Exact Eigenstates for Contact Interactions

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We show that in $d \geqslant 2$ dimensions the N-particle kinetic energy operator with periodic boundary conditions has symmetric eigenfunctions which vanish at particle encounters, and give a full description of these functions. In two and three dimensions they represent common eigenstates of bosonic Hamiltonians with any kind of contact interactions, and illustrate a partial "multi-dimensional Bethe Ansatz" or "quantum KAM theorem." The lattice analogs of these functions exist for $N \leqslant L^{[d/2]}$ where L is the linear size of the box, and are common eigenstates of Bose–Hubbard Hamiltonians and spin-$\frac{1}{2}$ XXZ Heisenberg models.

1. INTRODUCTION

In this paper we construct eigenstates to Hamiltonians of the form

$$H_N = -\sum_{i=1}^{N} \Delta_i + V(\mathbf{r}_1, ..., \mathbf{r}_N) - \mu N \tag{1}$$

$$V(\mathbf{r}_1, ..., \mathbf{r}_N) = 0 \qquad \text{if all } \mathbf{r}_i \text{ are different,}$$

that is, Hamiltonians with real symmetric contact interactions. The definition of such operators with the use of Dirac deltas is straightforward in one dimension and leads to integrable systems.[1] In higher dimensions the mere definition becomes mathematically tricky. The two- and three-dimensional realization of (1) needs renormalization to zero of the interaction strength,[2] while in four dimensions and above the family (1) reduces

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to a unique element with $V \equiv 0$, i.e., the kinetic energy operator (ref. 3, Theorem X.11). One can gain an impression about how this conclusion emerges by observing that the existence of contact interactions is closely related to the existence of a Green's function for the Laplacian, i.e., an L^2-solution $G_z(\cdot - \mathbf{r}')$ of the inhomogeneous equation

$$(-\Delta_{\mathbf{r}} - z) G_z(\mathbf{r} - \mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}') \tag{2}$$

for any complex (non-real) z. Any Hamiltonian with a contact interaction is a self-adjoint extension of the N-particle Laplacian defined on C^∞-functions whose support avoids the set $\{\mathbf{r}_i = \mathbf{r}_j, i \neq j\}$. This symmetric operator must have non-vanishing deficiency indices, i.e., its adjoint must have eigenstates with complex eigenvalues. For two particles, these eigenstates are the Green's functions for complex values of z. If an L^2-solution exists for Eq. (2), it has a Fourier representation

$$G_z(\mathbf{r} - \mathbf{r}') = \frac{1}{(2\pi)^d} \int \frac{e^{i\mathbf{p}(\mathbf{r} - \mathbf{r}')}}{\mathbf{p}^2 - z} \, d\mathbf{p}. \tag{3}$$

In one dimension this integral is convergent for any $\mathbf{r} - \mathbf{r}'$ and yields a bounded continuous function. In two and three dimensions $\int |\mathbf{p}^2 - z|^{-2} \, d\mathbf{p}$ is finite. Therefore, by Plancherel's theorem, $(\mathbf{p}^2 - z)^{-1}$ is the Fourier transform of an L^2-function which, however, diverges at $\mathbf{r} = \mathbf{r}'$ as $\ln |\mathbf{r} - \mathbf{r}'|$ and $|\mathbf{r} - \mathbf{r}'|^{-1}$, respectively. In four dimensions and above $\int |\mathbf{p}^2 - z|^{-2} \, d\mathbf{p} = \infty$ and, thus, (2) has no square-integrable solution. Now by separating off the motion of the center of mass, the two-body problem with a δ-interaction can be reduced to a one-body problem in a potential $\alpha\delta$. Multiplication of a suitable function f with $\alpha\delta$ has to be interpreted as $\alpha\langle\delta, f\rangle\delta$, where $\langle\delta, \cdot\rangle$ denotes the action of the linear functional δ. If we want to define $A = -\Delta + \alpha\langle\delta, \cdot\rangle\delta$ as a self-adjoint operator on $L^2(\mathbb{R}^d)$, we have to restrict it to functions $\psi \in L^2$ such that $A\psi$ is also in L^2 and $(\psi, A\psi)$ is real. So $A\psi$ cannot contain a δ, and this is why G_z has to be included in ψ. Actually $z = i$ suffices, and a straightforward computation yields that a general ψ in the domain of A is of the form

$$\psi(\mathbf{r}) = \tilde{\psi}(\mathbf{r}) + a\tilde{\psi}(0) \, \text{Re} \, G_i(\mathbf{r}) \tag{4}$$

with

$$a = -\frac{\alpha}{1 + \alpha\langle\delta, \text{Re} \, G_i\rangle} \tag{5}$$

and then

$$A\psi = -\Delta\tilde{\psi} + a\tilde{\psi}(0) \operatorname{Re} iG_i. \tag{6}$$

Here $\tilde{\psi}$ is any vector from the domain of the kinetic energy $-\Delta$. The problem appears in the denominator of a, with $\langle\delta, \operatorname{Re} G_i\rangle$. This is well-defined in one dimension and yields $\operatorname{Re} G_i(0) = \frac{1}{2\sqrt{2}}$. In dimensions two and three δ is not defined on $\operatorname{Re} G_i$. One can proceed at least in two different ways. One may define δ so that it does not feel the singularity of G_i and set $\langle\delta, \operatorname{Re} G_i\rangle = c$. Then different constants yield different operators, e.g., $c = \infty$ gives $A = -\Delta$. This more recent method was followed in ref. 4. The original procedure of ref. 2 replaced δ by a sequence δ_n of regular approximants and α by α_n. When $\delta_n \to \delta$, $\langle\delta_n, \operatorname{Re} G_i\rangle \to \infty$. In order to obtain a nonvanishing limit for a, α_n then has to go to zero; otherwise we get back the kinetic energy operator.

The general, N-particle case is much more involved since it requires considering multiple collisions and operators with infinite deficiency indices. The crucial question is to find the physically meaningful (lower semibounded) self-adjoint extensions. For this purpose generalized contact interactions have to be introduced.[5, 7] For an exhaustive mathematical treatment the reader can consult the monographs[6, 7] which also contain a detailed bibliography of the abundant mathematical and physical literature. As an example from the latter, we mention the use of contact interactions as "Fermi pseudopotentials" for an approximate treatment of the hard-core Bose gas.[8] They also appear in connection with the Laughlin wavefunction[9] and the trapped boson gas,[10, 11] in which case the ground state of the projected (to the lowest oscillator level) Hamiltonian for fixed non-vanishing angular momenta was found. Projection to the lowest oscillator level has a regularizing effect on the interaction, which is however not sufficient to settle all problems of definition. To avoid the lower unboundedness of the projected Hamiltonian and to make sure that the ground state energy does not *decrease* with an increasing angular momentum, the interaction strength still has to decrease as $1/N$ with the number of particles, see Eqs. (4) and (5) of ref. 10. We note that apparently all existing mathematical results concern systems of particles in infinite space, and cannot but anticipate the extension of these results to confined systems.

We are interested in the construction of eigenstates to the Hamiltonians (1) for the following reason. The delta-gas in one dimension is an integrable system, and we would like to see whether in two and three dimensions it preserves some trace of integrability. A partial survival of integrability could be viewed either as a remnant of the Bethe Ansatz when

the dimensionality is increased or as a germ of a quantum-KAM theorem when, in the free Bose-gas, a contact interaction is switched on. The Bethe Ansatz solution of the one-dimensional delta-gas assigns N wave numbers to each eigenfunction. The two and three dimensional analogy would be the existence of eigenstates which can be expressed in terms of finitely many wave vectors. From the point of view of the KAM theory, surviving, maybe slightly distorted, free-particle eigenstates would correspond to classical KAM tori.[12] What we actually find are eigenstates of N bosons in a box of linear size L which remain unperturbed by contact interactions, are characterized by $2N$ wave vectors and have an energy at least of order N^3/L^2.

A common feature of the operators (1) is that, on smooth functions which vanish at particle encounters, all act as the pure kinetic energy operator. Therefore, if this latter has eigenstates vanishing whenever $\mathbf{r}_i = \mathbf{r}_j$ for some $i \neq j$, these will be common eigenstates of all members of the family (1). For two particles in two dimensions it is very easy to give examples. Probably the simplest of them are

$$\sin\frac{2n\pi}{L}(x_1 - x_2)\sin\frac{2m\pi}{L}(y_1 - y_2) \text{ and } \cos\frac{2n\pi}{L}(x_1 - x_2) - \cos\frac{2n\pi}{L}(y_1 - y_2).$$

We will show that such eigenstates exist for any $N \geqslant 2$ in any dimension $d \geqslant 2$ and will find all of them for a system of bosons confined in a $L \times \cdots \times L$ torus Λ. That is, we will describe all N-particle eigenstates $\psi(\mathbf{r}_1,\ldots,\mathbf{r}_N)$ of the $d \geqslant 2$-dimensional kinetic energy operator with the following properties: (P1) ψ is *L-periodic separately in each of the dN coordinates*, (P2) ψ is *a symmetric function of* $\mathbf{r}_1,\ldots,\mathbf{r}_N$, and (P3) $\psi(\ldots,\mathbf{r},\ldots,\mathbf{r},\ldots) \equiv 0$. To satisfy (P2) and (P3) at the same time, a very large number of degenerate free-particle eigenstates will have to be combined. This becomes possible because the kinetic energy operator is unbounded and so is the degeneracy of the eigensubspaces. On the other hand, this explains why the energy of these states must increase so fast with N. As the proof of Theorem 2 will show, an interesting interpretation can be given to these functions: they can be considered as stationary states of N impenetrable bosons on the d-torus which interact with each other through elastic collisions, see Eqs. (19) and (25) later. If $\psi_1, \psi_2,\ldots$ is an orthonormal basis for (P1)–(P3) eigenstates with corresponding energy eigenvalues $E_1 \leqslant E_2 \leqslant \cdots$, we can define a self-adjoint operator

$$H_{\text{elastic}} = \sum_{i=1}^{\infty} E_i \, |\psi_i\rangle\langle\psi_i| \tag{7}$$

which, hence, is associated to such a system. Also, every member of the family (1) can be decomposed as $H_N = H'_N + H_{elastic}$, with H'_N depending on the interaction and living on the orthogonal complement of the subspace of (P1)–(P3) eigenstates.

The problem in continuous space, that we have discussed above, will be presented in Section 2. In Section 3 we separately treat the lattice case. We shall consider only hypercubic lattices. The analog of (1) is obtained by interpreting Δ_i as the lattice Laplacian. In lattices contact interactions mean on-site interactions which exist in any dimension and define the so-called Bose–Hubbard Hamiltonians. Incidentally, we shall obtain common exact eigenstates in any dimension $d \geqslant 2$ for a larger family of Hamiltonians,

$$H_{lattice} = \pm \sum_{\langle \mathbf{rr}' \rangle} (a^*_{\mathbf{r}'} - a^*_{\mathbf{r}})(a_{\mathbf{r}'} - a_{\mathbf{r}}) + \sum_{\mathbf{r}} f_{\mathbf{r}}(n_{\mathbf{r}}) - \mu \sum_{\mathbf{r}} n_{\mathbf{r}}$$
$$+ \sum_{i=1}^{d} \sum_{(\mathbf{r}-\mathbf{r}') \| \mathbf{e}_i} f_{\mathbf{r},\mathbf{r}'}(n_{\mathbf{r}}, n_{\mathbf{r}'}). \tag{8}$$

In the first term the summation goes over nearest neighbor pairs, $a^*_{\mathbf{r}}$ and $a_{\mathbf{r}}$ create, resp., annihilate a boson at site $\mathbf{r}$, $n_{\mathbf{r}} = a^*_{\mathbf{r}} a_{\mathbf{r}}$, $\mathbf{e}_i$ is the unit vector along the ith coordinate axis, μ is the chemical potential and $f_{\mathbf{r}}$ and $f_{\mathbf{r},\mathbf{r}'}$ are real functions with $f_{\mathbf{r}}(n) = 0$ if $n = 0, 1$ and $f_{\mathbf{r},\mathbf{r}'}(m, n) = 0$ if $mn = 0$. Among others, every spin-$\frac{1}{2}$ nearest-neighbor XXZ Heisenberg model, including the planar and the ferro- and antiferromagnetic isotropic models, is a member of this family (with $f_{\mathbf{r}}(t) = +\infty$ if $t \geqslant 2$). However, there are two limitations in the lattice case that we do not meet in the continuous one. First, the condition for finding the eigenstates is a set of transcendental Diophantine equations, in contrast with the algebraic ones in the continuous space version. We find *some* solutions but cannot pretend to find all. Second, the solutions we find are only for $N \leqslant L^{[d/2]}$ where $[\cdot]$ means integer part, and this seems to be an intrinsic limitation, due to the boundedness of $H_{lattice}$. In hard-core models, particle-hole transformation yields eigenstates also for $N \geqslant |A| - L^{[d/2]}$.

Finally, we note that both in the continuum and on lattices there is a family of exact eigenstates whose energy tends to zero as the volume increases. In two and three dimensions these states may contain $N = o(L^{2/3})$ particles. They correspond to gapless excitations above the grand canonical ground state if this latter belongs to $N = 0$ and, thus, has zero energy. This is the case, e.g., if the interaction is repulsive and the chemical potential is zero or negative (and we take the plus sign in (8)), but may also occur with attractive interactions, as in the isotropic Heisenberg ferromagnet.

2. BOSONS IN CONTINUOUS SPACE

2.1. Theorems and Proofs

For spinless fermions all states share the property (P3). This observation is the starting point of the construction of such eigenstates for (spinless) bosons in more than one dimension.

We introduce the short-hands $\mathbf{R} = (\mathbf{r}_1,...,\mathbf{r}_N)$ and $\mathbf{K} = (\mathbf{k}_1,...,\mathbf{k}_N)$. A pair $\mathbf{K}, \mathbf{K}'$ will be called *allowed* if both sets contain N different vectors and for any i and j, $\mathbf{k}_i + \mathbf{k}'_j$ is in $A^d \equiv (2\pi/L)\, Z^d$, where Z^d denotes the set of d-dimensional integers. We have the following.

Lemma 1. A pair $\mathbf{K}, \mathbf{K}'$ is allowed if and only if both sets contain N different vectors, and there exist d-dimensional integers $\mathbf{n}_i$, $\mathbf{n}'_i$ and a (complex) vector ξ such that $\mathbf{k}_i = (2\pi/L)\, \mathbf{n}_i + \xi$ and $\mathbf{k}'_i = (2\pi/L)\, \mathbf{n}'_i - \xi$ for every i.

If both $\mathbf{K}$ and $\mathbf{K}'$ contain N different vectors of the above form, the pair is clearly allowed. On the other hand, if the pair $\mathbf{K}, \mathbf{K}'$ is allowed, choose, e.g., $\xi = \mathbf{k}_1$. Then $\mathbf{k}'_i + \xi = \mathbf{k}_1 + \mathbf{k}'_i$ is in A^d for every i and $\mathbf{k}_i - \xi = (\mathbf{k}_i + \mathbf{k}'_1) - (\mathbf{k}'_1 + \mathbf{k}_1)$ is also in the Abelian group A^d for every i.

Let us consider the product of two Slater determinants,

$$\psi_{\mathbf{K}, \mathbf{K}'}(\mathbf{R}) = \det[e^{i\mathbf{k}_l \mathbf{r}_m}]\, \det[e^{i\mathbf{k}'_l \mathbf{r}_m}] = \sum_{\pi, \pi' \in S_N} (-)^\pi\, (-)^{\pi'}\, e^{i\sum_{j=1}^N (\mathbf{k}_{\pi(j)} + \mathbf{k}'_{\pi'(j)})\, \mathbf{r}_j}. \quad (9)$$

For any allowed pair $\mathbf{K}, \mathbf{K}'$, $\psi_{\mathbf{K}, \mathbf{K}'}$ has the properties (P1)–(P3). It is also an eigenstate of $-\sum \Delta_i$, provided that $\mathbf{k}_i \cdot \mathbf{k}'_j = 0$ for any i, j, a condition which can be satisfied above one dimension: Since $\sum_i (\mathbf{k}_{\pi(i)} + \mathbf{k}'_{\pi'(i)})^2 = \sum_i (\mathbf{k}_i + \mathbf{k}'_{\pi'\pi^{-1}(i)})^2$, the $(N!)^2$ plane waves in (9) may belong to at most $N!$ different eigenvalues. Thus, $\psi_{\mathbf{K}, \mathbf{K}'}$ is an eigenstate if $\sum_i (\mathbf{k}_i + \mathbf{k}'_{\pi(i)})^2 = \sum_i (\mathbf{k}_i + \mathbf{k}'_i)^2$ or, equivalently,

$$\sum_{i=1}^N \mathbf{k}_i \cdot \mathbf{k}'_{\pi(i)} = \sum_{i=1}^N \mathbf{k}_i \cdot \mathbf{k}'_i \quad (10)$$

for all permutations $\pi \in S_N$, which trivially holds if every $\mathbf{k}_i$ is orthogonal to every $\mathbf{k}'_j$. The following theorem suggests that there can be a huge redundancy in these equations. It extends the above example to further eigenstates and shows that for $\mathbf{K}$ and $\mathbf{K}'$ it suffices to satisfy only $(N-1)^2$ equations.

Below we use the notation $(i_1 i_2 \cdots i_m)$ for the cyclic permutation carrying i_1 into i_2, etc., i_m into i_1.

Theorem 1. Let $\mathbf{K}$, $\mathbf{K}'$ be an allowed pair. The following assertions are equivalent.

(i) Equation (10) holds for $\pi = (j\ j+1)$ with $1 \leqslant j \leqslant N-1$, for $\pi = (j\ j+1\ j+2)$ and $(j\ j+2\ j+1)$ with $1 \leqslant j \leqslant N-2$ and for $\pi = (j\ l\ j+1\ l+1)$ and $(j\ l+1\ j+1\ l)$ with $1 < j+1 < l < N$.

(ii)

$$(\mathbf{k}_{j+1} - \mathbf{k}_j) \cdot (\mathbf{k}'_{l+1} - \mathbf{k}'_l) = 0, \qquad 1 \leqslant j, l \leqslant N-1. \tag{11}$$

(iii) Equation (10) holds true for all permutations. As a consequence, $\psi_{\mathbf{K}, \mathbf{K}'}$ is an eigenstate of the kinetic energy belonging to the eigenvalue $\sum (\mathbf{k}_i + \mathbf{k}'_i)^2$ whose degeneracy is at least $(N!)^2$: $\psi_{\mathbf{K}, \mathbf{K}'}$ is the linear combination of $(N!)^2$ different, pairwise orthogonal, N-particle plane waves. Furthermore, each occurring plane wave is associated with N different wave vectors chosen from $\{\mathbf{k}_i + \mathbf{k}'_j\}_{i,j=1}^{N}$ whose all the N^2 elements are different.

Since (iii) obviously implies (i), it suffices to show that (ii) follows from (i) and implies (iii).

(i) $\Rightarrow$ (ii). Observe that we impose (10) for $(N-1)^2$ different permutations, and this is just the number of Eqs. (11) we want to prove. Writing (10) for $\pi = (j\ j+1)$ we immediately obtain $(\mathbf{k}_{j+1} - \mathbf{k}_j) \cdot (\mathbf{k}'_{j+1} - \mathbf{k}'_j) = 0$. If E_π denotes the Eq. (10) then $E_{(j\ j+1\ j+2)} - E_{(j\ j+1)} - E_{(j+1\ j+2)}$ yields $(\mathbf{k}_{j+2} - \mathbf{k}_{j+1}) \cdot (\mathbf{k}'_{j+1} - \mathbf{k}'_j) = 0$ and $E_{(j\ j+2\ j+1)} - E_{(j\ j+1)} - E_{(j+1\ j+2)}$ yields $(\mathbf{k}_{j+1} - \mathbf{k}_j) \cdot (\mathbf{k}'_{j+2} - \mathbf{k}'_{j+1}) = 0$. Moreover, $E_{(j\ l\ j+1\ l+1)} - E_{(j\ l)} - E_{(j+1\ l+1)}$ is equivalent with $(\mathbf{k}_{l+1} - \mathbf{k}_l) \cdot (\mathbf{k}'_{j+1} - \mathbf{k}'_j) = 0$ from which the last equation follows by interchanging j and l.

(ii) $\Rightarrow$ (iii). First, we note that (11) implies $(\mathbf{k}_j - \mathbf{k}_l) \cdot (\mathbf{k}'_m - \mathbf{k}'_n) = 0$ for all j, l, m, n. If $\pi = (j\ l)$, (10) is equivalent with $(\mathbf{k}_j - \mathbf{k}_l) \cdot (\mathbf{k}'_j - \mathbf{k}'_l) = 0$. For a general π different from the identity we write down the Eq. (10) for π and for π^{-1} (which may be the same) and rearrange them as $\sum \mathbf{k}_i \cdot (\mathbf{k}'_{\pi(i)} - \mathbf{k}'_i) = 0$ and $\sum \mathbf{k}_{\pi(i)} \cdot (\mathbf{k}'_i - \mathbf{k}'_{\pi(i)}) = 0$, respectively. The sum of them yields $\sum (\mathbf{k}_i - \mathbf{k}_{\pi(i)}) \cdot (\mathbf{k}'_{\pi(i)} - \mathbf{k}'_i) = 0$ which holds because each term separately vanishes. The difference gives $\sum (\mathbf{k}_i + \mathbf{k}_{\pi(i)}) \cdot (\mathbf{k}'_{\pi(i)} - \mathbf{k}'_i) = 0$ from which we subtract $2\mathbf{k}_1 \cdot \sum (\mathbf{k}'_{\pi(i)} - \mathbf{k}'_i) = 0$. Again, the resulting equation holds because each term equals zero. It remains to show that in $\psi_{\mathbf{K}, \mathbf{K}'}$ there are $(N!)^2$ different plane waves and in each of them N different wave vectors. For this we note that all the N^2 wave vectors $\mathbf{k}_i + \mathbf{k}'_j$ are different: $\mathbf{k}_i + \mathbf{k}'_j = \mathbf{k}_l + \mathbf{k}'_m$ with $(i, j) \neq (l, m)$ would be in conflict with (11). Now the coincidence of two plane waves would mean $\mathbf{k}_{\pi_1(i)} + \mathbf{k}'_{\pi'_1(i)} = \mathbf{k}_{\pi_2(i)} + \mathbf{k}'_{\pi'_2(i)}$

for $\pi_1 \neq \pi_2$, $\pi_1' \neq \pi_2'$ and for all i, which is impossible; nor can we have $\mathbf{k}_i + \mathbf{k}_{\pi(i)}' = \mathbf{k}_j + \mathbf{k}_{\pi(j)}'$ unless $i = j$. This ends the proof.

Let us remark that (11) is equivalent with

$$\epsilon(\mathbf{k}_j + \mathbf{k}_l') + \epsilon(\mathbf{k}_{j+1} + \mathbf{k}_{l+1}') = \epsilon(\mathbf{k}_j + \mathbf{k}_{l+1}') + \epsilon(\mathbf{k}_{j+1} + \mathbf{k}_l') \tag{12}$$

where $\epsilon(\mathbf{p})$ is the one-particle energy, $\mathbf{p}^2$. That is, the two-particle energy is conserved during an elastic collision of two particles, see also later.

The general solution of (11) can easily be obtained. The vectors $\mathbf{k}_{i+1} - \mathbf{k}_i$ and $\mathbf{k}_{j+1}' - \mathbf{k}_j'$ must be in different, orthogonal, subspaces of $\mathbf{R}^d$. One vector from each set, for example $\mathbf{k}_1$ and $\mathbf{k}_1'$, can be arbitrarily chosen from $\mathbf{A}^d$. In two dimensions both subspaces are one-dimensional and we have

$$\mathbf{k}_i = \mathbf{k}_1 + \frac{2\pi}{L} p_i(l_0, m_0), \qquad \mathbf{k}_i' = \mathbf{k}_1' + \frac{2\pi}{L} p_i'(m_0, -l_0) \quad (i = 2,..., N). \tag{13}$$

Here l_0 and m_0 are integers at least one of which is different from zero, $p_2,..., p_N$ are different nonzero integers and the same holds for $p_2',..., p_N'$. In three dimensions one of the subspaces is one-, the other is two-dimensional. Without restricting generality we may suppose that $\mathbf{k}_j - \mathbf{k}_i$ are in a one-dimensional subspace. Let $\mathbf{n}_0$ be any nonzero integer vector. Since the subspace orthogonal to $\mathbf{n}_0$ has an infinite intersection with $\mathbf{Z}^3$, there is no problem to choose the vectors of $\mathbf{K}'$. So we have

$$\mathbf{k}_i = \mathbf{k}_1 + \frac{2\pi}{L} p_i \mathbf{n}_0, \qquad \mathbf{k}_i' = \mathbf{k}_1' + \frac{2\pi}{L} \mathbf{n}_i' \quad (i = 2,..., N), \tag{14}$$

where p_i are different nonzero integers and $\mathbf{n}_i'$ are different nonzero integer vectors orthogonal to $\mathbf{n}_0$.

A complex vector ξ (the same one which has appeared in Lemma 1) can be added to $\mathbf{k}_1$ and subtracted from $\mathbf{k}_1'$ without changing the eigenvalue or the eigenfunction: it is a kind of gauge variable which affects only the decomposition of $\psi_{\mathbf{K}, \mathbf{K}'}$ in the product of two determinants.

We note that the two examples given in the Introduction correspond to $\psi_{\mathbf{K}, \mathbf{K}'}$ with $\mathbf{K} = \pm\frac{2\pi}{L}(n, 0)$, $\mathbf{K}' = \pm\frac{2\pi}{L}(0, m)$ and $\mathbf{K} = \pm\frac{\pi}{L}(n, n)$, $\mathbf{K}' = \pm\frac{\pi}{L}(n, -n)$, respectively.

The question naturally arises whether with Theorem 1 we have described all the eigenstates of the kinetic energy operator satisfying (P1)–(P3). For the moment we cannot even exclude the existence of other eigenstates $\psi_{\mathbf{K}, \mathbf{K}'}$ which do not fall under the authority of Theorem 1. For a general $\psi_{\mathbf{K}, \mathbf{K}'}$ with an allowed pair $\mathbf{K}, \mathbf{K}'$, some elements of $\{\mathbf{k}_i + \mathbf{k}_j'\}_{i, j}$

may coincide and, thus, the number of different wave vectors can be less than N^2. This may also imply that, by cancellation, the number of different N-particle plane waves contributing to $\psi_{\mathbf{K},\mathbf{K}'}$ is less than $(N!)^2$. (Cancellation occurs if $\{\mathbf{k}_i + \mathbf{k}'_{\alpha(i)}\}_{i=1}^N = \{\mathbf{k}_i + \mathbf{k}'_{\beta(i)}\}_{i=1}^N$ for two permutations α and β of different parity. It is easily verified that for $N = 2$ and 3 this is not possible but can take place for $N \geqslant 4$. An example for $d = 2$ and $N = 4$ is $\mathbf{K} = \frac{2\pi}{L}((0,-1), (1,0), (0,1), (-1,0))$ and $\mathbf{K}' = \frac{2\pi}{L}((-2,1), (1,1), (-1,0), (0,0))$ with $\alpha = (2\ 4)$ and $\beta = (1\ 2)(3\ 4)$.) As a consequence, some of the Eqs. (10) could not be satisfied but $\psi_{\mathbf{K},\mathbf{K}'}$ still could be an eigenstate. In the following, we exclude this and all other possibilities.

Theorem 2. For $d > 1$, among the eigenstates of the kinetic energy which satisfy the conditions (P1)–(P3) those described in Theorem 1 provide a basis. In one dimension such eigenstates do not exist.

To begin the proof, we note that an eigenstate of the kinetic energy satisfying (P1) and (P2) is a finite linear combination of symmetrized plane waves,

$$\psi(\mathbf{R}) = \sum_{\alpha \in I} a_\alpha \psi_{\mathbf{P}^\alpha}^+(\mathbf{R}). \tag{15}$$

In this expression α goes over some index set I, $\mathbf{P}^\alpha = (\mathbf{p}_1^\alpha, ..., \mathbf{p}_N^\alpha)$,

$$\psi_{\mathbf{P}^\alpha}^+(\mathbf{R}) = \sum_{\pi \in S_N} e^{i \sum_j \mathbf{p}_{\pi(j)}^\alpha \mathbf{r}_j} \tag{16}$$

and, for each α, all $\mathbf{p}_i^\alpha$ are in A^d and $\sum_i (\mathbf{p}_i^\alpha)^2$ is independent of α. If a_α are complex, $\psi = \psi_{\mathrm{Re}} + i\psi_{\mathrm{Im}}$ where $\psi_{\mathrm{Re}} = \sum_{\alpha \in I} (\mathrm{Re}\, a_\alpha)\, \psi_{\mathbf{P}^\alpha}^+$ and $\psi_{\mathrm{Im}} = \sum_{\alpha \in I} (\mathrm{Im}\, a_\alpha)\, \psi_{\mathbf{P}^\alpha}^+$. It is easily seen that (P3) holds for ψ if and only if it holds both for ψ_{Re} and ψ_{Im}. Therefore, when looking for a basis among (P1)–(P3) eigenstates, we can limit our considerations to functions (15) with real coefficients. To further specialize our choice of a basis, we need the notion of minimality. When writing (15), we understand that all the possible contractions in ψ have been made, so that $a_\alpha \neq 0$ if $\alpha \in I$ and the sets $\{\mathbf{p}_i^\alpha\}_{i=1}^N$ are different for different α (but may overlap with each other). We call the orthogonal set $\{\psi_{\mathbf{P}^\alpha}^+\}_{\alpha \in I}$ of (P1), (P2) eigenstates, all belonging to the same energy, the *support* of ψ and denote it by $\mathrm{supp}\,\psi$. A (P1)–(P3) eigenstate will be called a *minimal function* if it is the unique (P1)–(P3) eigenfunction (apart from a constant multiplier) in the linear span of its own support.

It will suffice to study only minimal functions because of the following.

Lemma 2. Among the (P1)–(P3) eigenstates there exists a basis formed by minimal functions.

Suppose that ϕ is a non-minimal (P1)–(P3)-eigenfunction. It is enough to show that it can be decomposed as $\phi = a\phi_1 + b\phi_2$ where ϕ_1 and ϕ_2 are (P1)–(P3)-eigenfunctions whose support is strictly smaller than that of ϕ. Then, if ϕ_i is not minimal, it can be decomposed in the same manner as ϕ and, in a finite number of steps, we arrive at an expression of ϕ as a sum of minimal functions. Now, because $\phi = \sum_{\alpha \in I} a_\alpha \psi_{\mathbf{P}^\alpha}^+$ is not minimal, its support spans an at least two-dimensional subspace of (P3)-eigenstates. Take here a $\phi' = \sum_{\alpha \in I} b_\alpha \psi_{\mathbf{P}^\alpha}^+$ which is linearly independent of ϕ (and may have vanishing coefficients). Choose a β such that $b_\beta \neq 0$ and define $\phi_1 = \phi - \frac{a_\beta}{b_\beta} \phi'$. Take a $\gamma \neq \beta$ and define $\phi_2 = \phi' - \frac{b_\gamma}{a_\gamma} \phi$. Then

$$\phi = \left(1 - \frac{a_\beta b_\gamma}{a_\gamma b_\beta}\right)^{-1} \phi_1 + \left(\frac{b_\beta}{a_\beta} - \frac{b_\gamma}{a_\gamma}\right)^{-1} \phi_2 \tag{17}$$

is the decomposition we were looking for.

From now on, we shall suppose that ψ also satisfies (P3) and is minimal. We are going to prove that *the minimal functions are precisely the eigenstates described in Theorem 1.*

First we consider $N = 2$. The simplest (P1)–(P3)-eigenstates are of the form

$$\psi(\mathbf{r}_1, \mathbf{r}_2) = e^{i(\mathbf{p}_1\mathbf{r}_1 + \mathbf{p}_2\mathbf{r}_2)} + e^{i(\mathbf{p}_2\mathbf{r}_1 + \mathbf{p}_1\mathbf{r}_2)} - e^{i(\mathbf{q}_1\mathbf{r}_1 + \mathbf{q}_2\mathbf{r}_2)} - e^{i(\mathbf{q}_2\mathbf{r}_1 + \mathbf{q}_1\mathbf{r}_2)}$$

$$= \psi_{\mathbf{P}}^+(\mathbf{r}_1, \mathbf{r}_2) - \psi_{\mathbf{Q}}^+(\mathbf{r}_1, \mathbf{r}_2) \tag{18}$$

where $\mathbf{p}_1, \mathbf{p}_2, \mathbf{q}_1, \mathbf{q}_2 \in A^d$ and

$$\mathbf{p}_1 + \mathbf{p}_2 = \mathbf{q}_1 + \mathbf{q}_2, \qquad \mathbf{p}_1^2 + \mathbf{p}_2^2 = \mathbf{q}_1^2 + \mathbf{q}_2^2 \tag{19}$$

or equivalently,

$$\mathbf{p}_1 + \mathbf{p}_2 = \mathbf{q}_1 + \mathbf{q}_2, \qquad \mathbf{p}_1 \cdot \mathbf{p}_2 = \mathbf{q}_1 \cdot \mathbf{q}_2. \tag{20}$$

These eigenstates are certainly minimal, because a (P3)-eigenstate must contain at least two symmetrized plane waves.

In any dimension Eqs. (19) have trivial solutions, $\mathbf{p}_1 = \mathbf{q}_1$ and $\mathbf{p}_2 = \mathbf{q}_2$ with $\mathbf{p}_i \in A^d$ arbitrary, which are useless because they yield $\psi(\mathbf{r}_1, \mathbf{r}_2) \equiv 0$. Thus, we must impose $\{\mathbf{p}_1, \mathbf{p}_2\} \cap \{\mathbf{q}_1, \mathbf{q}_2\} = \varnothing$, since an overlap would imply coincidence of the two sets. Moreover, if $\mathbf{p}_1 = \mathbf{p}_2 = \mathbf{p}$ then

$\mathbf{q}_1 = \mathbf{q}_2 = \mathbf{p}$, a solution already discarded. Hence, in any nontrivial solution of (19), $\mathbf{p}_1$, $\mathbf{p}_2$, $\mathbf{q}_1$ and $\mathbf{q}_2$ are four different vectors.

In one dimension, if any of the four numbers is zero, we obtain a trivial solution. In the opposite case $q_2 = p_1 p_2 / q_1$. This we insert in the first of Eqs. (19) to find $(p_1 - q_1)(q_1 - p_2) = 0$ which, again, leads to a trivial solution.

For $d > 1$ let $\mathbf{p}_1$, $\mathbf{p}_2$, $\mathbf{q}_1$ and $\mathbf{q}_2$ be any nontrivial solution of Eqs. (20). Choose an arbitrary vector $\mathbf{k}_2'$ and introduce $\mathbf{k}_1 = \mathbf{q}_1 - \mathbf{k}_2'$, $\mathbf{k}_2 = \mathbf{p}_2 - \mathbf{k}_2'$ and $\mathbf{k}_1' = \mathbf{p}_1 - \mathbf{q}_1 + \mathbf{k}_2'$. Then $\mathbf{k}_1 \neq \mathbf{k}_2$ and $\mathbf{k}_1' \neq \mathbf{k}_2'$. The original vectors can be written in the form $\mathbf{p}_1 = \mathbf{k}_1 + \mathbf{k}_1'$, $\mathbf{p}_2 = \mathbf{k}_2 + \mathbf{k}_2'$, $\mathbf{q}_1 = \mathbf{k}_1 + \mathbf{k}_2'$ and, because of the first of Eqs. (20), $\mathbf{q}_2 = \mathbf{k}_2 + \mathbf{k}_1'$. Furthermore, (20) implies $(\mathbf{k}_2 - \mathbf{k}_1) \cdot (\mathbf{k}_2' - \mathbf{k}_1') = (\mathbf{p}_2 - \mathbf{q}_1) \cdot (\mathbf{q}_1 - \mathbf{p}_1) = 0$. Thus, the eigenstate (18) takes on the form prescribed in Theorem 1. Clearly, $\mathbf{k}_2'$ plays the role of the gauge vector ξ.

It remains to show that minimal eigenfunctions, being the sum of more than two symmetrized plane waves, do not exist for $N = 2$. Let us suppose the opposite, i.e., that for some $n > 2$ there is a minimal eigenfunction $\psi(\mathbf{r}_1, \mathbf{r}_2) = \sum_{m=1}^{n} a_m \psi_{\mathbf{P}^m}^{+}$, where $\mathbf{P}^m = (\mathbf{p}_1^m, \mathbf{p}_2^m)$ and $(\mathbf{p}_1^m)^2 + (\mathbf{p}_2^m)^2$ is independent of m. Because of the minimality, identical vanishing of $\psi(\mathbf{r}, \mathbf{r}) = 2 \sum_{m=1}^{n} a_m e^{i(\mathbf{p}_1^m + \mathbf{p}_2^m) \cdot \mathbf{r}}$ implies that also $\mathbf{p}_1^m + \mathbf{p}_2^m$ is independent of m (indeed possible for $n > 2$, see Lemma 3 later), and $\sum_{m=1}^{n} a_m = 0$. But then $\psi(\mathbf{r}_1, \mathbf{r}_2) = \sum_{m=1}^{n-1} a_m [\psi_{\mathbf{P}^m}^{+}(\mathbf{r}_1, \mathbf{r}_2) - \psi_{\mathbf{P}^n}^{+}(\mathbf{r}_1, \mathbf{r}_2)]$, where each term of the sum is a minimal eigenfunction of the type (18), so ψ could not be minimal. Thus we have shown the theorem for $N = 2$.

We complete the study of the case $N = 2$ by answering the following question: Given $\mathbf{p}_1$ and $\mathbf{p}_2 \neq \mathbf{p}_1$, both in A^d, how to obtain all the solutions of Eqs. (19) for $\mathbf{q}_1$ and $\mathbf{q}_2$?

Lemma 3. Let $\mathbf{p}_1 \neq \mathbf{p}_2$, both in A^d, and consider the sphere S in $\mathbf{R}^d$ drawn over $\mathbf{p}_1 - \mathbf{p}_2$ as a diameter. There is a one-to-one correspondence between nonzero orthogonal pairs of vectors in the intersection of S with A^d and the solutions of Eq. (19) for $\{\mathbf{q}_1, \mathbf{q}_2\}$. If $\mathbf{a}$ and $\mathbf{b}$ form such a pair, the corresponding solution is $\mathbf{q}_1 = \mathbf{p}_1 - \mathbf{a} = \mathbf{p}_2 + \mathbf{b}$ and $\mathbf{q}_2 = \mathbf{p}_2 + \mathbf{a} = \mathbf{p}_1 - \mathbf{b}$.

If there is a pair $\{\mathbf{q}_1, \mathbf{q}_2\} \neq \{\mathbf{p}_1, \mathbf{p}_2\}$ which solves (20), we use the parametrization with an allowed pair $\mathbf{K}, \mathbf{K}'$ described above and define $\mathbf{a} = \mathbf{k}_1' - \mathbf{k}_2'$ and $\mathbf{b} = \mathbf{k}_1 - \mathbf{k}_2$. Then $\mathbf{q}_1$ and $\mathbf{q}_2$ are as asserted, $\mathbf{a} \cdot \mathbf{b} = 0$ and $\mathbf{p}_1 - \mathbf{p}_2 = \mathbf{a} + \mathbf{b}$. As we have seen in Lemma 1, both $\mathbf{a}$ and $\mathbf{b}$ are in A^d and, because they are orthogonal and sum up to $\mathbf{p}_1 - \mathbf{p}_2$, they are also on the sphere

$$S = \{\mathbf{r} \in \mathbf{R}^d : |\mathbf{r} - \tfrac{1}{2}(\mathbf{p}_1 - \mathbf{p}_2)| = \tfrac{1}{2}|\mathbf{p}_1 - \mathbf{p}_2|\}. \tag{21}$$

Oppositely, let $\mathbf{a} \in \mathrm{A}^d \cap S$ and define $\mathbf{q}_1 = \mathbf{p}_1 - \mathbf{a}$ and $\mathbf{q}_2 = \mathbf{p}_2 + \mathbf{a}$. Then $\mathbf{q}_1 + \mathbf{q}_2 = \mathbf{p}_1 + \mathbf{p}_2$ and $\mathbf{q}_1 \cdot \mathbf{q}_2 = \mathbf{p}_1 \cdot \mathbf{p}_2 + \mathbf{a} \cdot (\mathbf{p}_1 - \mathbf{p}_2) - \mathbf{a}^2 = \mathbf{p}_1 \cdot \mathbf{p}_2$ because $\mathbf{a} \in S$. Now along with $\mathbf{a}$, $\mathbf{b} = \mathbf{p}_1 - \mathbf{p}_2 - \mathbf{a}$ is also in the intersection and $\mathbf{a} \cdot \mathbf{b} = 0$. So vectors in $\mathrm{A}^d \cap S$ occur in orthogonal pairs whose elements add up to $\mathbf{p}_1 - \mathbf{p}_2$ and provide the same solution.

Any nontrivial partition of $(2\pi/L)^{-2} |\mathbf{p}_1 - \mathbf{p}_2|^2$ into the sum of the square of $2d$ integers gives rise to at least one solution of (19). Therefore, if $\mathbf{p}_1 - \mathbf{p}_2$ has two nonvanishing coordinates, there exists at least one orthogonal pair of vectors described in the lemma. On the other hand, if only a single coordinate is nonvanishing, there may not be any nontrivial solution for $\mathbf{q}_1, \mathbf{q}_2$ (take, e.g., $d = 2$ and $\mathbf{p}_1 - \mathbf{p}_2 = (2\pi/L)(0, 3)$).

We turn to the case $N > 2$. Since $\psi(\mathbf{R})$ is a symmetric function, for (P3) to hold $\psi(\mathbf{r}, \mathbf{r}, \mathbf{r}_3,...) \equiv 0$ suffices. To see how $\psi(\mathbf{r}, \mathbf{r}, \mathbf{r}_3,...)$ can vanish, we write

$$\psi_{\mathbf{P}^\alpha}^+(\mathbf{R}) = \sum_{1 \leqslant l < m \leqslant N} \psi_{\mathbf{P}^\alpha}^{lm}(\mathbf{R}) \tag{22}$$

with

$$\psi_{\mathbf{P}}^{lm}(\mathbf{R}) = [e^{i(\mathbf{p}_l \mathbf{r}_1 + \mathbf{p}_m \mathbf{r}_2)} + e^{i(\mathbf{p}_m \mathbf{r}_1 + \mathbf{p}_l \mathbf{r}_2)}] \sum_{\pi \in S_N : \pi(1) = l, \pi(2) = m} e^{i \sum_{n=3}^N \mathbf{p}_{\pi(n)} \mathbf{r}_n}$$
$$= \psi_{\{\mathbf{p}_l, \mathbf{p}_m\}}^+(\mathbf{r}_1, \mathbf{r}_2) \, \psi_{\{\mathbf{p}_j\}_{j \neq l, m}}^+(\mathbf{r}_3,..., \mathbf{r}_N). \tag{23}$$

Here we have used again the notation (16) for symmetrized plane waves. Now $\psi_{\mathbf{P}^\alpha}^{lm}(\mathbf{r}, \mathbf{r}, \mathbf{r}_3,...)$ can be cancelled as a whole by an identically equal $\psi_{\mathbf{P}^\beta}^{st}(\mathbf{r}, \mathbf{r}, \mathbf{r}_3,...)$. The condition of an identical equality imposes

$$\{\mathbf{p}_j^\alpha\}_{j \neq l, m} = \{\mathbf{p}_j^\beta\}_{j \neq s, t} \tag{24}$$

and

$$\mathbf{p}_l^\alpha + \mathbf{p}_m^\alpha = \mathbf{p}_s^\beta + \mathbf{p}_t^\beta, \qquad (\mathbf{p}_l^\alpha)^2 + (\mathbf{p}_m^\alpha)^2 = (\mathbf{p}_s^\beta)^2 + (\mathbf{p}_t^\beta)^2 \tag{25}$$

where we have added the last equality which comes from the fact that $\psi_{\mathbf{P}^\beta}^+$ must belong to the same energy eigenvalue as $\psi_{\mathbf{P}^\alpha}^+$. So for the vectors $\mathbf{p}_l^\alpha, \mathbf{p}_m^\alpha, \mathbf{p}_s^\beta, \mathbf{p}_t^\beta$ we find precisely Eqs. (19). Again, we have to discard the trivial solutions. They would yield $\mathbf{P}^\alpha = \mathbf{P}^\beta$, so $\psi_{\mathbf{P}^\alpha}^+(\mathbf{R}) \equiv \psi_{\mathbf{P}^\beta}^+(\mathbf{R})$, which contradicts the supposed contracted form of ψ. Considering Eq. (25) for every pair $l < m$, we conclude that for each α the set $\{\mathbf{p}_j^\alpha\}_{j=1}^N$ contains N different vectors. Furthermore, if $\psi_{\mathbf{P}^\alpha}^{l_1 m_1}(\mathbf{r}, \mathbf{r}, \mathbf{r}_3,...) \equiv \psi_{\mathbf{P}^\beta}^{s_1 t_1}(\mathbf{r}, \mathbf{r}, \mathbf{r}_3,...)$ then $\{\mathbf{p}_j^\alpha\}_{j=1}^N \cap \{\mathbf{p}_j^\beta\}_{j=1}^N = \{\mathbf{p}_j^\alpha\}_{j \neq l_1, m_1} = \{\mathbf{p}_j^\beta\}_{j \neq s_1, t_1}$, and for the same α and β no

other choice of $l < m$ and $s < t$ can yield the equality (24). Thus, to annihilate $\psi_{\mathbf{P}^\alpha}^+(\mathbf{r}, \mathbf{r}, \mathbf{r}_3,...)$ we need one term from the decomposition (22) of $N(N-1)/2$ different $\psi_{\mathbf{P}^\beta}^+$. Solving the $N(N-1)/2$ Eqs. (25) for $\{\mathbf{p}_s^\beta, \mathbf{p}_t^\beta\}$, one for each pair $l < m$, we may (but for the moment we cannot say we really do) obtain $N(N-1)$ different vectors which, together with the N vectors of $\mathbf{P}^\alpha$, form a set of N^2 wave vectors. Recall that $\psi_{\mathbf{K}, \mathbf{K}'}$ of Theorem 1 are also constructed with the help of N^2 vectors $\mathbf{k}_i + \mathbf{k}_j'$. So far we have found that minimal eigenfunctions share some attributes of $\psi_{\mathbf{K}, \mathbf{K}'}$, but have not seen as yet that these latter themselves are minimal.

Lemma 4. $\psi_{\mathbf{K}, \mathbf{K}'}$ of Theorem 1 are minimal (P1)–(P3)-eigenfunctions.

In the present case the index set is S_N. Let $(\mathbf{K} + \alpha\mathbf{K}')_j = \mathbf{k}_j + \mathbf{k}_{\alpha^{-1}(j)}'$. We have to prove that

$$\psi_{\mathbf{K}, \mathbf{K}'} = \sum_{\alpha \in S_N} (-)^\alpha \psi_{\mathbf{K}+\alpha\mathbf{K}'}^+ \tag{26}$$

is the unique (P1)–(P3)-eigenstate that can be obtained as a linear combination of the functions $\{\psi_{\mathbf{K}+\alpha\mathbf{K}'}^+\}_{\alpha \in S_N}$. According to Eqs. (15), (22) and (23), a general function over the above basis reads

$$\psi(\mathbf{R}) = \sum_{\alpha \in S_N} a_\alpha \psi_{\mathbf{K}+\alpha\mathbf{K}'}^+(\mathbf{R})$$

$$= \sum_{\alpha \text{ even}} \sum_{l < m} \left[a_\alpha \psi_{\{(\mathbf{K}+\alpha\mathbf{K}')_j\}_{j=l,m}}^+(\mathbf{r}_1, \mathbf{r}_2) \right.$$

$$\left. + a_{(lm)\alpha} \psi_{\{(\mathbf{K}+(lm)\alpha\mathbf{K}')_j\}_{j=l,m}}^+(\mathbf{r}_1, \mathbf{r}_2) \right] \psi_{\{(\mathbf{K}+\alpha\mathbf{K}')_j\}_{j \neq l,m}}^+(\mathbf{r}_3,...). \tag{27}$$

We may suppose that the coefficient of the identity is nonzero—this can always be achieved by renumbering the vectors of $\mathbf{K}'$, if necessary—and normalize ψ so as to have $a_{\text{id.}} = 1$. In (27) we have regrouped the terms which can cancel each other if $\mathbf{r}_1 = \mathbf{r}_2$. The point is that, given $(\alpha, l < m)$, there is a unique $(\beta, s < t)$ such that Eqs. (24) and (25) hold true, namely, $\beta = (l\,m)\,\alpha$, $s = l$ and $t = m$. This is because $\mathbf{k}_i + \mathbf{k}_j'$ uniquely determines (i, j). Thus, if ψ is a (P3)-eigenstate then for every α and every pair $l < m$, $a_{(lm)\alpha} = -a_\alpha$. Starting with $(l\,m) \in S_N$, $a_{(lm)} = -1$, and the products of any two, three, etc. of them appear with coefficients $(-)^2$, $(-)^3$, etc., respectively. Since the inversions generate S_N, we conclude that $a_\alpha = (-)^\alpha$ for each $\alpha \in S_N$ and, thus, $\psi = \psi_{\mathbf{K}, \mathbf{K}'}$, proving that the latter is minimal.

The last step is to show that no other type of minimal eigenfunctions exists. This we have seen for two particles and will prove for $N \geq 3$ by

induction. Suppose the claim is verified for any $n < N$. Let $\mathscr{P} = \bigcup_{\alpha \in I} \{\mathbf{p}_i^\alpha\}_{i=1}^N$, i.e., the full set of wave vectors used to define the minimal (P1)–(P3) eigenfunction (15). After resummation this function reads

$$\psi(\mathbf{R}) = \sum_{\mathbf{p} \in \mathscr{P}} b_{\mathbf{p}} e^{i\mathbf{p} \cdot \mathbf{r}_N} \phi_{\mathbf{p}}(\mathbf{r}_1, ..., \mathbf{r}_{N-1}). \tag{28}$$

Here every $\phi_{\mathbf{p}}$ is a uniquely determined (P1)–(P3) eigenfunction of $-\sum_{i=1}^{N-1} \Delta_i$ which, by the induction hypothesis, is a linear combination of $N-1$-variable eigenfunctions of the type described in Theorem 1. (That $\phi_{\mathbf{p}}$ is actually minimal and, thus, equals a single function of this type, will follow from the proof.) The sum (28) can be considered as an embedding of any given of its terms into a minimal (P1)–(P3) eigenfunction. The $(N-1)^2$ wave vectors appearing in each minimal component of $\phi_{\mathbf{p}}$ are of the form $\mathbf{k}_i + \mathbf{k}_j'$ with $1 \leqslant i, \ j \leqslant N-1$ and satisfy the orthogonality relations (11). Consider the function

$$\sum_{\pi, \pi' \in S_{N-1}} (-)^{\pi\pi'} \exp\left\{ i\mathbf{p}\mathbf{r}_N + i\sum_{j=1}^{N-1} (\mathbf{k}_{\pi(j)} + \mathbf{k}_{\pi'(j)}') \mathbf{r}_j \right\}$$

in the term $\mathbf{p}$ of (28). The symmetrical embedding of the plane wave belonging to (π, π') implies the presence, in the expansion of ψ, $N-1$ other plane waves, one for each j, in which $\mathbf{p}$ and $\mathbf{k}_{\pi(j)} + \mathbf{k}_{\pi'(j)}'$ are interchanged. So $\mathbf{k}_{\pi(j)} + \mathbf{k}_{\pi'(j)}' \in \mathscr{P}$ for $j = 1, ..., N-1$ and embedding of the $(N-1)$-particle plane wave $\exp\{i\mathbf{p}\mathbf{r}_j + \sum_{l \neq j}^{N-1} (\mathbf{k}_{\pi(l)} + \mathbf{k}_{\pi'(l)}') \mathbf{r}_l\}$ in $\phi_{\mathbf{k}_{\pi(j)} + \mathbf{k}_{\pi'(j)}'}(\mathbf{r}_1, ..., \mathbf{r}_{N-1})$ implies that $\mathbf{p} = \mathbf{k} + \mathbf{k}'$, and $\{(\mathbf{k}, \mathbf{k}')\} \cup \{(\mathbf{k}_j, \mathbf{k}_j')\}_{j=1}^{N-1}$ satisfy (11). We conclude that in $\mathscr{P}$ there is a subset parametrized by an allowed pair $\mathbf{K}, \mathbf{K}'$, both members containing N vectors such that (11) holds, and all the corresponding symmetrized plane waves $\psi_{\mathbf{K}+\alpha\mathbf{K}'}^+$ occur in the support of ψ. Since ψ is minimal, this *is* the support of ψ, and $\psi = \psi_{\mathbf{K}, \mathbf{K}'}$. This ends the proof of the theorem.

2.2. Remarks

1. The representation of a bosonic state as the product of two Slater determinants is, in a certain sense, natural. Intuitively, we can imagine a spinless boson to be built up of two coinciding half-spin fermions of opposite spins, and the two Slater determinants as wavefunctions of the two kinds of fermions. Also, the eigenstates we are looking for are twice continuously differentiable (C^2, in fact, analytic) functions of all coordinates and vanish, therefore, at least quadratically at $\mathbf{r}_i = \mathbf{r}_j$. The C^2-functions of all coordinates satisfying (P1)–(P3) form a linear space $\mathscr{L}$, and one may

suspect that $\psi_{\mathbf{K}, \mathbf{K}'}$ with allowed pairs is a generating system of this space. A way to prove it would be to take an arbitrary function of $\mathscr{L}$, divide and re-multiply it with a "nice" antisymmetric function and expand both—now antisymmetric—factors as a linear combination of Slater determinants which are known to form a basis in the antisymmetric subspace. The crux is the choice of the auxiliary antisymmetric function. It should yield an at least L^2-convergent expansion for both factors, and the product of the two expansions should still be L^2-convergent. Because $\mathscr{L}$ is dense in the symmetric subspace of $L^2(\Lambda^N)$, a successful proof would imply that $\psi_{\mathbf{K}, \mathbf{K}'}$ with allowed pairs linearly span the symmetric subspace. Note, however, that this would be a very bad basis for proving off-diagonal long-range order, see Remark 9 later.

2. The form of $\psi_{\mathbf{K}, \mathbf{K}'}$, corresponding to (28), is

$$\psi_{\mathbf{K}, \mathbf{K}'}(\mathbf{R}) = \sum_{l, m = 1}^{N} (-)^{2N-l-m} e^{i(\mathbf{k}_l + \mathbf{k}_m') \cdot \mathbf{r}_N} \phi_{\mathbf{k}_l + \mathbf{k}_m'}(\mathbf{r}_1, ..., \mathbf{r}_{N-1}), \tag{29}$$

where $\phi_{\mathbf{k}_l + \mathbf{k}_m'} = \psi_{\mathbf{K} \backslash \{\mathbf{k}_l\}, \mathbf{K}' \backslash \{\mathbf{k}_m'\}}$.

3. Theorem 2 is not claiming that eigenstates, being, for instance, the product of more than two Slater determinants, do not exist. It is easily seen that in $d \geqslant n$ dimensions, with n pairwise orthogonal k-sets one can obtain eigenstates in the form of a product of n Slater determinants. However, for n even these states can be expanded in the basis $\{\psi_{\mathbf{K}, \mathbf{K}'}\}$ (as for n odd they can be expanded in the basis of Slater determinants). As an example, the expansion of a product of four determinants belonging to $\mathbf{K}$, $\mathbf{K}^1$, $\mathbf{K}^2$ and $\mathbf{K}^3$, respectively, reads

$$\psi_{\mathbf{K}, \mathbf{K}^1, \mathbf{K}^2, \mathbf{K}^3} = \sum_{\alpha, \beta \in S_N} (-)^{\alpha\beta} \psi_{\mathbf{K}, \mathbf{K}^1 + \alpha \mathbf{K}^2 + \beta \mathbf{K}^3}, \tag{30}$$

irrespective of the space dimension or whether the product is an eigenfunction.

4. The energy of the eigenstates $\psi_{\mathbf{K}, \mathbf{K}'}$ is easy to estimate. In two and three dimensions the length of the vectors in one of the two sets has to increase at least linearly, so the energy is at least of the order of N^3/L^2 (because of the orthogonality (11), at the same time

$$\sum \mathbf{k}_i \cdot \mathbf{k}_i' = \mathbf{k}_1 \cdot \sum (\mathbf{k}_i' - \mathbf{k}_1') + \mathbf{k}_1' \cdot \sum (\mathbf{k}_i - \mathbf{k}_1) + N\mathbf{k}_1 \cdot \mathbf{k}_1'$$

is only of order N^2/L^2). At fixed positive densities this is much larger than the ground state energy of any physically meaningful H_N (which is smaller than a multiple of N), and these states play no role in thermodynamics

either. However, in cases when the grand-canonical ground state is the vacuum, $N = 0$, as, e.g., for repulsive pair interactions and zero or negative chemical potentials, we obtain gapless excitations in the form of $N = o(L^{2/3})$-particle eigenstates whose energy vanishes with the increasing volume.

5. Lemma 3 shows that degeneracy of minimal states can occur. Because of nonvanishing overlaps, within a degenerate subspace the minimal states may not be linearly independent and one may not choose an orthogonal basis of them.

6. $\psi_{\mathbf{K},\mathbf{K}'}$ are eigenstates of the total momentum operator with eigenvalue $N\mathbf{q} = \sum (\mathbf{k}_i + \mathbf{k}'_i)$. Multiplying and dividing $\psi_{\mathbf{K},\mathbf{K}'}$ by $\exp i\mathbf{q} \sum \mathbf{r}_j$ yields

$$\psi_{\mathbf{K},\mathbf{K}'}(\mathbf{R}) = e^{i\mathbf{q}\sum \mathbf{r}_j}\psi_{\mathbf{K}-\bar{\mathbf{k}},\mathbf{K}'-\bar{\mathbf{k}}'}(\mathbf{R}) \tag{31}$$

with $\bar{\mathbf{k}} = N^{-1}\sum \mathbf{k}_i$ and $\mathbf{K} - \bar{\mathbf{k}} = (\mathbf{k}_j - \bar{\mathbf{k}})_{j=1}^N$ and similar for the primed variables. If $\psi_{\mathbf{K},\mathbf{K}'}$ is an eigenstate of the kinetic energy then $\psi_{\mathbf{K}-\bar{\mathbf{k}},\mathbf{K}'-\bar{\mathbf{k}}'}$ is a zero-momentum eigenstate whose k-sets satisfy not only (11) but also the more specific equations $(\mathbf{k}_i - \bar{\mathbf{k}}) \cdot (\mathbf{k}'_j - \bar{\mathbf{k}}') = 0$ which are easy to verify. Replacing $\mathbf{k}_i - \bar{\mathbf{k}}$ by $\mathbf{k}_i$ and $\mathbf{k}'_i - \bar{\mathbf{k}}'$ by $\mathbf{k}'_i$ we obtain the canonical form of minimal functions:

Corollary. A basis of (P1)–(P3) eigenstates can be chosen among the functions

$$\psi_{\mathbf{q},\mathbf{K},\mathbf{K}'}(\mathbf{R}) = e^{i\mathbf{q}\sum \mathbf{r}_j}\psi_{\mathbf{K},\mathbf{K}'}(\mathbf{R}) \tag{32}$$

where $\mathbf{q} \in A^d$, $N\mathbf{q}$ is the total momentum and $\psi_{\mathbf{K},\mathbf{K}'}$ is a zero-momentum minimal eigenfunction. Namely, $\mathbf{K}, \mathbf{K}'$ is an allowed pair with $\mathbf{k}_i \cdot \mathbf{k}'_j = 0$ for any i and j and $\sum \mathbf{k}_i = \sum \mathbf{k}'_i = 0$.

In the right-hand side of Eq. (32) $\mathbf{R}$ can be replaced by $(\mathbf{r}_i - \bar{\mathbf{r}})_{i=1}^N$ where $\bar{\mathbf{r}} = N^{-1}\sum_{i=1}^N \mathbf{r}_i$.

7. Equations (19) and (25) suggest to interpret the (P1)–(P3) eigenstates of the kinetic energy operator as stationary states of a system of impenetrable, pointlike bosons which interact with each other through elastic collisions. Clearly, there exists no self-adjoint Hamiltonian with a dense domain in the symmetric subspace of $L^2(\Lambda^N)$ which would describe such a system! The states we have found cover only a very small fraction (roughly $\sim (N!)^{-2}$) of the Hilbert space. Since the suitable operator would be H_N with infinite repulsive delta-interactions, Theorem 2 provides an independent proof of the otherwise known fact, cf. the Introduction, that above one dimension $-\sum \Delta_i$, defined as a symmetric operator H^0 on

$C_0^\infty(\Lambda^N \setminus \bigcup_{i \neq j} \{\mathbf{r}_i = \mathbf{r}_j\})$, has no self-adjoint extension describing such an interaction. The states characterized in the above theorems are in the domain of $\overline{H^0}$, the closure of H^0. In two and three dimensions they are eigenstates of any Hamiltonian H_N with a properly defined contact interaction, and the only eigenstates in the domain of $\overline{H^0}$. Any such H_N is a self-adjoint extension of H^0 or $\overline{H^0}$, so densely defined in $L^2(\Lambda^N)$, and having infinitely many other symmetric eigenstates, which do *not* vanish (even diverge) at particle encounters. As suggested in the Introduction, we can orthogonally decompose any H_N in an interaction-dependent part and H_{elastic}, cf. Eq. (7).

8. Because of their simple form, some basic properties of minimal functions can be studied easily. Nodal surfaces, for example, can be identified if the function is written in the canonical form (32). Let V and V' be the orthogonal subspaces containing $\mathbf{k}_j$ and $\mathbf{k}'_j$, respectively. Since $\det[e^{i\mathbf{k}_l\mathbf{r}_m}] \equiv 0$ if $\mathbf{r}_i - \mathbf{r}_j$ is in V' and $\det[e^{i\mathbf{k}'_l\mathbf{r}_m}] \equiv 0$ if $\mathbf{r}_i - \mathbf{r}_j$ is in V, both for any $i \neq j$, we find that $\psi_{\mathbf{K},\mathbf{K}'}(\mathbf{R}) \equiv 0$ if $\mathbf{r}_i - \mathbf{r}_j$ is in $V \cup V'$ for a pair $i \neq j$. So there is a regular long-range exclusion effect, although it concerns only a set of zero Lebesgue measure in the configuration space. This effect can be amplified by particular choices of $\mathbf{K}$ or $\mathbf{K}'$, that we can see easier on the two-point correlation function. A straightforward computation of this latter yields

$$\rho_2(0, \mathbf{r}) \equiv N(N-1)\langle \delta(\mathbf{r}_1)\, \delta(\mathbf{r}_2 - \mathbf{r}) \rangle$$
$$= \rho^2 \frac{N}{N-1}\left(1 - \frac{1}{N^2}\left|\sum_l e^{i\mathbf{k}_l\mathbf{r}}\right|^2\right)\left(1 - \frac{1}{N^2}\left|\sum_l e^{i\mathbf{k}'_l\mathbf{r}}\right|^2\right) \tag{33}$$

where $\rho = N/|\Lambda|$ is the uniform value of $\rho_1(\mathbf{r}) = N\langle \delta(\mathbf{r}_1 - \mathbf{r}) \rangle$ and averaging means integration over $\mathbf{r}_1,\ldots,\mathbf{r}_N$ in Λ with the weight function $|\psi_{\mathbf{K},\mathbf{K}'}|^2/\|\psi_{\mathbf{K},\mathbf{K}'}\|^2$. In the derivation of (33) the minimality of $\psi_{\mathbf{K},\mathbf{K}'}$ is exploited via the property that $\mathbf{k}_i + \mathbf{k}'_j = \mathbf{k}_l + \mathbf{k}'_m$ implies $i = l$ and $j = m$. For most choices of $\mathbf{K}$ and $\mathbf{K}'$, $\rho_2(0, \mathbf{r}) \approx \rho^2$ outside a small neighborhood of $V \cup V'$ where it vanishes. In general, let $\mathscr{G}_{\mathbf{K}}$ be the set of points $\mathbf{r}$ in Λ such that $\mathbf{k}_l \cdot \mathbf{r}$ is an integer multiple of 2π for every l. $\mathscr{G}_{\mathbf{K}}$ is an Abelian group with respect to addition modulo Λ which contains V' as a subgroup and may contain translates of V'. For example, for $i = 1,\ldots,d$ let M_i be the greatest common divisor of $\{(L/2\pi)\, k_{ni}\}_{n=1}^N$ where k_{ni} is the ith component of $\mathbf{k}_n$. Then $\mathscr{G}_{\mathbf{K}}$ contains the points with coordinates $x_i = m_i L/M_i$, where m_i is any integer between $-M_i/2$ and $M_i/2$. Defining $\mathscr{G}_{\mathbf{K}'}$ analogously, we get another Abelian group containing V and maybe some translates of it. Now $\rho_2(0, \mathbf{r}) = 0$ if and only if $\mathbf{r}$ is in $\mathscr{G}_{\mathbf{K}} \cup \mathscr{G}_{\mathbf{K}'}$ and, as we can check also directly, $\psi_{\mathbf{K},\mathbf{K}'}(\mathbf{R}) = 0$ if (and only if) $\mathbf{r}_i - \mathbf{r}_j$ is in $\mathscr{G}_{\mathbf{K}} \cup \mathscr{G}_{\mathbf{K}'}$ for a pair $i \neq j$.

9.   In the eigenstates $\psi_{K, K'}$ there is no off-diagonal long-range order: The associated one-particle reduced density matrix, σ, has N^2 nonvanishing eigenvalues, each of which is equal to $1/N$. Indeed, using that all $k_l + k'_m$ are different, a straightforward calculation of the integral kernel of σ yields

$$\sigma(\mathbf{r}, \mathbf{r}') = N \, \|\psi_{K, K'}\|^{-2} \int_{A^{N-1}} \psi_{K, K'}(\mathbf{r}, \mathbf{r}_2, \dots) \, \psi^*_{K, K'}(\mathbf{r}', \mathbf{r}_2, \dots) \, d\mathbf{r}_2 \cdots d\mathbf{r}_N$$

$$= \frac{1}{N \, |A|} \sum_{l, m = 1}^{N} e^{-i(\mathbf{k}_l + \mathbf{k}'_m)(\mathbf{r} - \mathbf{r}')}. \tag{34}$$

Because $\psi_{K, K'}$ is a momentum eigenstate as well, σ is diagonal in momentum representation and its eigenvalues are the diagonal elements. Fourier transforming $\sigma(\mathbf{r}, \mathbf{r}')$,

$$\sigma(\mathbf{p}, \mathbf{p}) = \frac{1}{N} \sum_{l, m = 1}^{N} \delta_{\mathbf{p}, \, \mathbf{k}_l + \mathbf{k}'_m}. \tag{35}$$

Since $\mathbf{p} = \mathbf{k}_l + \mathbf{k}'_m$ can hold for at most a single pair (l, m), the result follows.

10.   The results extend to systems in $L_1 \times \cdots \times L_d$ rectangles with periodic boundary conditions. The appropriate definition of A^d is $(2\pi/L_1) \, \mathbb{Z} \times \cdots \times (2\pi/L_d) \, \mathbb{Z}$. The orthogonality relation (11) holds for example if $\{\mathbf{k}_i - \mathbf{k}_j\}$ and $\{\mathbf{k}'_i - \mathbf{k}'_j\}$ have disjoint subsets of nonvanishing coordinates. The existence of other solutions depends on the rationality of the ratios among L_i.

3. EIGENSTATES FOR LATTICE MODELS

We consider the same problem as before on an $L \times \cdots \times L$ part (now L is a positive integer) of $\mathbb{Z}^d$ with periodic boundary conditions. Defining the lattice Laplacian as

$$(\varDelta \psi)(\mathbf{r}) = \sum_{|\mathbf{r}' - \mathbf{r}| = 1} [\psi(\mathbf{r}') - \psi(\mathbf{r})], \tag{36}$$

$e^{i\mathbf{k}\mathbf{r}}$ with $\mathbf{k} = (k_1, \dots, k_d)$ is an eigenfunction of $-\varDelta$ belonging to the eigenvalue $\epsilon(\mathbf{k}) = 2 \sum_{i=1}^{d} (1 - \cos k_i)$. A pair $\mathbf{K}, \mathbf{K}'$ is called allowed if both $\{\mathbf{k}_j\}_{j=1}^{N}$ and $\{\mathbf{k}'_j\}_{j=1}^{N}$ contain N incongruent vectors modulo 2π and $\mathbf{k}_i + \mathbf{k}'_j$ is in A^d for all i, j. Now for an allowed pair $\mathbf{K}, \mathbf{K}'$, $\psi_{K, K'}$ as given by (9) is an eigenstate of $-\sum_{i=1}^{N} \varDelta_i$ if

$$\sum_{i=1}^{N} \epsilon(\mathbf{k}_i + \mathbf{k}'_{\pi(i)}) = \sum_{i=1}^{N} \epsilon(\mathbf{k}_i + \mathbf{k}'_i) \tag{37}$$

for all $\pi \in S_N$, in which case (37) provides the eigenvalue. The analog of Theorem 1 can be derived, based on the following observation. For $2d$-dimensional complex vectors $\mathbf{u}$ and $\mathbf{v}$ let us introduce the dot product $\mathbf{u} \cdot \mathbf{v} = \sum_{j=1}^{2d} u_j v_j$, that is, without taking the complex conjugate in one of the factors. Then, setting

$$\mathbf{v}(\mathbf{k}) = (\cos k_1, \ldots, \cos k_d, i \sin k_1, \ldots, i \sin k_d), \tag{38}$$

the condition (37) is equivalent with

$$\sum_{i=1}^{N} \mathbf{v}(\mathbf{k}_i) \cdot \mathbf{v}(\mathbf{k}'_{\pi(i)}) = \sum_{i=1}^{N} \mathbf{v}(\mathbf{k}_i) \cdot \mathbf{v}(\mathbf{k}'_i). \tag{39}$$

The analog of the particular solution $\mathbf{k}_i \cdot \mathbf{k}'_j = 0$ in the continuum case has to satify $\mathbf{v}(\mathbf{k}_i) \cdot \mathbf{v}(\mathbf{k}'_j) = 0$ or $\sum_{l=1}^{d} \cos(k_{il} + k'_{jl}) = 0$ for all i, j. For L odd no allowed pair can solve these equations. For L even, in two dimensions, a family of solutions is obtained by choosing $k_{i2} = \pi/2 - k_{i1}$ and $k'_{i2} = \pi/2 - k'_{i1}$. If 4 is a divisor of L, the same choice works in three dimensions if $k_{i3} + k'_{j3} = \pi/2$ for all i, j, e.g., $k_{i3} = k'_{i3} = \pi/4$ for all i. More solutions, in particular, solutions also for L odd are provided by the following theorem.

Theorem 3. Let $\mathbf{K}, \mathbf{K}'$ be an allowed pair. The following assertions are equivalent.

(i) Equation (39) holds for the permutations listed in part (i) of Theorem 1.

(ii)

$$[\mathbf{v}(\mathbf{k}_{i+1}) - \mathbf{v}(\mathbf{k}_i)] \cdot [\mathbf{v}(\mathbf{k}'_{j+1}) - \mathbf{v}(\mathbf{k}'_j)] = 0, \qquad 1 \leqslant i, j \leqslant N-1. \tag{40}$$

(iii) Equation (39) holds for all permutations. As a consequence, $\psi_{\mathbf{K}, \mathbf{K}'}$ is a (P1)–(P3) eigenfunction of the kinetic energy and, thus, of all Bose–Hubbard Hamiltonians with purely on-site interactions. The eigenvalue is given by (37).

The proof is exactly the same as that of Theorem 1; it suffices to replace everywhere $\mathbf{k}_i$ by $\mathbf{v}(\mathbf{k}_i)$ and $\mathbf{k}'_i$ by $\mathbf{v}(\mathbf{k}'_i)$. Also, condition (40) expresses energy conservation in two-particle collisions, and is the same as Eq. (12), if we use the suitable expression for the one-particle energy.

To find solutions of (40), it is convenient to rewrite it as

$$\sum_{l=1}^{d} [\cos(k_{i+1\,l} + k'_{j+1\,l}) + \cos(k_{il} + k'_{jl}) - \cos(k_{i+1\,l} + k'_{jl}) - \cos(k_{il} + k'_{j+1\,l})] = 0. \tag{41}$$

We will consider two families of solutions. Type 1 solutions exist for any L. In two dimensions they are obtained by choosing an allowed pair with k_{i1} and k'_{i2} independent of i. In three dimensions we can choose, e.g., k_{i1}, k_{i2} and k'_{i3} independent of i. In these examples Eq. (41) holds by a separate cancellation of the d terms. Also, notice that the pair $\mathbf{K}, \mathbf{K}'$ satisfies the Eqs. (11). Rewriting the solution in the canonical form (31) or (32), the constant components of the transformed vectors vanish and $\mathbf{k}_i \cdot \mathbf{k}'_j = 0$ for all i, j. Recalling Remark 8 of the former section, this implies that $\psi_{\mathbf{K}, \mathbf{K}'}(\mathbf{R}) = 0$ whenever for some i, j the vector $\mathbf{r}_i - \mathbf{r}_j$ is parallel to a coordinate axis. Thus we obtain:

Corollary. Type 1 solutions of Eq. (40) are eigenstates of the more general lattice Hamiltonian (8).

Type 2 solutions exist only for L even and are given by $k_{i2} = \vartheta - k_{i1}$ and $k'_{i2} = \pi - \vartheta - k'_{i1}$ which, in three dimesions, is completed with, e.g., k_{i3} chosen to be independent of i. Since the choice of ϑ does not influence the solution, we can fix $\vartheta = \pi/2$, as earlier.

The solutions of (41) we have presented above exist only for $N \leqslant L$. Indeed, in all these examples either in $\mathbf{K}$ or in $\mathbf{K}'$ a single component specifies the vector. Since in both sets all the vectors must be incongruent, the defining component must take on N different values out of L possible ones. In higher dimensions the same kind of solutions can easily be given—for example, in four dimensions we can fix the first two components in the $\mathbf{K}$ set and the second two in the $\mathbf{K}'$ set. In general, we can freely choose N incongruent vectors from a $[d/2]$ dimensional subspace, which limits the number of particles to $N \leqslant L^{[d/2]}$. If $N \ll L^{[d/2]}$, it is possible to choose $\mathbf{K}, \mathbf{K}'$ such that $|\mathbf{k}_i|, |\mathbf{k}'_i| \ll 1$ for each i. Then, in (37) we can expand the cosine functions up to second order, and find that the smallest attainable energy is of order $L^{-2}N^{1+\frac{2}{[d/2]}}$. Thus, for $N = o(L^{\frac{2[d/2]}{2+[d/2]}})$ there are eigenstates whose energy tends to zero as L goes to infinity. They correspond to gapless excitations above the grand canonical ground state when this is the vacuum ($N = 0$ or parallel spins).

The reader may notice that part (iii) of Theorem 3 claims less than that of Theorem 1. It is because Eq. (40) does not imply that $\mathbf{k}_i + \mathbf{k}'_j$ are different for different pairs (i, j). This nevertheless follows from (11) for type 1 solutions, but a counterexample of type 2 is easily obtained. Let L be even and choose $k_{i2} = \pi/2 - k_{i1}$, (k_{i3} independent of i if $d = 3$) and $\mathbf{k}'_i = \mathbf{k}_i$. As a special choice of type 2, the pair $\mathbf{K}, \mathbf{K}' = \mathbf{K}$ solves Eq. (41) and, for any (i, j), $\mathbf{k}_i + \mathbf{k}'_j = \mathbf{k}_j + \mathbf{k}'_i$. The same example shows that in the sum over the $N!$ symmetrized plane waves yielding the (P1)–(P3) eigenstate $\psi_{\mathbf{K}, \mathbf{K}}$ (cf. Eq. (26)) there are coinciding terms: $\psi^+_{\mathbf{K}+\alpha\mathbf{K}'} = \psi^+_{\alpha^{-1}\mathbf{K}+\mathbf{K}'}$ implies that

$\psi_{\mathbf{K}+\alpha\mathbf{K}}^{+} = \psi_{\mathbf{K}+\beta\mathbf{K}}^{+}$ if $\beta = \alpha^{-1}$. Now α differs from its inverse if and only if it contains at least one cycle longer than two. Thus, our example works for all such α (but we need $N > 2$) and $\beta = \alpha^{-1}$. As a permutation and its inverse have the same parity, the two occurrences of the same symmetrized plane wave arrive with the same sign in $\psi_{\mathbf{K},\mathbf{K}}$.

Keeping the earlier definition of minimality, Lemma 2 remains valid: Minimal functions form a basis among the (P1)–(P3) eigenstates of $-\sum \Delta_i$. Type 1 eigenfunctions are minimal, as it is seen by applying Lemma 4. We believe that all solutions of Eqs. (40), and only them, are minimal functions. However, we cannot prove this and have only a weaker analog of Theorem 2.

Theorem 4. If ψ is a minimal eigenfunction of $-\sum \Delta_i$ then supp ψ $\subset \{\psi_{\mathbf{K}+\alpha\mathbf{K}'}^{+}\}_{\alpha \in S_N}$ for some allowed pair $\mathbf{K}, \mathbf{K}'$ satisfying Eqs. (40).

For $N = 2$ the assertion is equivalent with the stronger claim of Theorem 2. The second of Eqs. (19) is to be replaced by

$$\sum_{j=1}^{d} (\cos p_{1j} + \cos p_{2j}) = \sum_{j=1}^{d} (\cos q_{1j} + \cos q_{2j}). \tag{42}$$

Again, the trivial solution $\{\mathbf{p}_1, \mathbf{p}_2\} = \{\mathbf{q}_1, \mathbf{q}_2\}$ is to be excluded, but now the four vectors need not be different. Indeed, with our earlier example $k_{i2} = \pi/2 - k_{i1}$ and $\mathbf{k}_i' = \mathbf{k}_i$ for $i = 1, 2$, $\mathbf{p}_i = 2\mathbf{k}_i$ and $\mathbf{q}_1 = \mathbf{q}_2 = \mathbf{k}_1 + \mathbf{k}_2$ is a nontrivial solution. When parametrizing a solution (18) with an allowed pair $\mathbf{K}, \mathbf{K}'$, Eq. (42) coincides with (40) written for $i = j = 1$. The minimality of such a solution is trivial, and the proof that no other minimal function exists is the same as in Theorem 2. The weaker assertion for a general N can be shown as in Theorem 2 by starting with a weaker induction hypothesis.

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