, k, x) + x - \mathfrak{b}(k), \quad (k, x) \in \mathcal{O}. \quad (113)$$

By Corollary 4.13, note that $\Phi(\infty, \cdot) : \mathcal{O} \rightarrow \mathbb{R}$ is nothing else than the pointwise limit of the function $\Phi(U, \cdot) : \mathcal{O} \rightarrow \mathbb{R}$ defined by (91):

$$\lim_{U \rightarrow \infty} \Phi(U, k, x) = \Phi(\infty, k, x). \quad (114)$$

The function $\Phi(\infty, \cdot, \cdot)$ is a continuously differentiable function satisfying

$$\partial_x \Phi(\infty, k, x) \geq 1/3 > 0, \quad (k, x) \in \mathcal{O},$$

thanks to Inequality (112). Observe also that $\Phi(\infty, \cdot) \in C^d(\mathcal{O})$ if \hat{v} is of class C^d on $\mathbb{S}^2 \subseteq \mathbb{R}^2$ with $d \in \mathbb{N} \cup \{\omega, a\}$. Therefore, by repeating essentially the same argument used in the proof of Theorem 4.9, one concludes that $E(\infty, \cdot) \in C^d(\mathbb{S}^2)$ whenever \hat{v} is of class C^d on $\mathbb{S}^2 \subseteq \mathbb{R}^2$ with $d \in \mathbb{N} \cup \{\omega, a\}$.

Finally, assume that $r_p > 0$; that is, $\mathfrak{p}_1 \notin \mathbb{C}e_0$ or $\mathfrak{p}_2 \notin \mathbb{C}e_0$. For $k \neq 0$, we deduce from (111) and Lemma 4.12 that

$$E(\infty, k) = \mathfrak{b}(k) \Leftrightarrow \hat{v}(k)^2 \mathfrak{T}(\infty, k, E(\infty, k)) = 0 \Leftrightarrow \hat{v}(k) = 0.$$

To conclude the proof of Assertion (v), it remains to show that $\hat{v}(0) \neq 0$ implies $E(\infty, 0) < \mathfrak{b}(0)$. Assume on the contrary that

$$\lim_{U \rightarrow \infty} E(U, 0) = \mathfrak{b}(0), \quad (115)$$

keeping in mind that $\mathfrak{b}(0) = \mathfrak{z}(0) = 0$. Then, we infer from Theorems 4.5 and 4.8 that the following equality must be true:

$$\lim_{U \rightarrow \infty} \mathfrak{T}(U, 0, E(U, 0)) = \lim_{U \rightarrow \infty} \hat{v}(0)^{-2} (\mathfrak{b}(0) - E(U, 0)) = 0.$$

By Lemma 4.12, it follows that

$$\lim_{U \rightarrow \infty} \frac{R_{\mathfrak{b}, \mathfrak{b}}(U)}{UR_{\mathfrak{s}, \mathfrak{s}}(U) + 1} = 0, \quad (116)$$

where, by a slight abuse of notation,

$$\begin{aligned} R_{\mathfrak{s},\mathfrak{s}}(\mathbf{U}) &\doteq R_{\mathfrak{s},\mathfrak{s}}(0, E(\mathbf{U}, 0)), \\ R_{\mathfrak{d},\mathfrak{d}}(\mathbf{U}) &\doteq R_{\mathfrak{d},\mathfrak{d}}(0, E(\mathbf{U}, 0)), \\ R_{\mathfrak{s},\mathfrak{d}}(\mathbf{U}) &\doteq R_{\mathfrak{s},\mathfrak{d}}(0, E(\mathbf{U}, 0)). \end{aligned}$$

Therefore, we deduce from Corollary 4.13 that

$$\lim_{\mathbf{U} \rightarrow \infty} \frac{R_{\mathfrak{d},\mathfrak{d}}(\mathbf{U})R_{\mathfrak{s},\mathfrak{s}}(\mathbf{U}) - |R_{\mathfrak{s},\mathfrak{d}}(\mathbf{U})|^2}{R_{\mathfrak{s},\mathfrak{s}}(\mathbf{U})} = \lim_{\mathbf{U} \rightarrow \infty} \mathfrak{T}(\infty, 0, E(\mathbf{U}, 0)) = 0. \quad (117)$$

Now, observe that

$$\begin{aligned} &\frac{R_{\mathfrak{d},\mathfrak{d}}(\mathbf{U})R_{\mathfrak{s},\mathfrak{s}}(\mathbf{U}) - |R_{\mathfrak{s},\mathfrak{d}}(\mathbf{U})|^2}{R_{\mathfrak{s},\mathfrak{s}}(\mathbf{U})} \\ &= \frac{1}{R_{\mathfrak{s},\mathfrak{s}}(\mathbf{U})} \langle (R_{\mathfrak{s},\mathfrak{s}}(\mathbf{U})\mathfrak{d}(0) - R_{\mathfrak{s},\mathfrak{d}}(\mathbf{U})\mathfrak{s}), (B_{1,1}(0) - E(\mathbf{U}, 0)\mathbf{1})^{-1} (R_{\mathfrak{s},\mathfrak{s}}(\mathbf{U})\mathfrak{d}(0) - R_{\mathfrak{s},\mathfrak{d}}(\mathbf{U})\mathfrak{s}) \rangle \\ &= \langle \mathfrak{d}(0) - \alpha(\mathbf{U})\mathfrak{s}, (B_{1,1}(0) - E(\mathbf{U}, 0)\mathbf{1})^{-1} (\mathfrak{d}(0) - \alpha(\mathbf{U})\mathfrak{s}) \rangle \end{aligned} \quad (118)$$

where

$$\alpha(\mathbf{U}) \doteq R_{\mathfrak{s},\mathfrak{s}}(\mathbf{U})^{-1} R_{\mathfrak{s},\mathfrak{d}}(\mathbf{U}).$$

Let $\varphi_{\mathbf{U}} = \mathfrak{d}(0) - \alpha(\mathbf{U})\mathfrak{s} \neq 0$ and $W_{\mathbf{U}} = B_{1,1}(0) - E(\mathbf{U}, 0)\mathbf{1}$. Since $W_{\mathbf{U}}$ is strictly positive, it has an unique square root, which is also strictly positive. Then

$$\begin{aligned} \|\varphi_{\mathbf{U}}\|^4 &= |\langle W_{\mathbf{U}}^{-1/2} \varphi_{\mathbf{U}}, W_{\mathbf{U}}^{1/2} \varphi_{\mathbf{U}} \rangle|^2 \leq \|W_{\mathbf{U}}^{-1/2} \varphi_{\mathbf{U}}\|^2 \|W_{\mathbf{U}}^{1/2} \varphi_{\mathbf{U}}\|^2 \leq \\ &\leq \|W_{\mathbf{U}}\|_{\text{op}} \|\varphi_{\mathbf{U}}\|^2 \langle \varphi_{\mathbf{U}}, W_{\mathbf{U}}^{-1} \varphi_{\mathbf{U}} \rangle \leq \|\varphi_{\mathbf{U}}\|^2 \langle \varphi_{\mathbf{U}}, W_{\mathbf{U}}^{-1} \varphi_{\mathbf{U}} \rangle (\|B_{1,1}(0)\|_{\text{op}} + |E(0, 0)|). \end{aligned}$$

As $\langle \varphi_{\mathbf{U}}, W_{\mathbf{U}}^{-1} \varphi_{\mathbf{U}} \rangle$ tends to 0 when $\mathbf{U} \rightarrow \infty$, it follows that also $\varphi_{\mathbf{U}}$ vanishes in this limit; that is,

$$\lim_{\mathbf{U} \rightarrow \infty} \alpha(\mathbf{U})\mathfrak{s} = \mathfrak{d}(0). \quad (119)$$

As $\mathbb{C}\mathfrak{s}$ is a closed subspace of $L^2(\mathbb{T}^2)$, we get that $\mathfrak{d}(0) \in \mathbb{C}\mathfrak{s}$, which is a contradiction. Therefore, Assertion (v) holds true. \square

Remark 4.16. Under the additional conditions that $r_{\mathfrak{p}} > 0$ (i.e., $\mathfrak{p}_1 \notin \mathbb{C}e_0$ or $\mathfrak{p}_2 \notin \mathbb{C}e_0$) and $\hat{v}(0) \neq 0$, Assertion (iv) remains valid with $(-\pi, \pi)^2$ instead of \mathbb{S}^2 (i.e., by including the zero quasi-momentum case $k = 0$). Also, Assertion (iii) holds true for $k = 0$. In fact, under these further conditions, we know from Assertion (v) that $E(\infty, 0) < \mathfrak{z}(0) = 0$.

Corollary 4.17 (Hard-core dispersion relation). *Let $h_{\mathfrak{b}} \in [0, 1/2]$ and \hat{v} be of class C^2 on \mathbb{S}^2 . Then, $E(\infty, \cdot) \in C(\mathbb{T}^2)$ and is of class C^2 on \mathbb{S}^2 . In this case, for any $k \in \mathbb{S}^2$,*

$$\mathbf{v}_{E,\infty}(k) \doteq \vec{\nabla}_k E(\infty, k) = -(\partial_x \Phi(\infty, k, E(\infty, k)))^{-1} \vec{\nabla}_k \Phi(\infty, k, E(\infty, k)) = \lim_{\mathbf{U} \rightarrow \infty} \mathbf{v}_{E,\mathbf{U}}(k).$$

Moreover, if \hat{v} is real analytic (of class C^a , in our terminology) on \mathbb{S}^2 , then either $\mathfrak{M}_{E(\infty, \cdot)}$ has full measure or is empty.

Proof. Recall that \mathcal{O} is the open set (92) and $\Phi(\cdot, \cdot) : \mathbb{R}_0^+ \times \mathcal{O} \rightarrow \mathbb{R}$ is the real-valued function defined by (91). Note that, for any $\mathbf{U} \in \mathbb{R}_0^+$, the function $\Phi(\mathbf{U}, \cdot)$ is a smooth function on \mathcal{O} , and we estimate its

derivatives with respect to the parameter k , at fixed $U \in \mathbb{R}_0^+$ and x , where $(k, x) \in \mathcal{O}$: For any $(k, x) \in \mathcal{O}$ and $U \in \mathbb{R}_0^+$, Equations 37–38 together with the second resolvent formula yield the derivative

$$\partial_{k_j}(A_{1,1}(U, k) - x\mathbf{1})^{-1} = -(A_{1,1}(U, k) - x\mathbf{1})^{-1}\{\partial_{k_j}M_{\mathfrak{f}(k)}\}(A_{1,1}(U, k) - x\mathbf{1})^{-1}$$

for any $j \in \{1, 2\}$, where $k = (k_1, k_2) \in \mathbb{S}^2$. Therefore, by (33) and (91), for any $(k, x) \in \mathcal{O}$ and $U \in \mathbb{R}_0^+$,

$$|\partial_{k_j}\Phi(U, k, x)| \leq 8\epsilon\hat{v}(k)^2|\mathfrak{z}(k) - x|^{-2} \quad (120)$$

for any $j \in \{1, 2\}$, where $k = (k_1, k_2) \in \mathbb{S}^2$. Taking the second derivative, one can easily check that

$$|\partial_{k_j}^2\Phi(U, k, x)| \leq 8\epsilon\hat{v}(k)^2|\mathfrak{z}(k) - x|^{-3} \quad (121)$$

for $j \in \{1, 2\}$, where $k = (k_1, k_2) \in \mathbb{S}^2$. In the same way, we deduce from the identities

$$\begin{aligned} \partial_x\Phi(U, k, x) &= \hat{v}(k)^2\left\langle \mathfrak{d}(k), (A_{1,1}(U, k) - x\mathbf{1})^{-2}\mathfrak{d}(k) \right\rangle + 1 \\ \partial_x^2\Phi(U, k, x) &= 2\hat{v}(k)^2\left\langle \mathfrak{d}(k), (A_{1,1}(U, k) - x\mathbf{1})^{-3}\mathfrak{d}(k) \right\rangle \end{aligned}$$

the following inequalities:

$$|\partial_x\Phi(U, k, x)| \leq \hat{v}(k)^2|\mathfrak{z}(k) - x|^{-2} + 1, \quad (122)$$

$$|\partial_x^2\Phi(U, k, x)| \leq 2\hat{v}(k)^2|\mathfrak{z}(k) - x|^{-3}, \quad (123)$$

for any $(k, x) \in \mathcal{O}$ and $U \in \mathbb{R}_0^+$.

Now, fix $(k_0, x_0) \in \mathcal{O}$. The function \mathfrak{z} of Corollary 4.3 is continuous with respect to k_1, k_2 , where $k = (k_1, k_2) \in \mathbb{S}^2$. Then, there is a closed cube centered at (k_0, x_0) with side length $\delta \in \mathbb{R}^+$ contained in \mathcal{O} . Suppose that $\partial_x\Phi(U, k_0, x_0)$ does not converge to $\partial_x\Phi(\infty, k_0, x_0)$. Then we can find $r_0 \in \mathbb{R}^+$ and a sequence $(U_n)_{n \in \mathbb{N}}$ of positive numbers such that $U_n \rightarrow \infty$ as $n \rightarrow \infty$ and, for every $n \in \mathbb{N}$,

$$|\partial_x\Phi(U_n, k_0, x_0) - \partial_x\Phi(\infty, k_0, x_0)| \geq r_0.$$

Let

$$\mathfrak{F} = \{\partial_x\Phi(U_n, k_0, \cdot) \upharpoonright [x_0 - \delta, x_0 + \delta] : n \in \mathbb{N}\}.$$

By combining Equation (123) with the mean value theorem, we see that \mathfrak{F} is Lipschitz equicontinuous. In particular, this family of functions is equicontinuous. Moreover, it follows from (122) that \mathfrak{F} is bounded in the supremum norm. We can hence apply the (Arzelà-) Ascoli theorem [44, Theorem A5], according to which $\partial_x\Phi(U_n, k_0, \cdot)$, when restricted to the compact interval $[x_0 - \delta, x_0 + \delta]$, converges uniformly along some subsequence. Assume, for simplicity and without loss of generality, that the (full) sequence of functions converges itself. By Equation (114), recall that $\Phi(U, \cdot, \cdot)$ converges pointwise to the function $\Phi(\infty, \cdot, \cdot)$ on \mathcal{O} , which is the real-valued function defined by (113). Then, by [93, Theorem 7.17],

$$\partial_x\Phi(\infty, k_0, x) = \lim_{n \rightarrow \infty} \partial_x\Phi(U_n, k_0, x), \quad x \in [x_0 - \delta, x_0 + \delta].$$

For $x = x_0$, this lead us to a contradiction. Thus,

$$\partial_x\Phi(\infty, k, x) = \lim_{U \rightarrow \infty} \partial_x\Phi(U, k, x)$$

for every $(k, x) \in \mathcal{O}$. In the same way, we invoke Equations (120) and (121) together with the mean value theorem and the (Arzelà-) Ascoli theorem [44, Theorem A5] to deduce that

$$\partial_{k_j} \Phi(\infty, k, x) = \lim_{U \rightarrow \infty} \partial_{k_j} \Phi(U, k, x), \quad j = 1, 2.$$

for every $(k, x) \in \mathcal{O}$. To prove the corollary, we eventually use these observations together with Theorem 4.15 (i), Corollary 4.10 and the equicontinuity of

$$\{\partial_\mu \Phi(U, k_0, \cdot) \upharpoonright (-\infty, \mathfrak{b}(k_0)] : U \in \mathbb{R}^+\},$$

with μ standing for the variables k_1, k_2 or x . Note that the last assertion concerning $\mathfrak{M}_{E(\infty, \cdot)}$ is a direct consequence of the fact that the zeros of any nonconstant real analytic function have null Lebesgue measure [49]; see the proof of the same assertion for $U < \infty$ in Corollary 4.10. \square

Note that no additional condition is required for E to have a well-defined hard-core limit. Compare Corollary 4.10 with Theorem 4.15. Moreover, by Corollary 4.17, $E(\infty, \cdot)$ can be viewed as the (effective) dispersion relation of the dressed bound fermion pairs, with lowest energy, in the hard-core limit.

We close this section by showing the convergence of the low-energy eigenvector of $A(U, k)$ for large Hubbard couplings. This refers to the (hard-core) limit $U \rightarrow \infty$ of the vector

$$\Psi(U, k) \equiv \Psi(k) \doteq \left(\hat{v}(k) (A_{1,1}(U, k) - E(U, k) \mathbf{1})^{-1} \mathfrak{d}(k), -1 \right) \in \mathcal{H}$$

see Equation (130).

Proposition 4.18 (Hard-core limit of eigenvectors). *Let $h_b \in [0, 1/2]$. Fix $k \in \mathbb{T}^2 \setminus \{0\}$. The following limit exists:*

$$\Psi(\infty, k) \doteq \lim_{U \rightarrow \infty} \Psi(U, k) \in \mathcal{H} \setminus \{0\}.$$

This statement remains valid for $k = 0$ provided that $\hat{v}(0) \neq 0$ and $r_p > 0$ (i.e., $\mathfrak{p}_1 \notin \mathbb{C}e_0$ or $\mathfrak{p}_2 \notin \mathbb{C}e_0$).

Proof. Fix $k \in \mathbb{T}^2$ with $k \neq 0$. By using the first resolvent formula together with Theorem 4.8, Theorem 4.15 (i) and (v), we find that

$$\|(A_{1,1}(U, k) - E(\infty, k) \mathbf{1})^{-1} - (A_{1,1}(U, k) - E(U, k) \mathbf{1})^{-1}\|_{\text{op}} \leq \frac{|E(U, k) - E(\infty, k)|}{|\mathfrak{z}(k) - E(\infty, k)|^2} \rightarrow 0.$$

Note that $E(\infty, k) \leq \mathfrak{b}(k) < \mathfrak{z}(k)$ for any $k \neq 0$. (When $\hat{v}(0) \neq 0$ and $\mathfrak{p}_1 \notin \mathbb{C}e_0$ or $\mathfrak{p}_2 \notin \mathbb{C}e_0$, we also have that $E(\infty, 0) < \mathfrak{b}(0) = \mathfrak{z}(0)$.) However, by Proposition A.14, $\{(A_{1,1}(U, k) - E(\infty, k) \mathbf{1})^{-1}\}_{U \geq 0}$ is a decreasing family of positive operators, and by Proposition A.15, it converges strongly as $U \rightarrow \infty$. Consequently, $(A_{1,1}(U, k) - E(U, k) \mathbf{1})^{-1}$ also converges strongly. \square

4.5. Spectral gap and Anderson localization

By Equation (90), the spectral gap of fiber Hamiltonians is equal to

$$\mathfrak{g}(U, k) \doteq \min \sigma_{\text{ess}}(A(U, k)) - E(U, k) \geq 0, \quad k \in \mathbb{T}^2, \quad (124)$$

for any Hubbard coupling constant $U \in \mathbb{R}_0^+$. When $r_p > 0$ (i.e., $\mathfrak{p}_1 \notin \mathbb{C}e_0$ or $\mathfrak{p}_2 \notin \mathbb{C}e_0$) and $\hat{v}(0) \neq 0$, this quantity turns out to be strictly positive, uniformly with respect to the parameter U :

Proposition 4.19 (Uniform spectral gap of fiber Hamiltonians). *Fix $h_b \in [0, 1/2]$. If $r_p > 0$ (i.e., $p_1 \notin \mathbb{C}e_0$ or $p_2 \notin \mathbb{C}e_0$) and $\hat{v}(0) \neq 0$, then*

$$\inf_{U \in \mathbb{R}_0^+} \min_{k \in \mathbb{T}^2} g(U, k) > 0.$$

Proof. The family $\{E(U, \cdot)\}_{U \in \mathbb{R}_0^+}$ of real-valued functions on \mathbb{T}^2 is equicontinuous, thanks to Theorem 4.9 (i). Since Proposition 4.2 says that, for any $k \in \mathbb{T}^2$,

$$\min \sigma_{\text{ess}}(A(U, k)) = \mathfrak{z}(k) \doteq 4\epsilon - 2\epsilon \cos(k/2), \quad (125)$$

we thus deduce from (124) that the family $\{g(U, \cdot)\}_{U \in \mathbb{R}_0^+}$ of real-valued functions on \mathbb{T}^2 is equicontinuous. It follows that the function

$$\mathbb{R}_0^+ \ni U \longmapsto \min_{k \in \mathbb{T}^2} g(U, k) \in \mathbb{R} \quad (126)$$

is continuous. Moreover, from the compactness of \mathbb{T}^2 , $g(U, \cdot)$ has a global minimizer, say $k_U \in \mathbb{T}^2$ for all $U \in \mathbb{R}_0^+$. Since $\hat{v}(0) \neq 0$, by Theorem 4.8,

$$E(U, k_U) < \min \sigma_{\text{ess}}(A(U, k_U)) = 0$$

when $k_U = 0$, while in the case $k_U \neq 0$,

$$E(U, k_U) \leq \mathfrak{b}(k_U) < \mathfrak{z}(k) = \min \sigma_{\text{ess}}(A(U, k_U)).$$

In particular,

$$\min_{k \in \mathbb{T}^2} g(U, k) = g(U, k_U) > 0, \quad U \in \mathbb{R}_0^+.$$

Using this together with the continuity of the function (126), we arrive at the inequality

$$\inf_{U \in [0, c]} \min_{k \in \mathbb{T}^2} g(U, k) > 0 \quad (127)$$

for any positive parameter $c \in \mathbb{R}_0^+$. Now, we perform the limit $U \rightarrow \infty$. Since \mathbb{T}^2 is compact, the net $(k_U)_{U \in \mathbb{R}_0^+}$ converges along subnets (in fact, subsequences). Assume without loss of generality that $(k_U)_{U \in \mathbb{R}_0^+}$ converges to some $k_\infty \in \mathbb{T}^2$ (otherwise, one uses all the following arguments on subsequences). If $k_\infty \neq 0$, then

$$\lim_{U \rightarrow \infty} \min_{k \in \mathbb{T}^2} g(U, k) \geq \lim_{U \rightarrow \infty} \mathfrak{z}(k_U) - \mathfrak{b}(k_U) = \mathfrak{z}(k_\infty) - \mathfrak{b}(k_\infty) > 0, \quad (128)$$

thanks to Theorem 4.8 and the continuity of the functions \mathfrak{z} and \mathfrak{b} . Assume now that $k_\infty = 0$. Since, for all $U \in \mathbb{R}_0^+$,

$$|E(U, k_U) - E(\infty, 0)| \leq |E(U, k_U) - E(U, 0)| + |E(U, 0) - E(\infty, 0)|,$$

we infer from the equicontinuity of the family $\{E(U, \cdot)\}_{U \in \mathbb{R}_0^+}$ (Theorem 4.9 (i)) and Theorem 4.15 (i) that

$$\lim_{U \rightarrow \infty} E(U, k_U) = E(\infty, 0).$$

Combined with Theorem 4.15 (v) and $\hat{v}(0) \neq 0$, this last limit in turn implies that

$$\lim_{U \rightarrow \infty} \min_{k \in \mathbb{T}^2} g(U, k) = \lim_{U \rightarrow \infty} \{\mathfrak{z}(k_U) - E(U, k_U)\} = \mathfrak{z}(0) - E(\infty, 0) = -E(\infty, 0) > 0. \quad (129)$$

The assertion is therefore a combination of Inequalities (127), (128) and (129). \square

We study now the space localization of the (dressed) bound pair with total quasi-momentum $k \in \mathbb{T}^2$ and energy $E(U, k)$. Assume that $\hat{v}(0) \neq 0$. By Corollary 4.6, for any fixed $k \in \mathbb{T}^2$, it corresponds to study the fermionic part of the eigenvector

$$\Psi(U, k) \doteq g(k, E(U, k)) = \left(\hat{v}(k)(A_{1,1}(U, k) - E(U, k)\mathbf{1})^{-1} \mathfrak{d}(k), -1 \right) \in \mathcal{H}, \quad (130)$$

written in the real space \mathbb{Z}^2 via the inverse Fourier transform \mathcal{F}^{-1} (see (31)). This function is denoted by

$$\psi_{U,k} \doteq \mathcal{F}^{-1} \left[\hat{v}(k)(A_{1,1}(U, k) - E(U, k)\mathbf{1})^{-1} \mathfrak{d}(k) \right] \in \ell^2(\mathbb{Z}^2) \quad (131)$$

for any fixed $k \in \mathbb{T}^2$. One should not be confused here by the parameter k . Recall, for instance, that, given $k \in \mathbb{T}^2$, $\mathfrak{d}(k) \in C(\mathbb{T}^2)$ is itself a function on the torus \mathbb{T}^2 , defined by

$$\mathfrak{d}(k)(p) \doteq \hat{\mathfrak{p}}_1(k+p) + \hat{\mathfrak{p}}_2(k/2+p), \quad p \in \mathbb{T}^2 \quad (132)$$

see Equation (34). In particular, observe that

$$\psi_{U,k} = \hat{v}(k) \mathcal{F}^{-1} \left[(A_{1,1}(U, k) - E(U, k)\mathbf{1})^{-1} \mathfrak{d}(k) \right]. \quad (133)$$

We now show that this function is exponentially localized in the real space:

Theorem 4.20 (Exponentially localized dressed bound fermion pairs). *Fix $h_b \in [0, 1/2]$, $k \in \mathbb{T}^2$ and suppose that $r_p > 0$ (i.e., $p \notin \mathbb{C}e_0$) and $\hat{v}(0) \neq 0$. There exist positive constants $C, \alpha > 0$ such that, for all $k \in \mathbb{T}^2$ and $U \in \mathbb{R}_0^+$,*

$$|\psi_{U,k}(x)| \leq Ce^{-\alpha|x|}, \quad x \in \mathbb{Z}^2.$$

Proof. By (36), we compute that

$$\begin{aligned} & \mathcal{F}^{-1} \left[(A_{1,1}(U, k) - E(U, k)\mathbf{1})^{-1} \mathfrak{d}(k) \right] \\ &= (\mathcal{F}^{-1} A_{1,1}(U, k) \mathcal{F} - E(U, k)\mathbf{1})^{-1} \mathcal{F}^{-1} [\mathfrak{d}(k)] \\ &= \sum_{y \in \mathbb{Z}^2} \left(e^{ik \cdot y} \mathfrak{p}_1(y) + e^{i\frac{k}{2} \cdot y} \mathfrak{p}_2(y) \right) (\mathcal{F}^{-1} A_{1,1}(U, k) \mathcal{F} - E(U, k)\mathbf{1})^{-1} \mathfrak{e}_y. \end{aligned} \quad (134)$$

By Equation (133), it suffices to estimate the exponential decay of this particular function. This is done by using the celebrated Combes-Thomas estimates, which correspond here to Theorem A.13. To this end, several quantities, one of them being related to the spectral gap $g(U, k)$ (124), have to be controlled and, as in Section A.6, we use the notation (A.22), that is,

$$\Delta(\lambda; T) \doteq \min\{|\lambda - a| : a \in \sigma(T)\} \quad (135)$$

for the distance between a complex number $\lambda \in \mathbb{C}$ and the spectrum $\sigma(T)$ of an operator $T \in \mathcal{B}(\ell^2(\mathbb{Z}^2))$, as well as (A.20), which, in the present case, refers to the quantity

$$\mathbf{S}(T, \mu) \doteq \sup_{x \in \mathbb{Z}^2} \sum_{y \in \mathbb{Z}^2} \left(e^{\mu|x-y|} - 1 \right) |\langle \mathfrak{e}_x, T \mathfrak{e}_y \rangle| \in [0, \infty] \quad (136)$$

for any $T \in \mathcal{B}(\ell^2(\mathbb{Z}^2))$ and $\mu \in \mathbb{R}_0^+$. We do it in three steps: The first one controls the spectral gap $\mathfrak{g}(\mathbf{U}, k)$ (124) and a quantity like (135) for $\lambda = \mathbf{E}(\mathbf{U}, k)$, while the second step is an analysis of quantities like (136). These two steps allow us to apply, in the last step, Theorem A.13 in order to get the desired result.

Step 1: Observe from Equation (124) and Proposition 4.19 that we can find $\alpha > 0$ such that, for all $k \in \mathbb{T}^2$ and $\mathbf{U} \in \mathbb{R}_0^+$,

$$0 < 4\epsilon(e^\alpha - 1) < \inf_{\mathbf{U} \in \mathbb{R}_0^+} \min_{k \in \mathbb{T}^2} \mathfrak{g}(\mathbf{U}, k) \leq \mathfrak{g}(\mathbf{U}, k) \doteq \min \sigma_{\text{ess}}(A(\mathbf{U}, k)) - \mathbf{E}(\mathbf{U}, k).$$

Using now Proposition 4.2 and the fact that

$$\min \sigma_{\text{ess}}(A_{1,1}(\mathbf{U}, k)) = \min \sigma(A_{1,1}(\mathbf{U}, k)),$$

for all $k \in \mathbb{T}^2$ and $\mathbf{U} \in \mathbb{R}_0^+$, we deduce from the last inequalities that

$$0 < 4\epsilon(e^\alpha - 1) < \inf_{\mathbf{U} \in \mathbb{R}_0^+} \min_{k \in \mathbb{T}^2} \mathfrak{g}(\mathbf{U}, k) \leq \Delta(\mathbf{E}(\mathbf{U}, k); A_{1,1}(\mathbf{U}, k)) = \min \sigma(A_{1,1}(\mathbf{U}, k)) - \mathbf{E}(\mathbf{U}, k)$$

see also Equation (135). Since \mathcal{F} is a unitary transformation, $A_{1,1}(\mathbf{U}, k)$ and $\mathcal{F}^* A_{1,1}(\mathbf{U}, k) \mathcal{F}$ have the same spectrum, and it follows that

$$0 < 4\epsilon(e^\alpha - 1) < \inf_{\mathbf{U} \in \mathbb{R}_0^+} \min_{k \in \mathbb{T}^2} \mathfrak{g}(\mathbf{U}, k) \leq \Delta(\mathbf{E}(\mathbf{U}, k); \mathcal{F}^* A_{1,1}(\mathbf{U}, k) \mathcal{F}) \quad (137)$$

for all $k \in \mathbb{T}^2$ and $\mathbf{U} \in \mathbb{R}_0^+$.

Step 2: By Equations (5) and (31), one easily checks that

$$\hat{\mathbf{e}}_y(p) \doteq \sum_{x \in \mathbb{Z}^2} e^{ip \cdot x} \mathbf{e}_y(x) = e^{ip \cdot y}, \quad p \in \mathbb{T}^2, y \in \mathbb{Z}^2,$$

while, for any fixed $k \in \mathbb{T}^2$, the real-valued functions $\mathfrak{f}(k)$, defined by (33) and (35) on the torus \mathbb{T}^2 , can be rewritten as

$$\mathfrak{f}(k)(p) \doteq \epsilon \{4 - \cos(p + k) - \cos(p)\} = 4\epsilon - \frac{\epsilon}{2} \sum_{z \in \mathbb{Z}^2, |z|=1} \left(e^{i(p+k) \cdot z} + e^{ip \cdot z} \right), \quad p \in \mathbb{T}^2.$$

Therefore, since $M_{\mathfrak{f}(k)}$ stands for the multiplication operator by $\mathfrak{f}(k) \in C(\mathbb{T}^2)$, for every $p, k \in \mathbb{T}^2$ and $y \in \mathbb{Z}^2$,

$$M_{\mathfrak{f}(k)} \hat{\mathbf{e}}_y(p) = 4\epsilon e^{ip \cdot y} \epsilon - \frac{\epsilon}{2} \sum_{z \in \mathbb{Z}^2, |z|=1} \left(e^{ik \cdot z} + 1 \right) e^{ip \cdot (y+z)} = 4\epsilon \hat{\mathbf{e}}_y(p) - \frac{\epsilon}{2} \sum_{z \in \mathbb{Z}^2, |z|=1} \left(e^{ik \cdot z} + 1 \right) \hat{\mathbf{e}}_{y+z}(p),$$

which, by (37)–(38), in turn implies that

$$\begin{aligned} \mathcal{F}^* A_{1,1}(\mathbf{U}, k) \mathcal{F} \mathbf{e}_y &= \mathcal{F}^* \left(M_{\mathfrak{f}(k)} \hat{\mathbf{e}}_y + \mathbf{U} P_0 \hat{\mathbf{e}}_y + \sum_{z \in \mathbb{Z}^2} \mathbf{u}(z) P_z \hat{\mathbf{e}}_y \right) \\ &= \mathcal{F}^* (M_{\mathfrak{f}(k)} \hat{\mathbf{e}}_y + (\mathbf{U} \delta_{y,0} + \mathbf{u}(y)) \hat{\mathbf{e}}_y) \\ &= 4\epsilon \mathbf{e}_y - \frac{\epsilon}{2} \sum_{z \in \mathbb{Z}^2, |z|=1} \left(e^{ik \cdot z} + 1 \right) \mathbf{e}_{y+z} + (\mathbf{U} \delta_{y,0} + \mathbf{u}(y)) \mathbf{e}_y, \end{aligned}$$

keeping in mind that P_x is the orthogonal projection onto the one-dimensional subspace $\mathbb{C}\hat{\mathbf{e}}_x \subseteq L^2(\mathbb{T}^2)$. Recall that $\mathcal{F}^* = \mathcal{F}^{-1}$, the Fourier transform being unitary. Thus, since $\alpha > 0$, for each $x \in \mathbb{Z}^2$, we obtain that

$$\sum_{y \in \mathbb{Z}^2} \left| e^{\alpha|x-y|} - 1 \right| \left| \langle \mathbf{e}_x, \mathcal{F}^* A_{1,1}(\mathbf{U}, k) \mathcal{F} \mathbf{e}_y \rangle \right| = \frac{\epsilon}{2} (e^\alpha - 1) \sum_{y \in \mathbb{Z}^2, |x-y|=1} \left| e^{ik \cdot (x-y)} + 1 \right| \leq 4\epsilon(e^\alpha - 1).$$

Hence, taking the supremum over all $x \in \mathbb{Z}^2$ in this equation and using the notation given by (136) as well as (137), we arrive at

$$\mathbf{S}(\mathcal{F}^* A_{1,1}(\mathbf{U}, k) \mathcal{F}, \alpha) \leq 4\epsilon(e^\alpha - 1) < \inf_{\mathbf{U} \in \mathbb{R}_0^+} \min_{k \in \mathbb{T}^2} \mathbf{g}(\mathbf{U}, k) \leq \Delta(\mathbf{E}(\mathbf{U}, k); \mathcal{F}^* A_{1,1}(\mathbf{U}, k) \mathcal{F}) \quad (138)$$

for any fixed $k \in \mathbb{T}^2$ and $\mathbf{U} \in \mathbb{R}_0^+$.

Step 3: Thanks to (138), we are now in a position to apply Theorem A.13 for $H = \mathcal{F}^* A_{1,1}(\mathbf{U}, k) \mathcal{F}$ and $\mu = \alpha$ to obtain that, for any $x, y \in \mathbb{Z}^2$,

$$\begin{aligned} & \left| \left\langle \mathbf{e}_x, (\mathcal{F}^* A_{1,1}(\mathbf{U}, k) \mathcal{F} - \mathbf{E}(\mathbf{U}, k) \mathbf{1})^{-1} \mathbf{e}_y \right\rangle \right| \\ & \leq \frac{e^{-\alpha|x-y|}}{\Delta(\mathbf{E}(\mathbf{U}, k); \mathcal{F}^* A_{1,1}(\mathbf{U}, k) \mathcal{F}) - \mathbf{S}(\mathcal{F}^* A_{1,1}(\mathbf{U}, k) \mathcal{F}, \alpha)} \\ & \leq \frac{e^{-\alpha|x-y|}}{\inf_{\mathbf{U} \in \mathbb{R}_0^+} \min_{k \in \mathbb{T}^2} \mathbf{g}(\mathbf{U}, k) - 4\epsilon(e^\alpha - 1)}. \end{aligned}$$

Combined with Equations (133)–(134) and the triangle inequality as well as the reverse one $|x - y| \geq |x| - |y|$, we then arrive at

$$\begin{aligned} |\psi_{\mathbf{U},k}(x)| &= \left| \langle \mathbf{e}_x, \psi_{\mathbf{U},k} \rangle \right| \\ &\leq |\hat{\nu}(k)| \sum_{y \in \mathbb{Z}^2} (|\mathbf{p}_1(y)| + |\mathbf{p}_2(y)|) \left| \left\langle \mathbf{e}_x, (\mathcal{F}^{-1} A_{1,1}(\mathbf{U}, k) \mathcal{F} - \mathbf{E}(\mathbf{U}, k) \mathbf{1})^{-1} \mathbf{e}_y \right\rangle \right| \\ &\leq \frac{|\hat{\nu}(k)|}{\inf_{\mathbf{U} \in \mathbb{R}_0^+} \min_{k \in \mathbb{T}^2} \mathbf{g}(\mathbf{U}, k) - 4\epsilon(e^\alpha - 1)} \sum_{y \in \mathbb{Z}^2} (|\mathbf{p}_1(y)| + |\mathbf{p}_2(y)|) e^{-\alpha|x-y|} \\ &\leq \frac{|\hat{\nu}(k)| e^{-\alpha|x|}}{\inf_{\mathbf{U} \in \mathbb{R}_0^+} \min_{k \in \mathbb{T}^2} \mathbf{g}(\mathbf{U}, k) - 4\epsilon(e^\alpha - 1)} \sum_{y \in \mathbb{Z}^2} (|\mathbf{p}_1(y)| + |\mathbf{p}_2(y)|) e^{\alpha|y|} \quad (139) \end{aligned}$$

for all $x \in \mathbb{Z}^2$, $k \in \mathbb{T}^2$ and $\mathbf{U} \in \mathbb{R}_0^+$. By choosing α sufficiently small (more precisely $\alpha \leq \alpha_0$), we can assume, without loss of generality, that the above sum is finite; see (12). This completes the proof, because the Fourier transform $\hat{\nu}$ of ν is a continuous function on the torus \mathbb{T}^2 , which is compact, and is consequently bounded. \square

4.6. Scattering channels

4.6.1. Unbound pair scattering channel

Recall that \mathfrak{H}_f is defined by (53) and H_f is the operator defined by (54) for any $\mathbf{V} \in \mathbb{R}_0^+$ and absolutely summable function $\mathbf{v} : \mathbb{Z}^2 \rightarrow \mathbb{R}_0^+$.

For any operator Y acting on a Hilbert space \mathcal{Y} , $P_{ac}(Y)$ denotes the orthogonal projection on the absolutely continuous space of Y , defined by (49). In order to show the existence of a unbound pair scattering channel, we need the following technical lemma:

Lemma 4.21 (Absolute continuous space of fermionic Hamiltonians). *For any $V \in \mathbb{R}_0^+$ and every absolutely summable function $v : \mathbb{Z}^2 \rightarrow \mathbb{R}_0^+$, the orthogonal projection $P_{ac}(H_f)$ on the absolutely continuous space of H_f , defined by (49), is equal to $\mathbf{1}$.*

Proof. Take any $\psi \in \mathfrak{H}_f$ and observe from Corollary A.5 that

$$\psi(k) \in \text{ran}(P_{ac}(M_{\mathfrak{f}(k)})), \quad k \in \mathbb{T}^2,$$

where $M_{\mathfrak{f}(k)}$ is the fiber Hamiltonian defined as the multiplication operator associated with the continuous function $\mathfrak{f}(k) \in C(\mathbb{T}^2)$ (see (33)). For any $V \in \mathbb{R}_0^+$ and absolutely summable function $v : \mathbb{Z}^2 \rightarrow \mathbb{R}_0^+$, the operator defined by (55); that is,

$$R(V, v) \doteq \sum_{x \in \mathbb{Z}^2} v(x) P_x + V P_0 \in \mathcal{B}(L^2(\mathbb{T}^2))$$

is a trace-class operator, where we recall that P_x is the orthogonal projection on the one-dimensional subspace $\mathbb{C}\hat{e}_x \subseteq L^2(\mathbb{T}^2)$. By [40, Theorem 4.4, Chapter X], it follows in this case that

$$\psi(k) \in \text{ran}(P_{ac}(M_{\mathfrak{f}(k)} + R(V, v))), \quad k \in \mathbb{T}^2.$$

Let $B \subseteq \mathbb{R}$ be an arbitrary Borel set with zero Lebesgue measure. By using (54), we deduce that

$$\begin{aligned} \langle \psi, \chi_B(M_{\mathfrak{f}})\psi \rangle_{\mathfrak{H}_f} &= \left\langle \psi, \left(\int_{\mathbb{T}^2}^{\oplus} \chi_B(M_{\mathfrak{f}(k)} + R(V, v)) v(dk) \right) \psi \right\rangle_{\mathfrak{H}_f} \\ &= \int_{\mathbb{T}^2} \langle \psi(k), \chi_B(M_{\mathfrak{f}(k)} + R(V, v)) \psi(k) \rangle_{L^2(\mathbb{T}^2)} v(dk) = 0. \end{aligned}$$

For the first equality, note that we apply Theorem A.3 (iii). □

The following results imply that the dynamic generated by the Hamiltonian H (i.e., included the exchange interaction and extended Hubbard repulsions) asymptotically far in the past or future approaches the purely fermionic dynamics for two unbound fermions. This is, of course, physically expected, since all interaction strengths get weak as the distance between the fermions increases. This is a consequence of the next assertions.

To shorten the notation, for any $V \in \mathbb{R}_0^+$ and every absolutely summable function $v : \mathbb{Z}^2 \rightarrow \mathbb{R}_0^+$, we define the Hamiltonian

$$H^{(1)} \equiv H^{(1)}(V, v) \doteq \int_{\mathbb{T}^2}^{\oplus} H^{(1)}(k) \oplus A_{2,2}(k) v(dk) \in \mathcal{B}(L^2(\mathbb{T}^2, \mathcal{H}))$$

with

$$H^{(1)}(k) \doteq M_{\mathfrak{f}(k)} + R(V, v) \in \mathcal{B}(\mathcal{H}), \quad k \in \mathbb{T}^2. \quad (140)$$

Here, $M_{\mathfrak{f}(k)}$, $R(V, v)$ and $A_{2,2}(k)$ are respectively the multiplication operator associated with the continuous function $\mathfrak{f}(k) \in C(\mathbb{T}^2)$ (see (33)), the trace-class operator (55) and the operator defined on \mathbb{C} by (41). We start with the unbounded pair scattering channel in each fiber:

Lemma 4.22 (Fiberwise unbound pair (scattering) channel). *For any $V \in \mathbb{R}_0^+$, every absolutely summable function $v : \mathbb{Z}^2 \rightarrow \mathbb{R}_0^+$ and all $k \in \mathbb{T}^2$, the wave operators*

$$W^{\pm}(A(k), H^{(1)}(k) \oplus A_{2,2}(k)) = s - \lim_{t \rightarrow \pm\infty} e^{itA(k)} e^{-itH^{(1)}(k) \oplus A_{2,2}(k)},$$

as defined by Equation (51), exist and are complete with

$$\operatorname{ran}\left(W^{\pm}\left(A(k), H^{(1)}(k) \oplus A_{2,2}(k)\right)\right) = \operatorname{ran}\left(P_{\mathrm{ac}}\left(H^{(1)}(k) \oplus A_{2,2}(k)\right)\right).$$

Proof. Note that $P_{\mathrm{ac}}(H_f) = \mathbf{1}$, thanks to Lemma 4.21. By (51), it justifies the strong limit given in the lemma. As we discuss in the proof of Proposition 4.2, for any $k \in \mathbb{T}^2$, the operator $A(k)$ is the sum of $M_{\mathfrak{f}(k)} \oplus A_{2,2}(k)$ and a compact operator T . In fact, as the function $u : \mathbb{Z}^2 \rightarrow \mathbb{R}$ (defining the fiber Hamiltonian $A(k)$) is absolutely summable (see (7)), the operator difference T is even trace-class. As explained in Lemma 4.21, $R(V, v)$ is also a trace-class operator, because $v : \mathbb{Z}^2 \rightarrow \mathbb{R}_0^+$ is absolutely summable, again by assumption. By using the Kato-Rosenblum theorem (41, Theorem XI.8), it thus follows that the wave operators

$$W^{\pm}\left(A(k), H^{(1)}(k) \oplus A_{2,2}(k)\right) = W^{\pm}\left(A(k), (M_{\mathfrak{f}(k)} + R(V, v)) \oplus A_{2,2}(k)\right)$$

exist and are complete for every $k \in \mathbb{T}^2$. □

We are now in a position to prove Theorem 3.11. Recall that $\mathfrak{U} : \mathfrak{H}_f \rightarrow L^2(\mathbb{T}^2, \mathcal{H})$ is the operator defined by (56), while $A_{2,2}(k)$ and $H^{(1)}(k)$ are respectively defined by (41) and (140). The definition of wave operators W^{\pm} are given by Equations 50–51.

Theorem 4.23 (Unbound pair (scattering) channel). *For any $V \in \mathbb{R}_0^+$ and every absolutely summable function $v : \mathbb{Z}^2 \rightarrow \mathbb{R}_0^+$,*

$$W^{\pm}(\mathfrak{U}H\mathfrak{U}^*, H_f; \mathfrak{U}) = \left(\int_{\mathbb{T}^2}^{\oplus} W^{\pm}\left(A(k), H^{(1)}(k) \oplus A_{2,2}(k)\right) v(dk) \right) \mathfrak{U}$$

with

$$\operatorname{ran}(W^{\pm}(\mathfrak{U}H\mathfrak{U}^*, H_f; \mathfrak{U})) = \int_{\mathbb{T}^2}^{\oplus} L^2(\mathbb{T}^2) \oplus \{0\} v(dk).$$

Proof. For almost every $k \in \mathbb{T}^2$ and every $\psi \in \mathfrak{H}_f$,

$$(H^{(1)}\mathfrak{U}\psi)(k) = H^{(1)}(k) \oplus A_{2,2}(k)(\mathfrak{U}\psi)(k) = (H^{(1)}(k)\psi(k), 0) = (\mathfrak{U}H_f\psi)(k).$$

In other words, \mathfrak{U} is an intertwining operator for H_f and $H^{(1)}$, and hence, for their respective complex exponential:

$$\mathfrak{U}e^{-itH_f} = e^{-itH^{(1)}}\mathfrak{U}, \quad t \in \mathbb{R}. \quad (141)$$

We also observe that, for any $z \in \mathbb{C}$ and any Borel set $B \subseteq \mathbb{R}$ containing $\mathfrak{b}(k) \in \mathbb{R}$ (see (32)),

$$\langle z, \chi_B(A_{2,2}(k))z \rangle_{\mathbb{C}} = |z|^2 \chi_B(\mathfrak{b}(k)) \neq 0$$

even if the Lebesgue measure of B is zero. This last observation, together with Remark 3.10 and Lemma 4.21, yields

$$\operatorname{ran}\left(P_{\mathrm{ac}}\left(H^{(1)}(k) \oplus A_{2,2}(k)\right)\right) = L^2(\mathbb{T}^2) \oplus \{0\}, \quad k \in \mathbb{T}^2. \quad (142)$$

In particular,

$$\int_{\mathbb{T}^2}^{\oplus} P_{\mathrm{ac}}\left(H^{(1)}(k) \oplus A_{2,2}(k)\right) \mathfrak{U} = \mathfrak{U}. \quad (143)$$

We can then apply Proposition A.6 together with Lemmata 4.21, 4.22, Theorem A.3 and Equations (141)–(143) to arrive at

$$\begin{aligned}
 W^\pm(\mathbb{U}H\mathbb{U}^*, M_f; \mathfrak{U}) &\doteq s - \lim_{t \rightarrow \mp\infty} e^{it\mathbb{U}H\mathbb{U}^*} \mathfrak{U} e^{-itH_f} P_{\text{ac}}(H_f) \\
 &= s - \lim_{t \rightarrow \mp\infty} e^{it\mathbb{U}H\mathbb{U}^*} \mathfrak{U} e^{-itH_f} \\
 &= s - \lim_{t \rightarrow \mp\infty} e^{it\mathbb{U}H\mathbb{U}^*} e^{-itH^{(1)}} \mathfrak{U} \\
 &= s - \lim_{t \rightarrow \mp\infty} \left(\int_{\mathbb{T}^2}^\oplus e^{itA(k)} \nu(\mathrm{d}k) \right) \left(\int_{\mathbb{T}^2}^\oplus e^{-it(H^{(1)}(k) \oplus A_{2,2}(k))} \nu(\mathrm{d}k) \right) \mathfrak{U} \\
 &= s - \lim_{t \rightarrow \mp\infty} \left(\int_{\mathbb{T}^2}^\oplus e^{itA(k)} e^{-it(H^{(1)}(k) \oplus A_{2,2}(k))} P_{\text{ac}}(H^{(1)}(k) \oplus A_{2,2}(k)) \nu(\mathrm{d}k) \right) \mathfrak{U} \\
 &= \left(\int_{\mathbb{T}^2}^\oplus W^\pm(A(k), H^{(1)}(k) \oplus A_{2,2}(k)) \nu(\mathrm{d}k) \right) \mathfrak{U}.
 \end{aligned}$$

Note that Lemma 4.22 combined with (142) implies that

$$\text{ran}\left(W^\pm\left(A(k), H^{(1)}(k) \oplus A_{2,2}(k)\right)\right) = L^2(\mathbb{T}^2) \oplus \{0\}.$$

In particular,

$$\text{ran}(W^\pm(\mathbb{U}H\mathbb{U}^*, H_f; \mathfrak{U})) = \int_{\mathbb{T}^2}^\oplus L^2(\mathbb{T}^2) \oplus \{0\} \nu(\mathrm{d}k). \quad \square$$

Observe that Lemma A.1 allows one to write

$$e^{itX} e^{i(s-t)(X+Y)} e^{-isX}, \quad s, t \in \mathbb{R}$$

as a Dyson series for all bounded operators X, Y . This can be applied to $X = H^{(1)}$ and $Y = \mathbb{U}H\mathbb{U}^* - X$, or in each fiber $k \in \mathbb{T}^2$ to $X = H^{(1)}(k) \oplus A_{2,2}(k)$ and $Y = A(k) - X$. When $\mathbb{U} = \mathbb{V} \in \mathbb{R}_0^+$ and $\nu = \mathfrak{u} : \mathbb{Z}^2 \rightarrow \mathbb{R}_0^+$ in $H^{(1)}$, this result is particularly advantageous because the operator family $(Y_t)_{t \in \mathbb{R}}$ appearing in Lemma A.1 can be represented in a relatively simple way in this situation:

Lemma 4.24 (Finite-time scattering and wave operators). *For $\mathbb{U} \in \mathbb{R}_0^+$ and all $s, t \in \mathbb{R}$,*

$$\begin{aligned}
 &e^{itH^{(1)}(\mathbb{U}, \mathfrak{u})} e^{i(s-t)\mathbb{U}H\mathbb{U}^*} e^{-isH^{(1)}(\mathbb{U}, \mathfrak{u})} \\
 &= \int_{\mathbb{T}^2}^\oplus \begin{pmatrix} \cos_{>}(B_{1,2}(k)B_{2,1}(k); s, t) & -i \sin_{>}(B_{1,2}(k)B_{2,1}(k); s, t) \\ -i \sin_{>}(B_{2,1}(k)B_{1,2}(k); s, t) & \cos_{>}(B_{2,1}(k)B_{1,2}(k); s, t) \end{pmatrix} \nu(\mathrm{d}k),
 \end{aligned}$$

where $B_{1,2}(k)$ and $B_{2,1}(k)$ are the operator families defined by (60) for any $k \in \mathbb{T}^2$, while $\cos_{>}$ and $\sin_{>}$ are respectively defined by (61) and (62).

Proof. Let $H^{(1)} \equiv H^{(1)}(\mathbb{U}, \mathfrak{u})$. We infer from Lemma A.1 applied to $X = H^{(1)}$ and $Y = \mathbb{U}H\mathbb{U}^* - X$ that

$$e^{itH^{(1)}} e^{i(s-t)\mathbb{U}H\mathbb{U}^*} e^{-isH^{(1)}} = V_{t,s} \doteq \mathbf{1} + \sum_{n=1}^{\infty} (-i)^n \int_s^t \mathrm{d}\tau_1 \cdots \int_s^{\tau_{n-1}} \mathrm{d}\tau_n B^{(\tau_1)} \cdots B^{(\tau_n)},$$

with $(B^{(t)})_{t \in \mathbb{R}} \subseteq \mathcal{B}(L^2(\mathbb{T}^2, \mathcal{H}))$ being the norm-continuous family defined by

$$\begin{aligned} B^{(t)} &= e^{itH^{(1)}} \left(\mathbb{U}H\mathbb{U}^* - H^{(1)} \right) e^{-itH^{(1)}} \\ &= \int_{\mathbb{T}^2}^{\oplus} \begin{pmatrix} e^{itA_{1,1}(\mathbb{U},k)} & 0 \\ 0 & e^{itA_{2,2}(k)} \end{pmatrix} \begin{pmatrix} 0 & A_{1,2}(k) \\ A_{2,1}(k) & 0 \end{pmatrix} \begin{pmatrix} e^{-itA_{1,1}(\mathbb{U},k)} & 0 \\ 0 & e^{-itA_{2,2}(k)} \end{pmatrix} \nu(dk) \\ &= \int_{\mathbb{T}^2}^{\oplus} \begin{pmatrix} 0 & B_{1,2}^{(t)}(k) \\ B_{2,1}^{(t)}(k) & 0 \end{pmatrix} \nu(dk), \end{aligned}$$

the operators $B_{2,1}^{(t)}(k)$ and $B_{1,2}^{(t)}(k)$ being defined by (60) for any $t \in \mathbb{R}$ and $k \in \mathbb{T}^2$. Then, one combines explicit computations together with Proposition A.6 and A.7 to arrive at the assertion. Notice that the above integrals are Riemann ones, $(B^{(t)})_{t \in \mathbb{R}}$ being a continuous family in the Banach space $\mathcal{B}(L^2(\mathbb{T}^2, \mathcal{H}))$. \square

4.6.2. Bound pair scattering channel

We start by studying the wave operator (50) with respect to the operators $X = \mathbb{U}H\mathbb{U}^*$ and $Y = M_{E(\mathbb{U}, \cdot)}$ (66), the identification operator J being $\mathfrak{P}_{\mathbb{U}}$ (65) for any fixed Hubbard coupling constant $\mathbb{U} \in \mathbb{R}_0^+$.

Proposition 4.25 (Wave operators in the bound pair channel). *Let $h_b \in [0, 1/2]$ and $\mathbb{U} \in \mathbb{R}_0^+$. Then, $\mathbb{U}H\mathbb{U}^*\mathfrak{P}_{\mathbb{U}} = \mathfrak{P}_{\mathbb{U}}M_{E(\mathbb{U}, \cdot)}$, and for every bounded continuous function $f \in C_b(\mathbb{R})$,*

$$f(\mathbb{U}H\mathbb{U}^*)\mathfrak{P}_{\mathbb{U}} = \mathfrak{P}_{\mathbb{U}} \int_{\mathbb{T}^2}^{\oplus} f(E(\mathbb{U}, k)) \nu(dk).$$

Proof. Using Proposition 2.1 and Theorem 4.8, we note that, for any $\varphi \in L^2(\mathbb{T}^2)$ and almost every $k \in \mathbb{T}^2$,

$$(\mathbb{U}H\mathbb{U}^*\mathfrak{P}_{\mathbb{U}}\varphi)(k) = A(k)(\mathfrak{P}_{\mathbb{U}}\varphi)(k) = E(\mathbb{U}, k)\varphi(k)\|\Psi(\mathbb{U}, k)\|^{-1}\Psi(\mathbb{U}, k) = (\mathfrak{P}_{\mathbb{U}}M_{E(\mathbb{U}, \cdot)}\varphi)(k)$$

(i.e., $\mathbb{U}H\mathbb{U}^*\mathfrak{P}_{\mathbb{U}} = \mathfrak{P}_{\mathbb{U}}M_{E(\mathbb{U}, \cdot)}$), keeping in mind Equations (65) and (66). We then obtain the last assertion by using the Stone-Weierstrass theorem and the spectral theorem. \square

We now study the (dressed) bound pair channel of lowest energy in the hard-core limit. This is a consequence of the following assertion:

Proposition 4.26 (Bound pair channel in the hard-core limit). *Fix $h_b \in [0, 1/2]$. Then,*

$$s - \lim_{\mathbb{U} \rightarrow \infty} \mathfrak{P}(\mathbb{U}) = \mathfrak{P}_{\infty}, \quad (144)$$

and for every bounded continuous function $f \in C_b(\mathbb{R})$,

$$s - \lim_{\mathbb{U} \rightarrow \infty} f(\mathbb{U}H\mathbb{U}^*)\mathfrak{P}_{\mathbb{U}} = \mathfrak{P}_{\infty} \int_{\mathbb{T}^2}^{\oplus} f(E(\infty, k)) \nu(dk).$$

Proof. Fix $\varphi \in L^2(\mathbb{T}^2)$. For any $\mathbb{U} \in \mathbb{R}_0^+$ and almost every $k \in \mathbb{T}^2$, one has that

$$\|\mathfrak{P}_{\mathbb{U}}\varphi(k) - \mathfrak{P}_{\infty}\varphi(k)\| \leq 2\|\Psi(\infty, k)\|^{-1}\|\Psi(\mathbb{U}, k) - \Psi(\infty, k)\|\|\varphi(k)\|.$$

Thus, by Lebesgue's dominated convergence theorem, we arrive at

$$\lim_{\mathbb{U} \rightarrow \infty} \|\mathfrak{P}_{\mathbb{U}}\varphi(k) - \mathfrak{P}_{\infty}\varphi(k)\|_{L^2(\mathbb{T}^2, \mathcal{H})}^2 = \lim_{\mathbb{U} \rightarrow \infty} \int_{\mathbb{T}^2} \|\mathfrak{P}_{\mathbb{U}}\varphi(k) - \mathfrak{P}_{\infty}\varphi(k)\|^2 \nu(dk) = 0.$$

Take now a bounded continuous function $f \in C_b(\mathbb{R})$. In particular, there exists $L \in \mathbb{R}^+$ such that

$$\sup_{U \in \mathbb{R}_0^+} \sup_{k \in \mathbb{T}^2} |f(E(U, k))| \leq L.$$

By Theorem 4.15 (i) and continuity of the function f , one has that

$$\lim_{U \rightarrow \infty} f(E(U, k)) = f(E(\infty, k)), \quad k \in \mathbb{T}^2.$$

Moreover,

$$\mathbb{T}^2 \ni k \mapsto f(E(U, k)) \in \mathcal{L}(\mathbb{C}) (= \mathcal{B}(\mathbb{C}))$$

is a composition of continuous functions and is in particular strongly measurable. Using Proposition A.6 (or Lebesgue's dominated convergence theorem), we arrive at the limit

$$s - \lim_{U \rightarrow \infty} \int_{\mathbb{T}^2}^{\oplus} f(E(U, k)) \nu(dk) = \int_{\mathbb{T}^2}^{\oplus} f(E(\infty, k)) \nu(dk). \quad (145)$$

By using Equations (144), (145), Proposition 4.25, Theorem A.3 (iii) and the fact that $\|\mathfrak{P}(U)\|_{\text{op}} = 1$ for all $U \in \mathbb{R}_0^+$, we find that

$$\begin{aligned} s - \lim_{U \rightarrow \infty} f(UH U^*) \mathfrak{P}_U &= s - \lim_{U \rightarrow \infty} \mathfrak{P}_U f(M_{E(U, \cdot)}) \\ &= s - \lim_{U \rightarrow \infty} \mathfrak{P}_U \int_{\mathbb{T}^2}^{\oplus} f(E(U, k)) \nu(dk) \\ &= \mathfrak{P}_{\infty} \int_{\mathbb{T}^2}^{\oplus} f(E(\infty, k)) \nu(dk). \end{aligned} \quad \square$$

A. Appendix

A.1. Toward a microscopic theory for cuprate superconductivity

Superconductivity was discovered in 1911 through the study of the resistance of solid mercury at very low temperatures, which was found to disappear below the critical temperature $T_c = 4.2$ K. This phenomenon was subsequently observed in several other materials, such as lead (in this case, $T_c = 7$ K). The first microscopic explanation of this unexpected, but very interesting physical behavior was given in 1957 by J. Bardeen, L. Cooper and J. R. Schrieffer with what is now known as the BCS theory. They were awarded the Nobel Prize in Physics in 1972. Their theory explained all the superconductors known at the time, named today 'conventional' superconductors. For more details, see [51, Chapter 10].

These superconductors not only have zero resistivity (below some critical current value), but also repel magnetic fields. This is the Meissner effect (or Meissner-Ochsenfeld effect). See, for example, the popular images showing a superconducting piece levitating above a magnet. However, when the magnetic field exceeds a critical value, superconductivity can be broken and the Meissner effect disappears abruptly. This is referred to as type I superconductivity, while type II superconductors manifests the appearance of vortices beyond a first critical magnetic field and the disappearance of any Meissner effect beyond a second critical field. The BCS theory refers to conventional superconductors but applies for both type I and II superconductors.

Superconductors are characterized not only by the critical temperature but also their superconducting coherence length, which quantifies the characteristic exponent that describes variations in the density of the superconducting component. It is often several hundred nanometers for conventional superconductors. More precisely, from (51, Chapter 10, Table 5), we have the following coherence lengths ξ and critical temperatures T_c for the following conventional superconductors:

	ξ in nm	T_c in K	Type
Tin (Sn)	230	3.72	I
Aluminium (Al)	1600	1.2	I
Lead (Pb)	83	7.19	I
Cadmium (Cd)	760	0.52	I
Niobium (Nb)	38	9.26	II

(A.1)

Note that the superconducting coherence length of a Niobium superconductor is much smaller than others, which is consistent with the type-II property, which requires shorter coherence lengths compared to type I superconductors.

In 1986, there was a major breakthrough in physics with the discovery of a new class of superconductors by G. Bednorz and K. A. Müller [16]. They were awarded the Nobel Prize in Physics in 1987. Physically, these materials are antiferromagnetic and insulating at low temperatures, but as with semiconductors, one dopes them with impurities that provide extra charge carriers and break the perfect Mott insulator phase, which is characterized by an integer number of charge carriers on each lattice site. As doping increases, the antiferromagnetic phase turns into a superconducting phase. This was the discovery of high- T_c superconductors in ceramics materials (i.e., cuprates) for critical temperatures T_c that today range in the interval [39, 164] K (approximately).

These superconductors are nonconventional, and the BCS theory fails to explain their properties. Indeed, while the conventional superconductivity results from an effective attraction between fermions (electrons or holes, depending on the charge carriers in each material) via phonons (i.e., lattice excitations), it soon became apparent that this kind of explanation could not work for cuprates, and the question of the mediator that could produce such an attraction has remained an open problem ever since. In fact, even if a large amount of numerical and experimental data is available, there is no pairing mechanism firmly established (through, for instance, antiferromagnetic spin fluctuations, phonons, etc.). See, for example, [13, Section 7.6]. The debate is strongly polarized [54] between researchers using a purely electronic/magnetic microscopic mechanism and those using electron-phonon mechanisms.

This is undoubtedly one of the most important questions in condensed matter physics, even if current research seems to have shown less interest in this fundamental issue in recent years. Quoting the Nobel Prize winner Müller in 2007 [17]: “... *It is a remarkable fact that in these 20 years since the discovery of high temperature superconductivity no other class of materials has been found which exhibits this property above the boiling point of liquid nitrogen. With a view to finding another class, it would be rewarding to understand why these exceptional properties occur, which per se are regarded as among the important unsolved problems in present day physics.*”

Our theoretical approach differs from all others and stems from a microscopic model – first proposed in 1985 by Ranninger-Robaszkiewicz [55] (see also [56, 57] or [13, Section 7.4.3]) and independently by Ionov [58] – which, before our works, was *never* investigated in the presence of strong Coulomb repulsions.

The cuprates are a class of compounds containing copper (Cu) atoms in an anion, and cuprate superconductors are oxide-based cuprates with two-dimensional CuO_2 layers made of Cu^{++} (cf. ‘cuprate’) and O^{--} (cf. ‘oxide’) ions, which generally possess the symmetries of the square, at least for the important family of tetragonal cuprates such as $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ (LaSr 214) and $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$. See, for example, [31, Section 9.1.2], [12, Section 2.3] and [14, Section 6.3.1].

As stressed in [15, Part VII], the very strong Jahn-Teller (JT) effect associated with copper ions (Cu^{++}) and its consequences for polaron formation are largely neglected in much of the physics literature, even though it was the JT effect that led to the discovery of superconductivity in cuprates [16]. See also [17, 18, 19]. For nonexperts, let us explain that the JT effect (or JT distortion) is a spontaneous symmetry breaking of molecules and ions that occurs via a geometrical distortion that suppresses the spatial degeneracy of the electronic ground state and lowers the overall energy of the system. See [15]. In this context, it can produce JT n -polarons. Polarons, bipolarons or more generally, n -polarons, $n \in \mathbb{N}$, are charge carriers that are self-trapped inside a strong and local lattice deformation that surrounds them. They are quasi-particle formed from fermions ‘dressed with phonons’. For example, a *bipolaron* involves *two*

fermions dressed with phonons. A JT polaron is a polaron for which the local lattice deformation is associated with the (geometrical) JT distortion. The existence of JT (bi)polarons in cuprates is attested in numerous experiments on cuprate superconductors [59, 17, 18, 19], and we have the following experimental facts:

- Superconducting transport in cuprates occurs in two-dimensional CuO_2 layers and only on oxygen atoms – a fact well established experimentally from 1987 by Bianconi and others [60, 61, 62, 63, 65, 64, 66] – while bipolarons are related to the strong JT effect of copper ions.
- Because of the presence of strong **antiferromagnetic** correlations of copper-oxides, experimentally proven even outside the antiferromagnetic phase (see, for example, [68, 67] and (13, Chapter 3)), it can be concluded that JT bipolarons have **zero total spin** and that other types of polaronic configuration are disadvantaged. This is, for instance, stressed in [17, Sect. 5.2].
- There is also an experimental evidence of the short lifetime of polarons in cuprates [69], decaying into fermions (pairs of holes or electrons). Expressed in terms of a length ℓ , one sees a lifetime comparable to the lattice spacing [69]. Remarkably, near the critical temperature, ℓ is actually close to the coherence length in cuprate superconductors.

The most straightforward approach would therefore be to consider the JT bipolarons as the charge carriers of cuprate superconductors. That is exactly what Alexandrov and coauthors have done in their bipolaron theory, based on light bipolarons [70] as charge carriers. Quoting [71, p. 4]: “*cuprate bipolarons are relatively light because they are intersite rather than on-site pairs due to the strong on-site repulsion, and because mainly c-axis polarized optical phonons are responsible for the in-plane mass renormalization.*” See, for instance, [71, 72, 73, 74] and references therein. However, this approach does not seem consistent with superconducting transport in cuprates occurring on oxygen ions in CuO_2 layers:

In fact, a priori, (strong and local) lattice deformations (or JT distortions) attached to n -polarons should barely move, and this is not in accordance with the known mobility of superconducting charge carriers. This is confirmed in experiments:

- Experimental evidence (still controversial [52]) of a large mass (approx. 700 electronic masses) of polarons in cuprates [37].
- Experimental evidence (apparently not controversial) of the small mass (approx. 3–4 electronic masses) of superconducting carriers in cuprates [75, Fig. 2.].

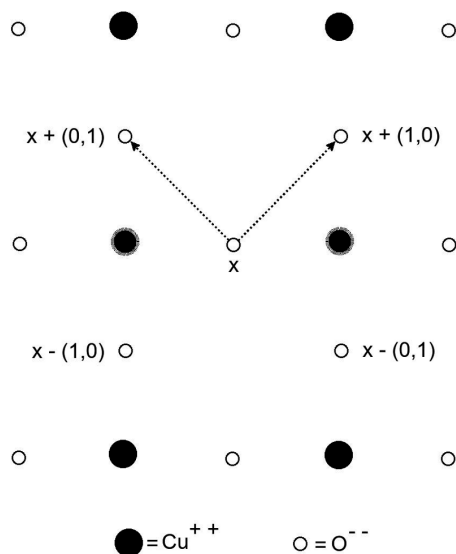
For more recent discussions on the (im)mobility of (bi)polarons in cuprates, we recommend, for instance, [34, 35, 36].

We bypass this problem by using the exchange interaction (10), while seeing the fermions as the true charge carriers. In other words, we use exchange interactions like (10) to define a simplified model for cuprates, taking into account a large mass of bipolarons but **non**-polaronic superconducting carriers. Since the lifetime of bipolarons in terms of a length ℓ is comparable to the coherence length in cuprate superconductors near the critical temperature, this suggests a strong exchange interaction between the (Bose-like, zero-spin) bipolaronic state and fermion pairs (electrons or holes).

As shown in Figure A1, bipolarons are formed around an oxygen ion (x) binding an adjacent pair of copper ions, because of the JT effect associated with Cu^{++} . It leads to JT ‘intersite bipolarons’. That is why we consider an annihilation (creation) operator c_x (c_x^*) of a fermion pair of zero total spin at $x \in \mathbb{Z}^2$ as defined by Equation (11). One simple example of such an operator is

$$c_x \doteq \sum_{z \in \mathbb{Z}^2, |z| \leq 1} (a_{x+z, \uparrow} a_{x, \downarrow} + a_{x+z, \uparrow} a_{x-z, \downarrow}) \quad (\text{A.2})$$

with $a_{z,s}$ ($a_{z,s}^*$) being the annihilation (creation) operator of a single fermion of spin $s \in \{\uparrow, \downarrow\}$ at lattice site $z \in \mathbb{Z}^2$. In this example, we set $\mathbf{p}_2(2z) = \mathbf{p}_1(z) = 1$ when $|z| \leq 1$ and $\mathbf{p}_1(z) = \mathbf{p}_2(z) = 0$ otherwise. Of course, one can also assign other weights to each space configuration of fermion pairs in Equation (11), as soon as at least one intersite configuration has a nonzero weight.

**Figure A1.** CuO₂ layer.

There is also an undeniable experimental evidence of **strong** on-site Coulomb repulsions (cf. the Mott insulator phase at zero doping), which forces us to consider terms like

$$U \sum_{x \in \mathbb{Z}^2} n_{x,\uparrow} n_{x,\downarrow}, \quad U \gg 1,$$

in Equation (6), where we recall that $n_{x,s} \doteq a_{x,s}^* a_{x,s}$ is the number operator of fermions at $x \in \mathbb{Z}^2$ and spin $s \in \{\uparrow, \downarrow\}$. It justifies our strong interest in studying in this paper the hard-core limit $U \rightarrow \infty$. See, for example, Theorem 3.5 and, more generally, related results that hold for $U \in [0, \infty]$.

The exchange interaction as formally given by (10); that is,

$$2^{-1/2} \sum_{x,y \in \mathbb{Z}^2} v(x-y) c_y^* b_x$$

with b_x (b_x^*) being the annihilation (creation) operator of a JT (intersite) bipolaron, is inspired by an interband interaction proposed by Kondo in 1963 for superconducting transition metals. In [55, 58], only an on-site version (i.e., $c_y = a_{y,\uparrow} a_{y,\downarrow}$) was proposed in 1985. Our version (A.2) of c_y captures the ‘intersite’ character of the bipolarons present in cuprates, and in [21], we specify the form of the coupling function v in (11) based on the presence of large electron-phonon anomalies²¹ in cuprates at optimum doping for the following points in the normalized Brillouin zone $\mathbb{T}^2 \doteq [-\pi, \pi)^2$:

$$(0, -\pi), (-\pi, 0) \quad [76, 77] \quad \text{and} \quad (0, \pm\pi/2), (\pm\pi/2, 0) \quad [77, 78, 79].$$

The anomalies at $(0, \pm\pi/2)$ and $(\pm\pi/2, 0)$ are correctly predicted by the Density Functional Theory (DFT) involving electrons and phonons [80, Fig. 1 (a)], in contrast to those of $(0, -\pi), (-\pi, 0)$. Moreover, when no superconducting phase appears, DFT works very well at all quasi-momenta, including $(0, -\pi), (-\pi, 0)$ [79, Fig. 18 (b)].

The above anomalies at quasi-momenta $(0, -\pi), (-\pi, 0)$ in the superconducting phase, which cannot be reproduced by the DFT, is expected to be a consequence of the existence of polaronic quasiparticles. Indeed, the DFT used in [80, Fig. 1 (a)] does not take into account the formation of compound particles

²¹The so-called softening of phonon dispersion and the broadening of phonon lines.

out of phonons and fermions like polaronic modes. In our theory, they are interpreted as being JT (intersite) bipolarons which should then interact strongly with charge carriers only at quasi-momenta $(-\pi, 0)$ and $(0, -\pi)$ (at moderate doping). The congruence between the DFT and experimental data for phonon dispersions at $(\pm\pi/2, 0)$ and $(0, \pm\pi/2)$ indeed makes the formation of such quasiparticles unlikely in this region of the (normalized) Brillouin zone \mathbb{T}^2 , and more generally in any other region relatively far from $(-\pi, 0)$ and $(0, -\pi)$. Consequently, the Fourier transform \hat{v} of v is chosen to take its maximum absolute value at the points $(-\pi, 0)$ and $(0, -\pi)$. This property is fundamental to explaining the superconductivity of cuprates in our microscopic theory.

There is indeed one very important property of superconducting carriers (pairs) in cuprates that differs from conventional superconductors, their d -wave symmetry. The (fiber) space of a fermion pair at constant quasimomentum K is the Hilbert space $L^2(\mathbb{T}^2, \mathbb{C}, \nu)$, see Section 2.3. Define by

$$[R_{\perp}|\varphi](k_x, k_y) \doteq \varphi(k_y, -k_x), \quad (k_x, k_y) \in \mathbb{T}^2$$

the unitary operator R_{\perp} implementing the $\pi/2$ -rotation on $L^2(\mathbb{T}^2, \mathbb{C}, \nu)$. Then define the mutually orthogonal projectors

$$\begin{aligned} P_s &\doteq \frac{R_{\perp}^4 + R_{\perp}^3 + R_{\perp}^2 + R_{\perp}}{4}, \\ P_d &\doteq \frac{R_{\perp}^4 - R_{\perp}^3 + R_{\perp}^2 - R_{\perp}}{4}, \\ P_p &\doteq \frac{R_{\perp}^4 - R_{\perp}^2}{2}. \end{aligned}$$

Since $P_s + P_d + P_p = \mathbf{1}$, any wave function $\Psi_f \in L^2(\mathbb{T}^2, \mathbb{C}, \nu)$ of a fermion pair can be uniquely decomposed into orthogonal s -, d - and p -wave components as

$$\Psi_f = \Psi_f^{(s)} + \Psi_f^{(d)} + \Psi_f^{(p)}, \quad \Psi_f^{(\#)} \doteq P_{\#}\Psi_f.$$

In other words, an arbitrary (fermionic pair) function Ψ_f can be uniquely decomposed into ‘ s -, d - and p -wave’ components, denoted respectively by $\Psi_f^{(s)}$, $\Psi_f^{(d)}$, $\Psi_f^{(p)}$. Observe that

$$R_{\perp}\Psi_f^{(s)} = \Psi_f^{(s)}, \quad R_{\perp}\Psi_f^{(d)} = -\Psi_f^{(d)}, \quad R_{\perp}^2\Psi_f^{(p)} = -\Psi_f^{(p)}. \quad (\text{A.3})$$

So, each component has a well-defined parity with respect to the group $\{0, \pi/2, \pi, 3\pi/2\}$ of rotations: The s -wave component $\Psi_f^{(s)}$ is invariant under these 4 rotations, the d -wave one $\Psi_f^{(d)}$ is antisymmetric with respect to the $\pi/2$ -rotation and the p -wave one $\Psi_f^{(p)}$ is antisymmetric with respect to the π -rotation (reflection over the origin), just like ‘ s ’, ‘ d ’ and ‘ p ’ atomic orbitals.

In conventional superconductivity, one has s -wave symmetry. For superconducting cuprates, it is more complex. It is firmly established that fermion pairs in cuprate superconductors have zero total spin [33], which is believed to lead to s - or d -wave superconductivity only. The s -wave symmetry is expected to correspond to fermion pairs on same lattice sites, which should be problematic in the presence of the strong on-site Coulomb repulsion. Therefore, d -wave superconductivity is anticipated in cuprate superconductors. This prediction is experimentally confirmed. See [33, 30, 13]. In cuprates, d -wave pairing is therefore predominant, but experiments (involving bulk properties) still indicate the presence of a non-negligible s -wave superconducting part; see [17, 59]. This is what our theory demonstrates, using the fact that the Fourier transform \hat{v} of v is maximal at the points $(-\pi, 0)$ and $(0, -\pi)$, but first we need to say a few words about the quantitative choice of its parameters. For example, if we take the hard-core limit $U \rightarrow \infty$, we get pure d -wave superconductivity, as shown in the first article [22].

In the second paper [21], we study the ground state $\Psi(U, k) \doteq (\hat{\psi}_k(U), -1)$ of Theorem 3.1 to give estimates on key features of cuprate superconductors by using **real** parameters taken from experiments

on the prototypical cuprates based on hole-doped cuprates La_2CuO_4 (e.g., LaSr 214) and $\text{YBa}_2\text{Cu}_3\text{O}_7$ (YBCO), near optimal doping:

- The hopping amplitude ϵ of charge carriers (here holes) in (6) is accessible using the lattice spacing and the effective mass of charge carriers. Both quantities are known for cuprates: The lattice spacing is $\mathbf{a} = 0.2672 \text{ nm}$ (14, Section 6.3.1) of the oxygen ions and the effective mass of mobile holes $m^* \simeq 4m_e$ [75, Fig. 2.], where m_e is the electron mass. This corresponds to $\epsilon = \hbar^2 / (m^* \mathbf{a}^2) \simeq 0.266 \text{ eV}$.
- In the same way, the hopping amplitude ϵh_b of JT bipolarons in (8) is accessible using the lattice spacing and the effective mass of bipolarons. The former is known, and the latter is estimated [37]. It leads to $h_b \simeq 0.00575 \ll 1$. That is, JT bipolarons can barely move, compared to fermions.
- The coefficient U in (6) can be fixed by using the first electronic affinity of oxygen – that is, the energy difference between the O^- anion state (one hole added to the O^{--} anion) and the neutral state (two holes added to O^{--}). These values are known with great precision: By [81], $U \simeq 1.461 \text{ eV}$. Note that $U\epsilon^{-1} \simeq 5.5$, which refers to a strong coupling regime, but it is not the hard-core limit $U \rightarrow \infty$ yet, from the perspective of real physical estimates.
- The intersite repulsion represented by the function $u : \mathbb{Z}^2 \rightarrow \mathbb{R}_0^+$ in (6) results from the screening of the Coulomb repulsion, usually estimated via the Thomas-Fermi screening length λ_{TF} . However, in two dimensions, the decay of the screened Coulomb repulsion is not exponential but rather polynomial [82, Eq. (5.41)]. In particular, even if $\lambda_{\text{TF}} \leq \mathbf{a}$, we consider the Coulomb repulsion for a few neighboring sites, with, of course, decaying strengths (for $z \neq 0$). For example, $u(z) = 0$ only when $|z| \geq r$ for some $r \leq 2$, with $u(0) = 0$ and $u(z) < U$.

It remains to fix the exchange strength function $v : \mathbb{Z}^2 \rightarrow \mathbb{R}$ in (10), taking into account the special choice (A.2) for the annihilation and creation operators of a fermion pair of zero total spin. We already know that the absolute value of the Fourier transform \hat{v} of v takes its maximum at the points $(-\pi, 0)$ and $(0, -\pi)$, but its precise amplitude has to be still determined. This is performed indirectly through a phenomenological relationship with the density of the superconducting charge carriers (also named superfluid): From recent experimental data [53], for optimum doping, around 90% of the charge carriers inserted via the doping do not form superfluid. If $\hat{\psi}_K(U)$ and -1 are respectively the fermionic and bosonic parts of the eigenvector $\Psi(U, k) \doteq (\hat{\psi}_K(U), -1)$ associated with the eigenvalue $E(U, K)$ and $K = (\pi, 0), (0, \pi)$, then we can interpret

$$\varrho = \frac{100\%}{\|\hat{\psi}_K(U)\|_2^2 + 1}$$

as the proportion of charge carriers forming JT bipolarons. Computing this quantity, we can identify the unique value $\hat{v}(K) \simeq 0.11 \text{ eV}$ making $\varrho = 90\%$. Similar to [83, 84], note that we choose \hat{v} of the form

$$\left[\alpha \left((k_x - \pi)^2 + k_y^2 \right) + 1 \right]^{-1} \quad (\text{resp.} \quad \left[\alpha \left(k_x^2 + (k_y - \pi)^2 \right) + 1 \right]^{-1})$$

for quasimomenta $(k_x, k_y) \in \mathbb{T}^2$ near $(\pi, 0)$ or $(0, \pi)$, where $\alpha > 0$ determines the effective mass m^{***} of (dressed) bound fermion pairs. Conversely, α can be recovered from m^{***} .

Using our mathematical results and rigorous numerical computations, we show in [21] that the model gives the following quantitative estimates in relation with properties of hole-doped cuprates La_2CuO_4 (LaSr 214 or LSCO) and $\text{YBa}_2\text{Cu}_3\text{O}_7$ (YBCO):

- **Pairing symmetry.**
 - Prediction: 16.5% *s*-wave, 83.5% *d*-wave, 0% *p*-wave. See [21, p. 10 and Corollary 1.1].
 - Experimental data: $\sim 20 - 25\%$ *s*-wave, $\sim 75 - 80\%$ *d*-wave, $\sim 0\%$ *p*-wave. Indirect measurement with rough estimates for the *s*-wave/*d*-wave ratio, see [17, 59].
- **Pseudogap temperature T_*** (i.e., pair dissociation energy).
 - Prediction of the binding energy of (*d*-wave) pairs: $E = 1250 \text{ K}$ found for the quasi-momenta $(-\pi, 0)$ and $(0, -\pi)$. See Theorem 3.1 (ii)–(iii) and [21, Fig. 6].

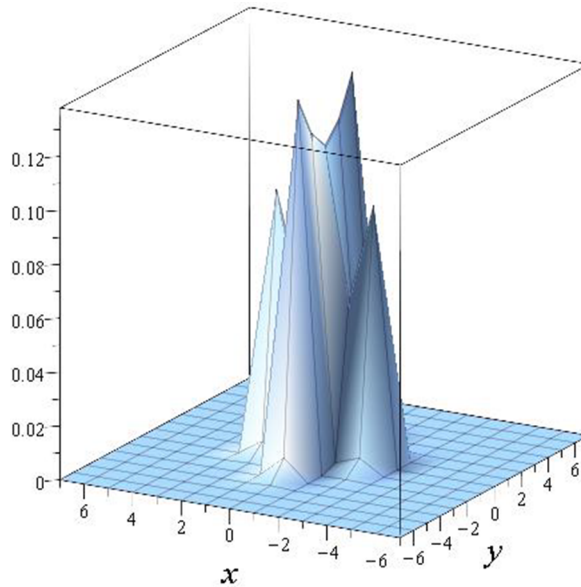


Figure 5. Normalized density $|\mathcal{F}^{-1}[\hat{\psi}_{1.461, (0, -\pi)}]|^2$ of the dressed bound fermion pair as a function of the (relative) position space at total quasimomentum $(0, -\pi)$ for the prototypical parameters. It is a reproduction of (21, Fig. 5).

– Experimental data:

- * Experiments on cuprates demonstrates a pseudogap appears at $(-\pi, 0)$ and $(0, -\pi)$. See [30, Fig. 4] and references therein.
- * $T_* \simeq 100 - 750$ K, depending on the doping [85, Fig. 26]. For example, $T_* \simeq 400$ K around optimal doping for $\text{La}_{1.85}\text{Sr}_{0.16}\text{CuO}_4$ and $T_* \simeq 200$ K for $\text{La}_{1.8}\text{Sr}_{0.2}\text{CuO}_4$. The ratio between the theoretical bond energy (in K) and the dissociation temperature²² of dressed fermion pairs should be between E/T_* and E/T_c . For $\text{La}_{1.8}\text{Sr}_{0.2}\text{CuO}_4$, the coherence length of which perfectly matches our prediction below, $E/T_* \simeq 6.2$ and $E/T_c = 34.247$, with an average ratio of around 20.
- * Binding energy of bipolarons [87, Fig. 2]: 1500 K at zero doping and 500 K at optimal doping for LaSr 214.
- * To compare with, for standard diatomic molecules, the ratio between the bond energy (in K) and their dissociation temperatures ranges²³ from 10 to 40, with an average of around 20.

○ **Superconducting coherence length ξ** (i.e., pair radius).

- Prediction: $\xi_a = 1.6$ nm in one direction, $\xi_b = 2.1$ nm in the orthogonal one at quasi-momenta $(-\pi, 0)$ and $(0, -\pi)$. See Figure 5 (in lattice units), reproducing [21, Fig. 5]. It refers approximately to 6 lattice sites in one direction and 8 lattice sites in the other one. Compare this result with the exponential localization of the fermionic component $\mathcal{F}^{-1}[\hat{\psi}_{U,k}]$ of the eigenstate given by Theorem 3.1 (iii).

²²How to theoretically determine the dissociation temperature of a dressed fermionic pair is not entirely clear to us. Clearly, this temperature must be higher than the critical temperature T_c and lower than the pseudogap temperature T_* .

²³For example, a quick internet search reveals that the dissociation temperatures T_d (in K) and bond energies E (in K) of ten common diatomic molecules are as follows: H_2 : $T_d = 4000$ K, $E = 52438$ K, $E/T_d \simeq 13$; N_2 : $T_d = 9500$ K, $E = 1.1330 \times 10^5$ K, $E/T_d \simeq 12$; O_2 : $T_d = 6000$ K, $E = 59895$ K, $E/T_d \simeq 10$; F_2 : $T_d = 1300$ K, $E = 19003$ K, $E/T_d \simeq 14.6$; Cl_2 : $T_d = 1200$ K, $E = 29226$ K, $E/T_d \simeq 24.3$; Br_2 : $T_d = 800$ K, $E = 23212$ K, $E/T_d \simeq 29$; I_2 : $T_d = 700$ K, $E = 18161$ K, $E/T_d \simeq 25.9$; CO : $T_d = 5000$ K, $E = 51356$ K, $E/T_d \simeq 10.3$; NO : $T_d = 4100$ K, $E = 75891$ K, $E/T_d \simeq 18.5$; HCl : $T_d = 3000$ K, $E = 1.2893 \times 10^5$ K, $E/T_d \simeq 43$.

- – Experimental data:

- * $\xi_{ab} = 1.6$ nm is obtained for an optimally doped $\text{YBa}_2\text{Cu}_3\text{O}_{6.9}$ for which $T_c = 95$ K. See [89, above the “Summary and conclusion”].
- * $\xi_{ab} = 2.1$ nm is obtained for $\text{La}_{1.8}\text{Sr}_{0.2}\text{CuO}_4$ for which $T_c = 36.5$ K. See [86, Table II].
- * $\xi_{ab} = 3.8$ nm is obtained for an optimally doped $\text{La}_{1.85}\text{Sr}_{0.16}\text{CuO}_4$ for which $T_c = 38$ K. See [89, above the “Summary and conclusion”].
- * More generally, ξ_{ab} is in the nanometer range, between 1 nm and 3.8 nm for various other examples of La_2CuO_4 and $\text{YBa}_2\text{Cu}_3\text{O}_7$. See, for example, [14, Table 9.1] and (88, Table 3.2 on page 60). The coherence length is **very small** compared to conventional superconductors, for which it is generally several tens or hundreds of nanometers. See, for example, the table in (A.1).

The pseudo-gap temperature is the temperature below which the Fermi surface of a material exhibits a partial energy gap, in fact a gap in a particular direction, as in the quasi-momenta $(-\pi, 0)$ and $(0, -\pi)$. Compare with Theorem 3.1 (iii). The 2-fermion 1-boson problem studied here and in [21] cannot a priori explain the superconducting phase, which is a **collective** phenomenon, but only the pseudogap regime which is expected to be related to the formation of fermion pairs (mainly for quasi-momenta $(-\pi, 0)$ and $(0, -\pi)$).

To conclude, this paper together with [22, 21] contributes a **mathematically rigorous** microscopic model for cuprate superconductors that includes Jahn-Teller-type bipolarons with zero spin and local repulsions. This model captures the following phenomenological aspects of these materials:

- *d*-wave pairing not based on anisotropy.
- Low density superconducting superfluid.
- Pseudogap temperature.
- Very accurate coherence lengths.
- Solution to the ‘large bipolaron mass vs. small mass of superconducting carrier pairs’.

In addition, as proven in the Ph.D. thesis [24], in a mean-field-like approximation, the many-body version of the model considered here also explains another very special feature of cuprate superconductors – namely, the density waves [23]. We therefore think that the model we present here deserves to be studied in much more detail, in view of a microscopic theory for cuprate superconductivity.

A.2. The Fock-space formalism

In quantum mechanics, one generally starts with a (one-particle) Hilbert space \mathfrak{h} , often realized as a space $L^2(\mathcal{M})$ of square-integrable, complex-valued functions on a measure space $(\mathcal{M}, \mathfrak{a})$. The states of a quantum system of $n \in \mathbb{N}$ quantum particles are then represented within the n -fold tensor product $\mathfrak{h}^{\otimes n}$ of \mathfrak{h} . However, identical quantum particles are indistinguishable, meaning that they cannot be differentiated from one another, not even in principle. In this situation, the states of these indistinguishable quantum particles are only taken from a subspace of $\mathfrak{h}^{\otimes n}$.

Recall meanwhile that all quantum particles possess an intrinsic form of angular momentum known as spin, characterized by a quantum number $s \in \mathbb{N}/2$. If s is half-integer, then the corresponding particles are named fermions; otherwise, we have bosons. By the celebrated spin-statistics theorem, fermionic wave functions are antisymmetric with respect to permutations of particles, whereas the bosonic ones are symmetric. The states of a system of $n \in \mathbb{N}$ fermions correspond then to vectors in the subspace $\wedge^n \mathfrak{h}$ of totally antisymmetric n -particle wave functions in $\mathfrak{h}^{\otimes n}$, while the states of a system of $n \in \mathbb{N}$ bosons are vectors in the subspace $\vee^n \mathfrak{h}$ of totally symmetric n -particle wave functions in $\mathfrak{h}^{\otimes n}$.

In most many-body quantum systems, the exact number of particles is not known. In quantum statistical mechanics, physical properties are typically studied in the limit $n \rightarrow \infty$ of infinite number of particles. Quantum field theory deals with situations where the particle number and species vary with time. The so-called Fock spaces are used to encode both situations. For fermionic systems, the Fock space is, by definition, the Hilbert space

$$\mathfrak{F}_- \equiv \mathfrak{F}(\mathfrak{h}) \doteq \bigoplus_{n=0}^{\infty} \wedge^n \mathfrak{h}, \quad \wedge^0 \mathfrak{h} \doteq \mathbb{C}, \quad (\text{A.4})$$

while, for bosonic systems,

$$\mathfrak{F}_+ \equiv \mathfrak{F}(\mathfrak{h}) \doteq \bigoplus_{n=0}^{\infty} \vee^n \mathfrak{h}, \quad \vee^0 \mathfrak{h} \doteq \mathbb{C}. \quad (\text{A.5})$$

The respective scalar products are denoted by $\langle \cdot, \cdot \rangle_{\mathfrak{F}_{\pm}}$. The two scalar products are the sum over $n \in \mathbb{N}$ of each canonical scalar product on the sector $\wedge^n \mathfrak{h}$ and $\vee^n \mathfrak{h}$, respectively. In both cases, we denote the vacuum state by $\Omega \doteq (1, 0, \dots)$.

The Fock space proved very useful, not least because it allows so-called creation and annihilation operators:

Fermionic case. The annihilation operator $a(\varphi) \in \mathcal{B}(\mathfrak{F}_-)$ of a fermion with wave function $\varphi \in \mathfrak{h}$ is the (linear) bounded operator uniquely defined by the conditions $a(\varphi)\Omega = 0$ and

$$a(\varphi)(\psi_1 \wedge \dots \wedge \psi_n) \doteq \frac{\sqrt{n}}{n!} \sum_{\pi \in \Pi_n} \text{sgn}(\pi) \langle \varphi, \psi_{\pi(1)} \rangle_{\mathfrak{h}} \psi_{\pi(2)} \wedge \dots \wedge \psi_{\pi(n)} \quad (\text{A.6})$$

for any $n \in \mathbb{N}$ and $\psi_1, \dots, \psi_n \in \mathfrak{h}$, where Π_n is the set of all permutations π of n elements and $\text{sgn} : \Pi_n \rightarrow \{-1, 1\}$ denotes the sign of these permutations, while $\Omega = (1, 0, 0, \dots)$ is the vacuum state and $\psi_1 \wedge \dots \wedge \psi_n$ is the orthogonal projection of $\psi_1 \otimes \dots \otimes \psi_n \in \mathfrak{h}^{\otimes n}$ onto the subspace of antisymmetric n -particle wave functions:

$$\psi_1 \wedge \dots \wedge \psi_n \doteq \frac{1}{n!} \sum_{\pi \in \Pi_n} \text{sgn}(\pi) \psi_{\pi(1)} \otimes \dots \otimes \psi_{\pi(n)} \in \wedge^n \mathfrak{h}.$$

The creation operator of a fermion with wave function $\varphi \in \mathfrak{h}$ is the adjoint $a^*(\varphi) \doteq a(\varphi)^*$ of $a(\varphi)$ – namely, $a^*(\varphi)\Omega = \varphi$ and

$$a^*(\varphi)(\psi_1 \wedge \dots \wedge \psi_n) = \sqrt{n+1} \varphi \wedge \psi_1 \wedge \dots \wedge \psi_n. \quad (\text{A.7})$$

Such operators are known to satisfy the so-called Canonical Anticommutation Relations (CAR): For all $\varphi_1, \varphi_2 \in \mathfrak{h}$,

$$a(\varphi_1)a(\varphi_2) + a(\varphi_2)a(\varphi_1) = 0, \quad a(\varphi_1)a(\varphi_2)^* + a(\varphi_2)^*a(\varphi_1) = \langle \varphi_1, \varphi_2 \rangle_{\mathfrak{h}} \mathbf{1}.$$

See [90, p. 10]. Here, $\mathbf{1}$ stands for the identity operator on the Fock space \mathfrak{F}_- .

Bosonic case. The annihilation operator $b(\varphi)$ of a boson with wave function $\varphi \in \mathfrak{h}$ is the (linear) unbounded operator acting on \mathfrak{F}_+ and uniquely defined by the conditions $b(\varphi)\Omega = 0$ and

$$b(\varphi)(\psi_1 \vee \dots \vee \psi_n) \doteq \frac{\sqrt{n}}{n!} \sum_{\pi \in \Pi_n} \langle \varphi, \psi_{\pi(1)} \rangle_{\mathfrak{h}} \psi_{\pi(2)} \vee \dots \vee \psi_{\pi(n)} \quad (\text{A.8})$$

for any $n \in \mathbb{N}$ and $\psi_1, \dots, \psi_n \in \mathfrak{h}$, where $\psi_1 \vee \dots \vee \psi_n$ is the orthogonal projection of $\psi_1 \otimes \dots \otimes \psi_n \in \mathfrak{h}^{\otimes n}$ onto the subspace of symmetric n -particle wave functions:

$$\psi_1 \vee \dots \vee \psi_n \doteq \frac{1}{n!} \sum_{\pi \in \Pi_n} \psi_{\pi(1)} \otimes \dots \otimes \psi_{\pi(n)} \in \vee^n \mathfrak{h}.$$

As in the fermionic case, the creation operator of a boson with wave function $\varphi \in \mathfrak{h}$ is the adjoint $b^*(\varphi) \doteq b(\varphi)^*$ of $b(\varphi)$, where $b^*(\varphi)\Omega = \varphi$ and

$$b^*(\varphi)(\psi_1 \vee \cdots \vee \psi_n) = \sqrt{n+1} \varphi \vee \psi_1 \vee \cdots \vee \psi_n. \quad (\text{A.9})$$

Such operators are known to satisfy the so-called Canonical Commutation Relations (CCR): For all $\varphi_1, \varphi_2 \in \mathfrak{h}$,

$$b(\varphi_1)b(\varphi_2) - b(\varphi_2)b(\varphi_1) = 0, \quad b(\varphi_1)b(\varphi_2)^* - b(\varphi_2)^*b(\varphi_1) = \langle \varphi_1, \varphi_2 \rangle_{\mathfrak{h}} \mathbf{1}.$$

See [90, p. 10]. Here, $\mathbf{1}$ stands again for the identity operator on the Fock space \mathfrak{F}_+ .

The interest of Fock spaces lies in the use of creation and annihilation operators, which not only give a mathematically rigorous definition for precesses of creation or annihilation of physical particles, but also possess essential algebraic properties: the CAR and CCR relations given above. Although Fock spaces and the creation and annihilation operators are not strictly necessary for our proofs, we use them in this paper because they allow us to define the model in a very intuitive way, which makes its physical meaning easy to understand once the Fock-space formulation is familiar.

A.3. Non-autonomous evolution equations and scattering theory

This section collects simple results on wave and scattering operators (50)–(52) for bounded Hamiltonians, related to their approximation by Dyson series. We start with the following elementary lemma, resulting from the theory of non-autonomous evolution equations:

Lemma A.1 (Finite-time scattering and wave operators). *For any self-adjoint $X, Y \in \mathcal{B}(\mathcal{X})$ acting on a Hilbert space \mathcal{X} and all $s, t \in \mathbb{R}$,*

$$e^{itX} e^{i(s-t)(X+Y)} e^{-isX} = \mathbf{1} + \sum_{n=1}^{\infty} (-i)^n \int_s^t d\tau_1 \cdots \int_s^{\tau_{n-1}} d\tau_n Y_{\tau_1} \cdots Y_{\tau_n} \quad (\text{A.10})$$

with $(Y_t)_{t \in \mathbb{R}} \subseteq \mathcal{B}(\mathcal{X})$ being the norm-continuous family

$$Y_t \doteq e^{itX} Y e^{-itX}, \quad t \in \mathbb{R}. \quad (\text{A.11})$$

Proof. We compute that, for any $s, t \in \mathbb{R}$,

$$\partial_t \left\{ e^{itX} e^{i(s-t)(X+Y)} e^{-isX} \right\} = -i \left(e^{itX} Y e^{-itX} \right) \left(e^{itX} e^{i(s-t)(X+Y)} e^{-isX} \right)$$

as well as

$$\partial_s \left\{ e^{itX} e^{i(s-t)(X+Y)} e^{-isX} \right\} = \left(e^{itX} e^{i(s-t)(X+Y)} e^{-isX} \right) \left(i e^{isX} Y e^{-isX} \right)$$

both in $\mathcal{B}(\mathcal{X})$. In other words, the family

$$V_{t,s} \doteq e^{itX} e^{i(s-t)(X+Y)} e^{-isX}, \quad s, t \in \mathbb{R}, \quad (\text{A.12})$$

of (uniformly) bounded operators is a norm-continuous two-parameter family of unitary operators solving the non-autonomous evolution equations

$$\forall s, t \in \mathbb{R} : \quad \partial_t Z_{t,s} = -i Y_t Z_{t,s}, \quad \partial_s Z_{t,s} = i Z_{t,s} Y_s, \quad Z_{s,s} = \mathbf{1}, \quad (\text{A.13})$$

in $\mathcal{B}(\mathcal{X})$, where $(Y_t)_{t \in \mathbb{R}} \subseteq \mathcal{B}(\mathcal{X})$ is the norm-continuous family defined by (A.11). As is well-known, there is a unique solution to this non-autonomous evolution equation (A.13), which is given by the Dyson

series (A.10). This series is absolutely summable in $\mathcal{B}(\mathcal{X})$. Notice that the integrals appearing in it are Riemann integrals, for their arguments are continuous functions taking values in a Banach space. \square

Corollary A.2 (Approximation of scattering and wave operators). *Let $X, Y \in \mathcal{B}(\mathcal{X})$ be two self-adjoint operators acting on a Hilbert space \mathcal{X} . Assume that the waves operators*

$$W^\pm(X+Y, X) \doteq s - \lim_{t \rightarrow \pm\infty} e^{it(X+Y)} e^{-itX} P_{ac}(X)$$

exist. Let $\varepsilon \in \mathbb{R}^+$. Then

i.) *For any $\varphi \in \text{ran}(P_{ac}(X))$, there is $T > 0$ such that*

$$T < t \implies \|(W^+(X+Y, X) - V_{0,t})\varphi\|_{\mathcal{X}} \leq \varepsilon,$$

whereas

$$t < -T \implies \|(W^-(X+Y, X) - V_{0,t})\varphi\|_{\mathcal{X}} \leq \varepsilon.$$

ii.) *For any $\varphi, \psi \in \text{ran}(P_{ac}(X))$, there is $T > 0$ such that*

$$\langle \psi, S(X+Y, X)\varphi \rangle_{\mathcal{X}} = \langle \psi, W^+(X+Y, X)^* W^-(X+Y, X)\varphi \rangle_{\mathcal{X}} = \langle \psi, V_{t,s}\varphi \rangle_{\mathcal{X}} + \mathcal{O}(\varepsilon)$$

uniformly for $s < -T < T < t$.

Here,

$$V_{t,s} \doteq \mathbf{1} + \sum_{n=1}^{\infty} (-i)^n \int_s^t d\tau_1 \cdots \int_s^{\tau_{n-1}} d\tau_n Y_{\tau_1} \cdots Y_{\tau_n},$$

the norm-continuous family $(Y_t)_{t \in \mathbb{R}} \subseteq \mathcal{B}(\mathcal{X})$ being defined by (A.11).

Proof. Assertion (i) is a direct consequence of Lemma A.1. Concerning the scattering operator, remark in particular that, for any $r, s, t \in \mathbb{R}$, $V_{t,s}V_{s,r} = V_{t,r}$ and $V_{t,s}^* = V_{s,t}$. Given $\varphi, \psi \in \text{ran}(P_{ac}(Y))$, we have that

$$\begin{aligned} & |\langle \psi, (S(X+Y, X) - V_{t,s})\varphi \rangle_{\mathcal{X}}| \\ &= \left| \left\langle \psi, \left(W^+(X+Y, X)^* W^-(X+Y, X) - V_{0,t}^* V_{0,s} \right) \varphi \right\rangle_{\mathcal{X}} \right| \\ &= \left| \left\langle \psi, (W^+(X+Y, X) - V_{0,t})^* W^-(X+Y, X)\varphi \right\rangle_{\mathcal{X}} \right. \\ &\quad \left. + \left\langle \psi, V_{0,t}^* (W^-(X+Y, X) - V_{0,s})\varphi \right\rangle_{\mathcal{X}} \right| \\ &\leq \| (W^+(X+Y, X) - V_{0,t})\psi \|_{\mathcal{X}} \| W^-(X+Y, X)\varphi \|_{\mathcal{X}} \\ &\quad + \| (W^-(X+Y, X) - V_{0,s})\varphi \|_{\mathcal{X}} \| \psi \|_{\mathcal{X}}. \end{aligned}$$

Assertion (ii) therefore follows from assertion (i). \square

A.4. Constant fiber direct integrals

For more details, we refer to [38, Section XIII.16] as well as [45] for the general theory.

Let (\mathcal{X}, μ) be any semifinite measure space and \mathcal{Y} any separable Hilbert space. The constant fiber direct integral of \mathcal{Y} over \mathcal{X} is, by definition, the Hilbert space

$$\int_{\mathcal{X}}^{\oplus} \mathcal{Y} \mu(dx) \equiv L^2(\mathcal{X}, \mathcal{Y}, \mu) \doteq \{F \in \mathcal{Y}^{\mathcal{X}} : \|F(\cdot)\|_{\mathcal{Y}}^2 \in L^1(\mathcal{X}, \mu)\}$$

of equivalence classes of square-integrable \mathcal{Y} -valued functions with scalar product²⁴

$$\langle \varphi, \psi \rangle \equiv \langle \varphi, \psi \rangle_{L^2(\mathcal{X}, \mathcal{Y}, \mu)} \doteq \int_{\mathcal{X}} \langle \varphi(x), \psi(x) \rangle_{\mathcal{Y}} \mu(\mathrm{d}x), \quad \varphi, \psi \in L^2(\mathcal{X}, \mathcal{Y}, \mu),$$

and the pointwise vector space operations

$$(\varphi + \psi)(x) = \varphi(x) + \psi(x), \quad (\alpha\varphi)(x) = \alpha\varphi(x), \quad \alpha \in \mathbb{C}, \quad \varphi, \psi \in L^2(\mathcal{X}, \mathcal{Y}, \mu).$$

If $\mathcal{Y} = \mathbb{C}$, then we use the shorter notation $L^2(\mathcal{X}, \mu) \equiv L^2(\mathcal{X}, \mathbb{C}, \mu)$.

A mapping $A : \mathcal{X} \rightarrow \mathcal{B}(\mathcal{Y})$ is strongly measurable whenever the mapping $x \mapsto \langle \varphi, A(x)\psi \rangle_{\mathcal{Y}}$ from \mathcal{X} to \mathbb{C} is measurable for all $\varphi, \psi \in \mathcal{Y}$. Let $L^\infty(\mathcal{X}, \mathcal{Y}, \mu)$ be the C^* -algebra of equivalence classes of strongly measurable functions $A : \mathcal{X} \rightarrow \mathcal{B}(\mathcal{Y})$ with

$$\|A\|_\infty \doteq \operatorname{ess-sup} \{ \|A(x)\|_{\operatorname{op}} : x \in \mathcal{X} \} < \infty. \quad (\text{A.14})$$

Here, $\operatorname{ess-sup}$ denotes the essential supremum and $\|\cdot\|_{\operatorname{op}}$ stands for the operator norm. If $\mathcal{Y} = \mathbb{C}$, then we use the shorter notation $L^\infty(\mathcal{X}, \mu) \equiv L^\infty(\mathcal{X}, \mathbb{C}, \mu)$.

A bounded operator D on $L^2(\mathcal{X}, \mathcal{Y}, \mu)$ is decomposable if there is $A \in L^\infty(\mathcal{X}, \mathcal{Y}, \mu)$ such that, for all $\psi \in L^2(\mathcal{X}, \mathcal{Y}, \mu)$,

$$(D\psi)(x) = A(x)\psi(x), \quad x \in \mathcal{X} \quad (\mu\text{-a.e.}).$$

If such an A exists, then it is unique. Moreover, the mapping $A \mapsto D$ defined by the above equality is a $*$ -homomorphism which is isometric. See [38, Theorem XIII.83]. The operators $A(x) \in \mathcal{B}(\mathcal{Y})$, $x \in \mathcal{X}$, are called the fibers of D and we write

$$D = \int_{\mathcal{X}}^{\oplus} A(x) \mu(\mathrm{d}x).$$

For the reader's convenience, we now give three essential properties of decomposable operators used in the paper, referring to [38, Theorem XIII.85 (a), (c) and (d)]. Note that $\sigma(X)$ denotes below the spectrum of any operator X acting on some Hilbert space, as is usual.

Theorem A.3 (Properties of decomposable operators). *Let D be a decomposable operator on $L^2(\mathcal{X}, \mathcal{Y}, \mu)$, the fibers $A(x) \in \mathcal{B}(\mathcal{Y})$, $x \in \mathcal{X}$, of which are all self-adjoint. Then*

- i.) D is self-adjoint.
- ii.) $\lambda \in \sigma(D)$ iff, for all $\varepsilon \in \mathbb{R}^+$,

$$\mu(\{x \in \mathcal{X} : \sigma(A(x)) \cap (\lambda - \varepsilon, \lambda + \varepsilon) \neq \emptyset\}) > 0.$$

- iii.) For any bounded Borel function f on \mathbb{R} , $f(D)$ is decomposable and has fibers $f(A(x))$, $x \in \mathcal{X}$; that is,

$$f(D) = \int_{\mathcal{X}}^{\oplus} f(A(x)) \mu(\mathrm{d}x).$$

The above theorem can be used to elegantly prove the following well-known results about multiplication operators M_φ by any bounded measurable function $\varphi \in L^\infty(\mathcal{X}, \mu)$, defined for any $\psi \in L^2(\mathcal{X}, \mu)$, by

$$(M_\varphi\psi)(x) = \varphi(x)\psi(x), \quad x \in \mathcal{X} \quad (\mu\text{-a.e.}).$$

²⁴The scalar product is well-defined, by the polarization identity and the Cauchy-Schwarz inequality. See for instance (46, Section 7.3.2).

Corollary A.4 (Properties of multiplication operators). *The multiplication operators M_φ by $\varphi \in L^\infty(\mathcal{X}, \mu)$ have the following properties:*

- i.) *For any bounded Borel function f on \mathbb{R} , one has $f(M_\varphi) = M_{f \circ \varphi}$.*
- ii.) *$\sigma(M_\varphi)$ is the essential range $\text{ess-im}(\varphi)$ of φ .*
- iii.) *Its operator norm $\|M_\varphi\|_{\text{op}}$ is equal to $\|\varphi\|_\infty$.*

Proof. Noting that M_φ is a decomposable operator on

$$L^2(\mathcal{X}, \mu) = \int_{\mathcal{X}}^{\oplus} \mathbb{C} \mu(dx)$$

with $\varphi(x)$, seen as a linear operator on \mathbb{C} , being its fibers, we can use Theorem A.3 (iii) to get the equality

$$f(M_\varphi) = \int_{\mathcal{X}}^{\oplus} f(\varphi(x)) \mu(dx) = M_{f \circ \varphi}.$$

This proves Assertion (i). For the second one, we use that $\sigma(\varphi(x)) = \{\varphi(x)\}$ for all $x \in \mathcal{X}$ and thus infer from Theorem A.3 (ii) that $\lambda \in \sigma(M_f)$ iff, for all $\varepsilon \in \mathbb{R}^+$,

$$\mu(\{x \in \mathcal{X} : |\lambda - \varphi(x)| < \varepsilon\}) > 0.$$

In other words, one gets Assertion (ii). Assertion (iii) is an elementary application of [38, Theorem XIII.83]. \square

Below, we study the special case of multiplication operators on $L^2(\mathbb{T}^2, \nu)$, where $\mathbb{T}^2 \doteq [-\pi, \pi)^2$ is the torus and ν is the normalized Haar measure (23) on \mathbb{T}^2 . It is again an elementary result, used in the paper. To this end, we recall that, for any self-adjoint operator Y acting on a Hilbert space \mathcal{Y} , $P_{\text{ac}}(Y)$ is the orthogonal projection onto the absolutely continuous space of Y , which is defined by (49).

Corollary A.5 (Absolutely continuous space of multiplication operators on $L^2(\mathbb{T}^2, \nu)$). *Let $\varphi : \mathbb{T}^2 \rightarrow \mathbb{R}$ be a bounded Borel function with the property that, for every Borel set $\Omega \subseteq \mathbb{R}$ with zero Lebesgue measure, one has $\nu(\varphi^{-1}(\Omega)) = 0$. Then, $P_{\text{ac}}(M_\varphi) = \mathbf{1}$; that is,*

$$\text{ran}(P_{\text{ac}}(M_\varphi)) = L^2(\mathbb{T}^2, \nu).$$

Proof. Given any Borel set $\Omega \subseteq \mathbb{R}$, we deduce from Corollary A.4 (i) that

$$\chi_\Omega(M_\varphi) = M_{\chi_{\Omega \circ \varphi}} = M_{\chi_{\varphi^{-1}(\Omega)}},$$

which in turn implies that, for any $\psi \in L^2(\mathbb{T}^2, \nu)$,

$$\langle \psi, \chi_\Omega(M_\varphi)\psi \rangle = \int_{\varphi^{-1}(\Omega)} |\psi(k)|^2 \nu(dk).$$

Hence, if $\Omega \subseteq \mathbb{R}$ has zero Lebesgue measure, then under the conditions of the corollary,

$$\langle \psi, \chi_\Omega(M_\varphi)\psi \rangle = 0.$$

In other words, for any $\psi \in L^2(\mathbb{T}^2, \nu)$, $\langle \psi, \chi_{(\cdot)}(M_\varphi)\psi \rangle$ is absolutely continuous with respect to the Lebesgue measure. \square

We next provide a result on the strong operator convergence and a version of Fubini's theorem for (constant fiber) direct integrals, which are also used in our proofs.

Proposition A.6 (Strong operator convergence). *Let $(A_n)_{n \in \mathbb{N}}$ be any bounded sequence in $L^\infty(\mathcal{X}, \mathcal{Y}, \mu)$. If*

$$s - \lim_{n \rightarrow \infty} A_n(x) = A(x), \quad x \in \mathcal{X},$$

then $A \in L^\infty(\mathcal{X}, \mathcal{Y}, \mu)$ and

$$s - \lim_{n \rightarrow \infty} \int_{\mathcal{X}}^{\oplus} A_n(x) \mu(dx) = \int_{\mathcal{X}}^{\oplus} A(x) \mu(dx).$$

Proof. The assertion is well-known, but for the reader's convenience, we give here its complete proof. For any $\varphi, \psi \in \mathcal{Y}$, it follows from the fact that $A_n(x)\psi \rightarrow A(x)\psi$ everywhere and the continuity of $\langle \varphi, \cdot \rangle \in \mathcal{Y}^*$ that

$$\lim_{n \rightarrow \infty} \langle \varphi, A_n(x)\psi \rangle_{\mathcal{Y}} = \langle \varphi, A(x)\psi \rangle_{\mathcal{Y}}, \quad x \in \mathcal{X}.$$

This shows that A is strongly measurable, because the pointwise limit of a sequence of real-valued measurable functions is measurable as well. Now, let

$$M \doteq \sup_{n \in \mathbb{N}} \|A_n\|_{\infty} < \infty.$$

For μ -a.e. $x \in \mathcal{X}$ and any $\varphi \in \mathcal{Y}$,

$$\|A_n(x)\varphi\|_{\mathcal{Y}} \leq \|A_n(x)\|_{\text{op}} \|\varphi\|_{\mathcal{Y}} \leq M \|\varphi\|_{\mathcal{Y}}, \quad n \in \mathbb{N}. \quad (\text{A.15})$$

Taking the limit $n \rightarrow \infty$, one thus gets that, for μ -a.e. $x \in \mathcal{X}$ and any $\varphi \in \mathcal{Y}$,

$$\|A(x)\varphi\|_{\mathcal{Y}} = \lim_{n \rightarrow \infty} \|A_n(x)\varphi\|_{\mathcal{Y}} \leq M \|\varphi\|_{\mathcal{Y}}. \quad (\text{A.16})$$

Hence, M is an essential upper bound for $\{\|A(x)\|_{\text{op}}\}_{x \in \mathcal{X}}$ and, therefore, $A \in L^\infty(\mathcal{X}, \mathcal{Y}, \mu)$. Finally, given any element $\varphi \in L^2(\mathcal{X}, \mathcal{Y}, \mu)$, by (A.15)–(A.16) and the triangle inequality, we have the estimate

$$\|A_n(x)\varphi(x) - A(x)\varphi(x)\|_{\mathcal{Y}} \leq 2M \|\varphi(x)\|_{\mathcal{Y}}, \quad x \in \mathcal{X} \quad (\mu\text{-a.e.}).$$

Since $A_n(x)\varphi(x) \rightarrow A(x)\varphi(x)$ for all $x \in \mathcal{X}$, we can therefore apply Lebesgue's dominated convergence theorem to conclude that, for any $\varphi \in L^2(\mathcal{X}, \mathcal{Y}, \mu)$,

$$\lim_{n \rightarrow \infty} \left\| \left(\int_{\mathcal{X}}^{\oplus} A_n(x) \mu(dx) \right) \varphi - \left(\int_{\mathcal{X}}^{\oplus} A(x) \mu(dx) \right) \varphi \right\|_{L^2(\mathcal{X}, \mathcal{Y}, \mu)} = 0. \quad \square$$

Before proving a version of Fubini's theorem for constant fiber direct integrals, we fix some terminology concerning the Riemann integral: A partition of the interval $[a, b]$ is a finite set $P = \{t_0 < t_1 < \dots < t_k\}$ where $t_0 = a$ and $t_k = b$. The norm of the partition P is the number $|P| = \max_{1 \leq i \leq k} (t_i - t_{i-1})$. A tagged partition is a pair $P^* = (P, \xi)$ where P is a partition and $\xi = (\xi_1, \dots, \xi_k)$ is such that $t_{i-1} \leq \xi_i < t_i$ for every $i = 1, \dots, k$. If P^* is a tagged partition of $[a, b]$, the corresponding Riemann sum for $f : [a, b] \rightarrow \mathcal{Z}$, with \mathcal{Z} being a vector space, is

$$\Sigma(f; P^*) = \sum_{i=1}^k (t_i - t_{i-1}) f(\xi_i) \in \mathcal{Z}.$$

Proposition A.7 (Fubini's Theorem for direct integrals). *Let $A_{(\cdot)} : [a, b] \rightarrow L^\infty(\mathcal{X}, \mathcal{Y}, \mu)$ be a continuous function. Then*

i.) The mapping

$$\mathcal{X} \ni x \mapsto \int_a^b A_t(x) \, dt \in \mathcal{B}(\mathcal{Y})$$

is an element of $L^\infty(\mathcal{X}, \mathcal{Y}, \mu)$;

ii.) The mapping

$$[a, b] \ni t \mapsto \int_{\mathcal{X}}^{\oplus} A_t(x) \, \mu(dx) \in \mathcal{B}\left(\int_{\mathcal{X}}^{\oplus} \mathcal{Y} \, \mu(dx)\right)$$

is continuous and

$$\int_a^b \int_{\mathcal{X}}^{\oplus} A_t(x) \, \mu(dx) \, dt = \int_{\mathcal{X}}^{\oplus} \int_a^b A_t(x) \, dt \, \mu(dx).$$

Proof. If $A_{(\cdot)} : [a, b] \rightarrow L^\infty(\mathcal{X}, \mathcal{Y}, \mu)$ is continuous, then so is $A_{(\cdot)}(x) : [a, b] \rightarrow \mathcal{B}(\mathcal{Y})$ for $x \in \mathcal{X}\mu$ -a.e. For simplicity, we may assume that $A_{(\cdot)}(x)$ is even continuous for all $x \in \mathcal{X}$. If fact, as this is true for $x \in \mathcal{X}\mu$ -a.e., for some Borel set $\mathcal{X}_0 \subseteq \mathcal{X}$ with $\mu(\mathcal{X}_0) = 0$, $\mathbf{1}_{[x \notin \mathcal{X}_0]} A_{(\cdot)}(x)$ is continuous for all $x \in \mathcal{X}$. Note that, for all $t \in [a, b]$, the functions A_t and $\mathbf{1}_{[\cdot \notin \mathcal{X}_0]} A_t$ are strongly measurable and represent the same element (i.e., equivalence class of strongly measurable functions $\mathcal{X} \rightarrow \mathcal{B}(\mathcal{Y})$) of $L^\infty(\mathcal{X}, \mathcal{Y}, \mu)$. Moreover, as $[a, b]$ is compact, $\{A_t\}_{t \in [a, b]}$ is bounded as a subset of the metric space $(L^\infty(\mathcal{X}, \mathcal{Y}, \mu), \|\cdot\|_\infty)$. Thus,

$$\begin{aligned} \left\| \int_a^b A_t(x) \, dt \right\|_{\text{op}} &\leq \int_a^b \|A_t(x)\|_{\text{op}} \, dt \leq \int_a^b \|A_t\|_\infty \, dt \\ &\leq (b-a) \sup_{t \in [a, b]} \|A_t\|_\infty < \infty \quad (\mu\text{-a.e.}). \end{aligned}$$

Let P_n^* be a tagged partition whose norm of the corresponding partition P_n goes to zero as $n \rightarrow \infty$. Then for every $\varphi, \psi \in \mathcal{Y}$ and $x \in \mathcal{X}\mu$ -a.e.,

$$\left\langle \varphi, \left(\int_a^b A_t(x) \, dt \right) \psi \right\rangle_{\mathcal{Y}} = \int_a^b \langle \varphi, A_t(x) \psi \rangle_{\mathcal{Y}} \, dt = \lim_{n \rightarrow \infty} \Sigma(\langle \psi, A_{(\cdot)}(x) \varphi \rangle_{\mathcal{Y}}; P_n^*).$$

For the first equality, we used the fact that the Riemann integral commutes with bounded linear transformations. Observing that for $x \in \mathcal{X}\mu$ -a.e., the right-hand side is a pointwise limit of a linear combination of continuous (hence Riemann integrable) functions, this proves assertion (i).

Note that the mapping defined in Assertion (ii) is a composition of two continuous functions – namely, $A_{(\cdot)} : [a, b] \rightarrow L^\infty(\mathcal{X}, \mathcal{Y}, \mu)$ and

$$L^\infty(\mathcal{X}, \mathcal{Y}, \mu) \ni B \mapsto \int_{\mathcal{X}}^{\oplus} B(x) \, \mu(dx) \in \mathcal{B}\left(\int_{\mathcal{X}}^{\oplus} \mathcal{Y} \, \mu(dx)\right).$$

Given any $\varphi, \psi \in L^2(\mathcal{X}, \mathcal{Y}, \mu)$, observe that the function

$$\mathcal{X} \times [a, b] \ni (x, t) \mapsto f(x, t) = \langle \varphi(x), A_t(x) \psi(x) \rangle_{\mathcal{Y}} \in \mathbb{C}$$

is measurable when $A_{(\cdot)}(x) \in C([a, b], \mathcal{B}(\mathcal{Y}))$ for any $x \in \mathcal{X}$.

To prove this, for each $n \in \mathbb{N}$, define the function $f_n : \mathcal{X} \times [a, b] \rightarrow \mathbb{C}$ by $f_n(x, t) = f(x, s_t)$, with $s_t = \min\{m_{t,n}/n, b\}$ and $m_{t,n} \in \mathbb{Z}$ being such that $(m_{t,n} - 1)/n \leq t < m_{t,n}/n$. In particular,

$$f_n(x, t) = \sum_{m \in \mathbb{Z}: m \geq na} \mathbf{1}[t \in n^{-1}[m-1, m)] f(x, \min\{m/n, b\}).$$

Characteristic functions are measurable on $[a, b]$, and $f(\cdot, t)$ is also measurable on \mathcal{X} for every $t \in [a, b]$. So, f_n is measurable for all $n \in \mathbb{N}$. It is easy to check that $m_{t,n}/n \rightarrow t$ for any $t \in [a, b]$, which in turn implies that f_n pointwise converges to f , as $n \rightarrow \infty$, because of the continuity of $f(x, \cdot)$ for any fixed $x \in \mathcal{X}$. The last continuity property is a direct consequence of the assumption $A_{(\cdot)}(x) \in C([a, b], \mathcal{B}(\mathcal{Y}))$ together with elementary estimates using the Cauchy-Schwarz inequality.

As a consequence, f is measurable on $\mathcal{X} \times [a, b]$. Note also that

$$\int_{\mathcal{X}} \int_a^b |f(x, t)| \, dt \, \mu(dx) \leq (b-a) \|\varphi\|_{L^2(\mathcal{X}, \mathcal{Y}, \mu)}^2 \|\psi\|_{L^2(\mathcal{X}, \mathcal{Y}, \mu)}^2 \sup_{t \in [a, b]} \|A_t\|_{\infty} < \infty,$$

thanks to the Cauchy-Schwarz inequality for both spaces \mathcal{Y} and $L^2(\mathcal{X}, \mathcal{Y}, \mu)$. We can then apply (usual) Fubini's theorem to obtain

$$\begin{aligned} \left\langle \varphi, \left(\int_{\mathcal{X}}^{\oplus} \int_a^b A_t(x) \, dt \, \mu(dx) \right) \psi \right\rangle_{L^2(\mathcal{X}, \mathcal{Y}, \mu)} &= \int_{\mathcal{X}} \left\langle \varphi(x), \left(\int_a^b A_t(y) \, dt \right) \psi(x) \right\rangle_{\mathcal{Y}} \mu(dx) = \\ &= \int_{\mathcal{X}} \int_a^b \langle \varphi(x), A_t(x) \psi(x) \rangle_{\mathcal{Y}} \, dt \, \mu(dx) = \int_a^b \int_{\mathcal{X}} \langle \varphi(x), A_t(x) \psi(x) \rangle_{\mathcal{Y}} \mu(dx) \, dt = \\ &= \int_a^b \left\langle \varphi, \left(\int_{\mathcal{X}}^{\oplus} A_t(x) \mu(dx) \right) \psi \right\rangle_{\mathcal{Y}} \, dt = \left\langle \varphi, \left(\int_a^b \int_{\mathcal{X}}^{\oplus} A_t(x) \mu(dx) \, dt \right) \psi \right\rangle_{L^2(\mathcal{X}, \mathcal{Y}, \mu)}. \end{aligned}$$

As φ, ψ are arbitrary, we arrive at Assertion (ii). \square

We conclude this short account on constant fiber direct integrals by providing a representation of them as tensor products:

Proposition A.8 (Direct integrals and tensor products). *There is a unique unitary transformation $\mathbf{V} : L^2(\mathcal{X}, \mu) \otimes \mathcal{Y} \rightarrow L^2(\mathcal{X}, \mathcal{Y}, \mu)$ such that*

$$\mathbf{V}(f \otimes \varphi)(x) = f(x)\varphi, \quad f \in L^2(\mathcal{X}, \mu), \varphi \in \mathcal{Y}, x \in \mathcal{X} \quad (\mu\text{-a.e.}).$$

Proof. See [45, Proposition 5.2]. \square

A.5. The Birman-Schwinger principle

There are various versions of the Birman-Schwinger principle in the literature, and we give below the precise version that is used in our proofs. To this end, we first define *Birman-Schwinger operators*: For any operator T acting on some complex vector space, recall that $\rho(T) \subseteq \mathbb{C}$ denotes its resolvent set. Given two (bounded) operators T, V acting on some complex vector space and any $\lambda \in \rho(T)$, we define the associated Birman-Schwinger operator to be

$$\mathbf{B}(\lambda) \equiv \mathbf{B}(\lambda, T, V) \doteq V(T - \lambda \mathbf{1})^{-1} V. \quad (\text{A.17})$$

It turns out that, for all $\lambda \in \rho(T)$, 1 is an eigenvalue of $\mathbf{B}(\lambda)$ iff λ is an eigenvalue of $T - V^2$:

Lemma A.9 (The eigenvalues of Birman-Schwinger operators). *Let T, V be two bounded operators acting on a vector space \mathcal{X} over \mathbb{C} . Assume that $\lambda \in \rho(T)$ is an eigenvalue of $T - V^2$ and let $\{\varphi_i\}_{i \in I}$ denote any basis of the corresponding eigenspace. Define $\gamma_i \doteq V\varphi_i$, $i \in I$. Then,*

$$\varphi_i = (T - \lambda \mathbf{1})^{-1} V^2 \varphi_i = (T - \lambda \mathbf{1})^{-1} V \gamma_i, \quad i \in I, \quad (\text{A.18})$$

and $\{\gamma_i\}_{i \in I}$ is a linearly independent set satisfying

$$B(\lambda) \gamma_i = V \varphi_i = \gamma_i, \quad i \in I. \quad (\text{A.19})$$

Proof. Suppose that λ is an eigenvalue of $T - V^2$ and let $\{\varphi_i\}_{i \in I}$ be a basis of the corresponding eigenspace. Set $\gamma_i = V\varphi_i$, $i \in I$. Then

$$(T - \lambda \mathbf{1}) \varphi_i = (T - V^2) \varphi_i + (V^2 - \lambda \mathbf{1}) \varphi_i = \lambda \varphi_i + (V^2 - \lambda \mathbf{1}) \varphi_i = V^2 \varphi_i$$

so that (A.18) holds true. By (A.18), γ_i is a nonzero vector for any $i \in I$ since $\varphi_i \neq 0$ for all $i \in I$. As linear transformations map a linearly dependent set onto a linearly dependent set, we conclude that $\{\gamma_i\}_{i \in I}$ is a linearly independent set. Equation (A.19) is a direct consequence of (A.17) and (A.18). \square

This last lemma is explicitly used in the proof of Corollary 4.6 and allows meanwhile to prove the Birman-Schwinger principle for eigenvalues. Below, for any operator T , we use the notation $\mathcal{E}_T(\lambda)$ for the eigenspace associated with the eigenvalue λ of T .

Theorem A.10 (Birman-Schwinger). *Let T, V be two linear operators acting on a vector space \mathcal{X} over \mathbb{C} and $\lambda \in \rho(T)$. Then λ is an eigenvalue of $T - V^2$ iff 1 is an eigenvalue of $B(\lambda) \equiv B(\lambda, T, V)$. In this case,*

$$\dim \mathcal{E}_{T-V^2}(\lambda) = \dim \mathcal{E}_{B(\lambda)}(1);$$

that is, the corresponding (geometric) multiplicities of eigenvalues are equal to each other.

Proof. If λ is an eigenvalue of $T - V^2$, then Lemma A.9 implies that 1 is an eigenvalue of $B(\lambda)$ and the eigenspace of $B(\lambda)$ corresponding to the eigenvalue 1 has at least dimension $|I| = \dim \mathcal{E}_{T-V^2}(\lambda)$. Conversely, if $\{\phi_j\}_{j \in J}$ is a basis of the eigenspace of $B(\lambda)$ corresponding to the eigenvalue 1, then we set

$$\psi_j \doteq (T - \lambda \mathbf{1})^{-1} V \phi_j, \quad j \in J.$$

Then, by (A.17),

$$\phi_j = B(\lambda) \phi_j = V \psi_j, \quad j \in J,$$

which implies that $\{\psi_j\}_{j \in J}$ is a linearly independent set. Thus,

$$(T - V^2) \psi_j = (T - \lambda \mathbf{1}) \psi_j + (\lambda \mathbf{1} - V^2) \psi_j = V \phi_j + (\lambda \mathbf{1} - V^2) \psi_j = \lambda \psi_j, \quad j \in J,$$

and hence, the eigenspace of $T - V^2$ corresponding to the eigenvalue λ has at least dimension $|J| = \dim \mathcal{E}_{B(\lambda)}(1)$. \square

A.6. Combes-Thomas estimates

We give here a version of the celebrated Combes-Thomas estimates, first proven in 1973 [47], which is well-adapted to our framework. For the nonexpert reader, we provide also its proof, which is relatively short and easy to understand in the particular situation we are interested in.

Fix a countable set Λ and a pseudometric $d : \Lambda \times \Lambda \rightarrow \mathbb{R}_0^+$ on Λ . Let $\ell^2(\Lambda)$ be the (separable) Hilbert space of square summable functions $\Lambda \rightarrow \mathbb{C}$. Similar to (5), its canonical orthonormal basis is defined by

$$\mathbf{e}_x(y) \doteq \delta_{x,y}, \quad x, y \in \Lambda,$$

where $\delta_{i,j}$ is the Kronecker delta. For simplicity, as before, we use the shorter notation $\langle \cdot, \cdot \rangle \equiv \langle \cdot, \cdot \rangle_{\ell^2(\Lambda)}$ for its scalar product.

For each bounded operator $T \in \mathcal{B}(\ell^2(\Lambda))$ and positive parameter $\mu \in \mathbb{R}_0^+$, we define the quantity

$$\mathbf{S}(T, \mu) \doteq \sup_{x \in \Lambda} \sum_{y \in \Lambda} \left(e^{\mu d(x,y)} - 1 \right) |\langle \mathbf{e}_x, T \mathbf{e}_y \rangle| \in [0, \infty]. \quad (\text{A.20})$$

Compare with (136). By definition of a pseudometric, the function d is symmetric with respect to the variables x and y . The same occurs with the factor $|\langle \mathbf{e}_x, T \mathbf{e}_y \rangle|$, provided that T is self-adjoint. Thus, in this particular case, $\mathbf{S}(T, \mu)$ is equal to

$$\mathbf{S}(T, \mu) = \sup_{y \in \Lambda} \sum_{x \in \Lambda} \left(e^{\mu d(x,y)} - 1 \right) |\langle \mathbf{e}_x, T \mathbf{e}_y \rangle| \in [0, \infty]. \quad (\text{A.21})$$

The lemma below provides an estimate of the operator norm of T in terms of quantities that are similar to (A.20) and (A.21):

Lemma A.11. *For any bounded operator $T \in \mathcal{B}(\ell^2(\Lambda))$,*

$$\|T\|_{\text{op}}^2 \leq \left(\sup_{y \in \Lambda} \sum_{x \in \Lambda} |\langle \mathbf{e}_x, T \mathbf{e}_y \rangle| \right) \left(\sup_{x \in \Lambda} \sum_{y \in \Lambda} |\langle \mathbf{e}_x, T \mathbf{e}_y \rangle| \right).$$

Proof. Assume without loss of generality that the above bound is finite for $T \in \mathcal{B}(\ell^2(\Lambda))$. Otherwise the assertion would be trivial. Let $V : \ell^1(\Lambda) + \ell^\infty(\Lambda) \rightarrow \ell^1(\Lambda) + \ell^\infty(\Lambda)$ be the mapping defined by

$$Vf(x) \doteq \sum_{y \in \Lambda} f(y) \langle \mathbf{e}_x, T \mathbf{e}_y \rangle, \quad x \in \Lambda, \quad f \in \ell^1(\Lambda) + \ell^\infty(\Lambda).$$

If $f \in \ell^\infty(\Lambda)$, then $Vf \in \ell^\infty(\Lambda)$ because

$$\sup_{x \in \Lambda} \sum_{y \in \Lambda} |f(y)| |\langle \mathbf{e}_x, T \mathbf{e}_y \rangle| \leq \|f\|_\infty \sup_{x \in \Lambda} \sum_{y \in \Lambda} |\langle \mathbf{e}_x, T \mathbf{e}_y \rangle| < \infty,$$

while, for any $f \in \ell^1(\Lambda)$, we also have $Vf \in \ell^1(\Lambda)$ because

$$\|Vf\|_{\ell^1(\Lambda)} \sum_{x \in \Lambda} |Vf(x)| \leq \sum_{x,y \in \Lambda} |f(y)| |\langle \mathbf{e}_x, T \mathbf{e}_y \rangle| \leq \|f\|_{\ell^1(\Lambda)} \sup_{y \in \Lambda} \sum_{x \in \Lambda} |\langle \mathbf{e}_x, T \mathbf{e}_y \rangle| < \infty,$$

using Tonelli's theorem. It then follows from the Riesz-Thorin theorem [94, Theorem 6.27] that, for any function $f \in \ell^2(\Lambda) \subseteq \ell^1(\Lambda) + \ell^\infty(\Lambda)$,

$$\|Vf\|_{\ell^2(\Lambda)}^2 \leq \|f\|_{\ell^2(\Lambda)}^2 \left(\sup_{y \in \Lambda} \sum_{x \in \Lambda} |\langle \mathbf{e}_x, T \mathbf{e}_y \rangle| \right) \left(\sup_{x \in \Lambda} \sum_{y \in \Lambda} |\langle \mathbf{e}_x, T \mathbf{e}_y \rangle| \right).$$

Finally, we observe that

$$(Tf)(x) = \langle \mathbf{e}_x, Tf \rangle = \sum_{y \in \Lambda} f(y) \langle \mathbf{e}_x, T\mathbf{e}_y \rangle = (Vf)(x)$$

whenever $x \in \Lambda$ and $f \in \ell^2(\Lambda)$. \square

We now state another, well-known, technical lemma, which is given here for completeness. Recall that, here, $\rho(T) \subseteq \mathbb{C}$ and $\sigma(T) \doteq \mathbb{C} \setminus \rho(T)$ respectively denote the resolvent set and the spectrum of any element T in some unital C^* -algebra (like the space of bounded operators on some Hilbert space). Similar to (135), we use the notation

$$\Delta(\lambda; T) \doteq \min\{|\lambda - a| : a \in \sigma(T)\} \quad (\text{A.22})$$

for the distance between a complex number $\lambda \in \mathbb{C}$ and the spectrum $\sigma(T)$ of any element T in some unital C^* -algebra.

Lemma A.12 (Norm estimates of resolvents). *Let \mathcal{X} be an unital C^* -algebra with norm $\|\cdot\|$. Take $T, B \in \mathcal{X}$ with T being self-adjoint and let $\lambda \in \rho(T)$. If $\|B\| < \Delta(\lambda; T)$, then $\lambda \in \rho(T + B)$ and*

$$\|(T + B - \lambda \mathbf{1})^{-1}\| \leq \frac{1}{\Delta(\lambda; T) - \|B\|}.$$

Proof. Assume all conditions of the lemma, in particular that $\|B\| < \Delta(\lambda; T)$. Then,

$$\|(T - \lambda \mathbf{1})^{-1}B\| \leq \Delta(\lambda; T)^{-1}\|B\| < 1,$$

and using the Neumann series [46, Lemma 4.24] for $-(T - \lambda \mathbf{1})^{-1}B$, the element $\mathbf{1} + (T - \lambda \mathbf{1})^{-1}B$ is invertible with norm bounded by

$$\begin{aligned} \left\| \left(\mathbf{1} + (T - \lambda \mathbf{1})^{-1}B \right)^{-1} \right\| &\leq \sum_{n=0}^{\infty} \|(T - \lambda \mathbf{1})^{-1}B\|^n = \frac{1}{1 - \|(T - \lambda \mathbf{1})^{-1}B\|} \\ &\leq \frac{1}{1 - \Delta(\lambda; T)^{-1}\|B\|} = \frac{\Delta(\lambda; T)}{\Delta(\lambda; T) - \|B\|}. \end{aligned}$$

Finally, one uses the equality

$$T + B - \lambda \mathbf{1} = (T - \lambda \mathbf{1}) \left(\mathbf{1} + (T - \lambda \mathbf{1})^{-1}B \right)$$

for any $\lambda \in \rho(T)$ to deduce that $\lambda \in \rho(T + B)$ and

$$\|(T + B - \lambda \mathbf{1})^{-1}\| = \left\| \left(\mathbf{1} + (T - \lambda \mathbf{1})^{-1}B \right)^{-1} (T - \lambda \mathbf{1})^{-1} \right\| \leq \frac{1}{\Delta(\lambda; T) - \|B\|}. \quad \square$$

We can now prove the following version of Combes-Thomas estimates:

Theorem A.13 (Combes-Thomas estimates). *Let $T \in \mathcal{B}(\ell^2(\Lambda))$ be a self-adjoint operator. Given $\mu \in \mathbb{R}_0^+$ and $\lambda \in \mathbb{C}$ with $\Delta(\lambda; T) > \mathbf{S}(T, \mu)$, the following inequality holds true:*

$$|\langle \mathbf{e}_x, (T - \lambda \mathbf{1})^{-1} \mathbf{e}_y \rangle| \leq \frac{e^{-\mu d(x, y)}}{\Delta(\lambda; T) - \mathbf{S}(T, \mu)}, \quad x, y \in \Lambda.$$

Proof. Fix $y \in \Lambda$ and $R \in \mathbb{R}^+$. Define the function $\varphi : \Lambda \rightarrow [1, e^{\mu R}]$ by

$$\varphi(x) \doteq \exp(\mu \min\{d(x, y), R\}), \quad x \in \Lambda.$$

Clearly, φ and $1/\varphi$ are bounded, and the inverse of the multiplication operator $M_\varphi \in \mathcal{B}(\ell^2(\Lambda))$ by φ is nothing else than $M_{1/\varphi}$. Because φ is a real-valued function, $M_\varphi^* = M_\varphi$ and, for any $x \in \Lambda$, \mathbf{e}_x is of course an eigenvector of M_φ with associated eigenvalue $\varphi(x)$. In particular,

$$\langle \mathbf{e}_x, M_\varphi T M_\varphi^{-1} \mathbf{e}_z \rangle = \frac{\varphi(x)}{\varphi(z)} \langle \mathbf{e}_x, T \mathbf{e}_z \rangle, \quad x, z \in \Lambda.$$

Since $(x, z) \mapsto \min\{d(x, z), R\}$ is another pseudometric on Λ , for all $x, z \in \Lambda$, we have that

$$\min\{d(x, y), R\} - \min\{d(z, y), R\} \leq \min\{d(x, z), R\} \leq d(x, z).$$

In particular, the operator $B \doteq M_\varphi T M_\varphi^{-1} - T$ satisfies the bound

$$|\langle \mathbf{e}_x, B \mathbf{e}_z \rangle| \leq \left(e^{\mu d(x, z)} - 1 \right) |\langle \mathbf{e}_x, T \mathbf{e}_z \rangle|, \quad x, z \in \Lambda.$$

By Lemma A.11 together with Equations (A.20) and (A.21), it follows that

$$\|B\|_{\text{op}} \leq \mathbf{S}(T, \mu) < \Delta(\lambda; T).$$

Applying now Lemma A.12, we then arrive at the bound

$$\left\| \left(M_\varphi T M_\varphi^{-1} - \lambda \mathbf{1} \right)^{-1} \right\|_{\text{op}} \leq \frac{1}{\Delta(\lambda; T) - \|B\|_{\text{op}}} \leq \frac{1}{\Delta(\lambda; T) - \mathbf{S}(T, \mu)}.$$

Finally, for any $x \in \Lambda$ such that $d(x, y) \leq R$, we observe from the last upper bound that

$$\begin{aligned} e^{\mu d(x, y)} |\langle \mathbf{e}_x, (T - \lambda \mathbf{1})^{-1} \mathbf{e}_z \rangle| &= \frac{\varphi(x)}{\varphi(1)} |\langle \mathbf{e}_x, (T - \lambda \mathbf{1})^{-1} \mathbf{e}_z \rangle| = \left| \left\langle \mathbf{e}_x, \left(M_\varphi T M_\varphi^{-1} - \lambda \mathbf{1} \right)^{-1} \mathbf{e}_z \right\rangle \right| \\ &\leq \frac{1}{\Delta(\lambda; T) - \mathbf{S}(T, \mu)}. \end{aligned}$$

Since $y \in \Lambda$ and $R \in \mathbb{R}^+$ are arbitrary parameters, the above inequality in fact holds true for all $x, y \in \Lambda$. \square

A.7. Elementary observations

For completeness and the reader's convenience, we conclude the appendix by given a few elementary results related to the space of bounded operators on a Hilbert space.

Proposition A.14 (Monotonicity of the inverse on operators). *Let B and C be two positive bounded operators on a Hilbert space with bounded (positive) inverse. If $B \leq C$, then $C^{-1} \leq B^{-1}$.*

Proof. The proof is standard. Since it is very short, we give it for completeness. If B and C commute, then

$$B^{-1} - C^{-1} = B^{-1}(C - B)C^{-1} \geq 0,$$

because B^{-1} , C^{-1} and $C - B$ are positive commuting operators. If B and C do not commute, then we observe that $B \leq C$ yields

$$C^{-\frac{1}{2}} B C^{-\frac{1}{2}} \leq \mathbf{1},$$

which in turn implies that

$$C^{\frac{1}{2}}B^{-1}C^{\frac{1}{2}} \geq \mathbf{1},$$

because $\mathbf{1}$ and $C^{-\frac{1}{2}}BC^{-\frac{1}{2}}$ commute. From the last inequality it follows that $B^{-1} \geq C^{-1}$. \square

Proposition A.15 (Monotone convergence theorem for operators). *Let \mathcal{X} be any complex Hilbert space. Any increasing (decreasing) monotone net $(A_i)_{i \in I}$ of self-adjoint elements in $\mathcal{B}(\mathcal{X})$ that is bounded from above (below) has a supremum (infimum) in $\mathcal{B}(\mathcal{X})$. The supremum (infimum) is itself also self-adjoint and is the strong operator limit of the net.*

Proof. [46, Proposition 2.17] already tells us that any increasing (decreasing) monotone net $(A_i)_{i \in I}$ of self-adjoint elements in $\mathcal{B}(\mathcal{X})$ that is bounded from above (below) has a supremum (infimum) A_∞ in $\mathcal{B}(\mathcal{X})$. The supremum (infimum) A_∞ is itself also self-adjoint and is the weak operator limit of the net. This is proven by using the polarization identity and the Riesz representation theorem together with elementary estimates. To conclude the proof, it remains to show that $A_\infty \in \mathcal{B}(\mathcal{X})$ is the limit of the increasing net $(A_i)_{i \in I}$ also in the strong operator topology. To this end, assume that $(A_i)_{i \in I}$ is an increasing net and define the (decreasing) net $(B_i)_{i \in I}$ of positive operators by $B_i \doteq A_\infty - A_i \geq 0$. By construction, this net converges in the weak operator topology to $0 \in \mathcal{B}(\mathcal{X})$, which in turn implies that the net $(B_i^{1/2})_{i \in I}$ converges in the strong operator topology to $0 \in \mathcal{B}(\mathcal{X})$. As the net $(B_i^{1/2})_{i \in I}$ is norm-bounded and $B_i = B_i^{1/2}B_i^{1/2}$, we then conclude that also $(B_i)_{i \in I}$ converges in the strong operator topology to $0 \in \mathcal{B}(\mathcal{X})$; that is, A_∞ is the strong operator limit of the net $(A_i)_{i \in I}$. If $(A_i)_{i \in I}$ is a decreasing net, then we consider the increasing net $(-A_i)_{i \in I}$ to conclude that $(A_i)_{i \in I}$ has a infimum $A_\infty = A_\infty^* \in \mathcal{B}(\mathcal{X})$, which is again the strong operator limit of the net $(A_i)_{i \in I}$. \square

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