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Pair theory of the Hubbard Hamiltonian

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A detailed account is given of a recently developed pair theory of the Hubbard Hamiltonian for the case of a half-filled band. The resulting pair Hamiltonian is an exact reformulation of the original Hubbard Hamiltonian in terms of pair operators which satisfy elementary boson commutation relations. The Hamiltonian takes the familiar form of a sum of a quadratic part representing independent-pair energies and a quartic part representing pair interactions. The matrix elements entering the pair Hamiltonian are the pair energies and products of pair wave functions, which are formally given as the solutions of a certain eigenvalue equation. By the solving of the eigenvalue problem, explicit analytical expressions are obtained for both pair energies and wave functions for an arbitrary number of dimensions. For the case $M=1$, where M is the number of spin-down electrons, pair interactions do not enter since there is only one electron-hole pair, and the exact energies of the Hubbard Hamiltonian are obtained. This will be explicitly verified for the one-dimensional case; here we demonstrate that the pair energies agree with the exact energies found by other authors for this case.

I. INTRODUCTION

The one-band Hubbard model[1] has been widely studied in connection with correlation effects in narrow-band solids. The general interest in this model was further stimulated by the discovery of the exact solution for the one-dimensional ground-state energy by Lieb and Wu.[2] Although the results of Ref. 2 are important for a proper understanding of correlation effects in one-dimensional systems such as long polyenes, they cannot be generalized to more than one dimension. Despite the relative simplicity of the model, only few exact theorems for certain limiting cases exist so far. The significance and usefulness of these results have been critically reviewed by Cyrot.[3] Further references to previous work in this field can be found in the review articles by Bari[4] and Ovchinnikov *et al.*[5]

A novel approach, completely different from all previous ones, has been recently proposed by the present author.[6] This approach is basically a pair-theory method, and it leads to an *exact* reformulation of the original Hamiltonian in terms of pair operators. The latter obey ordinary boson commutation relations and the resulting pair Hamiltonian takes the familiar form of a sum of a quadratic part representing independent pair energies and a quartic part representing pair interactions. Owing to the simplicity of the Hubbard model, the independent pair energies and wave functions can all be obtained explicitly.[6]

The purpose of the present work is to give a detailed account of the ideas developed in Ref. 6 and to add a few new results. As in Ref. 6, only the case of a half-filled band will be considered here. The paper is organized as follows.

In Sec. II particle-hole (p-h) operators are introduced and the Hubbard Hamiltonian is rewritten in terms of these operators. Owing to the fact that p-h operators do not obey simple Bose or Fermi commutation relations, some mathematical problems arise such as nonorthogonality and overcompleteness of state vectors generated by the p-h creation operators. These mathematical problems are analyzed in Sec. III. There it will also be shown how these difficulties can be overcome by imposing certain subsidiary conditions on the space of wave functions. The results of this section provide a proper basis for an expansion of the Hamiltonian in terms of ordinary ("ideal") boson operators; this will be done in Sec. IV. In the past several boson-expansion methods have been proposed, the earliest one being that developed by Dyson.[7] Here we have preferred to follow the method of Girardeau,[8] which is ideally suited for application to the present problem. In Sec. V the band limit and the atomic limit of the Hubbard model are reconsidered. These limits will serve mainly as test cases to show the equivalence of the Hubbard Hamiltonian with the one derived in Sec. IV. The final pair Hamiltonian is obtained in Sec. VI. The independent pair energies and wave functions entering this Hamiltonian are derived in an explicit form for an arbitrary number of dimensions. By specifying our solutions to one dimension, we recover the solutions derived by Lieb and Wu[2] for the particular case $M=1$. The main results of the present work are summarized in Sec. VII.

II. TRANSFORMATION TO PARTICLE-HOLE OPERATORS

The main purpose of this section is to reformulate the Hubbard Hamiltonian in terms of (p-h) operators. We begin with a brief discussion of the Hubbard model[1-3] and its main properties.

The one-band Hubbard Hamiltonian may be written as

$$H=\sum_{\sigma,k}\epsilon_k a^{\dagger}_{k\sigma}a_{k\sigma}+\frac{U}{N}\sum_{k,p,q}a^{\dagger}_{k+q,\uparrow}a_{p\uparrow}a^{\dagger}_{p-q,\downarrow}a_{k\downarrow}\,, \tag{2.1a}$$

where $a_{k\sigma}^{\dagger}, a_{k\sigma}$ are, respectively, the creation and annihilation operators for an electron with spin σ and reduced wave vector k. The first term of (2.1a) is usually referred to as the hopping term, where the energies ϵ_k are given by

$$\epsilon_k = -t\sum_{\alpha} \exp(ik\cdot R_\alpha) \ . \tag{2.1b}$$

Here $t>0$ is the hopping matrix element and R_α denotes a nearest-neighbor lattice vector. The second term in (2.1a) describes an effective short-range Coulomb interaction. In the one-band Hubbard model, it is assumed that each site is capable of accommodating only two electrons of opposite spins with an interaction energy $U>0$. All matrix elements other than those for which both interacting electrons are on the same site are neglected. We specify the model further by restricting ourselves to the case of a half-filled band, where the total number N_e of electrons equals the number N of lattice sites.

It is an important property of the Hubbard Hamiltonian that it commutes with $N_\sigma = \sum_k a_{k\sigma}^{\dagger} a_{k\sigma}$. Hence the eigenvalues M of $N_\downarrow$ and M' of $N_\uparrow$ are good quantum numbers; here M and M' can assume all integral values between zero and N so that $M+M'=N$ is fulfilled. Moreover, as has been shown by Lieb and Wu,[2] one may restrict the range of M to $0\le M\le N/2$ without loss of generality. We next define a new vacuum by

$$|\Psi_0\rangle = \prod_k a_{k\uparrow}^{\dagger}|0\rangle \ , \tag{2.2}$$

where the product extends over all wave vectors of the reduced zone, and we redefine the operator $a_{k\sigma}$ as

$$a_{k\sigma} = \begin{cases} b_k & \text{for } \sigma=\downarrow \ \text{(particles)} \\ c_k^{\dagger} & \text{for } \sigma=\uparrow \ \text{(holes)}. \end{cases} \tag{2.3}$$

It is easy to show that $|\Psi_0\rangle$ is an eigenvector of both $N_\downarrow$ and H with respective eigenvalues $M=0$ and $E_0=\sum_k \epsilon_k = 0$. We mention in passing that the particle and hole destruction operators both annihilate the new vacuum: $b_k|\Psi_0\rangle = c_k|\Psi_0\rangle = 0$. It should also be clear from the definition that all particle operators anticommute with all hole operators because they refer to different spin components. The Hubbard Hamiltonian may now be rewritten in terms of the new operators as

$$H = U\sum_k b_k^{\dagger} b_k + \sum_k \epsilon_k (b_k^{\dagger} b_k - c_k^{\dagger} c_k) - \frac{U}{N}\sum_{k,p,q} b_k^{\dagger} c_{k+q}^{\dagger} c_{p+q} b_p \ . \tag{2.4}$$

Since $N = N_\uparrow + N_\downarrow$, we have in addition that

$$N_\downarrow = \sum_k b_k^{\dagger} b_k = \sum_k c_k^{\dagger} c_k \ . \tag{2.5}$$

The latter equation expresses the well-known fact that, for a fixed total number of fermions, particles and holes necessarily have to occur in pairs.

The new fermion operators will now be used to construct p-h operators. These are defined by

$$\rho_k(q) = c_{k+q} b_k, \quad \rho_k^{\dagger}(q) = b_k^{\dagger} c_{k+q}^{\dagger} \ , \tag{2.6}$$

where k refers to the particle momentum and q is the total quasimomentum of the p-h pair. The operators obey the following commutation relations:

$$[\rho_k(q), \rho_{k'}(q')] = [\rho_k^{\dagger}(q), \rho_{k'}^{\dagger}(q')] = 0 \ , \tag{2.7a}$$

$$[\rho_k(q), \rho_{k'}^{\dagger}(q')] = \delta_{kk'}\delta_{qq'} - \delta_{kk'} c_{k'+q'}^{\dagger} c_{k+q} - \delta_{k+q,k'+q'} b_{k'}^{\dagger} b_k \ , \tag{2.7b}$$

$$[[\rho_k(q), \rho_{k'}^{\dagger}(q')], \rho_{k''}^{\dagger}(q'')] = -\delta_{kk''}\delta_{k+q,k'+q'}\rho_{k'}^{\dagger}(q''+k-k') - \delta_{kk'}\delta_{k+q,k''+q''}\rho_{k''}^{\dagger}(q'+k-k'') \ . \tag{2.7c}$$

Equations (2.7a) and (2.7b) strongly resemble the commutation relations of "ideal boson" operators. For this reason, particles obeying commutation rules like those of Eqs. (2.7) are sometimes referred to as "physical bosons." The additional terms by which (2.7b) differs from an ideal boson commutator simply reflect the fact that the p-h operators are composite particles whose constituents obey Fermi-Dirac statistics rather than being really independent Bose-Einstein particles. It may already be mentioned here that Eqs. (2.7) will also entail some mathematical difficulties such as nonorthogonality and overcompleteness of state vectors generated by the p-h creation operators. These mathematical problems will be dealt with in some detail in the following section where it will also be shown how they can be overcome.

The physical meaning of the p-h operators becomes obvious by considering the vector $\rho_k^{\dagger}(q)|\Psi_0\rangle$. As follows from (2.6), this vector describes a state where a hole has been created (a spin-up electron has been annihilated) at wave vector $k+q$ with subsequent creation of a particle (creation of a spin-down electron) at wave vector k. The $\rho_k^{\dagger}(q)$ operators can therefore be regarded as spin-deviation operators. The state vector is schematically depicted in Fig. 1.

Now let $\mathscr{U}_M$ denote the subspace spanned by all simultaneous eigenvectors of H and $N_\downarrow$ for some fixed eigenvalue M of $N_\downarrow$ (the spaces $\mathscr{U}_M$ will be explicitly constructed in Sec. III). Since $N_\downarrow|\Psi_M\rangle = M|\Psi_M\rangle$ for any vector of this subspace, the operator $N_\downarrow$ may be replaced by its eigenvalue M in $\mathscr{U}_M$. Hence, in the following, we will focus our attention on a definite subspace $\mathscr{U}_M$ for some $0<M\le N/2$ (the trivial case $M=0$ will be excluded from our further considerations since it has already been solved at the beginning of this section). Consider now the following relation:

$$c_k^{\dagger} c_k N_\downarrow = \sum_q \rho_q^{\dagger}(k-q)\rho_q(k-q) \ , \tag{2.8}$$

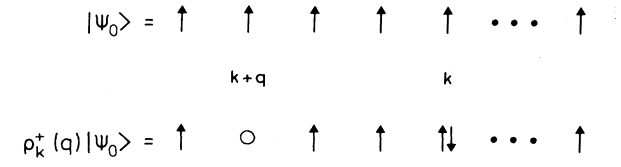

FIG. 1. Graphical illustration of the state vector $\rho_k^\dagger(q)\,|\,\Psi_0\rangle$.

which is readily verified with the help of Eqs. (2.5) and (2.6). It then follows from the above discussion that on any subspace $\mathscr{U}_M$ $(0<M\leq N/2)$, Eq. (2.8) may be rewritten as

$$c_k^\dagger c_k = M^{-1}\sum_q \rho_q^\dagger(k-q)\rho_q(k-q),\quad 0<M\leq N/2\ . \tag{2.9}$$

With the help of Eq. (2.9) and a similar relation for $b_k^\dagger b_k$,[6] the Hamiltonian (2.4) can now be completely rewritten in terms of p-h operators. One obtains:

$$H_M=\sum_{k,k'}\sum_q\left[\frac{1}{M}\omega_k(q)\delta_{kk'}-\frac{U}{N}\right]\rho_k^\dagger(q)\rho_{k'}(q)\ , \tag{2.10a}$$

where

$$\omega_k(q)=\epsilon_k(q)+U \tag{2.10b}$$

and

$$\epsilon_k(q)=\epsilon_k-\epsilon_{k+q},\quad 0<M\leq N/2\ . \tag{2.10c}$$

Because of Eqs. (2.5) and (2.9), we can also express the particle-number operator $N_\downarrow$ in terms of p-h operators as follows:

$$N_\downarrow = M^{-1}\sum_{k,q}\rho_k^\dagger(q)\rho_k(q),\quad 0<M\leq N/2\ . \tag{2.11}$$

In view of the rather complicated commutation rules obeyed by the p-h operators, it would be very helpful if there existed some formalism allowing one to expand the physical boson operators in terms of ideal boson operators. Such methods do, in fact, exist, the earliest one being that developed by Dyson[7] in connection with the theory of spin-wave interactions. Later Girardeau[8] presented a theory for composite particles which, in this author's opinion, is ideally suited to apply to the present problem, and it is essentially this method that will be used in the present work. A brief outline of Girardeau's method and its application to the present problem may also be found in Ref. 6. Before we can express the Hubbard Hamiltonian in terms of ideal boson creation and annihilation operators, however, it is first necessary to examine more closely the spaces $\mathscr{U}_M$ mentioned above.

III. PHYSICAL-STATE SPACE

In the preceding section the space $\mathscr{U}_M$ was defined to be the subspace spanned by all simultaneous eigenvectors of H and $N_\downarrow$ for some fixed eigenvalue M of $N_\downarrow$, where $0<M\leq N/2$. Here we wish to show how the space $\mathscr{U}_M$, also denoted as *physical-state space,* is actually constructed. In view of the importance of this section for the theory presented here, we find it necessary to rephrase the essential elements of Girardeau's[8] treatment, which as previously mentioned, form the basis of the subsequent development.

Consider an arbitrary vector $|\,\Psi_M\rangle$ of $\mathscr{U}_M$, which may be written as

$$|\,\Psi_M\rangle=\sum_{k_1,\ldots,k_M}\sum_{q_1,\ldots,q_M}\psi_{k_1,\ldots,k_M}(q_1,\ldots,q_M)\times|\,(k_1,q_1);\ldots;(k_M,q_M)\rangle\ , \tag{3.1}$$

where

$$|\,(k_1,q_1);\ldots;(k_M,q_M)\rangle=\rho_{k_1}^\dagger(q_1)\cdots\rho_{k_M}^\dagger(q_M)\,|\,\Psi_0\rangle\ , \tag{3.2}$$

and each of the $2M$ summations in (3.1) extends over the whole first Brillouin zone. We will show in Appendix A that $|\,\Psi_M\rangle$ is an eigenvector of $N_\downarrow$ with eigenvalue M. Since $|\,\Psi_M\rangle$ of Eq. (3.1) is completely arbitrary, this implies that *any* vector of $\mathscr{U}_M$ (which is, by definition, an eigenvector of $N_\downarrow$) can be expressed in the form of Eq. (3.1). Hence the set of all M-pair product states (3.2) spans $\mathscr{U}_M$, i.e., any vector of $\mathscr{U}_M$ can be represented as some linear combination of such product states.

The wave functions ψ in Eq. (3.1) are required to be symmetric with respect to an arbitrary permutation of the p-h pairs. More formally, let P denote any permutation of the pair indices $\{1,2,\ldots,M\}$. We then require that

$$P\psi_{k_1,\ldots,k_M}(q_1,\ldots,q_M)=\psi_{k_1,\ldots,k_M}(q_1,\ldots,q_M)\ . \tag{3.3}$$

This requirement is the same as for a wave function describing a system of ideal bosons, and is due to the fact that all $\rho_k^\dagger(q)$ operators commute.

We now proceed to show that for $M\geq 2$ the set of all M-pair product states (3.2) is not linearly independent, i.e., that there exist linear relations among these states. Since we have already shown above that they span the space $\mathscr{U}_M$, it then follows that they form an overcomplete set (if they were merely complete, they would be linearly independent). This is the overcompleteness problem mentioned briefly in Sec. II. The physical reason for the linear dependency between the pair product states (3.2) rests upon the fact that, for $M\geq 2$, there is no unique assignment of particles or holes to the p-h pairs, i.e., there is the possibility of exchange of particles (or holes) between different p-h pairs. To see this explicitly, consider two different pairs labeled by the pair indices i and j, where we assume that $1\leq i<j\leq M$. These pairs are then described by

$$\rho_{k_i}^\dagger(q_i)\rho_{k_j}^\dagger(q_j)=b_{k_i}^\dagger c_{k_i+q_i}^\dagger b_{k_j}^\dagger c_{k_j+q_j}^\dagger\ . \tag{3.4}$$

An interchange of the particle operators $b^\dagger$ between the two pairs leads to

$$\rho^{\dagger}_{k_i}(q_i)\rho^{\dagger}_{k_j}(q_j)=-b^{\dagger}_{k_j}c^{\dagger}_{k_i+q_i}b^{\dagger}_{k_i}c^{\dagger}_{k_j+q_j}=-\rho^{\dagger}_{k_j}(q_i+k_i-k_j)\rho^{\dagger}_{k_i}(q_j+k_j-k_i)=-\rho^{\dagger}_{k_i}(q_j+k_j-k_i)\rho^{\dagger}_{k_j}(q_i+k_i-k_j)\ , \tag{3.5}$$

where use has been made of the anticommutation relations for fermions and Eq. (2.7a). One easily verifies that the same result is obtained by interchanging the hole operators instead of the particle operators. Inserting (3.5) into (3.2), one has

$$|(k_1,q_1);\ldots;(k_i,q_i);\ldots;(k_j,q_j);\ldots;(k_M,q_M)\rangle$$
$$=-|(k_1,q_1);\ldots;(k_i,q_j+k_j-k_i);\ldots;(k_j,q_i+k_i-k_j);\ldots;(k_M,q_M)\rangle\ , \tag{3.6}$$

showing explicitly the linear dependence between the pair product states. An immediate consequence is, of course, that a given vector $|\Psi_M\rangle$ of $\mathscr{U}_M$ $(M\geq 2)$ does not possess a unique expansion in terms of these product states. For if the right-hand side of Eq. (3.6) is inserted into (3.1) and the summation variables are appropriately changed, one obtains

$$|\Psi_M\rangle=-\sum_{k_1,\ldots,k_M}\sum_{q_1,\ldots,q_M}K_{ij}\psi_{k_1,\ldots,k_M}(q_1,\ldots,q_M)\,|(k_1,q_1);\ldots;(k_M,q_M)\rangle\ , \tag{3.7a}$$

where

$$K_{ij}\psi_{k_1,\ldots,k_M}(q_1,\ldots,q_i,\ldots,q_j,\ldots,q_M)$$
$$=\psi_{k_1,\ldots,k_M}(q_1,\ldots,q_{i-1},q_j+k_j-k_i,q_{i+1},\ldots,q_{j-1},q_i+k_i-k_j,q_{j+1},\ldots,q_M),\quad 1\leq i<j\leq M\ . \tag{3.7b}$$

A comparison of Eqs. (3.7a) and (3.1) clearly shows that the same vector $|\Psi_M\rangle$ can be expanded in two different ways, since $\psi\neq -K_{ij}\psi$, in general. There exist other similar relationships between the pair product states, which can be obtained by interchanging more than one pair of particle operators in Eq. (3.2). These additional relationships, however, are not independent since any permutation of particle operators is a product of particle interchanges K_{ij}.

There have been several attempts in the past to overcome the difficulties associated with the overcompleteness problem just discussed, which is a basic difficulty of all composite-particle theories in solid-state and nuclear physics. Some of these attempts are reviewed in a recent monograph by Ring and Schuck.[9] In a series of papers, Girardeau[8] has made a particularly thorough investigation of the many-body problem for composite particles. He solved the overcompleteness problem by imposing subsidiary conditions on the space of wave functions ψ so that the latter all represent physically possible many-pair states, i.e., states which have the correct symmetry under exchange of fermions (particles or holes) between different p-h pairs, and thus satisfy the Pauli principle. The subsidiary conditions imposed by Girardeau are

$$K_{ij}\psi_{k_1,\ldots,k_M}(q_1,\ldots,q_i,\ldots,q_j,\ldots,q_M)=-\psi_{k_1,\ldots,k_M}(q_1,\ldots,q_i,\ldots,q_j,\ldots,q_M),\quad 1\leq i<j\leq M\ , \tag{3.8}$$

where the left-hand side is defined by (3.7b). In order to show that any wave function satisfying Eqs. (3.8) obeys the exclusion principle, we first set $k_i=k_j=k$ in Eqs. (3.8). It then follows from (3.7b) that

$$\psi_{k_1,\ldots,k_{i-1},k,k_{i+1},\ldots,k_{j-1},k,k_{j+1},\ldots,k_M}(q_1,\ldots,q_{i-1},q_j,q_{i+1},\ldots,q_{j-1},q_i,q_{j+1},\ldots,q_M)$$
$$=-\psi_{k_1,\ldots,k_{i-1},k,k_{i+1},\ldots,k_{j-1},k,k_{j+1},\ldots,k_M}(q_1,\ldots,q_i,\ldots,q_j,\ldots,q_M)\ .$$

But from the symmetry property (3.3),

$$\psi_{k_1,\ldots,k,\ldots,k,\ldots,k_M}(q_1,\ldots,q_M)=0\ . \tag{3.9a}$$

Similarly, let $q_i+k_i=q_j+k_j=q+k$ in (3.8). Then from Eqs. (3.7b) and (3.3)

$$\psi_{k_1,\ldots,k_M}(q_1,\ldots,q+k-k_i,\ldots,q+k-k_j,\ldots,q_M)$$
$$=0\ . \tag{3.9b}$$

Equation (3.9a) obviously states that two particles cannot occupy the same state characterized by the wave vector k, whereas (3.9b) does not allow two holes to occupy the same state $q+k$. Hence any wave function satisfying Eqs. (3.8) obeys the exclusion principle.

Girardeau then proved that *the subsidiary conditions (3.8) just suffice to remove the redundancy of the product states (3.2),* but without destroying their property of spanning the space $\mathscr{U}_M$. The proofs of these assertions are clearly presented in Ref. 8(a) so they will be omitted here. It then follows immediately that *any given vector* $|\Psi_M\rangle$ *of* $\mathscr{U}_M$ *can be uniquely represented by an expansion such as (3.1), provided the wave function* ψ *satisfies the conditions (3.8).* In this context we note that the arguments given above to show the nonuniqueness of the expansion of $|\Psi_M\rangle$ fail if Eqs. (3.8) are satisfied. In summary, the subsidiary conditions (3.8) suffice to remove the redundancy of the pair product states (3.2) and, at the same time, ensures the proper statistics under exchange of particles and holes between different p-h pairs. This is no accident since, as was discussed above, the overcompleteness results precisely from the possibility of such exchanges.

We conclude this section by pointing out that the $M(M-1)/2$ subsidiary conditions (3.8) associated with different values of i and j are not independent. Using the symmetry (3.3) of ψ with respect to interchanges of whole pairs, one can readily show that these conditions for one

pair of values for i and j (e.g., $i=1, j=2$) imply the conditions for all other values of i and j.

IV. BOSON EXPANSION OF THE HUBBARD HAMILTONIAN

The results of the preceding section enable us to express the Hamiltonian H_M of Eq. (2.10) in terms of ideal boson operators. These are defined by their commutation relations

$$[B_k(q),B_{k'}(q')]=[B_k^\dagger(q),B_{k'}^\dagger(q')]=0\ ,$$
$$[B_k(q),B_{k'}^\dagger(q')]=\delta_{kk'}\delta_{qq'}\ , \tag{4.1}$$

together with the condition $B_k(q)\,|\,\Psi_0\rangle=0$, where $|\,\Psi_0\rangle$ is the ideal boson vacuum.

Once these operators are defined, it is possible to construct an *ideal-state space* $\hat{\mathscr{U}}_M$ (the analog of the physical-state space $\mathscr{U}_M$ described in Sec. III). This will again be done along the lines developed by Girardeau in Ref. 8(a). In the preceding section it has been shown that any vector $|\,\Psi_M\rangle$ of the physical-state space can be represented in the form

$$|\,\Psi_M\rangle=\frac{1}{M!}\sum_{k_1,\ldots,k_M}\sum_{q_1,\ldots,q_M}\psi_{k_1,\ldots,k_M}(q_1,\ldots,q_M)\times|\,(k_1,q_1);\ldots;(k_M,q_M)\rangle\ , \tag{4.2a}$$

with wave functions ψ which are made unique by imposition of the subsidiary conditions (3.8). Here the factor $1/M!$ has been chosen so that $|\,\Psi_M\rangle$ is normalized to unity provided the wave function ψ satisfies the normalization condition

$$\sum_{k_1,\ldots,k_M}\sum_{q_1,\ldots,q_M}|\,\psi_{k_1,\ldots,k_M}(q_1,\ldots,q_M)\,|^2=1\ . \tag{4.2b}$$

Given any such $|\,\Psi_M\rangle$ of $\mathscr{U}_M$, we define its correspondent $|\,\Psi_M)$ in $\hat{\mathscr{U}}_M$ by

$$|\,\Psi_M)=\frac{1}{\sqrt{M!}}\sum_{k_1,\ldots,k_M}\sum_{q_1,\ldots,q_M}\psi_{k_1,\ldots,k_M}(q_1,\ldots,q_M)\times|\,(k_1,q_1);\ldots;(k_M,q_M))\ , \tag{4.3a}$$

with the *same* wave function ψ as in (4.2), and where

$$|\,(k_1,q_1);\ldots;(k_M,q_M))=B_{k_1}^\dagger(q_1)\cdots B_{k_M}^\dagger(q_M)\,|\,\Psi_0)\ . \tag{4.3b}$$

It can be easily shown that $|\,\Psi_M)$ is also normalized to unity provided ψ is normalized as in Eq. (4.2b). Moreover, one can prove that the inner product is conserved, i.e., we have $\langle\Psi'_M\,|\,\Psi_M\rangle=(\Psi'_M\,|\,\Psi_M)$.

The ideal-state space $\hat{\mathscr{U}}_M$ is then defined to be the set of all such states $|\,\Psi_M)$ as $|\,\Psi_M\rangle$ runs over all of $\mathscr{U}_M$, thereby establishing an isomorphism between $\mathscr{U}_M$ and $\hat{\mathscr{U}}_M$. We emphasize the importance of the subsidiary conditions (3.8) for the construction of $\hat{\mathscr{U}}_M$, since without them one state in $\mathscr{U}_M$ would have many images in $\hat{\mathscr{U}}_M$. These conditions will now be reformulated in terms of an eigenvalue problem in $\hat{\mathscr{U}}_M$. According to Eqs. (3.8), we require that

$$|\,\Psi_M)=-\frac{1}{\sqrt{M!}}\sum_{k_1,\ldots,k_M}\sum_{q_1,\ldots,q_M}K_{ij}\psi_{k_1,\ldots,k_M}(q_1,\ldots,q_M)\,|\,(k_1,q_1);\ldots;(k_M,q_M))\ . \tag{4.4}$$

Consider now the following Hermitian operator $\hat{K}$, hereafter referred to as *exchange operator:*

$$\hat{K}=\tfrac{1}{2}\sum_{k,k'}\sum_{q,q'}B_{k+k'}^\dagger(q)B_{k'}^\dagger(q')B_{k'}(q+k)B_{k+k'}(q'-k)\ . \tag{4.5}$$

It is not difficult to show that $\hat{K}\,|\,\Psi_M)$, where $|\,\Psi_M)$ is given by Eq. (4.3a), yields the following expression:

$$\hat{K}\,|\,\Psi_M)=\tfrac{1}{2}M(M-1)\frac{1}{\sqrt{M!}}\sum_{k_1,\ldots,k_M}\sum_{q_1,\ldots,q_M}K_{ij}\psi_{k_1,\ldots,k_M}(q_1,\ldots,q_M)\,|\,(k_1q_1);\ldots;(k_Mq_M))\ , \tag{4.6}$$

where use has been made of Eqs. (3.3) and (4.1). A comparison of Eqs. (4.6) and (4.4) shows that the latter equation and, hence, the subsidiary conditions (3.8) are fulfilled for all those vectors $|\,\Psi_M)$ satisfying the following eigenvalue equation:

$$\hat{K}\,|\,\Psi_M)=-\tfrac{1}{2}M(M-1)\,|\,\Psi_M)\ . \tag{4.7}$$

Equation (4.7) is completely equivalent to Eqs. (3.8) and one may, therefore, say that only those vectors $|\,\Psi_M)$ satisfying (4.7) can be vectors of the ideal space $\hat{\mathscr{U}}_M$. This implies that, for example, the product states (4.3b) themselves are not contained in $\hat{\mathscr{U}}_M$ because they do not satisfy Eq. (4.7).

In order to express H_M of Eq. (2.10a) in terms of ideal boson operators, we must find the image of H_M in $\hat{\mathscr{U}}_M$. Quite generally, the correspondence between operators O on $\mathscr{U}_M$ and those $\hat{O}$ and $\hat{\mathscr{U}}_M$ is determined by expressing $O\,|\,\Psi_M\rangle$ in the form (4.2a), using (4.3), and identifying the result as some operator $\hat{O}$ acting on $|\,\Psi_M)$. Our first task, therefore, is to calculate $H_M\,|\,\Psi_M\rangle$. A somewhat lengthy calculation, which is carried out in Appendix B, yields

$$H_M \mid \Psi_M \rangle = \frac{1}{M!} \sum_{k_1,\ldots,k_M} \sum_{q_1,\ldots,q_M} \{H_M \psi_{k_1,\ldots,k_M}(q_1,\ldots,q_M)\} \mid (k_1,q_1);\ldots;(k_M,q_M)\rangle \ . \tag{4.8a}$$

The expression in curly brackets is given by

$$\begin{aligned} H_M \psi_{k_1,\ldots,k_M}(q_1,\ldots,q_M) = & \sum_{i=1}^{M} \sum_{k} W_{k_i,k_i+k}(q_i)\psi_{k_1,\ldots,k_i+k,\ldots,k_M}(q_1,\ldots,q_M) \\ & - \frac{U}{N} \sum_{\substack{i,j=1 \\ i<j}}^{M} \sum_{k} \{ \psi_{k_1,\ldots,k_i+k,\ldots,k_M}(q_1,\ldots,q_i-k,\ldots,q_j+k,\ldots,q_M) \\ & + \psi_{k_1,\ldots,k_j+k,\ldots,k_M}(q_1,\ldots,q_i+k,\ldots,q_j-k,\ldots,q_M)\} \ , \end{aligned} \tag{4.8b}$$

where

$$W_{kk'}(q) = \omega_k(q)\delta_{kk'} - \frac{U}{N} \tag{4.8c}$$

and $\omega_k(q)$ is defined by (2.10b). The expansion (4.8a) is unique since $H_M\psi$, as given by (4.8b), satisfies the subsidiary conditions (3.8), which is also shown in Appendix B. To $H_M \mid \Psi_M\rangle$ there corresponds a vector $\hat{H} \mid \Psi_M)$ in $\hat{\mathscr{U}}_M$ which, according to (4.3), is given by

$$\hat{H} \mid \Psi_M) = \frac{1}{\sqrt{M!}} \sum_{k_1,\ldots,k_M} \sum_{q_1,\ldots,q_M} \{H_M \psi_{k_1,\ldots,k_M}(q_1,\ldots,q_M)\} \mid (k_1,q_1);\ldots;(k_M,q_M)) \ , \tag{4.9}$$

with the *same* function $H_M\psi$ as in Eq. (4.8b). Since $H_M\psi$ satisfies Eqs. (3.8), the mapping $H_M \mid \Psi_M\rangle \rightarrow \hat{H} \mid \Psi_M)$ is one to one as discussed above. We now ask what operator $\hat{H}$, expressed as an explicit function of the $B_k(q)$ and $B_k^\dagger(q)$ operators, leads to Eq. (4.9) with expression (4.8b) for $H_M\psi$. Subsequently, we will prove that the following operator has the desired properties:

$$\begin{aligned} \hat{H} = & \sum_{k,k',q} W_{kk'}(q) B_k^\dagger(q) B_{k'}(q) \\ & - \frac{U}{N} \sum_{k,k',k''} \sum_{q,q'} B_{k+k'}^\dagger(q) B_{k''}^\dagger(q') \\ & \times B_{k''}(q'-k) B_{k'}(q+k) \ . \end{aligned} \tag{4.10}$$

We note that $\hat{H}$ is Hermitian and that the quantum number M no longer explicitly occurs in (4.10). Moreover, since $\hat{H}$ is defined on $\hat{\mathscr{U}}_M$ and any vector of that space must satisfy Eq. (4.7), $\hat{H}$ and $\hat{K}$ possess common eigenvectors. This is only possible if these operators commute

$$[\hat{H},\hat{K}] = 0 \ . \tag{4.11}$$

In fact, it is not difficult to verify that Eq. (4.11) is fulfilled. Another useful way of writing $\hat{H}$ is as follows:

$$\hat{H} = \sum_{k,q} \omega_k(q) B_k^\dagger(q) B_k(q) - \hat{V} \ , \tag{4.12a}$$

where

$$\hat{V} = \frac{U}{N} \sum_{k,k',k''} \sum_{q,q'} B_{k+k'}^\dagger(q) B_{k'}(q+k) B_{k''}^\dagger(q') B_{k''}(q'-k) \ . \tag{4.12b}$$

Here it can be shown that $\hat{K}$ commutes separately with each term on the right-hand side of (4.12a). Equations (4.12) will now be used to prove that $\hat{H}$ leads to (4.9), where the expression in curly brackets is identical to that given by Eq. (4.8b). First, it is an easy exercise to show the validity of the following equation:

$$B_k(q) \mid (k_1,q_1);\ldots;(k_M,q_M)) = \sum_{i=1}^{M} \delta_{kk_i}\delta_{qq_i} \mid (k_1,q_1);\ldots;(k_{i-1},q_{i-1});(k_{i+1},q_{i+1});\ldots;(k_M,q_M)) \ . \tag{4.13}$$

A simple and straightforward calculation then yields

$$\sum_{k,q} \omega_k(q) B_k^\dagger(q) B_k(q) \mid (k_1,q_1);\ldots;(k_M,q_M)) = \sum_{i=1}^{M} \omega_{k_i}(q_i) \mid (k_1,q_1);\ldots;(k_M,q_M)) \tag{4.14}$$

and

$$\sum_{k'',q'} B_{k''}^\dagger(q') B_{k''}(q'-k) \mid (k_1,q_1);\ldots;(k_M,q_M)) = \sum_{i=1}^{M} \mid (k_1,q_1);\ldots;(k_i,q_i+k);\ldots;(k_M,q_M)) \ . \tag{4.15}$$

Using (4.13) again, we further obtain from (4.15)

$$B_{k'}(q+k)\sum_{i=1}^{M}|(k_1,q_1);\ldots;(k_i,q_i+k);\ldots;(k_M,q_M))$$

$$=\sum_{i=1}^{M}\delta_{k'k_i}\delta_{qq_i}|(k_1,q_1);\ldots;(k_{i-1},q_{i-1});(k_{i+1}q_{i+1});\ldots(k_M,q_M))$$

$$+\sum_{\substack{i,j=1\\ i>j}}^{M}\delta_{k'k_j}\delta_{q+k,q_j}|(k_1,q_1);\ldots;(k_{j-1},q_{j-1});(k_{j+1},q_{j+1});\ldots;(k_i,q_i+k);\ldots(k_m,q_M))$$

$$+\sum_{\substack{i,j=1\\ i<j}}^{M}\delta_{k'k_j}\delta_{q+k,q_j}|(k_1,q_1);\ldots;(k_i,q_i+k);\ldots;(k_{j-1}q_{j-1});(k_{j+1},q_{j+1});\ldots;(k_M,q_M))\ . \tag{4.16}$$

From (4.16) one then easily deduces the following result:

$$\hat{V}|(k_1,q_1);\ldots;(k_M,q_M))=\frac{U}{N}\sum_{i=1}^{M}\sum_{k}|(k_1,q_1);\ldots;(k_i-k,q_i);\ldots;(k_M,q_M))$$

$$+\frac{U}{M}\sum_{\substack{i,j=1\\ i<j}}^{M}\sum_{k}\{|(k_1,q_1);\ldots;(k_i-k,q_i+k);\ldots;(k_j,q_j-k);\ldots;(k_M,q_M))$$

$$+|(k_1,q_1);\ldots;(k_i,q_i-k);\ldots;(k_j-k,q_j+k);\ldots;(k_M,q_M))\}\ . \tag{4.17}$$

If Eqs. (4.14) and (4.16) are now multiplied by $(M!)^{-1/2}\psi$ and summed over all k_i and q_i $(i=1,\ldots,M)$, one ends up with Eq. (4.9), where $H_M\psi$ is precisely given by (4.8b). This completes the proof.

Equation (4.10) is not yet our final pair Hamiltonian, the latter being related to the former by a unitary transformation of the operators. Before we turn to the pair Hamiltonian, however, it is expedient first to investigate two well-known limiting cases of the Hubbard Hamiltonian. These will serve as test cases to show the equivalence of the original Hamiltonian (2.1) with its correspondent $\hat{H}$ of Eq. (4.10).

V. BAND LIMIT AND ATOMIC LIMIT

There are two limiting cases of the Hubbard Hamiltonian (2.1a), frequently referred to as "band limit" and "atomic limit," for which the eigenvalues and eigenvectors can be readily found. The band limit is obtained by setting $U=0$ in Eqs. (2.1), while the atomic limit results for $t=0$. These two cases and, in particular, the transition from band limit to atomic limit, were studied extensively by Hubbard[1] himself in order to explore the occurrence of the metal-insulator transition.[4] In the present section these two limits will be reconsidered, since they will serve as test cases to show the equivalence of the original Hamiltonian H of Eq. (2.1a) with its correspondent $\hat{H}$ in ideal boson space.

In terms of the fermion operators $a_{k\sigma}^{\dagger}$ and $a_{k\sigma}$ the band limit of the Hubbard Hamiltonian, Eq. (2.1a), is given by

$$H_0=\sum_{k,\sigma}\epsilon_k a_{k\sigma}^{\dagger}a_{k\sigma}\ \text{(band limit)}\ . \tag{5.1}$$

The atomic limit is more conveniently described by using Wannier operators $a_{n\sigma}$. These are related to the $a_{k\sigma}$ by

$$a_{k\sigma}=\frac{1}{\sqrt{N}}\sum_{n}a_{n\sigma}\exp(-ik\cdot R_n)\ , \tag{5.2}$$

where R_n is a lattice vector and n runs over all N lattice sites. In terms of Wannier operators the atomic limit of (2.1a) is then characterized by

$$H_U=U\sum_{n}N_{n\uparrow}N_{n\downarrow}\ \text{(atomic limit)}\ , \tag{5.1'}$$

where $N_{n\sigma}=a_{n\sigma}^{\dagger}a_{n\sigma}$.

In terms of ideal boson operators $B_k^{\dagger}(q)$ and $B_k(q)$ the band limit of $\hat{H}$, Eqs. (4.10) or (4.12), is described by

$$\hat{H}_0=\sum_{k,q}\epsilon_k(q)B_k^{\dagger}(q)B_k(q)\ \text{(band limit)}\ , \tag{5.3}$$

where $\epsilon_k(q)$ is given by (2.10c). Again the atomic limit of (4.12) is more conveniently described by using Wannier operators B_{nm} instead of the $B_k(q)$, these operators being related by

$$B_{nm}=\frac{1}{N}\sum_{k,q}B_k(q)\exp\{i[k\cdot R_m-(k+q)\cdot R_n]\}\ , \tag{5.4}$$

where Eqs. (5.2), (2.3), and (2.6) have been used. In terms of Wannier operators, the atomic limit of (4.12) is then obtained as

$$H_U=U\sum_{n,m}B_{nm}^{\dagger}B_{nm}-\hat{V}\ \text{(atomic limit)}\ , \tag{5.3'}$$

where $\hat{V}$ is now given by

$$\hat{V}=U\sum_{n,n'}\sum_{m}B_{nn'}^{\dagger}B_{nn'}B_{n'm}^{\dagger}B_{n'm}\ . \tag{5.3''}$$

For later purposes we also need the exchange operator $\hat{K}$ expressed in terms of Wannier operators. From Eqs. (4.5) and (5.4) one obtains

$$\hat{K}=\tfrac{1}{2}\sum_{n,n'}\sum_{m,m'} B^{\dagger}_{nm}B^{\dagger}_{n'm'}B_{nm'}B_{n'm} \ . \tag{5.5}$$

After these preliminary considerations, we will now show that the eigenvalues of the operators (5.1) are the same as those of the corresponding operators (5.3).

A. Band limit

One readily verifies that the eigenvectors of H_0 have the form

$$|\Psi^0_M\rangle = a^{\dagger}_{k_1,\downarrow}\cdots a^{\dagger}_{k_M,\downarrow}a_{k_1+q_1,\uparrow} \times\cdots a_{k_M+q_M,\uparrow}|\Psi_0\rangle \ , \tag{5.6}$$

while the corresponding eigenvalues are given by

$$E^0_M=\sum_{i=1}^{M}\epsilon_{k_i}(q_i) \ . \tag{5.7}$$

Here $|\Psi_0\rangle$ and $\epsilon_k(q)$ are defined by Eqs. (2.2) and (2.10c), respectively.

To solve the eigenvalue problem of $\hat{H}_0$, Eq. (5.3), we have to remember that since $\hat{H}_0$ and $\hat{K}$ commute, the eigenvectors of $\hat{H}_0$ also must be simultaneous eigenvectors of the exchange operator satisfying Eq. (4.7). Eigenvectors of $\hat{H}_0$ with the required properties are readily found and read

$$|\Psi^0_M)=\frac{1}{\sqrt{M!}}\sum_{q'_1,\ldots,q'_M}\chi_0\begin{bmatrix}k_1+q_1 & \cdots & k_M+q_M\\ k_1+q'_1 & \cdots & k_M+q'_M\end{bmatrix} \times|(k_1,q'_1);\ldots;(k_M,q'_M))\ , \tag{5.8}$$

where χ_0 is the following determinant:

$$\chi_0\begin{bmatrix}k_1+q_1 & \cdots & k_M+q_M\\ k_1+q'_1 & \cdots & k_M+q'_M\end{bmatrix}=\begin{vmatrix}\delta_{q'_1,q_1} & \delta_{k_1+q'_1,k_1+q_2} & \cdots & \delta_{k_1+q'_1,k_M+q_M}\\ \cdots & \cdots & \cdots & \cdots\\ \delta_{k_i+q'_i,k_1+q_1} & \delta_{k_i+q'_i,k_2+q_2} & \cdots & \delta_{k_i+q'_i,k_M+q_M}\\ \cdots & \cdots & \cdots & \cdots\\ \delta_{k_M+q'_M,k_1+q_1} & \delta_{k_M+q'_M,k_2+q_2} & \cdots & \delta_{q'_M,q_M}\end{vmatrix} \ . \tag{5.9}$$

We shall now prove that $|\Psi^0_M)$ satisfies Eq. (4.7) and is an eigenvector of $\hat{H}_0$. If we let $\hat{K}$ act on $|\Psi^0_M)$, a straightforward calculation yields

$$\hat{K}|\Psi^0_M)=\frac{1}{\sqrt{M!}}\sum_{\substack{i,j=1\\ i<j}}^{M}\sum_{q'_1,\ldots,q'_M}K_{ij}\chi_0 \times|(k_1,q'_1);\ldots;(k_M,q'_M))\ , \tag{5.10}$$

where $K_{ij}\chi_0$ is again a determinant similar to (5.9), differing from χ_0 only in that the ith and jth rows have been interchanged. Since $K_{ij}\chi_0=-\chi_0$, it follows immediately from (5.10) that $|\Psi^0_M)$ satisfies Eq. (4.7). To obtain $\hat{H}_0|\Psi^0_M)$, we use Eq. (4.14) and find

$$\hat{H}_0|\Psi^0_M)=\frac{1}{\sqrt{M!}}\sum_{i=1}^{M}\sum_{q'_1,\ldots,q'_M}\epsilon_{k_i}(q'_i)\chi_0 \times|(k_1,q'_1);\ldots;(k_M,q'_M))\ . \tag{5.11}$$

Here it is not immediately obvious that (5.11) is an eigenvalue equation for $|\Psi^0_M)$. By using elementary properties of determinants, however, one readily proves the following:

$$\sum_{i=1}^{M}\epsilon_{k_i}(q'_i)\chi_0=\sum_{i=1}^{M}\epsilon_{k_i}(q_i)\chi_0 \ . \tag{5.12}$$

If this result is now inserted into Eq. (5.11) we see at once that $|\Psi^0_M)$ is an eigenvector of $\hat{H}_0$ with eigenvalue E^0_M, where E^0_M is precisely given by Eq. (5.7). This then clearly shows the equivalence of the Hamiltonians (5.1) and (5.3) in the band limit.

B. Atomic limit

Here again an elementary calculation shows that the eigenvectors of H_U, Eq. (5.1′), have the form

$$|\Psi^U_M\rangle=a^{\dagger}_{n_1,\downarrow}\cdots a^{\dagger}_{n_M,\downarrow}a_{m_1,\uparrow}\cdots a_{m_M,\uparrow}|\Psi_0\rangle \ , \tag{5.13}$$

where the Wannier operators of Eq. (5.2) have been used. The corresponding eigenvalues are given by

$$E^U_M=U\left[M-\sum_{i,j=1}^{M}\delta_{n_i m_j}\right] \ . \tag{5.14}$$

As is evident from Eqs. (5.13) and (5.14), E^U_M can take the values $MU,(M-1)U,\ldots,0$ according to whether $M,M-1,\ldots$, etc., lattice sites are doubly occupied by a spin-up and a spin-down electron.

Turning now to the eigenvalue problem of $\hat{H}_U$, Eq. (5.3′), we again recall that since $\hat{H}_U$ and $\hat{K}$ commute, the eigenvectors of $\hat{H}_U$ must be simultaneous eigenvectors of $\hat{K}$ such that Eq. (4.7) is fulfilled. As in the band-limit case, it is not difficult to find eigenvectors with the required properties. Consider

$$|\Psi_M^U)=\frac{1}{\sqrt{M!}}\sum_{n_1',\ldots,n_M'}\chi_U\begin{bmatrix}n_1 & \cdots & n_M\\ n_1' & \cdots & n_M'\end{bmatrix}\times|(n_1',m_1);\ldots;(n_M',m_M))\,, \tag{5.15a}$$

where

$$|(n_1',m_1);\ldots;(n_M',m_M))=B^\dagger_{n_1',m_1}\cdots B^\dagger_{n_M'm_M}|\Psi_0) \tag{5.15b}$$

and χ_U is the determinant

$$\chi_U\begin{bmatrix}n_1 & \cdots & n_M\\ n_1' & \cdots & n_M'\end{bmatrix}=\begin{vmatrix}\delta_{n_1'n_1} & \delta_{n_1'n_2} & \cdots & \delta_{n_1'n_M}\\ \cdots & \cdots & \cdots & \cdots\\ \delta_{n_i'n_1} & \delta_{n_i'n_2} & \cdots & \delta_{n_i'n_M}\\ \cdots & \cdots & \cdots & \cdots\\ \delta_{n_M'n_1} & \delta_{n_M'n_2} & \cdots & \delta_{n_M'n_M}\end{vmatrix}\,. \tag{5.16}$$

In order to prove that $|\Psi_M^U)$ satisfies (4.7), let $\hat{K}$, as given by (5.5), act on $|\Psi_M^U)$. The result is similar to that of Eq. (5.10),

$$\hat{K}|\Psi_M^U)=\frac{1}{\sqrt{M!}}\sum_{\substack{i,j=1\\ i<j}}^{M}\sum_{n_1',\ldots,n_M'}K_{ij}\chi_U|(n_1',m_1);\ldots;(n_M',m_M))\,, \tag{5.17}$$

where $K_{ij}\chi_U$ is again a determinant differing from (5.16) only in that the ith and jth rows have been interchanged. Hence, by the same arguments as in the band-limit case, $|\Psi_M^U)$ satisfies Eq. (4.7). To obtain $H_U|\Psi_M^U)$, we first calculate $\hat{V}|(n_1',m_1);\ldots;(n_M',m_M))$, where $\hat{V}$ is given by (5.3''). This yields

$$\hat{V}|(n_1',m_1);\ldots;(n_M',m_M))=U\sum_{i,j=1}^{M}\delta_{n_i'm_j}|(n_1',m_1);\ldots;(n_M',m_M))\,. \tag{5.18}$$

From (5.18) we then easily get the expression for $H_U|\Psi_M^U)$:

$$H_U|\Psi_M^U)=MU|\Psi_M^U)-\frac{U}{\sqrt{M!}}\sum_{i,j=1}^{M}\sum_{n_1',\ldots,n_M'}\delta_{n_i'm_j}\chi_U|(n_1',m_1);\ldots;(n_M',m_M))\,. \tag{5.19}$$

As the last step, we again use elementary properties of determinants to obtain

$$\sum_{i=1}^{M}\delta_{n_i'm_j}\chi_U=\sum_{i=1}^{M}\delta_{n_im_j}\chi_U\,. \tag{5.20}$$

From Eqs. (5.19) and (5.20) it is now quite obvious that $|\Psi_M^U)$ is an eigenvector of $\hat{H}_U$ with the eigenvalue E_M^U, where E_M^U is the same as in Eq. (5.14). This result again shows the equivalence of the Hamiltonians (5.1') and (5.3') in the atomic limit.

In summary, the results of this section show that the original Hubbard Hamiltonian and its correspondent $\hat{H}$ in ideal boson space have identical eigenvalue spectra in two important limiting cases, namely the band limit and the atomic limit. As a by-product we have also obtained the eigenvectors of $\hat{H}$ for these limits. These might turn out to be useful in constructing trial eigenvectors of $\hat{H}$ for the intermediate region between the two limits.

VI. PAIR HAMILTONIAN

In Sec. V we have studied the limiting behavior of the boson expansion of the Hubbard Hamiltonian. We will now continue the development of Sec. IV by transforming the operators $B_k(q)$ so that the first term of Eq. (4.10) assumes diagonal form. The Hamiltonian resulting from this transformation will be our final pair Hamiltonian.

Let $A_p(q)$ be new boson operators related to the $B_k(q)$ by the unitary transformation

$$B_k(q)=\sum_p\phi_{kp}(q)A_p(q)\,. \tag{6.1}$$

Since (6.1) is required to be unitary, the coefficients must satisfy the following orthogonality and completeness relations:

$$\sum_p\phi^*_{kp}(q)\phi_{k'p}(q)=\delta_{kk'}\,,\qquad \sum_k\phi^*_{kp}(q)\phi_{kp'}(q)=\delta_{pp'}\,. \tag{6.2}$$

The new operators $A_p(q)$, hereafter referred to as *pair operators*, are then given by

$$A_p(q)=\sum_k\phi^*_{kp}(q)B_k(q)\,, \tag{6.1'}$$

and it is easy to show that they obey the ideal boson commutation relations (4.1). The *pair wave functions* $\phi_{kp}(q)$ will now be chosen such that the real symmetric matrix $W(q)$ of Eq. (4.8c) is brought to diagonal form. This will be the case if the pair wave functions satisfy the eigenvalue equation

$$\sum_{k'} W_{kk'}(q)\phi_{k'p}(q)=E_p(q)\phi_{kp}(q) . \tag{6.3}$$

Equation (4.10) is then transformed into the *pair Hamiltonian*[6]

$$\hat{H}=\sum_{p,q} E_p(q)A_p^{\dagger}(q)A_p(q) - \frac{U}{N}\sum_{p_1,\ldots,p_4}\sum_{k,q,q'} V_{p_1,\ldots,p_4}(k,q,q') \times A_{p_1}^{\dagger}(q)A_{p_2}^{\dagger}(q')A_{p_3}(q'-k) \times A_{p_4}(q+k) , \tag{6.4a}$$

where $E_p(q)$ are the *pair energies* and the interaction matrix elements are given by

$$V_{p_1,\ldots,p_4}(k,q,q')=\sum_{k',k''}\phi^*_{k+k',p_1}(q)\phi^*_{k'',p_2}(q') \times\phi_{k'',p_3}(q'-k)\phi_{k',p_4}(q+k) . \tag{6.4b}$$

The pair Hamiltonian (6.4) now has a form which one would intuitively expect: The first term represents independent pairs, while the second term describes the pair interactions. The exchange operator can be transformed similarly by inserting (6.1) into (4.5). This results in

$$\hat{K}=\tfrac{1}{2}\sum_{p_1,\ldots,p_4}\sum_{k,q,q'} K_{p_1,\ldots,p_4}(k,q,q') \times A_{p_1}^{\dagger}(q)A_{p_2}^{\dagger}(q')A_{p_3}(q'-k)A_{p_4}(q+k) , \tag{6.5a}$$

where the exchange matrix elements are given by

$$K_{p_1,\ldots,p_4}(k,q,q')=\sum_{k'}\phi^*_{k+k',p_1}(q)\phi^*_{k',p_2}(q') \times\phi_{k+k',p_3}(q'-k) \times\phi_{k',p_4}(q+k) . \tag{6.5b}$$

We emphasize once more that all eigenvectors of $\hat{H}$ must be simultaneous eigenvectors of $\hat{K}$ such that Eq. (4.7) is satisfied.

The pair energies $E_p(q)$ and wave functions $\phi_{kp}(q)$ entering the pair Hamiltonian, Eqs. (6.4), are formally given as the solutions of the eigenvalue equation (6.3). We will now show that these quantities can all be obtained in an *explicit* form.[6] From Eq. (6.3) we find that

$$\phi_{kp}(q)=(U/N)[\omega_k(q)-E_p(q)]^{-1}N_p(q) , \tag{6.6}$$

where $N_p(q)=\sum_k\phi_{kp}(q)$ is a normalization factor to be determined later. By summing Eq. (6.6) over k, one obtains the characteristic equation for the eigenvalues

$$D(E,q)=1+(U/N)\sum_k[E-\omega_k(q)]^{-1} . \tag{6.7}$$

The pair energies $E_p(q)$ are then given as the zeros of $D(E,q)$. We next multiply Eq. (6.6) by $\phi^*_{kp}(q)$, sum over all k, and make use of the orthogonality relations (6.2). This yields

$$U\frac{\partial D(E,q)}{\partial E}\bigg|_{E=E_p(q)}=-N\,|\,N_p(q)\,|^{-2} , \tag{6.8}$$

showing that the slopes of $D(E,q)$ at $E=E_p(q)$ are all negative. The qualitative behavior of this function is represented in Fig. 2.

The normalization factors $N_p(q)$ can be obtained from Eq. (6.8) and the easily proven relation

$$t\frac{\partial}{\partial t}[E_p(q)-\omega_k(q)]^{-1}+[E_p(q)-\omega_k(q)]^{-1} =\frac{E_p(q)-t\partial E_p(q)/\partial t-U}{[E_p(q)-\omega_k(q)]^2} ,$$

where t is the hopping matrix element of Eq. (2.1b). In this manner one obtains[6]

$$|\,N_p(q)\,|^2=\frac{N}{U}\left[U+t\frac{\partial E_p(q)}{\partial t}-E_p(q)\right] . \tag{6.9}$$

Equations (6.6) and (6.9) determine the pair wave functions once the energies $E_p(q)$ are known.

The pair energies can be determined by evaluating the characteristic function $D(E,q)$. A closer look at Fig. 2 reveals that the zeros of $D(E,q)$ fall into two distinct categories: There is one isolated zero (bound state), hereafter denoted as $E(q)$, which lies *below* the quasicontinuum of p-h energies $\omega_k(q)$. Since in this case none of the terms in Eq. (6.7) is divergent, $E(q)$ can be simply obtained by converting the sum in (6.7) to a k-space integral. Thus $E(q)$ is determined by[6]

$$\Omega_d\int_{\mathrm{BZ}}dk[\omega_k(q)-E]^{-1}=1, \quad \Omega_d=UV_c/(2\pi)^d , \tag{6.10}$$

where BZ indicates the Brillouin zone. Here V_c is the

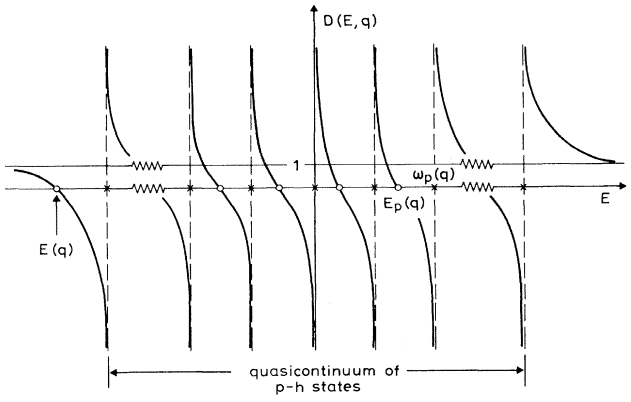

FIG. 2. Schematic plot of $D(E,q)$. The crosses ($\times$) and circles ($\circ$) indicate, respectively, the positions of the poles $\omega_p(q)$ and zeros $E_p(q)$ of $D(E,q)$ on the real E axis. The bound-state solution $E(q)$ is indicated by an arrow.

volume of the unit cell and d is the number of dimensions. All other solutions $E_p(q)$ (scattering states) of Eq. (6.7) fall inside the limits of the band in a way depicted in Fig. 2. To obtain these roots, much more care is needed in evaluating Eq. (6.7). In Appendix C we have demonstrated one possible method, based on Wentzel's[10] treatment, by which these roots may be obtained. According to Appendix C, these solutions are given by[6]

$$E_p(q)=\omega_p(q)-\frac{1}{\pi}\Delta_p(q)\tan^{-1}\left[\frac{\mathcal{N}[E_p(q)]}{D_0[E_p(q)]}\right], \tag{6.11a}$$

where

$$\mathcal{N}(E,q)=\pi\Omega_d\int_{\mathrm{BZ}}dk\,\delta[E-\omega_k(q)], \tag{6.11b}$$

$$D_0(E,q)=1+\Omega_d P\int_{\mathrm{BZ}}dk[E-\omega_k(q)]^{-1}, \tag{6.11c}$$

and $\Delta_p(q)$ is the spacing of two successive poles $\omega_k(q)$ at wave vector p. From Eqs. (6.10) and (6.11a) it is not difficult to see that in the limit $U/t\gg1$ (atomic limit), the energies $E(q)$ are separated from the $E_p(q)$ by a gap of $\sim U$. Hence, by the results of Sec. V B, the former energies correspond to low-energy states where all sites are singly occupied (homopolar states[5]), whereas the energies $E_p(q)$ belong to excited states where one site is doubly occupied (ionic states[5]).

The preceding expressions for the pair energies and wave functions are valid for any number of dimensions. Before we proceed to evaluate Eqs. (6.9), (6.10), and (6.11a) for the one-dimensional case, we wish to add a few remarks here: The pair energies and wave functions determined above are the exact eigenvalues and eigenfunctions of the full pair Hamiltonian (6.4a) for the particular case $M=1$. This is true because the interaction term of (6.4a) vanishes on the subspace $\hat{\mathcal{U}}_{M=1}$. Moreover, since the exchange operator $\hat{K}$ also vanishes on that subspace, the eigenvalue equation (4.7) is trivially fulfilled for any vector of this subspace. This implies that *the pair energies and wave functions are, at the same time, the exact solutions of the Hubbard Hamiltonian for* $M=1$, since (2.1a) is completely equivalent to (6.4a). Although this has been proved for general M in Sec. IV, the equivalence for $M=1$ can also be seen more directly by applying the Hubbard Hamiltonian (2.1a) on

$$|\Psi_p(q)\rangle=\sum_k\phi_{kp}(q)a^\dagger_{k,\downarrow}a_{k+q,\uparrow}|\Psi_0\rangle .$$

The requirement that $|\Psi_p(q)\rangle$ be an eigenvector of H leads to a condition for the $\phi_{kp}(q)$, which is exactly the same as Eq. (6.3). In particular, by specifying our solutions to one dimension we should recover the solutions derived by Lieb and Wu[2] for $M=1$. This will be verified below.

In one dimension, Eq. (2.1b) yields

$$\omega_p(q)=U-2t\{\cos(pa)-\cos[(p+q)a]\}, \tag{6.12}$$

where a is the lattice constant and the wave vectors p and q range over the one-dimensional Brillouin zone $(-\pi/a,\pi/a)$. From (6.12) the pole spacings $\Delta_p(q)$ are obtained as

$$\Delta_p(q)=(8\pi t/N)\,|\sin(\tfrac{1}{2}qa)\cos[(p+\tfrac{1}{2}q)a]|, \tag{6.13}$$

while Eqs. (6.11b) and (6.11c) yield the following:

$$\mathcal{N}(E,q)=U\{[4t\sin(\tfrac{1}{2}qa)]^2-(E-U)^2\}^{-1/2}, \tag{6.14a}$$

$$D_0(E,q)=1. \tag{6.14b}$$

By Eqs. (6.14a) and (6.14b), the pair energies[6] and wave functions are now readily calculated. Thus Eq. (6.10) becomes

$$E(q)=U-\{U^2+[4t\sin(\tfrac{1}{2}qa)]^2\}^{1/2}, \tag{6.15}$$

while Eqs. (6.11) lead to

$$E_p(q)=U-2t\{\cos(\varphi_p a)-\cos[(\varphi_p+q)a]\}, \tag{6.16a}$$

where the φ_p are pseudo-wave-vectors given by

$$\varphi_p=p\pm\frac{\pi}{Na}-\frac{2}{Na}\tan^{-1}\left[\frac{2t}{U}\{\sin[(p+q)a]-\sin(pa)\}\right]. \tag{6.16b}$$

Here the upper or lower sign applies according to whether the argument of the arctangent function is positive or negative, respectively. Equation (6.16b) is correct up to, and including, terms of the order $1/N$. Equations (6.15) and (6.16a) explicitly show that, for $U/t\gg1$, the energies $E(q)$ and $E_p(q)$ are separated by a gap of $\sim U$ since, in this limit, $E(q)$ tends to zero, while $E_p(q)$ approaches U.

The pair wave functions are given by Eq. (6.6), the normalization factors being determined by (6.9). From the latter equation we find that the normalization factor corresponding to the bound-state solution (6.15) is given by

$$|N(q)|^2=\frac{NU}{U-E(q)}, \tag{6.17}$$

while the one corresponding to (6.16a) is obtained as

$$|N_p(q)|^2=\frac{2\cos^2[(p+\frac{1}{2}q)a]}{\xi^2(q)+\cos^2[(p+\frac{1}{2}q)a]}, \tag{6.18a}$$

where

$$\xi^2(q)=U^2/[4t\sin(\tfrac{1}{2}qa)]^2. \tag{6.18b}$$

Having obtained the solutions for the one-dimensional case, we will now compare our results with those of Lieb and Wu[2] for $M=1$. According to Ref. 2, the ground-state energy of the one-dimensional Hubbard model for $M=1$ is determined by the coupled equations:

$$E(\Lambda)=-\frac{2t}{\pi}\int_{-\pi}^{\pi}dk(\sin k)\tan^{-1}[\xi^{-1}(\sin k-\Lambda)], \tag{6.19a}$$

$$Qa=\frac{1}{\pi}\int_{-\pi}^{\pi}dk\,\tan^{-1}[\xi^{-1}(\Lambda-\sin k)]. \tag{6.19b}$$

Here

$$\xi = U/(4t)$$

and (6.19c)

$$Q = \frac{2\pi}{Na} J ,$$

where J is integer (or half-odd integer) for N even (or odd). We will not attempt to solve Eqs. (6.19) for arbitrary values of Λ and ξ, but consider only two special cases for which these equations can be solved by a modest amount of labor. Consider first the case $\xi \gg 1$; here a Taylor-series expansion of the integrands leads to

$$E(\Lambda) = -\frac{2t\xi}{\xi^2+\Lambda^2}, \quad \Lambda = \xi \tan(\tfrac{1}{2}Qa) ,$$

where only terms of the order ξ^{-1} have been considered. By inserting Λ into the expression for the energy and replacing Q by $q \pm \pi/a$, we find

$$E(q) = -\frac{4t^2}{U}[1-\cos(qa)] . \tag{6.20}$$

It is now easy to verify that the same expression results from Eq. (6.15), if the square root is expanded to the same order of ξ. Consider next the case $\Lambda = 0$; here the integral in (6.19a) can be evaluated for arbitrary ξ yielding

$$E(0) = U - 4t(1+\xi^2)^{1/2} .$$

This again agrees with (6.15) for $qa = \pm\pi$.

We next turn to the energies $E_p(q)$ of Eq. (6.16a). According to our previous discussion, these belong to excited (or ionic-type[5]) states. As described in some detail by the authors of Ref. 5, such an excited state can be created by first adding an additional spin-down electron of wave vector k_+ to the system of N electrons in the state $|\Psi_0\rangle$ [see Eq. (2.2) and Fig. 1], and then removing one of the spin-up electrons with wave vector k_-. In the notation of Ref. 5, the energy of such a state is given by

$$E(k_+,k_-) = U - \mu(k_+) - \mu(k_-) , \tag{6.21a}$$

where

$$\mu(k_\pm) = E(N,0) - [E(N-1,0)]_{k_\pm} , \tag{6.21b}$$

and use has been made of the relation[2] $E(N,1) = U + E(0,N-1)$. We mention that Eqs. (6.21) differ from the exact expressions by terms of $O(1/N)$ since, in the chemical potentials μ, terms of the order $1/N$ have been neglected.[5] In Eq. (6.21b), $E(N,0)$ is the energy of the state $|\Psi_0\rangle$, which has been found to be zero in Sec. II, while

$$[E(N-1,0)]_{k_\pm} = -2t\sum_{j=1}^{N}{}' \cos(k_j a) . \tag{6.21c}$$

Here the prime on the summation sign indicates that the term $k_j = k_\pm$ is to be omitted. We further note that, for $M = 0$, the pseudo-wave-vectors k_j reduce to ordinary wave vectors [see Eq. (9) of Ref. 2] so that (6.21c) may be rewritten as

$$[E(N-1,0)]_{k_\pm} = 2t\cos(k_\pm a) , \tag{6.21d}$$

where we have used the fact that $\sum_k \cos(ka) = 0$. If we now set $k_+ = p \pm \pi/a$ and $k_- = p + q$, Eq. (6.21a) becomes

$$E(k_+,k_-) = \omega_p(q) ,$$

and we recover Eq. (6.16a), if terms of $O(1/N)$ are neglected in the latter equation. The preceding discussion should suffice to demonstrate that our pair energies are, in fact, identical to the energies found in Refs. 2 and 5 for the case $M = 1$.

In the present work we have restricted ourselves to the calculation of pair energies in one dimension since our primary purpose was to develop the general theory. The extension to higher dimensions presents no principal problems since the pair energies are given explicitly by Eqs. (6.10) and (6.11) for an arbitrary number of dimensions. Although the integrals, occurring in these equations can no longer be evaluated in closed form, they can be treated numerically. The numerical study of higher-dimensional lattices is planned to be considered in future work.

VII. SUMMARY AND CONCLUSION

In the present work a detailed account has been given of a recently[6] developed pair theory of the Hubbard Hamiltonian. The resulting pair Hamiltonian is an exact reformulation of the original Hubbard Hamiltonian in terms of pair operators, which satisfy elementary boson commutation relations. The Hamiltonian takes the familiar form of a sum of a quadratic part representing independent pair energies and a quartic part representing interactions between the pairs. The price one pays for this particularly simple formulation of the many-pair problem is that all eigenstates of the Hamiltonian are required to be simultaneous eigenstates of an exchange operator, which commutes with the Hamiltonian. Eigenvectors satisfying these requirements have been explicitly constructed for two limiting cases of the Hubbard model, the band limit and the atomic limit. We were also able to show that in these limits the eigenvalues of the pair Hamiltonian are the same as those of the original Hubbard Hamiltonian.

The energies and wave functions entering the pair Hamiltonian are formally given as the solutions of an eigenvalue equation. By solving the eigenvalue problem explicit analytical expressions for both pair energies and wave functions have been obtained for an arbitrary number of dimensions. The spectrum of pair energies is shown in Fig. 2 and may be described as follows: There is one eigenvalue (bound state), which lies below the quasicontinuum of p-h energies. In the atomic limit ($U/t \to \infty$), this eigenvalue corresponds to a homopolar state,[5] where all sites are singly occupied ($N-1$ sites by spin-up electrons and one site by a spin-down electron). All other eigenvalues (scattering states) fall inside the limits of the band of p-h states; in the atomic limit these eigenvalues are degenerate with each other and correspond to ionic states,[5] where one site is doubly occupied. In the same limit the ionic states are separated from the homopolar state by a gap of $\sim U$.

By a simple argument, we could further show that the pair energies and wave functions are the exact solutions of the Hubbard Hamiltonian for $M = 1$, where M is the num-

ber of spin-down electrons. This has been explicitly verified for the one-dimensional case, where we demonstrated that our pair energies are, in fact, identical to the exact energies found in Refs. 2 and 5 for the case $M=1$. In this connection, we mention a recent paper by Chui,[11] where he proposed the existence (in one dimension) of a bound state with an energy $\gtrsim U$, based on an extension of the Bethe-ansatz solution of Ref. 2 to complex wave vectors. Since, as demonstrated in Sec. VI, all solutions of the $M=1$ problem are given by the zeros of the characteristic function $D(E,q)$ of Eq. (6.7), where only real wave vectors occur, the existence of such a bound-state solution[11] seems to be ruled out, at least for $M=1$.

In this work we attempted to show that the pair-theory formalism possibly represents a very useful and interesting alternative to other methods of treating the Hubbard Hamiltonian, e.g., by more sophisticated Green's-function decoupling schemes. Further-reaching conclusions about the possibilities of the pair Hamiltonian approach can, however, only be drawn once a suitable variational (or perturbational) treatment of the pair Hamiltonian has been worked out.

So far we have restricted ourselves to the case of a half-filled band. We believe that the theory presented here can be extended to the case of arbitrary band filling, but preliminary considerations seem to indicate that such an extension is nontrivial. This question will be investigated in future work.

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APPENDIX A

In order to prove that $|\Psi_M\rangle$ of Eq. (3.1) is an eigenvector of $N_\downarrow$ with eigenvalue M, we start with the following equation which is readily proved by the use of induction:

$$\rho_k(q)\,|(k_1,q_1);\ldots;(k_M,q_M)\rangle=\sum_{i=1}^{M}\rho^\dagger_{k_1}(q_1)\cdots\rho^\dagger_{k_{i-1}}(q_{i-1})\rho^\dagger_{k_{i+1}}(q_{i+1})\cdots\rho^\dagger_{k_M}(q_M)[\rho_k(q),\rho^\dagger_{k_i}(q_i)]\,|\Psi_0\rangle$$
$$+\sum_{\substack{i,j=1\\ i<j}}^{M}\rho^\dagger_{k_1}(q_1)\cdots\rho^\dagger_{k_{i-1}}(q_{i-1})\rho^\dagger_{k_{i+1}}(q_{i+1})\cdots\rho^\dagger_{k_{j-1}}(q_{j-1})$$
$$\times\rho^\dagger_{k_{j+1}}(q_{j+1})\cdots\rho^\dagger_{k_M}(q_M)[[\rho_k(q),\rho^\dagger_{k_i}(q_i)],\rho^\dagger_{k_j}(q_j)]\,|\Psi_0\rangle\ . \tag{A1}$$

Here $|(k_1,q_1);\ldots;(k_M,q_M)\rangle$ is given by Eq. (3.2). We next multiply (A1) by $\psi/M!$, sum over all k_i and q_i $(1\le i\le M)$, and insert Eqs. (2.7) for the commutators. This yields

$$\rho_k(q)\,|\Psi_M\rangle=\frac{1}{M!}\sum_{i=1}^{M}\sum_{k_1,\ldots,k_M}\sum_{q_1,\ldots,q_M}\delta_{kk_i}\delta_{qq_i}\psi_{k_1,\ldots,k_M}(q_1,\ldots,q_M)$$
$$\times|(k_1,q_1);\ldots;(k_{i-1},q_{i-1});(k_{i+1},q_{i+1});\ldots;(k_M,q_M)\rangle$$
$$-\frac{1}{M!}\sum_{\substack{i,j=1\\ i<j}}^{M}\sum_{k_1,\ldots,k_M}\sum_{q_1,\ldots,q_M}\delta_{kk_j}\delta_{k+q,k_i+q_i}\psi_{k_1,\ldots,k_M}(q_1,\ldots,q_M)$$
$$\times|(k_1,q_1);\ldots;(k_i,q_j+k-k_i);\ldots;(k_{j-1},q_{j-1});(k_{j+1},q_{j+1});\ldots;(k_M,q_M)\rangle$$
$$-\frac{1}{M!}\sum_{\substack{i,j=1\\ i<j}}^{M}\sum_{k_1,\ldots,k_M}\sum_{q_1,\ldots,q_M}\delta_{kk_i}\delta_{k+q,k_j+q_j}\psi_{k_1,\ldots,k_M}(q_1,\ldots,q_M)$$
$$\times|(k_1,q_1);\ldots;(k_{i-1},q_{i-1});(k_{i+1},q_{i+1});\ldots;(k_j,q_i+k-k_j);\ldots;(k_M,q_M)\rangle\ , \tag{A2}$$

where the normalization factor $1/M!$ has already been included. In order to obtain $N_\downarrow|\Psi_M\rangle$, where $N_\downarrow$ is given by Eq. (2.11), we multiply (A2) by $\rho^\dagger_k(q)/M$ and sum over k and q. This results in

$$N_\downarrow \mid \Psi_M\rangle = \mid \Psi_M\rangle - \frac{2}{MM!}\sum_{\substack{i,j=1\\ i<j}}^{M}\sum_{k_1,\ldots,k_M}\sum_{q_1,\ldots,q_M}\psi_{k_1,\ldots,k_M}(q_1,\ldots,q_M)$$

$$\times \mid (k_1,q_1);\ldots;(k_i,q_j+k_j-k_i);\ldots;(k_j,q_i+k_i-k_j);\ldots;(k_M,q_M)\rangle\ .$$

The final step of the calculation consists in applying relation (3.6). This immediately yields the eigenvalue equation $N_\downarrow \mid \Psi_M\rangle = M \mid \Psi_M\rangle$, which we set out to prove.

APPENDIX B

In order to show that $H_M \mid \Psi_M\rangle$ has the form of Eq. (4.8a) with $H_M\psi$ given by (4.8b), we consider Eq. (A2) of Appendix A. On multiplying this equation by $M^{-1}\omega_k(q)\rho_k^\dagger(q)$ and summing over k and q, one obtains

$$\frac{1}{M}\sum_{k,q}\omega_k(q)\rho_k^\dagger(q)\rho_k(q)\mid\Psi_M\rangle = \frac{1}{MM!}\sum_{i=1}^{M}\sum_{k_1,\ldots,k_M}\sum_{q_1,\ldots,q_M}\omega_{k_i}(q_i)\psi_{k_1,\ldots,k_M}(q_1,\ldots,q_M)\mid(k_1,q_1);\ldots;(k_M,q_M)\rangle$$

$$-\frac{1}{MM!}\sum_{\substack{i,j=1\\ i<j}}^{M}\sum_{k_1,\ldots,k_M}\sum_{q_1,\ldots,q_M}[\omega_{k_i}(q_j+k_j-k_i)+\omega_{k_j}(q_i+k_i-k_j)]\psi_{k_1,\ldots,k_M}(q_1,\ldots,q_M)$$

$$\times \mid (k_1,q_1);\ldots;(k_i,q_j+k_j-k_i);\ldots;$$

$$\ldots;(k_j,q_i+k_i-k_j);\ldots;(k_M,q_M)\rangle\ . \tag{B1}$$

The second term of (B1) can be simplified by recalling Eq. (3.6) and by using the easily proven relations

$$\omega_{k_i}(q_j+k_j-k_i)+\omega_{k_j}(q_i+k_i-k_j)=\omega_{k_i}(q_i)+\omega_{k_j}(q_j)\ , \tag{B2a}$$

$$\sum_{\substack{i,j=1\\ i<j}}^{M}[\omega_{k_i}(q_i)+\omega_{k_j}(q_j)]=(M-1)\sum_{i=1}^{M}\omega_{k_i}(q_i)\ . \tag{B2b}$$

Equation (B1) then asssumes the simple form

$$\frac{1}{M}\sum_{k,q}\omega_k(q)\rho_k^\dagger(q)\rho_k(q)\mid\Psi_M\rangle = \frac{1}{M!}\sum_{i=1}^{M}\sum_{k_1,\ldots,k_M}\sum_{q_1,\ldots,q_M}\omega_{k_i}(q_i)\psi_{k_1,\ldots,k_M}(q_1,\ldots,q_M)\mid(k_1,q_1);\ldots;(k_M,q_M)\rangle\ . \tag{B3}$$

We next multiply Eq. (A2) by $(U/N)\rho_{k'}^\dagger(q)$, sum over k,k' and q to obtain

$$\frac{U}{N}\sum_{k,k',q}\rho_{k'}^\dagger(q)\rho_k(q)\mid\Psi_M\rangle$$

$$=\frac{U}{NM!}\sum_{i=1}^{M}\sum_{k}\sum_{k_1,\ldots,k_M}\sum_{q_1,\ldots,q_M}\psi_{k_1,\ldots,k_i+k,\ldots,k_M}(q_1,\ldots,q_M)\mid(k_1,q_1);\ldots;(k_M,q_M)\rangle$$

$$-\frac{U}{NM!}\sum_{\substack{i,j=1\\ i<j}}^{M}\sum_{k}\sum_{k_1,\ldots,k_M}\sum_{q_1,\ldots,q_M}\psi_{k_1,\ldots,k_M}(q_1,\ldots,q_M)$$

$$\times[\ \mid(k_1,q_1);\ldots;(k_i,q_j+k_j-k_i);\ldots;(k_j+k,q_i+k_i-k_i);\ldots;(k_M,q_M)\rangle$$

$$+\mid(k_1,q_1);\ldots;(k_i+k,q_j+k_j-k_i);\ldots;(k_j,q_i+k_i-k_j);\ldots;(k_M,q_M)\rangle]\ . \tag{B4}$$

In the middle term of (B4) we now substitute k_j-k for k_j, q_i-k for q_i, and q_j+k for q_j, while in the last term k_i is replaced by k_i-k, q_i by q_i+k, and q_j by q_j-k. This leads to

$$\begin{aligned}\frac{U}{N}\sum_{k,k',q}\rho^{\dagger}_{k'}(q)\rho_k(q)\,|\,\Psi_M\rangle
&=\frac{U}{NM!}\sum_{i=1}^{M}\sum_{k}\sum_{k_1,\ldots,k_M}\sum_{q_1,\ldots,q_M}\psi_{k_1,\ldots,k_i+k,\ldots,k_M}(q_1,\ldots,q_M)\,|\,(k_1,q_1);\ldots;(k_M,q_M)\rangle\\
&-\frac{U}{NM!}\sum_{\substack{i,j=1\\ i<j}}^{M}\sum_{k}\sum_{k_1,\ldots,k_M}\sum_{q_1,\ldots,q_M}[\,\psi_{k_1,\ldots,k_j-k,\ldots,k_M}(q_1,\ldots,q_i-k,\ldots,q_j+k,\ldots,q_M)\\
&\qquad+\psi_{k_1,\ldots,k_i-k,\ldots,k_M}(q_1,\ldots,q_i+k,\ldots,q_j-k,\ldots,q_M)]\\
&\qquad\times|\,(k_1,q_1);\ldots;(k_i,q_j+k_j-k_i);\ldots;(k_j,q_i+k_i-k_j);\ldots;(k_M,q_M)\rangle\ .\end{aligned}\tag{B5}$$

The final step consists in recalling Eq. (3.6) again and to subtract the resulting expression from Eq. (B3). These operations immediately lead to Eq. (4.8a), where the wave function $H_M\psi$ is precisely that given by Eq. (4.8b).

To conclude our proof, we still have to show that $H_M\psi$ satisfies the subsidiary conditions (3.8), provided that ψ itself satisfies these conditions. In view of the discussion given at the end of Sec. III, it suffices to consider only the case $M=2$. We thus have to prove the equation

$$K_{12}H_2\psi_{k_1k_2}(q_1q_2)=H_2\psi_{k_1k_2}(q_2+k_2-k_1,q_1+k_1-k_2)=-H_2\psi_{k_1k_2}(q_1q_2)\ ,\tag{B6a}$$

where $K_{ij}\psi$ is defined by (3.7b) and $H_2\psi$ is given by

$$\begin{aligned}H_2\psi_{k_1k_2}(q_1q_2)&=[\omega_{k_1}(q_1)+\omega_{k_2}(q_2)]\psi_{k_1k_2}(q_1q_2)-\frac{U}{N}\sum_k[\psi_{k_1+k,k_2}(q_1q_2)+\psi_{k_1,k_2+k}(q_1q_2)]\\
&-\frac{U}{N}\sum_k[\psi_{k_1+k,k_2}(q_1-k,q_2+k)+\psi_{k_1,k_2+k}(q_1+k,q_2-k)]\ .\end{aligned}\tag{B6b}$$

From Eqs. (B6) and (3.7b) we then obtain

$$\begin{aligned}K_{12}H_2\psi_{k_1k_2}(q_1q_2)&=H_2\psi_{k_1k_2}(q_2+k_2-k_1,q_1+k_1-k_2)\\
&=[\omega_{k_1}(q_2+k_2-k_1)+\omega_{k_2}(q_1+k_1-k_2)]\psi_{k_1k_2}(q_2+k_2-k_1,q_1+k_1-k_2)\\
&-\frac{U}{N}\sum_k[\,\psi_{k_1+k,k_2}(q_2'+k_2-k_1,q_1+k_1-k_2)+\psi_{k_1,k_2+k}(q_2+k_2-k_1,q_1+k_1-k_2)\\
&\qquad+\psi_{k_1+k,k_2}(q_2+k_2-k_1-k,q_1+k_1-k_2+k)\\
&\qquad+\psi_{k_1,k_2+k}(q_2+k_2-k_1+k,q_1+k_1-k_2-k)]\ .\end{aligned}\tag{B7}$$

With the aid of Eqs. (B2a) and (3.7b), this equation can be rewritten as

$$\begin{aligned}K_{12}H_2\psi_{k_1k_2}(q_1q_2)&=[\omega_{k_1}(q_1)+\omega_{k_2}(q_2)]K_{12}\psi_{k_1k_2}(q_1q_2)\\
&-\frac{U}{N}\sum_k K_{12}[\psi_{k_1+k,k_2}(q_1-k,q_2+k)+\psi_{k_1,k_2+k}(q_1+k,q_2-k)]\\
&-\frac{U}{N}\sum_k K_{12}[\psi_{k_1+k,k_2}(q_1q_2)+\psi_{k_1,k_2+k}(q_1q_2)]\ .\end{aligned}\tag{B8}$$

Since by assumption ψ itself satisfies the subsidiary condition (i.e., we have $K_{12}\psi=-\psi$), Eq. (B8) immediately leads to Eq. (B6a). Hence $H_2\psi$ satisfies the subsidiary conditions, ensuring the uniqueness of the expansion (4.8a).

APPENDIX C

We wish to determine here the zeros $E_p(q)$ of the characteristic equation

$$D(E,q)=1+(U/N)\sum_k [E-\omega_k(q)]^{-1} , \tag{C1}$$

with the exception of the bound-state (homopolar) solution $E(q)$, which is determined by Eq. (6.10). A schematic plot of $D(E,q)$ is shown in Fig. 2.

In order to determine these roots we closely follow the treatment given by Wentzel in Ref. 10. Subsequently, we shall consider, instead of Eq. (C1), the complex function

$$D(z)=1+(U/N)\sum_k (z-\omega_k)^{-1} , \tag{C2}$$

where z ($\mathrm{Re}z=E$) is a complex variable and where, for simplicity, we have dropped the parametric dependence on the wave vector q. As follows from Eq. (C2) or Fig. 2, $D(z)$ is a meromorphic function with simple poles and zeros at $z=\omega_k$ and $z=E_k$, respectively, which are all located on the real axis. Moreover, there is an equal number of poles and zeros and, except for the bound-state solution $E(q)$, there is exactly one zero between two successive poles (see also Fig. 2). From these remarks we may infer that Eq. (C2) can also be written as

$$D(z)=\frac{\prod_k (z-E_k)}{\prod_k (z-\omega_k)} . \tag{C3}$$

Subsequently, we shall also need the logarithmic derivative of $D(z)$. From Eq. (C3) we obtain

$$\frac{d}{dz}\ln D(z)=\frac{D'(z)}{D(z)}=\sum_k \left[\frac{1}{z-E_k}-\frac{1}{z-\omega_k}\right] . \tag{C4}$$

Let now $g(z)$ be a function which is analytic in the vicinity of the real axis and let Γ be the rectangular path in the complex plane as indicated in Fig. 3. The contour Γ encircles one pole at ω_p and one neighboring zero E_p such that both $g(z)$ and the logarithmic derivative of $D(z)$ are analytic on Γ. Then by Cauchy's integral formula and Eq. (C4) one obtains

$$\begin{aligned}&\int_\Gamma dz\, g(z)\frac{d}{dz}\ln D(z)\\ &\quad=\sum_k \int_\Gamma dz\, g(z)\left[\frac{1}{z-E_k}-\frac{1}{z-\omega_k}\right]\\ &\quad=2\pi i\,[g(E_p)-g(\omega_p)] .\end{aligned}$$

In particular, for $g(z)=z$ the following equation results:

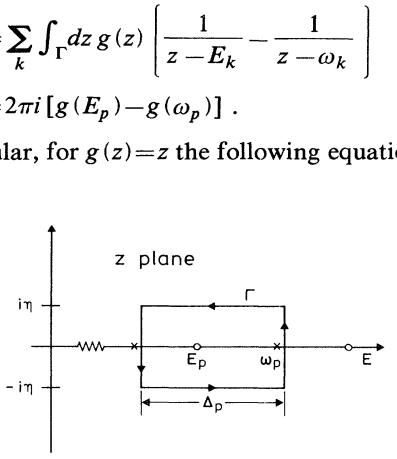

FIG. 3. Integration contour Γ in the complex plane. Γ encircles one pole ω_p and one zero E_p. Δ_p denotes the spacing of two successive poles at wave vector p.

$$E_p=\omega_p+\frac{1}{2\pi i}\int_\Gamma dz\, z\frac{d}{dz}\ln D(z) . \tag{C5}$$

According to the principle of argument, the variation in the argument of $\ln D(z)$ over the contour Γ is zero, since Γ contains exactly one pole and one zero; integration by parts then yields

$$E_p=\omega_p-\frac{1}{2\pi i}\int_\Gamma dz\,\ln D(z) . \tag{C6}$$

Thus the problem of finding the zeros of $D(z)$ is reduced to the evaluation of a contour integral over the function $\ln D(z)$.

As the next step, we let Γ approach the real axis by taking the limit $\eta\to 0+$, where $0+$ is a positive infinitesimal. In this limit the integral in (C6) becomes

$$\begin{aligned}\lim_{\eta\to 0+}\int_\Gamma dz\,\ln D(z)=\lim_{\eta\to 0+}\Big[&\int_{a-i\eta}^{b-i\eta} dz\,\ln D(z)\\ &+\int_{b+i\eta}^{a+i\eta} dz\,\ln D(z)\Big] .\end{aligned}$$

Here a and $b=a+\Delta_p$ are the points where Γ intersects the real axis and Δ_p denotes the spacing of two successive poles at wave vector p (see Fig. 3). We now substitute $z=E-i\eta$ in the first integral and $z=E+i\eta$ in the second integral on the right-hand side of the last equation. Equation (C6) then takes the form

$$E_p=\omega_p-\frac{1}{2\pi i}\lim_{\eta\to 0+}\int_0^b dE\,\ln\frac{D_-(E)}{D_+(E)} , \tag{C7a}$$

where

$$D_\pm(E)=D(E\pm i\eta)=1+(U/N)\sum_k (E-\omega_k\pm i\eta)^{-1} . \tag{C7b}$$

By recalling the standard expression

$$\lim_{\eta\to 0+}\frac{1}{x\pm i\eta}=\mathrm{P}\frac{1}{x}\mp i\pi\delta(x) ,$$

where P denotes Cauchy's principal value and $\delta(x)$ Dirac's δ function, we may rewrite the functions $D_\pm(E)$ as

$$D_\pm(E)=D_0(E)\mp i\mathcal{N}(E) , \tag{C8a}$$

where

$$D_0(E)=1+(U/N)\mathrm{P}\sum_k (E-\omega_k)^{-1} , \tag{C8b}$$

$$\mathcal{N}(E)=\pi(U/N)\sum_k \delta(E-\omega_k) . \tag{C8c}$$

Now insert Eqs. (C8) into (C7) to obtain

$$E_p=\omega_p-\frac{1}{\pi}\int_a^b dE\,\tan^{-1}\frac{\mathcal{N}(E)}{D_0(E)} . \tag{C9}$$

The final step of this analysis follows by application of the mean-value theorem, whence Eq. (C9) becomes

$$E_p=\omega_p-\frac{1}{\pi}\Delta_p\tan^{-1}\frac{\mathcal{N}(E_p)}{D_0(E_p)} . \tag{C10}$$

Here the variable E has been replaced by the zero E_p, which is located somewhere in the middle of the interval $(a, a+\Delta_p)$. Since the pole spacing Δ_p is of $\sim 1/N$, Eq. (C10) becomes exact in the large-N limit. This concludes the proof of Eqs. (6.11).

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