Pair Theory of the Hubbard Hamiltonian

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A pair theory of the Hubbard Hamiltonian is presented for the case of a half-filled band. The original Hamiltonian is reformulated exactly in terms of pair operators which satisfy boson commutation relations. The pair energies and wave functions are obtained explicitly. In the one-dimensional case, these reduce to the results derived by Lieb and Wu for $M = 1$. The pair Hamiltonian offers a better starting point for perturbation treatments or variational calculations.

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There is a common belief that the Hubbard model[1] incorporates the main physical effects which are due to electron correlation. Unfortunately, even this simplified model is not solvable by techniques available today. In one dimension, however, Lieb and Wu[2] were able to derive the exact solutions by generalizing Bethe's *Ansatz*[3] for the antiferromagnetic Heisenberg chain. Though this is an important first step towards an understanding of correlation effects in solids, not very much can be learned from this about the three-dimensional case. References to previous work in this field can be found in the review articles by Cyrot[4] and Ovchinnikov, Ukrainskii, and Kventsel.[5]

Since no obvious generalization of Bethe's *Ansatz* exists for more than one dimension, novel techniques are required. In this work we present a pair theory of the Hubbard Hamiltonian for the case of a half-filled band, which leads to an *exact* reformulation of the original Hamiltonian in terms of pair operators. These operators satisfy boson commutation relations and 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. Since the independent-pair energies already contain an appreciable amount of correlation energy, one may generally expect that the pair Hamiltonian offers a better starting point for perturbation treatments or variational calculations.

Pair theories have a long tradition,[6] and have been successfully applied to the high-density electron gas and other problems in solid-state physics.[7] It is also known, however, that exact pair theories are inevitably connected with serious mathematical difficulties. The origin of these difficulties lies in the fact that pair operators do not satisfy simple Bose or Fermi commutation relations. In 1963, Girardeau[8] presented a pair theory in which the pair operators do satisfy elementary boson commutation relations. The price one pays for this formulation is that all eigenstates of the Hamiltonian are required to be simultaneous eigenstates of a certain exchange operator, which commutes with the Hamiltonian. It is essentially Girardeau's method that will be used in the present work.

The one-band Hubbard Hamiltonian may be written as

$$H=\sum_{\sigma k}\epsilon_k a_{k\sigma}^{\dagger}a_{k\sigma}+\frac{U}{N}\sum_{kpq}a_{k+q\uparrow}^{\dagger}a_{p\uparrow}a_{p-q\downarrow}^{\dagger}a_{k\downarrow}, \quad (1)$$

where the energies ϵ_k are defined by

$$\epsilon_k=-t\sum_{\alpha}\exp(ik\cdot R_{\alpha}) \quad (t>0), \quad (1a)$$

and R_{α} denotes a nearest-neighbor lattice vector. Since H commutes with $N_{\sigma}=\sum_k a_{k\sigma}^{\dagger}a_{k\sigma}$, 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 0 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 $0\leq M\leq N/2$ without loss of generality. We next define a new vacuum by

$$|\Psi_0\rangle=\prod_k a_{k\uparrow}^{\dagger}|0\rangle, \quad (2)$$

and redefine the operator $a_{k\sigma}$ as

$$a_{k\sigma}=\begin{cases} b_k & \text{for } \sigma=\downarrow \text{ (particles)},\\ c_k^{\dagger} & \text{for } \sigma=\uparrow \text{ (holes)}.\end{cases} \quad (3)$$

It is easy to show that $|\Psi_0\rangle$ is an eigenvector of both $N_{\downarrow}$ and H with respective eigenvalues $M=0$ and $E_0=\sum_k\epsilon_k=0$. The Hubbard Hamiltonian may now be rewritten in terms of the new operators as

$$H=U\sum_k b_k^{\dagger}b_k+\sum_k\epsilon_k(b_k^{\dagger}b_k-c_k^{\dagger}c_k)-\frac{U}{N}\sum_{kpq}b_k^{\dagger}c_{k+q}^{\dagger}c_{p+q}b_p, \quad (4)$$

and we have, in addition, that $N_{\downarrow}=\sum_k b_k^{\dagger}b_k=\sum_k c_k^{\dagger}c_k$.

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

$$\rho_k(q)=c_{k+q}b_k,\quad \rho_k{}^\dagger(q)=b_k{}^\dagger c_{k+q}{}^\dagger, \tag{5}$$

and obey the following commutation relations:

$$[\rho_k(q),\rho_{k'}(q')]=[\rho_k{}^\dagger(q),\rho_{k'}{}^\dagger(q')]=0, \tag{6a}$$

$$[\rho_k(q),\rho_{k'}{}^\dagger(q')]=\delta_{kk'}\delta_{qq'}-\delta_{kk'}b_{k+q'}{}^\dagger b_{k+q}-\delta_{k+q,k'+q'}c_{k'}{}^\dagger c_k. \tag{6b}$$

Now let $\mathfrak{U}_M$ denote the subspace spanned by all simultaneous eigenvectors of H and $N_\downarrow$ for some fixed eigenvalue M of $N_\downarrow$. One can then readily show that the following relation holds on any subspace $\mathfrak{U}_M$ for $0<M\leq N/2$:

$$b_k{}^\dagger b_k=M^{-1}\textstyle\sum_q\rho_k{}^\dagger(q)\rho_k(q). \tag{7}$$

With the help of Eq. (7) and a similar relation for $c_k{}^\dagger c_k$, the Hamiltonian (4) can now be completely rewritten in terms of p-h operators. One obtains

$$H_M=\sum_{kk'}\sum_q\left\{\frac{1}{M}\,\omega_k(q)\delta_{kk'}-\frac{U}{N}\right\}\rho_k{}^\dagger(q)\rho_{k'}(q), \tag{8}$$

where

$$\omega_k(q)=\epsilon_k-\epsilon_{k+q}+U\quad(0<M\leq N/2). \tag{8a}$$

Consider now a general vector $|\Psi_M\rangle$ of the space $\mathfrak{U}_M$,

$$|\Psi_M\rangle=\sum_{k_1\cdots k_M}\sum_{q_1\cdots q_M}\psi_{k_1\cdots k_M}(q_1\cdots q_M)|(k_1q_1)\cdots(k_Mq_M)\rangle, \tag{9}$$

where

$$|(k_1q_1)\cdots(k_Mq_M)\rangle=\rho_{k_1}{}^\dagger(q_1)\cdots\rho_{k_M}{}^\dagger(q_M)|\Psi_0\rangle. \tag{10}$$

The above-mentioned mathematical difficulties now arise since, for $M\geq 2$, the set of all product states (10) is overcomplete.[8] This implies that a given vector $|\Psi_M\rangle$ of $\mathfrak{U}_M$ ($M\geq 2$) cannot be expanded in a unique way into the set of product states (10). The physical reason for the linear dependency between the pair product states rests upon the fact that 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 pairs. Girardeau[8] solved the overcompleteness problem by imposing subsidiary conditions on the space of wave functions ψ so that the latter all represent states having the correct symmetry under exchange of fermions between different pairs, and thus satisfy the Pauli principle. The subsidiary conditions imposed by Girardeau are

$$K_{ij}\psi_{k_1\cdots k_M}(q_1\cdots q_M)=-\psi_{k_1\cdots k_M}(q_1\cdots q_M), \tag{11}$$

where

$$K_{ij}\psi_{k_1\cdots k_M}(q_1\cdots q_M)=\psi_{k_1\cdots k_M}(q_1\cdots q_j+k_j-k_i\cdots q_i+k_i-k_j\cdots q_M)\quad(1\leq i<j\leq M). \tag{11a}$$

While it is not difficult to show that any wave function satisfying Eqs. (11) obeys the exclusion principle, it is by no means obvious that *the same conditions just suffice to remove the redundancy of the product states (10)*. For a proof of this assertion, the reader is again referred to Ref. 8. Hence, any given vector of $\mathfrak{U}_M$ can be uniquely represented by an expansion such as (9), provided the wave function ψ satisfies the conditions (11).

The preceding results enable us to express H_M of Eq. (8) in terms of "ideal-boson" operators $B_k(q)$ and $B_k{}^\dagger(q)$. These operators are defined to satisfy the usual boson commutation relations such as $[B_k(q),B_{k'}{}^\dagger(q')]=\delta_{kk'}\delta_{qq'}$, together with $B_k(q)|\Psi_0\rangle=0$, where $|\Psi_0\rangle$ is the ideal-boson vacuum. Once these operators have been defined, it is possible to construct an ideal state space $\hat{\mathfrak{U}}_M$. Given any vector $|\Psi_M\rangle$ of $\mathfrak{U}_M$, we define its unique image $|\Psi_M\rangle$ in $\hat{\mathfrak{U}}_M$ by

$$|\Psi_M\rangle=\sum_{k_1\cdots k_M}\sum_{q_1\cdots q_M}\psi_{k_1\cdots k_M}(q_1\cdots q_M)B_{k_1}{}^\dagger(q_1)\cdots B_{k_M}{}^\dagger(q_M)|\Psi_0\rangle, \tag{12}$$

with the *same* wave function ψ as in (9), which has been made unique by imposition of the subsidiary conditions (11). The ideal space $\hat{\mathfrak{u}}_M$ is then defined to be the set of all such states $|\Psi_M\rangle$ as $|\Psi_M\rangle$ runs over all of $\mathfrak{u}_M$. The conditions (11) can be more conveniently reformulated in terms of an eigenvalue problem in $\hat{\mathfrak{u}}_M$. Consider the following exchange operator:

$$\hat{K}=\tfrac{1}{2}\sum_{kk'}\sum_{qq'}B_{k+k'}{}^{\dagger}(q)B_{k}{}^{\dagger}(q')B_{k'}(q+k)B_{k+k'}(q'-k). \tag{13}$$

One can show[8,9] that imposition of the subsidiary conditions (11) is completely equivalent to the following eigenvalue equation:

$$\hat{K}|\Psi_M)=-\tfrac{1}{2}M(M-1)|\Psi_M). \tag{14}$$

In order to express H_M of Eq. (8) in terms of ideal-boson operators, one has to find the image of H_M in $\hat{\mathfrak{u}}_M$. A convenient way to do this is described in Refs. 8 and 9. In this manner, one ends up with the Hamiltonian

$$\hat{H}=\sum_{kk'q}W_{kk'}(q)B_{k}{}^{\dagger}(q)B_{k'}(q)-\frac{U}{N}\sum_{kk'k''}\sum_{qq'}B_{k+k'}{}^{\dagger}(q)B_{k''}{}^{\dagger}(q')B_{k''}(q'-k)B_{k'}(q+k), \tag{15}$$

where

$$W_{kk'}(q)=\omega_{k}(q)\delta_{kk'}-U/N. \tag{15a}$$

Since $\hat{H}$ is defined on $\hat{\mathfrak{u}}_M$ and any vector of that space has to satisfy Eq. (14), $\hat{H}$ and $\hat{K}$ possess common eigenvectors. This is only possible if these operators commute,

$$[\hat{H},\hat{K}]=0. \tag{16}$$

One readily verifies that Eq. (16) is fulfilled.

The final step consists in diagonalizing the first term of (15) by means of a unitary transformation of the operators. Let A and $A^{\dagger}$ be new boson operators related to the B and $B^{\dagger}$ operators by

$$B_{k}(q)=\sum_{p}\varphi_{kp}(q)A_{p}(q), \tag{17}$$

where the $\varphi_{kp}(q)$ are required to satisfy the eigenvalue equation

$$\sum_{k'}W_{kk'}(q)\varphi_{k'p}(q)=E_{p}(q)\varphi_{kp}(q). \tag{18}$$

Equation (15) is then transformed into the *pair Hamiltonian*

$$\hat{H}=\sum_{pq}E_{p}(q)A_{p}{}^{\dagger}(q)A_{p}(q)-\frac{U}{N}\sum_{p_1\ldots p_4}\sum_{kqq'}V_{p_1\ldots p_4}(kqq')A_{p_1}{}^{\dagger}(q)A_{p_2}{}^{\dagger}(q')A_{p_3}(q'-k)A_{p_4}(q+k), \tag{19}$$

where the first term represents the independent-pair energies, while the second term describes interactions between the pairs. Note that, because of the commutation rules, the interaction term of (19) vanishes identically on the subspace $\hat{\mathfrak{u}}_{M=1}$; evidently this result holds for any number of dimensions. The matrix elements are given by

$$V_{p_1\ldots p_4}(kqq')=\sum_{k'k''}\varphi_{k+k',p_1}{}^{*}(q)\varphi_{k''p_2}{}^{*}(q')\varphi_{k''p_3}(q'-k)\varphi_{k'p_4}(q+k). \tag{19a}$$

The exchange operator can be transformed similarly by inserting (17) into (13). Equations (19), (16), and (14) constitute the central results of this work.

For the applicability of the pair Hamiltonian (19), it is important that the energies $E_p(q)$ and wave functions $\varphi_{kp}(q)$ can all be given *explicitly*. I now show that this is indeed the case: Thus, from Eq. (18), we find that the energies are given as the zeros of the function

$$D(E,q)=1+(U/N)\sum_{k}\{E-\omega_{k}(q)\}^{-1}. \tag{20}$$

Further, the wave functions are obtained as

$$\varphi_{kp}(q)=(U/N)\{\omega_{k}(q)-E_{p}(q)\}^{-1}N_{p}(q), \tag{21}$$

where $N_p(q)=\sum_{k}\varphi_{kp}(q)$ is a normalization factor. The latter can be written more explicitly by making use of the orthonormality of the $\varphi_{kp}(q)$ and Eq. (20). This leads to

$$|N_{p}(q)|^{2}=(N/U)\{U+t\,\partial E_{p}(q)/\partial t-E_{p}(q)\}, \tag{21a}$$

where t is defined by Eq. (1a). A closer examination of Eq. (20) reveals that the zeros of $D(E,q)$

fall into two categories: There is one isolated zero, $E(q)$, which lies below the quasicontinuum of p-h states $\omega_k(q)$ and is determined by

$$\Omega_d \int dk/[\omega_k(q)-E]=1, \quad \Omega_d = UV_c/(2\pi)^d. \quad (22)$$

Here, V_c is the volume of the unit cell, d is the number of dimensions, and the integral extends over the whole Brillouin zone. All other zeros of (20) fall inside the limits of the band and can be obtained by contour integration.[6] One finds

$$E_p(q)=\omega_p(q)-\frac{1}{\pi}\Delta_p(q)\tan^{-1}\left\{\frac{\mathfrak{N}(E_p(q))}{D_0(E_p(q))}\right\}, \quad (23)$$

where

$$\mathfrak{N}(E,q)=\pi\Omega_d\int_{BZ} dk\,\delta\{E-\omega_k(q)\}, \quad (23a)$$

$$D_0(E,q)=1+\Omega_d \mathrm{P}\int_{BZ} dk\{E-\omega_k(q)\}^{-1}. \quad (23b)$$

In Eqs. (23), $\Delta_p(q)$ is the spacing of two successive poles $\omega_k(q)$ at wave vector p, and P denotes the principal value integral. Equations (21)–(23) are the desired expressions for the pair wave functions and energies. It can be seen from Eqs. (22) and (23) that for $U \gg t$ (atomic limit), the energies $E(q)$ (homopolar states[5]) are separated from the $E_p(q)$ (ionic states[5]) by a gap of $\sim U$.

In one dimension, where $\epsilon_k = -2t\cos(ka)$ (a is the lattice constant), Eqs. (22) and (23) reduce to

$$E(q)=U-\{U^2+(4t\sin\tfrac{1}{2}qa)^2\}^{1/2} \quad (24)$$

and

$$E_p(q)=U-2t\{\cos(\mathfrak{L}_p a)-\cos(\mathfrak{L}_p+q)a\}, \quad (25)$$

where

$$\mathfrak{L}_p = p \pm \frac{\pi}{Na} - \frac{2}{Na}\tan^{-1}\left\{\frac{2t}{U}[\sin(p+q)a-\sin(pa)]\right\}. \quad (25a)$$

In (25a), the upper or lower sign applies according to whether the argument of the arctangent is positive or negative, respectively. Equation (25a) is correct up to, and including, terms of the order $1/N$. It can be shown[9] that the energies given by (24) and (25) are identical to those derived by Lieb and Wu[2] for $M=1$. Although the details are too lengthy to present here, essentially this result follows because, as previously mentioned, the interaction term of (19) yields no contribution in this case. A more detailed account of the present work will be published elsewhere.[9]

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Coherent Transient Effects in Mössbauer Spectroscopy

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Coherent transient effects in Mössbauer spectroscopy due to phase modulation of recoilless γ radiation are considered both theoretically and experimentally. Absolute calibration of the source motion in the angstrom range and separation of the source and absorber contributions to the experimental linewidth were obtained from a single transient Mössbauer spectrum. A new phase-modulation method for generating short enhanced recoilless γ pulses is introduced.

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In a recent Letter[1] anomalous line shapes were reported in Mössbauer experiments with sinusoidal phase modulation at frequencies close to the linewidth of the Mössbauer state. Decaying interference oscillations appear in such transient Mössbauer (TM) spectra. Here, a general formula is derived for the time dependence of Mössbauer transmission due to phase modulation of γ