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Scalar Particles in a Narrow-Band Periodic Potential

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A system of an infinite number of spinless particles in a narrow-band periodic potential is treated. The dimension of the space is arbitrary, the tight-binding approximation is used, and it is assumed that the filling fraction is nearly one electron per atom. After a preliminary discussion of the Hartree approximation, the full Schrödinger equation is considered and a rigorous spectral perturbation theory in the kinetic energy term is set up. To get rid of the lack of relative boundedness of this perturbation, a vacuum state is constructed and its energy renormalized to zero, and passage is made to an excitonic representation in which the quasiparticles appear naturally as local perturbations of the vacuum. In this representation, relative boundedness is recovered and Rayleigh–Schrödinger expansions can be used to find cluster expansions for all local observables.

KEY WORDS: Mott localization; many-body systems; spectral perturbation theory.

The aim of this work is to study a problem of spectral perturbation theory for a quantum many-body system of particles in a narrow-band periodic potential. Unfortunately, the available tools are not suitable for studying the Hubbard model for spin-$\frac{1}{2}$ electrons, but can only deal with its version for scalar particles. Nonetheless, some of the qualitative properties of the system considered here should also characterize fermion systems. The reason is that I consider the limit in which the bandwidth for the one-particle problem is much smaller than the repulsion energy among the electrons. In such a limit, the particles are localized and have a small overlap. This phenomenon is generally known as Mott's localization.[5] The Pauli

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principle forbids two electrons with the same spin from sitting on the same site and this has major effects favoring an antiferromagnetic ordering of the spins and, perhaps, in inducing superconductivity. However, it should not compromise localization, but enhance it.

The first section of this paper is introductory and contains the statements of all the results proven in the subsequent sections. In the Appendix I prove some results about the Hartree approximation, which has the advantage of being easy to deal with and furnishing a correct picture of the situation. In Section 2 I give a convergent expansion for a family of eigenprojections which is complete in all finite-volume truncations. Each one of the relative eigenspaces can be seen as containing a number of excitonic quasiparticles proportional to the energy gap with the ground state. The radius of convergence for these expansions depends on the number of such quasiparticles and it shrinks to zero as this number tends to infinity. Moreover, I prove that the ground state in the sector in which there are as many particles as potential wells is nondegenerate and it is separated by a finite gap from the rest of the spectrum of the Hamiltonian restricted to this sector. This state plays an important role in the sequel and I shall refer to it as to the "vacuum state." The two-point function in the vacuum state decays exponentially fast and the momentum distribution function is smooth. This has to be contrasted with the noninteracting case in which the two-point function is not summable and the momentum distribution function is a delta function. Thus, somewhere, there must be a transition from a weakly interacting, extended regime to a strongly interacting, localized regime. Finally, I study the excitonic quasiparticles and prove analyticity of the dispersion law and a clustering property which means that the interactions among them decay exponentially with the separation. These applications will be discussed in Section 3.

With regard to the method I follow, I have used some new tools which have also been applied in ref. 1. In fact, a rigorous study of the Schrödinger equation requires that one faces the main technical difficulty of many-body perturbation theory: The lack of relative boundedness of the perturbation with respect to the unperturbed part. What I do is to perform a nonunitary transformation on the Hamiltonian whose aim is twofold: To construct the vacuum state and to pass to a representation in which the perturbation is relatively bounded. This permits us to use Rayleigh–Schrödinger expansions to construct analytic families of eigenprojections. The formalism is devised in such a way as to yield in the most natural way cluster expansions for all local observables. Also, Hubbard[9] considered a similar problem and ended up with cluster expansions in the hopping parameter. However, he worked with a finite-temperature formalism and did not address the question of convergence. I shall call the nonunitary transformation I use a "dressing transformation," because it resembles in some respects a transformation of this name introduced by Glimm in the 1960s to renormalize the two-dimensional Yukawa model.

1. INTRODUCTION, NOTATIONS, AND RESULTS

My aim in this work is to study a system consisting of an infinite number of scalar particles in a periodic background. The tight-binding Hamiltonian on the lattice $\mathbb{Z}^d$ is

$$H_\lambda = -\lambda \sum_i \Delta_i + \sum_{i \neq j} \delta(x_i - x_j) \equiv -\lambda \Delta + \delta \tag{1.1}$$

where λ is the dimensionless and small parameter in which we perturb. Δ is the discretized Laplacian without the diagonal terms and acts as follows:

$$(\Delta u)(x) = \sum_{|y-x|=1} u(y) \tag{1.2}$$

δ is the delta function

$$\delta(x) = \begin{cases} 1 & \text{if } x = 0 \\ 0 & \text{if } x \neq 0 \end{cases} \tag{1.3}$$

i and j are labels for the particles. It is convenient to restrict the Hamiltonian H_λ to a large but finite cube Λ with periodic boundary conditions. The Hilbert space $\mathfrak{H}$ is the Bose–Fock space of all completely symmetric wavefunctions, $S \otimes_{i=1}^{N} l^2(\Lambda) = \mathfrak{H}$, where N is the number of particles and S is the symmetrization operator. In the second quantization formalism, $\mathfrak{H}$ is seen as the tensor product $\mathfrak{H} = \otimes_{x \in \Lambda} l^2(n)$, a basis of the copy of $l^2(n)$ corresponding to the site x being $(|n\rangle_x, n \geqslant 0)$, where $|n\rangle_x$ denotes the state with n particles in the site x. I am interested in the properties of the spectrum of the operator (1.1) which hold for λ small and are independent of the size of Λ. I shall denote by $\mathfrak{H}_N$ the subspace of $\mathfrak{H}$ with N particles and with $|0\rangle$ the state with one and only one particle sitting on each site.

To begin with, it is instructive to consider the Hartree approximation in the case $N = |\Lambda|$. In ref. 3 a similar problem is studied without the simplifying passage to the tight-binding approximation. Let us consider the problem of minimizing the expectation value of the Hamiltonian (1.1) in the space of all the functions of the form $S \prod_{i \in \Lambda} u(x_i - i)$ with $u \in l^2(\mathbb{Z}^d)$ of norm one; then we find the following Euler–Lagrange equations:

$$\begin{gathered} -\lambda\, \Delta u(x) + \sum_{y \neq 0} u(x+y)^2\, u(x) = E u(x) \\ u \in l^2(\mathbb{Z}^d), \qquad \|u\|_2 = 1 \end{gathered} \tag{1.4}$$

If we make use of the normalization condition, we can rewrite (1.4) as follows:

$$-\lambda\, \Delta u(x) - u(x)^3 = \varepsilon u$$
$$u \in l^2(\mathbb{Z}^d); \qquad \|u\|_2 = 1 \tag{1.5}$$

where $\varepsilon = E - 1$. In the Appendix I prove that, for every dimension $d \geqslant 1$, there is a $\lambda_d > 0$ such that Eq. (1.5) has a solution u_λ, analytic in the disc $\{|\lambda| < \lambda_d\}$. This suggests that in all dimensions and for $|\lambda|$ small enough, we find a "Mott localized" regime in which each electron sits on a single atom. Of course, Mott in its papers considered only fermion systems and thus the use of his name may appear improper in the present context. However, one can extract from the solution (1.5) some information about fermion systems which appears to be correct at the first nonvanishing order in λ. In the Appendix I shall elaborate on this point in order to get closer to the physics of real systems. My aim in the main part of this paper will be to set up techniques to do perturbation theory for the original problem (1.1) in this localized regime.

I introduce some notations. Let

$$a^d(\lambda) = \sum_{n=1}^{\infty} a_n^d \lambda^n \tag{1.6}$$

be the function implicitly defined as the solution of the following equation:

$$a^d(\lambda) = 2d\lambda + \lambda \sum_{k=1}^{4} [16 d a^d(\lambda)]^k \tag{1.7}$$

Let $\rho_d > 0$ be its radius of analyticity around $\lambda = 0$ and let $c_d > 0$ be the minimum constant such that

$$\sum_{m=k}^{\infty} a_n^d \lambda^n \leqslant (c_d \lambda)^k \tag{1.8}$$

for all $k \geqslant 1$. Finally, if $x_1, \ldots, x_{|\Lambda|}$ are the points of Λ and $\psi \in \mathfrak{H} = \bigotimes_{x \in \Lambda} l^2(\mathbb{N})$ is the wavefunction

$$\psi = \sum_{n_{x_1}, \ldots, n_{x_{|\Lambda|}}} \psi(n_{x_1}, \ldots, n_{x_{|\Lambda|}})\, |n_{x_1}\rangle_{x_1} \otimes \cdots \otimes |n_{x_{|\Lambda|}}\rangle_{x_{|\Lambda|}} \tag{1.9}$$

its l^1-norm will be defined as follows:

$$\|\psi\|_1 = \sum_{n_{x_1}, \ldots, n_{x_{|\Lambda|}}} |\psi(n_{x_1}, \ldots, n_{x_{|\Lambda|}})| \tag{1.10}$$

I shall also use the corresponding l^1-operator norm and denote it by $\|\cdot\|_{\mathscr{L}^1(\mathfrak{H})}$.

In Section 2 I prove the following basic result

Theorem 1. For all Λ and all N, there is an operator $R(\lambda)$, analytic in a disc around $\lambda = 0$ of radius $\geqslant \rho_d$, such that

$$e^{-R(\lambda)} H_\lambda e^{R(\lambda)} = E_0(\lambda) + \delta + V(\lambda) \tag{1.11}$$

where $E_0(\lambda)$ is an analytic function for $|\lambda| < \rho_d$ and $V(\lambda)$ is an operator which annihilates the eigenstate $|0\rangle$ of H_0 with $E_n = 0$ and $N = |\Lambda|$ particles. $V(\lambda)$ is relatively bounded with respect to δ in the following sense:

$$\begin{aligned} &\|(\delta + P_0)^{-1/2} V(\lambda)(\delta + P_0)^{-1/2}\|_{\mathscr{L}^1(\mathfrak{H}_N)} \\ &\quad \leqslant \frac{2de\,|\lambda|}{1 - c_d e\,|\lambda|} (\max(0, |\Lambda| - N) + 2) \end{aligned} \tag{1.12}$$

where P_0 is the orthogonal projection onto the kernel of δ.

This theorem has a series of applications that will be considered in detail in Section 3. The first of them is the following result.

Theorem 2. For all Λ, all N, all integers $n \geqslant 0$, and for $|\lambda|$ small enough, there is an analytic family of spectral projections $P_{nN\lambda}$ of (1.1) such that P_{nN0} is the spectral projection of (1.1) for $\lambda = 0$ on the eigenspace with N particles and energy $E_n = n$. The radius of analyticity of $P_{nN\lambda}$ is not smaller than

$$e^{-1} \left\{ c_d + \frac{d}{2} (E_n + 1)[2 + \max(0, |\Lambda| - N)] \right\}^{-1} \tag{1.13}$$

Moreover, for $|\lambda|$ small, the ground state of the Hamiltonian H_λ restricted to the sector with $|\Lambda|$ particles is $e^{R(\lambda)}|0\rangle$ and its energy is separated by a finite gap from the rest of the spectrum of H_λ in that sector.

Notice that the radius of analyticity of $P_{nN\lambda}$ shrinks to zero as E_n or $|\Lambda| - N$ gets larger. This is due to the fact that the corresponding eigenspace contains $n + \max(0, |\Lambda| - N)$ quasiparticles, each of which has kinetic energy of order λ that interact with each other and move around the lattice. The width of the bands originating from the eigenvalues of $H_0 = \delta$ increases at a rate that should be proportional to the number of quasiparticles, i.e., to $n + \max(0, |\Lambda| - N)$. Thus, one expects that a level crossing occurs very soon for very excited states and this is likely to originate some point of nonanalyticity for complex λ, which compromises the convergence of power series expansions.

To state the next result, I introduce some notations. Let c_x and $c_x^\dagger$ be the Bose creation and annihilation operators for a particle in the site x and let $|\psi_\lambda\rangle = P_{0\,|\Lambda|\,\lambda}\,|0\rangle$, where $|0\rangle$ is the ground state of (1.1) for $\lambda = 0$ and $N = |\Lambda|$. The two-point function $\langle\psi_\lambda|\, c_y^\dagger c_x\, |\psi_\lambda\rangle / \|\psi_\lambda\|^2$ depends only on the difference $(x - y)$ and will be denoted by $W(x - y)$. Finally, the momentum distribution function

$$\hat{W}_\lambda(p) = \langle\psi_\lambda|\, c_p^\dagger c_p\, |\psi_\lambda\rangle / \|\psi_\lambda\|^2 \tag{1.14}$$

where

$$c_p^\dagger = \frac{1}{|\Lambda|^{1/2}} \sum_y e^{-ip\cdot y} c_y^\dagger, \qquad c_p = \frac{1}{|\Lambda|^{1/2}} \sum_x e^{ip\cdot x} c_x \tag{1.15}$$

is the Fourier transform of $W(x - y)$. We have the following result.

Theorem 3. For every Λ, $\varepsilon > 0$, $|\lambda| < \rho_d - \varepsilon$ and for $N = |\Lambda|$ there is a finite, positive constant $C(\varepsilon)$ such that

$$|W_\lambda(x - y)| \leqslant a^d(\lambda)\, C(\varepsilon) \exp[-m(\lambda, \varepsilon)\, |x - y|] \tag{1.16}$$

where

$$m(\lambda, \varepsilon) = -\frac{1}{2} \ln \left| \frac{\lambda}{\rho_d - \varepsilon} \right| \tag{1.17}$$

and $\hat{W}_\lambda(p)$ is analytic in the region $|\mathrm{Im}\, p| < m(\lambda)$ of $\mathbb{C}^d$.

Note that, for $\lambda = \infty$, $\hat{W}_\lambda(p)$ is equal to $\delta(p)$. For λ large but finite, there is no rigorous result, but I believe that, at least in dimension high enough, $\hat{W}_\lambda(p)$ still has some kind of singularity at zero momentum marking the existence of a Bose condensate. In this case, there must be a critical value of λ under which the interaction is so strong that the singularity is completely obliterated. This is reminiscent of what occurs in a model of interacting fermions in dimension one considered by Lieb and Mattis[(7)] (see also ref. 6). They proved that if the interaction is weak, then the momentum distribution function has a point of infinite steepness which defines the Fermi surface, while if the interaction is strong, it is analytic.

The last question I address concerns excitonic quasiparticles and their mutual interactions. I shall work with the following renormalized Hamiltonian:

$$H_\lambda^{\mathrm{ren}} \equiv e^{-R(\lambda)} H_\lambda e^{R(\lambda)} - E_0(\lambda) = \delta + V(\lambda) \tag{1.18}$$

Adopting the terminology of ref. 2, I shall refer to the transformation

$H_\lambda \mapsto H_\lambda^{\text{ren}}$ as to a "dressing transformation." Let $P_{nN\lambda}^{\text{ren}}$ be the (non-orthogonal) projection

$$e^{-R(\lambda)} P_{nN\lambda} e^{R(\lambda)}$$

The eigenspaces $P_{nN\lambda}^{\text{ren}} \mathfrak{H}$ of H_λ^{ren} contain a fixed number of quasiparticles and one can ask which are the properties of H_λ^{ren} restricted on such eigenspaces. An example of the kind of result that one can prove is given by the following theorem, which considers the cases of one and two hole-quasiparticles.

Theorem 4. Let $|x\rangle$ and $|x, y\rangle$ denote the states

$$|x\rangle_\lambda = P_{0,|\Lambda|-1,\lambda} c_x |0\rangle$$

and

$$|x, y\rangle_\lambda = P_{0,|\Lambda|-2,\lambda} c_x c_y |0\rangle$$

For every $|\lambda|$ small enough, there are constants $0 < c_1, c_2, m_1, m_2 < \infty$ such that, for every $x_1, y_1, x_2, y_2 \in \Lambda$ we have

$$|_\lambda\langle x_2| H_\lambda^{\text{ren}} |x_1\rangle_\lambda| \leqslant c_1 e^{-m_1 |x_1 - x_2|} \tag{1.19}$$

and

$$\begin{aligned} |_\lambda\langle x_2 y_2| H_\lambda^{\text{ren}} |x_1 y_1\rangle_\lambda - {}_\lambda\langle x^2| H_\lambda^{\text{ren}} |x_1\rangle_\lambda \delta_{y_1 y_2} \\ - {}_\lambda\langle y_2| H_\lambda^{\text{ren}} |y_1\rangle_\lambda \delta_{x_1 x_2}| \leqslant c_2 e^{-m_2 |x_1 - y_1|} \end{aligned} \tag{1.20}$$

2. EXISTENCE OF THE DRESSING TRANSFORMATION

In this section I prove Theorem 1, which was stated in Section 1. Let us rewrite the operator (1.1) as follows:

$$H_\lambda = \delta + \lambda \sum_{\langle xy \rangle} (\xi_y^1 \xi_x^{-1} + \eta_y^+ \xi_x^{-1} + \xi_y^1 \eta_x^- + \eta_y^+ \eta_x^-) \tag{2.1}$$

The operators ξ^n, $n = -1, 1, 2,\ldots$, η^+, and η^- appearing here are defined so that

$$\begin{aligned} &\xi^n: && |1\rangle \to |1+n\rangle && \text{for} \quad n = -1, 1, 2,\ldots \\ &\eta^+: && |n\rangle \to |1+n\rangle && \text{for} \quad n = 0, 2, 3,\ldots \\ &\eta^-: && |n\rangle \to |n-1\rangle && \text{for} \quad n = 2, 3, 4,\ldots \end{aligned} \tag{2.2}$$

while they annihilate all other basis vectors of $l^2(\mathbb{N})$. To prove Theorem 1, we must establish the existence of an operator $R(\lambda)$, analytic for $|\lambda|$ small, such that

$$e^{-R(\lambda)}H_\lambda e^{R(\lambda)}|0\rangle = E_0(\lambda)|0\rangle \tag{2.3}$$

where $E_0(\lambda)$ is a real-valued function and $|0\rangle$ is the state with $N = |\Lambda|$ particles, each one sitting on a different site. Equation (2.3) does not determine $R(\lambda)$ uniquely and it is possible to impose the following additional condition: The operators R_n such that

$$R(\lambda) = \sum_{n=1}^{\infty} \lambda^n R_n \tag{2.4}$$

have the following form:

$$R_n = \sum_\gamma r_n(\gamma)\,\xi_\gamma \tag{2.5}$$

Here γ is a function from Λ to the subset of integers $\{-1, 0, 1, 2,...\}$ with support $s(\gamma)$, and

$$\xi_\gamma = \prod_{x \in \Lambda} \xi_x^{\gamma(x)} \tag{2.6}$$

Moreover, the following clustering property holds:

$$r_n(\gamma) = 0 \qquad \text{if} \quad \operatorname{diam}(s(\gamma)) > n+1 \tag{2.7}$$

The operators (2.6) have two basic properties: First, they are complete in the sense that a suitable linear combination of them can map the state $|0\rangle$ to any other state in $\mathfrak{H}$. Second, they generate a commutative algebra. The first property is necessary to guarantee the solvability of the recurrence relations below for R_n. The second property is essential as well, because it keeps low the number of diagrams generated by those recurrence relations, thus permitting the control of the convergence of the perturbation expansions. Let us observe that apparently the three basic properties needed to apply the method below, i.e., clustering, completeness, and commutativity, are incompatible with the requirement that the dressing transformation is unitary.

Notice that

$$[\delta, R_n] = \sum_\gamma r_n(\gamma)\,\varepsilon(\gamma) \tag{2.8}$$

where

$$\varepsilon(\gamma) = \langle \xi_\gamma 0 | S | \xi_\gamma 0 \rangle \tag{2.9}$$

The operator R_1 must satisfy the condition

$$[\delta, R_1] |0\rangle = -\sum_{\langle xy \rangle} \xi_y^1 \xi_x^{-1} |0\rangle \tag{2.10}$$

whence

$$R_1 = -\sum_{\langle xy \rangle} \xi_y^1 \xi_x^{-1} \tag{2.11}$$

The operators R_n, for $n \geqslant 2$, are determined by the following recurrence relations:

$$[\delta, R_n] |0\rangle = -\sum_{\langle xy \rangle} \sum_{\substack{j_1 \leqslant \cdots \leqslant j_m \\ j_1 + \cdots + j_m = n-1}} \frac{1}{(j)!} \times [\cdots[\eta_y^+ \xi_x^{-1} + \xi_y^1 \eta_x^- + \eta_y^+ \eta_x^-, R_{j_1}], \ldots, R_{j_m}] |0\rangle \tag{2.12}$$

Note that in (2.12), only the terms with at most four commutators do not vanish. In fact, the only nonvanishing products of one η and two ξ operators are the following:

$$\begin{aligned} \xi^n \eta^+ \xi^{-1} &= \xi^n \eta^- \xi^1 = \xi^n \\ \xi^{-1} \eta^- \xi^{-1} &= \xi^{-1} \end{aligned} \tag{2.13}$$

where $n \geqslant 1$. We have

$$\begin{aligned} &\left\| \left[\left(\sum_{\langle xy \rangle} \eta_y^+ \xi_x^{-1} + \xi_y^1 \eta_x^- + \eta_y^+ \eta_x^- \right), R_{j_1} \right] |0\rangle \right\|_1 \\ &\leqslant 2d \sum_\gamma 4 \, |r_{j_1}(\gamma)| \, s(\gamma) \\ &\leqslant 16d \sum_\gamma |r_{j_1}(\gamma)| \, \varepsilon(\gamma) = 16d \, |\Lambda| \, r_{j_1}^* \end{aligned} \tag{2.14}$$

where

$$r_{j_1}^* = \sum_{\gamma: s(\gamma) \cap \langle xy \rangle} \varepsilon(\gamma) \, |r_{j_1}(\gamma)| \tag{2.15}$$

where the sum runs over all γ's such that $s(\gamma) \cap \langle x, y \rangle \neq \varnothing$ for some bond

$\langle x, y\rangle$. Due to the translation invariance of the problem, r_j^* does not depend on the bond $\langle x, y\rangle$. Analogously, one can find

$$\sum_{\langle xy\rangle} \|[\cdots[\eta_y^+\xi_x^{-1}+\xi_y^1\eta_x^- +\eta_y^+\eta_x^-, R_{j_1}]\cdots R_{j_k}]\,|0\rangle\| \leqslant (16d)^k\,|\Lambda|\, r_{j_1}^*\cdots r_{j_k}^* \tag{2.16}$$

for all $k=2, 3, 4$. In virtue of (2.9) and (2.12), we have

$$r_n^* \leqslant f(r_1^*,..., r_{n-1}^*) \tag{2.17}$$

for all $n \geqslant 2$, where

$$f(r_1^*,..., r_{n-1}^*) = \sum_{j_1+j_2+j_3+j_4=n-1} (16d)^{\# j}\, r_{j_1}^*\cdots r_{j_4}^* \tag{2.18}$$

where $\# j = \#\{j_k \neq 0, k=1, 2, 3, 4\}$ and we put $r_0^*=1$. Thus the radius of convergence of the power series (2.4) is not smaller than that of the series

$$a^d(\lambda) = \sum_{n=1}^{\infty} a_n^d \lambda^n \tag{2.19}$$

where $a_1^d = 2d$ and the a_n for $n \geqslant 2$ are determined by the recurrence relations

$$a_n^d = f(a_1^d,..., a_{n-1}^d) \tag{2.20}$$

To prove the convergence of the series (2.19), it suffices to notice that $a^d(\lambda)$ solves formally the equation

$$a^d(\lambda) = 2d\lambda + \lambda \sum_{k=1}^{4} [16da^d(\lambda)]^k \tag{2.21}$$

which has a solution analytic near $\lambda = 0$.

To conclude the proof of Theorem 1, we have to show that the operator $V(\lambda)$ such that

$$e^{-R(\lambda)} H_\lambda e^{R(\lambda)} = E_0(\lambda) + \delta + V(\lambda) \tag{2.22}$$

is relatively bounded with respect to δ in the following sense:

$$\|\delta^{-1/2} V(\lambda)\, \delta^{-1/2}\|_{\mathscr{L}^1(\mathfrak{H}_N)} \leqslant \frac{2de\lambda}{1-c_0 e\lambda}\,[2+\max(0, |\Lambda|-N)] \tag{2.23}$$

where $\tilde{\delta}=\delta+P_0$, and P_0 is the orthogonal projection onto the kernel of δ. We have

$$\|\tilde{\delta}^{-1/2}V(\lambda)\,\tilde{\delta}^{-1/2}\|_{\mathscr{L}^1(\mathfrak{H}_N)}\leqslant \sup_{\gamma:\,N(\gamma)=N} \|\tilde{\delta}^{-1/2}V(\lambda)\,\tilde{\delta}^{-1/2}\xi_\gamma\,|0\rangle\|_1 \quad (2.24)$$

where $N(\gamma)$ is the number of particles in the state $\xi_\gamma\,|0\rangle$. If γ describes an excitation such that $N(\gamma)=N$, we have

$$\|\tilde{\delta}^{-1/2}V(\lambda)\,\tilde{\delta}^{-1/2}\xi_\gamma\,|0\rangle\|_1\leqslant|\lambda|\sum_{x\in\overline{s(\gamma)}}\sum_{n=0}^{\infty}\sum_{\gamma':\,d(\gamma,\gamma')=n} \times|\langle\xi_{\gamma'}0|\,\tilde{\delta}^{-1/2}e^{-R(\lambda)}H_x e^{R(\lambda)}\tilde{\delta}^{-1/2}\,|\xi_\gamma 0\rangle| \quad (2.25)$$

where $\overline{s(\gamma)}=\{x\colon |x-y|\leqslant 1,\ \forall y\in s(\gamma)\}$ and

$$H_x=c_x^\dagger c_x+\frac{\lambda}{2d}\sum_{|y-x|=1} c_y^\dagger c_x+c_x^\dagger c_y$$

is defined so that $\sum_x H_x=H_\lambda$. Finally, if γ and γ' are two excitations, let us consider all families of operators of the form $\{c_{x_1}^\dagger c_{x_2},\ \langle x_1x_2\rangle\in\mathscr{F}\}$, where $\mathscr{F}$ is a connected set of bonds, such that

$$\prod_{\langle x_1x_2\rangle\in\mathscr{F}} c_{x_1}^\dagger x_{x_2}\xi_\gamma\,|0\rangle=\text{const}\cdot\xi_{\gamma'}\,|0\rangle$$

The minimum cardinality of a family like this is, by definition, $d(\gamma,\gamma')$. If we introduce the notations

$$Q_x(\lambda)=\sum_{n=1}^{\infty}\lambda^n Q_{x;n}=e^{-R(\lambda)}H_x e^{R(\lambda)}-c_x^\dagger c_x-\frac{1}{|\Lambda|}E_0(\lambda) \quad (2.26)$$

from the first part of the proof we get the bound. Hence,

$$(2.25)=|\lambda|\sum_{x\in\overline{s(\gamma)}}\sum_{n=0}^{\infty}\sum_{\gamma':\,d(\gamma,\gamma')=n}\sum_{m=n}^{\infty}|\lambda^m|\,|\langle\xi_{\gamma'}0|\,\tilde{\delta}^{-1/2}Q_{x,m}\tilde{\delta}^{-1/2}\,|\xi_\gamma 0\rangle|$$

$$\leqslant 2d\,|\lambda|\,|s(\gamma)|\sum_{n=0}^{\infty}(c_d\lambda)^n\,\varepsilon(\gamma)^{-1/2}[\max(1,(\varepsilon(\gamma)-n))]^{-1/2}$$

Since

$$|s(\gamma)|\leqslant 2\varepsilon(\gamma)+\max(0,|\Lambda|-N)$$

we have

$$(2.25) \leqslant 4d\,|\lambda| \sum_{n=0}^{\infty} (c_d\,|\lambda|)^n \left(\frac{\varepsilon(\gamma)}{\max(1, [\varepsilon(\gamma)-n])}\right)^{1/2}$$

$$+ 2d\,|\lambda| \max(0, |\Lambda| - N) \sum_{n=0}^{\infty} (c_d\lambda)^n$$

The following inequality is easy to obtain:

$$\left(\frac{\varepsilon(\gamma)}{\varepsilon(\gamma)-n}\right)^{1/2} \leqslant e^{1+n}$$

for all $n = 1, 2,..., \varepsilon(\gamma) - 1$. Thus, we have

$$(2.25) \leqslant \frac{4de\,|\lambda|}{1 - c_d e\,|\lambda|} + 2d \max(0, |\Lambda| - N) \frac{|\lambda|}{1 - c_0\,|\lambda|}$$

$$\leqslant \frac{2de\,|\lambda|}{1 - c_d e\,|\lambda|} [2 + \max(0, |\Lambda| - N)]$$

This completes the proof of Theorem 1.

3. SOME APPLICATIONS

This section contains the proof of Theorems 2–4 in Section 1.

Proof of Theorem 2. Our aim is to control the Rayleigh–Schrödinger expansion for the resolvent $[\zeta - \delta - V(\lambda)]^{-1}$ through which one can express the eigenprojections; see ref. 4. Let us assume that ζ belongs to the circle

$$\mathscr{C}_n = \{\zeta \colon |\zeta - E_n| = 1/4\}$$

for some n. We have

$$[\zeta - \delta - V(\lambda)]^{-1} = \bar{\delta}^{-1/2} \sum_{n=0}^{\infty} (\zeta\bar{\delta}^{-1} - \delta\bar{\delta}^{-1})^{-1} \times [\bar{\delta}^{-1/2} V(\lambda)\,\bar{\delta}^{-1/2} (\zeta\bar{\delta}^{-1} - \delta\bar{\delta}^{-1})^{-1}]^n\,\bar{\delta}^{-1/2} \quad (3.1)$$

This series converges in the l^1-operator norm if $|\lambda|$ is so small that

$$\|\bar{\delta}^{-1/2} V(\lambda)\,\bar{\delta}^{-1/2}\|_{\mathscr{L}^1(\mathfrak{H}_N)} \,\|(\zeta\bar{\delta}^{-1} - \delta\bar{\delta}^{-1})^{-1}\|_{\mathscr{L}^1(\mathfrak{H}_N)} < 1 \quad (3.2)$$

If γ is such that $\xi_\gamma\,|0\rangle \in \mathfrak{H}_N$ we have

$$\|(\zeta\delta^{-1}-\delta\delta^{-1})^{-1}\,\xi_\gamma\,|0\rangle\|_1 = |[\zeta-\varepsilon(\gamma)]^{-1}\,[\varepsilon(\gamma)+\|P_0\xi_\gamma\|_1]|$$
$$\leqslant \frac{\varepsilon(\gamma)+1}{|\zeta-\varepsilon(\gamma)|} \leqslant \frac{1}{4}(E_n+1) \tag{3.3}$$

By using the bound (1.12), we see that (3.2) holds and the series (3.1) converges if $|\lambda|$ is so small that

$$\frac{2de\,|\lambda|}{1-c_d e\,|\lambda|}\,[2+\max(0,|\Lambda|-N)]\,\frac{1}{4}(E_n+1)<1 \tag{3.4}$$

which is equivalent to the condition (1.13). Thus, if (1.13) holds, the contour integral which represents $P_{nN\lambda}$,

$$\oint_{\mathscr{C}_n} \frac{1}{\zeta-\delta-V(\lambda)}\,\frac{d\zeta}{2\pi i} \tag{3.5}$$

exists and is analytic in λ. Let us consider the following function:

$$\dim \operatorname{Ran} \oint_{\mathscr{C}_0} \frac{1}{\zeta-\delta-V(\lambda)}\,\frac{d\zeta}{2\pi i} \tag{3.6}$$

where the operator is restricted to the sector with $N=|\Lambda|$ particles. This function represents the number of eigenvalues in the sector $N=|\Lambda|$ lying inside the circle $\mathscr{C}_0$. Since this function is integer-valued and analytic for $|\lambda|$ small, it must be equal to one for all λ fulfilling (1.13) with $N=|\Lambda|$ and $n=0$. This concludes the proof of Theorem 2.

Proof of Theorem 3. Let us rewrite the two-point function as follows:

$$W(y-x)=\langle c_y e^R 0\,|\,c_x e^R 0\rangle\langle e^R 0\,|\,e^R 0\rangle^{-1} \tag{3.7}$$

Due to the fact that the product of any two ξ operators on the same site vanishes, we have

$$e^{R(\lambda)}=\prod_{n,\gamma}\,[1+\lambda^n r_n(\gamma)\,\xi_\gamma] \tag{3.8}$$

Hence

$$|W(y-x)| = \left|\sum \lambda^{n_1+n_2}\langle c_y r_{n_1}(\gamma_1)\,\xi_{\gamma_1} e^{R(\lambda)}0\,|\,c_x r_{n_1}(\gamma_2)\,\xi_{\gamma_2} e^{R(\lambda)}0\rangle\right|$$
$$\times\,|\langle e^{R(\lambda)}0\,|\,e^{R(\lambda)}0\rangle|^{-1}$$
$$\leqslant \sum |\lambda|^{n_1+n_2}\,|r_{n_1}(\gamma_1)|\,|r_{n_2}(\gamma_2)| \tag{3.9}$$

where the two sums run over all $n_1, n_2, \gamma_1, \gamma_2$, such that $y \in s(\gamma_1)$, $x \in s(\gamma)$, $s(\gamma_1) \cap s(\gamma_2) \neq 0$. In the last step we used a bound in norm for the operators $c_y \xi_{\gamma_1}$ and $c_x \xi_{\gamma_2}$. Thus, we find

$$|W(y-x)| \leqslant \left[\sum_{\substack{n \geqslant |x-y|/2 \\ \gamma}} |\lambda|^n \, |r_n(\gamma)| \right]^2 |a^d(\lambda)|$$
$$\leqslant \left| \frac{\lambda}{\rho_d - \varepsilon} \right|^{|x-y|} |a^d(\lambda)| \left[\sum_{\substack{n \geqslant |x-y|/2 \\ \gamma}} |\rho_d - \varepsilon|^n \, |r_n(\gamma)| \right]^2 \tag{3.10}$$

This proves Theorem 3. Note that one could have proven this theorem without using a bound in norm, but by a straightforward polymer expansion for the two-point function. However, I shall not discuss this point further here.

Proof of Theorem 4. We have

$$H_\lambda^{\text{ren}} P_{nN\lambda}^{\text{ren}} \xi_\gamma |0\rangle = H_\lambda^{\text{ren}} [P_{nN\lambda}^{\text{ren}}, \xi_\gamma] |0\rangle$$
$$= \{\delta[P_{nN\lambda}^{\text{ren}}, \xi_\gamma] + [V(\lambda), [P_{nN\lambda}^{\text{ren}}, \xi_\gamma]]\} |0\rangle$$

In virtue of the proof of Theorem 2, we can represent the projection $P_{nN\lambda}^{\text{ren}}$ with a convergent Rayleigh–Schrödinger expansion

$$P_{nN\lambda}^{\text{ren}} = \oint_{\mathscr{C}_n} \frac{d\zeta}{2\pi i} \sum_{n=0}^{\infty} [(\zeta - \delta)^{-1} V(\lambda)]^n (\zeta - \delta)^{-1} \tag{3.11}$$

We have

$$P_{nN\lambda}^{\text{ren}} \xi_\gamma |0\rangle = [P_{nN\lambda}^{\text{ren}}, \xi_\gamma] |0\rangle$$
$$= \sum_{k=0}^{\infty} \oint_{\mathscr{C}_n} \frac{d\zeta}{2\pi i \zeta} [(\zeta - \delta)^{-1} V(\lambda),..., [(\zeta - \delta)^{-1} V(\lambda), \xi_\gamma] \cdots] |0\rangle$$
$$= \left\{ \sum_{\substack{k=0,\infty \\ \gamma_0}} \lambda^k p_{nN\lambda}^{\text{ren}}(\gamma, \gamma_0; k) \, \xi_{\gamma_0} \right\} \xi_\gamma |0\rangle \tag{3.12}$$

where the series on the right-hand side converges and the coefficients $p_{nN\lambda}^{\text{ren}}(\gamma, \gamma_0; k)$ are nonzero only if $s(\gamma_0)$ is at a distance $\leqslant 2k$ from $s(\gamma)$. Relation (1.19) is an immediate consequence of this remark. To prove (1.20), it suffices to prove the exponential decay of the l^1-norm of the operators

$$Q(\lambda) = [P_{0,|\Lambda|-2,\lambda}^{\text{ren}}, \xi_x^{-1} \xi_y^{-1}] - [P_{0,|\Lambda|-1,\lambda}^{\text{ren}}, \xi_x^{-1}] \, \xi_y^{-1}$$
$$- [P_{0,|\Lambda|-1,\lambda}^{\text{ren}}, \xi_y^{-1}] \, \xi_x^{-1}$$

and

$$[V(\lambda), Q(\lambda)] \tag{3.13}$$

as $|x-y| \uparrow \infty$. But this follows from the cluster expansion (3.12), because from it we see that there is a convergent cluster expansion also for (3.13) with the first nonvanishing term of order $O(\lambda^{|x-y|})$ as $|x-y| \uparrow \infty$. QED

APPENDIX. THE HARTREE APPROXIMATION

The aim of this Appendix is to set up a strong coupling, i.e., small λ, expansion for the solutions of the eigenvalue problem

$$\begin{aligned} -\lambda\, \Delta u_\lambda - u_\lambda^3 &= \varepsilon_\lambda u_\lambda \\ u_\lambda \in l^2(\mathbb{Z}^d), \qquad \|u_\lambda\|_2 &= 1 \end{aligned} \tag{A.1}$$

The first result I prove is the following.

Theorem A.1. For every dimension $d \geqslant 1$, there is a $\lambda_d > 0$ such that Eq. (A.1) has a solution $(\varepsilon_\lambda, u_\lambda)$ for every $|\lambda| < \lambda_d$ $(\varepsilon_\lambda, u_\lambda)$ is analytic for $|\lambda| < \lambda_d$.

Proof. One can prove that $(\varepsilon_\lambda, u_\lambda)$ is a solution of (A.1) with $(\varepsilon_\lambda, u_\lambda)|_{\lambda=0} = (-1, \delta)$ if u_λ solves the initial value problem

$$\begin{aligned} \frac{du_\lambda}{d\lambda} &= [-\lambda\Delta - u_\lambda^2 - 2(1-P_{u_\lambda})\, u_\lambda^2 - \varepsilon_\lambda(u_\lambda)]^{-1}\, (1-P_{u_\lambda})\, \Delta u_x \\ u_\lambda|_{\lambda=0} &= \delta \end{aligned} \tag{A.2}$$

where

$$\varepsilon_\lambda(u_\lambda) \equiv (u_\lambda, (-\lambda\Delta + u_\lambda^2)\, u_\lambda) \tag{A.3}$$

In fact, if u_λ is a solution of (A.2), we have

$$[-\lambda\Delta - 3u_\lambda^2 - \varepsilon_\lambda(u_\lambda)]\, \frac{du_\lambda}{d\lambda} - \Delta u_\lambda = \alpha(\lambda)\, u_\lambda \tag{A.4}$$

where

$$\alpha(\lambda) = \left(u_\lambda, \left(2u_\lambda \frac{du_\lambda}{d\lambda} - \Delta\right) u_\lambda\right) = \frac{d}{d\lambda}\, \varepsilon_\lambda(u_\lambda) \tag{A.5}$$

Hence, we have

$$\frac{d}{d\lambda}\, (-\lambda\, \Delta u_\lambda - u_\lambda^3) = \frac{d}{d\lambda}\, (\varepsilon_\lambda(u_\lambda)\, u_\lambda) \tag{A.6}$$

From (A.6) it follows that $(\varepsilon_\lambda(u_\lambda), u_\lambda)$ solves (A.1). It remains to prove that (A.2) has a solution. The only fact to check is that the operator

$$[-\lambda\Delta - u_\lambda^2 - \varepsilon_\lambda(u_\lambda) - 2(1-P_{u_\lambda})\, u_\lambda^2]\,|_{(1-P_{u_\lambda})\, l^2(\mathbb{Z}^d)}$$

is invertible if u_λ is a solution of (A.1) and (λ, u_λ) is in a neighborhood of $(0, \delta)$. This can be seen by noticing that the operator $[-\lambda\Delta - u_\lambda^2 - \varepsilon_\lambda(u_\lambda)]$ is invertible in $(1-P_{u_\lambda})\, l^2(\mathbb{Z}^d)$ if u_λ is a solution of (A.1) with λ small and that the norm of $2(1-P_{u_\lambda})\, u_\lambda^2$ is small. QED

On the basis of this existence result, one can now make a digression on the spin-1/2 case and construct approximate solutions of the Hartree–Fock equations. Namely, one can do the following: Let $\chi: \mathbb{Z}^d \to \mathbb{C}^2$ be a spinor-valued function such that $\chi_x^* \chi_x = 1$, $\forall x \in \mathbb{Z}^d$, and introduce the spin orbitals

$$\psi_x^{\mathrm{H}}(\cdot) = \chi_x u_\lambda(\cdot - x) \tag{A.7}$$

where u_λ is a solution of (A.1) and H stands for Hartree. The wavefunctions (A.7) cannot be considered as an approximate HF solution because they are not mutually orthonormal. However, if one orthonormalizes them and computes the HF energy $\mathfrak{H}(\chi, \lambda)$, one finds a result independent of the orthonormalization process. We have

$$\varepsilon_\lambda = O(\lambda^4) \tag{A.8}$$

and

$$u_\lambda = \delta + \lambda\, \Delta\delta + \lambda^2(\Delta^2\delta - 3d\delta) + O(\lambda^3) \tag{A.9}$$

In this approximation, one can choose the approximate HF solution as follows:

$$\psi_x^{\mathrm{HF}}(y) = \begin{cases} \lambda[\chi_x - 2(\chi_y, \chi_x)\,\chi_y] + O(\lambda^3) & \text{if } |y-x| = 1,\ y \prec x \\ \chi_x(1-\lambda^2) + O(\lambda^4) & \text{if } y = x \\ \lambda\chi_x + O(\lambda^3) & \text{if } |y-x| = 1,\ y \succ x \\ O(\lambda^2) & \text{otherwise} \end{cases} \tag{A.10}$$

where $y \prec x$ ($\succ x$) means that $y_i \leqslant x_i$ ($\geqslant x_i$), $\forall i = 1,..., d$. The kinetic energy of ψ_x^{HF} is equal to

$$\mathscr{E}_{\mathrm{kin}}(\psi_x^{\mathrm{HF}}) = 2\lambda^2 \sum_{|y-x|=1} [2\,|(\chi_y, \chi_x)|^2 - 1] + O(\lambda^4) \tag{A.11}$$

while the contribution to the total energy coming from the exchange term relative to two electrons ψ_x^{HF} and ψ_y^{HF} sitting on neighboring sites is

$$J(\psi_x^{\mathrm{HF}}, \psi_y^{\mathrm{HF}}) = -2\lambda^2\,|(\chi_y, \chi_x)|^2 + O(\lambda^4) \tag{A.12}$$

Hence, the total energy corresponding to the spin configuration $\chi_.$ is given by

$$\mathfrak{H}(\chi, \lambda) = \sum_{\langle xy \rangle} 2\lambda^2 |(\chi_x, \chi_y)|^2 + O(\lambda^4) + \text{const} \tag{A.13}$$

The classical Hamiltonian (A.13) is equal to the expectation value in the state $\bigotimes_{x \in \mathbb{Z}^d} \chi_x$ of the quantum Heisenberg Hamiltonian

$$H(\lambda) = \sum_{\langle xy \rangle} 4\lambda^2 \left(\mathbf{s}_x \cdot \mathbf{s}_y + \frac{1}{4} \right) + O(\lambda^4) + \text{const} \tag{A.14}$$

This is consistent with the formal perturbative result of Anderson.[8] Thus, one can conclude that the approximation scheme above which starts by neglecting the spin and solving the Hartree equations and then incorporates the spin in such a way as to fulfill the orthonormality conditions gives a result which is correct at the first nonvanishing order of perturbation theory.

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