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New Model Hamiltonian for the Metal-Insulator Transition

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With use of the symmetry properties of the half-filled single-band Hubbard Hamiltonian, there is derived an effective Hamiltonian on a decimated lattice in which the spin and charge operators occur explicitly. Being a generalization of the Blume-Emery-Griffiths Hamiltonian for He^3-He^4 mixtures, this new statistical mechanical model permits one to give a preliminary discussion of the phase diagram of the correlated electron gas by establishing analogies with their results.

It is generally accepted that the metal-insulator transition, when described exclusively on the basis of electron correlation on a lattice with one electron per site, is due to a competition between the delocalizing effect of the hopping term and the localizing effect of the on-site repulsive Coulomb interaction as described by the Hubbard Hamiltonian[1]:

$$H=\sum_{i,j}\sum_{\sigma} t_{ij}\, c_{i\sigma}^{\dagger} c_{j\sigma} + U\sum_i n_{i\uparrow} n_{i\downarrow}. \tag{1}$$

Here $c_{i\sigma}^{\dagger}$ and $c_{i\sigma}$ are the creation and annihilation operators of an electron with spin σ in a Wannier state $\varphi_i(\vec{x})$ at site i and $n_{i\sigma}=c_{i\sigma}^{\dagger}c_{i\sigma}$ are the corresponding occupation numbers. We suppose that the hopping integrals $t_{ij}=t$ are nonzero only for nearest-neighbor sites.

It is still an open question whether this model is really capable of reproducing the anticipated phase diagram,[2,3] which is expected to show at least the following three features with the variation of the temperature: (1) a second-order phase transition from a paramagnetic insulator to an antiferromagnetic insulator when U is large in comparison with the bandwidth $W=2zt$ (z is the number of nearest neighbors in a simple cubic lattice); (2) a first-order phase transition from an antiferromagnetic insulator to a metal when U is small in comparison with W; (3) a first-order phase transition from a metal to a paramagnetic insulator when U is comparable with W.

So far nothing conclusive has been stated in the literature concerning the number and the nature of the intersection points of the various coexistence curves. In fact, only the first feature has been unquestionably established since for $U \gg W$, the Hubbard Hamiltonian becomes equivalent to the Heisenberg Hamiltonian.[2] The relevant quantities in this case are the local spin operators, each site being occupied by one electron with either spin up or spin down.

When the condition $U/W \gg 1$ does not hold, such a description is no longer valid and doubly occupied sites and empty sites will also occur. For a long time there has been a preoccupation with finding the relevant variables which would permit one to express the Hubbard Hamiltonian in the various regions of the parameters U/W and T/W (T being the temperature), so that the various competing mechanisms responsible for the spin ordering and the metalic and insulating state can be rendered directly apparent.

The normal procedure for achieving this goal has to a large extent been based, as it is usually done for other systems, on the functional formulation of the Hubbard problem with the purpose of deriving an effective Lagrangian in terms of classical spin and charge fields.[3] This approach has been shown[4] to encounter serious difficulties when it is required that the basic symmetry properties of the original Hubbard model (related to its fermion character) be maintained.

We shall here report on a derivation of a new effective Hamiltonian for the Hubbard problem based on an entirely different approach. This Hamiltonian represents a generalization of the Blume-Emery-Griffiths (BEG) Hamiltonian which was introduced in order to describe He^3-He^4 mixtures along the λ line and near the critical mixing point.[5]

Our new model Hamiltonian is constructed in such a way as to maintain the thermodynamics of the initial Hamiltonian at least as far as criticality is concerned. The underlying idea is to carry out a decimation procedure.[6] Decomposing the lattice (e.g., a simple cubic lattice) into two equivalent sublattices, we derive a partial trace partition function for the Hubbard Hamiltonian which corresponds to the elimination of the degrees of freedom of one sublattice. The effective Hamiltonian defined by the relation

$$\exp(-\beta H_{\text{eff}}) = \mathrm{Tr}_{\text{partial}}\, e^{-\beta(H-\mu N)} \tag{2}$$

will have the desired property of explicit occurrence of spin and charge fluctuation variables, with no limitation on the values of the parameters U/W and T/W. μ denotes the chemical potential, N is the operator for the total number of electrons, and $\beta = 1/kT$.

We are able to obtain the structure of our model Hamiltonian without carrying out the decimation procedure explicitly. In fact the following basic properties of the Hubbard model imply a definite structure of the decimated Hamiltonian: (1) The grand partition function associated with (1) is trivially invariant under a phase change of the Wannier representation $\varphi_i(\vec{x}) \to \varphi_i(\vec{x})\exp(i\alpha_i)$. The particular choice $\alpha_i - \alpha_j = \pi$ (i, j nearest-neighbor sites) implies

$$Z_\mu(t) = \mathrm{Tr}\, e^{-\beta(H-\mu N)} = Z_\mu(-t). \tag{3}$$

(2) Under particle-hole exchange, $c_{i\sigma}{}^\dagger \longleftrightarrow c_{i,-\sigma}$, we find that $H(t) - \mu N$ goes into $H(-t) - (U-\mu)N + (U-2\mu)N_s$ and consequently by means of (3)

$$Z_\mu(t) = \exp[-\beta(U-2\mu)N_s]\, Z_{U-\mu}(t); \tag{4}$$

N_s denotes the total number of sites. Taking the partial derivative of Eq. (4) with respect to μ, we obtain

$$\frac{1}{\beta}\frac{\partial}{\partial(U-\mu)} \ln Z_{U-\mu}(t) = 2N_s - \langle N\rangle. \tag{5}$$

If $\langle N\rangle = N_s$ (i.e., the system has on the average one electron per site), it follows that $U-\mu = \mu$ and hence $\mu = U/2$.

(3) We define the spin and charge operators as

$$\begin{aligned} &S_i{}^z = n_{i\uparrow} - n_{i\downarrow}; \quad S_i{}^+ = c_{i\uparrow}{}^\dagger c_{i\downarrow}; \\ &S_i{}^- = c_{i\downarrow}{}^\dagger c_{i\uparrow}; \quad \rho_i{}^z = n_{i\uparrow} + n_{i\downarrow} - 1; \\ &\rho_i{}^+ = c_{i\uparrow}{}^\dagger c_{i\downarrow}; \quad \rho_i{}^- = c_{i\downarrow} c_{i\uparrow}. \end{aligned} \tag{6}$$

Since the c's are fermion operators the following relations hold:

$$\begin{aligned} &(S_i{}^\nu)^2 + (\rho_i{}^{\nu'})^2 = 1, \\ &S_i{}^\nu \rho_i{}^{\nu'} = 0, \quad \nu, \nu' = x, y, z, \end{aligned} \tag{7}$$

where

$$\begin{aligned} &S_i{}^x = S_i{}^+ + S_i{}^-, \quad S_i{}^y = -i(S_i{}^+ - S_i{}^-), \\ &\rho_i{}^x = \rho_i{}^+ + \rho_i{}^-, \quad \rho_i{}^y = -i(\rho_i{}^+ - \rho_i{}^-). \end{aligned}$$

Considering the four possible states at any given site i ($|0\rangle$, $|\uparrow\downarrow\rangle$, $|\uparrow\rangle$, $|\downarrow\rangle$), we notice that the operators ρ are nonzero only when acting on the first two states (nonmagnetic sites), while the operators S are nonzero only when acting on the last two states (magnetic sites).

(4) We introduce the two unitary transformations

$$\begin{aligned} &U_s = \textstyle\prod_i \exp(i\alpha_i \vec{K}_i \cdot \vec{S}_i), \\ &U_\rho = \textstyle\prod_i \exp(i\gamma_i \vec{q}_i \cdot \vec{\rho}_i), \end{aligned} \tag{8}$$

where $\vec{K}_i$ and $\vec{q}_i$ are arbitrary unit vectors and α_i and γ_i are the parameters of the transformations. U_s represents a rotation in the "spin space" $|\uparrow\rangle$, $|\downarrow\rangle$ leaving the "charge space" $|0\rangle$, $|\uparrow\downarrow\rangle$ unaffected. It amounts to a local change of the quantization axis of the spin. Under U_s, $H - \mu N$ is invariant provided that a single vector $\vec{K}_i = \vec{K}$ and a single parameter $\alpha_i = \alpha$ are used for the whole lattice. U_ρ rotates the states $|0\rangle$ and $|\uparrow\downarrow\rangle$ and leaves the singly occupied states unchanged. The rotation in the x-y plane is a generalization of the particule-hole exchange considered above. The rotation around the z axis corresponds to a trivial change in the Wannier representation. It can be verified that under the transformation U_ρ, $H - \mu N$ is trivially invariant when $\vec{q}_i = \vec{q}$ is oriented in the z direction and $\gamma_i = \gamma$ for all lattice points. When $\vec{q}$ is in the x-y plane, $H - \mu N$ is still invariant provided that we subdivide the original lattice into two equivalent sublattices (each sublattice being made up by the nearest-neighbor sites of the other one) and that we carry out the rotation on the two sublattices with equal and opposite angles (i.e., $\gamma_i = \gamma$ and $\gamma_j = -\gamma$ with i, j being nearest-neighbor sites).

It is now easy to construct an effective Hamiltonian defined on a sublattice according to the decimation procedure outlined above. Because of the elimination of the degrees of freedom associated with one of the two sublattices, the effective Hamiltonian must be globally invariant under both of the transformations U_s and U_ρ given in (8). We shall limit ourselves to consideration of the one- and two-site interactions on the decimated lattice. The effective Hamiltonian must include a linear combination of the invariants which can be built in terms of the operator $\vec{S}_i$ and $\vec{\rho}_i$:

$$-\sum_{i,j} J_{ij}\vec{S}_i\cdot\vec{S}_j - \sum_{i,j} K_{ij} S_i^2 S_j^2 + \Delta\sum_i S_i^2 + \sum_{i,j} I_{ij}\vec{\rho}_i\cdot\vec{\rho}_j. \tag{9}$$

No other independent invariants can be built with the operators $\vec{S}_i$ and $\vec{\rho}_i$ because of the constraints (7), which reflect the fermion character of the original system.

The terms which are still missing are those which cannot be expressed in terms of $\vec{S}_i$ and $\vec{\rho}_i$ and must retain their form in terms of $c_i^\dagger$ and c_i. They are therefore necessarily odd in the number of $c^\dagger$ and c operators per site. The most general combination of these terms, which is invariant under the transformations U_s and U_ρ, is $\sum_{i,j}\sum_\sigma (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma})(1 - n_{i,-\sigma} - n_{j,-\sigma})$. If we consider only nearest-neighbor interactions, the most general expression for our model Hamiltonian therefore reads

$$H_{\text{eff}} = -J\sum_{i,j} \vec{S}_i\cdot\vec{S}_j - K\sum_{i,j} S_i^2 S_j^2 + \Delta\sum_i S_i^2 + I\sum_{i,j}\vec{\rho}_i\cdot\vec{\rho}_j + D\sum_{i,j}\sum_\sigma (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma})(1 - n_{i,-\sigma} - n_{j,-\sigma}). \tag{10}$$

The main new feature of this Hamiltonian, compared with the original Hubbard Hamiltonian (1) and its functional formulation, is that now the spin-spin interaction term leading to a magnetic order (which in the decimated Hamiltonian is of ferromagnetic rather than antiferromagnetic nature) and the interaction related to the charge fluctuations both appear explicitly. Moreover, this result is not confined to a limited region of the parameters U/W and T/W. The charge effect in (10) is included in the term proportional to I and via Eq. (7) in the terms proportional to K and Δ.

All the terms appearing in (10) derived purely from symmetry considerations are in fact present as has been explicitly verified by actually performing a decimation in a finite-lattice approximation in one dimension. The resulting expressions for the parameters entering (10) in terms of the original parameters U/W and T/W and the actual method of calculation will be reported elsewhere.

The effective Hamiltonian (10) is a generalization of the BEG Hamiltonian[5] given by expression (10) without the terms proportional to I and D. In the BEG model the spin-1 variable S_i is of Ising rather than Heisenberg type and assumes the value 0 if it is a He^3 atom that occupies the site i and ±1 if it is a He^4 atom. The two values for He^4 are introduced in order to allow for "superfluid ordering" described by the exchange term proprotional to J.

The physical analogy of the BEG model and the correlated electron-gas model described by our Hamiltonian (10) is the following: The sites occupied by the He^4 atoms correspond to magnetic sites with one electron with either spin up or spin down, which allows for ferromagnetic ordering. The sites occupied by He^3 atoms correspond to the nonmagnetic sites, which are either empty or doubly occupied and allow for electron itinerancy. In our case the He^3 concentration $x = 1 - \langle S_i^2\rangle$, corresponds to the number of nonmagnetic sites ($x = 1 - \langle (n_{i\uparrow} - n_{i\downarrow})^2\rangle = 2\langle n_{i\uparrow} n_{i\downarrow}\rangle$). This is a relevant parameter for describing the insulator-to-metal transition.[7]

The BEG analysis of the phase diagram for their Hamiltonian provides already in mean-field theory all the main features necessary for the phase diagram of the correlated electron system as outlined at the beginning. The BEG analysis has been essentially confirmed by the renormalization-group approach.[8] Depending on the relative values of the parameters, their model undergoes (1) a second-order phase transition to an ordered system starting from a normal mixture rich in He^4; (2) a first-order phase transition with a jump in both the order parameter and the concentration x; (3) a first-order phase transition ending in a critical point between two normal phases with a jump in the concentration from a He^4-rich phase to a He^3-rich phase. The intersection points of the coexistence curves vary in number and nature as illustrated in Fig. 6 of Ref. (5).

The second-order phase transition corresponds in our case to the analogous transition to a magnetically ordered insulating phase starting from a paramagnetic insulator. The He^4-rich phase corresponds to the predominance of the magnetic sites with one localized electron per site versus nonmagnetic sites, a situation which is realized when $U/W \gg 1$.

The first-order transitions are induced either by the superfluid ordering or by the interaction between the two components (He^3-He^4: nonmagnetic-magnetic sites). In our model the first mechanism accounts for the first-order phase transition from the magnetic insulator to the paramagnetic metal. This transition is the continuation of the second-order phase transition line into the region where the occurrence of magnetic sites is no longer dominant with respect to the nonmagnetic sites. The second mechanism accounts for the direct metal-insulator transition. This last statement will be further specified in the discussion of the two additional terms (proportional to I and D) present in our Hamiltonian.

As far as the first term is concerned, we should stress that the nonmagnetic sites have an internal structure which distinguishes between empty sites, $|0\rangle$, and doubly occupied sites, $|\uparrow\downarrow\rangle$. This feature is not present in the BEG model where only one state corresponds to $S_i = 0$. The interaction term $I\vec{p}_i \cdot \vec{p}_j$ acts within this internal structure in the same way that $J\vec{S}_i \cdot \vec{S}_j$ acts on the singly occupied spin-up or spin-down states $|\uparrow\rangle$, $|\downarrow\rangle$. Since there is no charge ordering in the physical region of the parameters of the Hamiltonian ($U \geq 0$), this term is important only in determining the relative occurrence of magnetic and nonmagnetic sites, resulting in a renormalization of the numerical values of K and Δ. It should therefore be irrelevant in determining the nature of the phase diagram in the physically relevant region.

The hopping term associated with D interchanges a site occupied by a He^4 atom with a site occupied by a He^3 atom, thus allowing for their relative motion. It is therefore important in determining the proper nature of the metallic phase.

We expect, therefore, that it will change the BEG results to take account of the specific metallic nature of the system under consideration. It should enrich the BEG structure in the sense that the first-order transition induced by the interaction between the two components should also allow for a transition from a phase where magnetic sites are dominant (insulator) to a phase where there is a balance between magnetic and nonmagnetic sites and which thus exhibits electron itinerancy.

A complete analysis of the phase diagram associated with our model Hamiltonian is now under study with use of various methods including a decoupling procedure of the equation of motion, a real-space renormalization-group approach, and the Migdal recurrence relations. However, it is already a firm result that the mechanisms leading to the various phases of the correlated electron system now have a clear physical interpretation.

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