Ground-state solutions of the Hubbard model

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The ground-state solutions of the Hubbard model are studied. A two-sublattice formalism is developed in order to allow ferromagnetic, ferrimagnetic, and antiferromagnetic solutions. The electronic structure is solved within the Bethe-lattice method and the size of the local moments on each sublattice are determinated in a self-consistent manner. We find that, for various values of the Coulomb repulsion (U) and as a function of the number of electrons (n), the ground state of the system may be that of a Pauli paramagnet, a ferromagnet, a ferrimagnet, or an antiferromagnet. It is also found that over a large region of the U-n phase diagram the ferrimagnetic state has a lower energy than the short-range-order phase reported by other authors.

The ground-state solutions of the Hubbard Hamiltonian have been extensively studied in recent years. By solving the local electronic structure within different methods,[1–4] several authors found four different phases in the Coulomb-repulsion (U)–electron-concentration (n) parameter space. These phases are as follows: the Pauli paramagnetic, the ferromagnetic, the antiferromagnetic, and the short-range ordered. The so-called short-range-ordered phase is characterized by a finite short-range order between the local magnetic moments, but with no long-range order. This phase could be visualized as a magnet above the Curie temperature where still some short-range order persists.

Here, we study the ground-state solutions within a model for itinerant-electron magnets, in which local moments are assumed to exist on each lattice site in both the magnetically ordered and in the short-range-ordered state.

In order to allow ferrimagnetic as well as antiferromagnetic solutions, we develop a two-sublattice formalism in which the local electronic structure is solved within the Bethe-lattice method and the local magnetic moments on each sublattice are obtained in a self-consistent manner.

We consider the Hubbard Hamiltonian in the unrestricted Hartree-Fock approximation

$$H=\sum_{i,j,\sigma} t_{ij}c_{i\sigma}^{\dagger}c_{j\sigma}+\sum_{i,\sigma}U\langle n_{i-\sigma}\rangle n_{i\sigma}-\sum_{i}U\langle n_{i\uparrow}\rangle\langle n_{i\downarrow}\rangle \quad , \tag{1}$$

where t_{ij} denotes the hopping integral for electronic transitions between lattice sites i and j, σ is the spin index, U is the Coulomb integral, $c_{i\sigma}^{\dagger}, c_{i\sigma}$ are the usual creation and annihilation operators for electrons on site i with spin σ, and $\langle n_{i\sigma}\rangle$ is the average number of electrons with spin σ at an atomic site i.

In order to allow ferromagnetic, ferrimagnetic, and antiferromagnetic solutions we subdivide a body-centered-cubic crystal into two equivalent sublattices, α and β. The magnetic moments at the two sublattices are defined by

$$\mu_{\nu}=\langle n_{\nu\uparrow}\rangle-\langle n_{\nu\downarrow}\rangle \quad , \quad \nu=\alpha,\beta \quad , \tag{2}$$

and the ferromagnetic, ferrimagnetic, and antiferromagnetic configurations correspond to $\mu_{\alpha}=\mu_{\beta}$, $|\mu_{\alpha}|\neq|\mu_{\beta}|$, and $\mu_{\alpha}=-\mu_{\beta}$, respectively. The short-range-ordered phase is characterized by magnetic moments of equal magnitude pointing parallel and antiparalled to a given direction. These magnetic moments are disordered from a long-range-order point of view but possess a finite short-range order.[2]

To calculate

$$\langle n_{\nu\sigma}\rangle=-\frac{1}{\pi}\int_{-\infty}^{\epsilon_F}d\omega\,\mathrm{Im}G_{0,0;\sigma}^{\nu}(\omega) \tag{3}$$

we determine the local Green's function for spin-σ electrons at a site of the sublattice ν from the set of equations

$$(\omega-\epsilon_{\nu\sigma})G_{0,0;\sigma}^{\nu}(\omega)=1-ZtG_{1,0;\sigma}^{\lambda}(\omega) \quad , \quad \nu,\lambda=\alpha,\beta \tag{4}$$

and

$$(\omega-\epsilon_{\lambda\sigma})G_{1,0;\sigma}^{\lambda}(\omega)=-tG_{0,0}^{\nu}(\omega)-(Z-1)tG_{2,0;\sigma}^{\nu} \quad , \tag{5}$$

$$\vdots$$

and so forth. Here, Z is the coordination number, $\epsilon_{\nu\sigma}$ is given by

$$\epsilon_{\nu\sigma}=\tfrac{1}{2}(n_{\nu}\pm\mu_{\nu}) \tag{6}$$

and

$$n_\nu = \langle n_{\nu\uparrow} \rangle + \langle n_{\nu\downarrow} \rangle \ . \tag{7}$$

In Eq. (6) the minus and the plus signs hold for spin-up and -down electrons, respectively.

The set of Eqs. (4) and (5) can be solved in the Bethe approximation by defining the transfer functions[5]

$$\gamma_{\alpha,\beta;\sigma} \equiv \frac{G^{\alpha}_{n,0;\sigma}}{G^{\beta}_{n-1,0;\sigma}}, \quad \gamma_{\beta,\alpha;\sigma} \equiv \frac{G^{\beta}_{n,0;\sigma}}{G^{\alpha}_{n-1,0;\sigma}} \ . \tag{8}$$

Substituting these definitions in Eqs. (4) and (5) we obtain for $\gamma_{\beta,\alpha;\sigma}$ the quadratic equation

$$(Z-1)t(\omega-\epsilon_{\beta\sigma})\gamma^2_{\beta,\alpha;\sigma}+(\omega-\epsilon_{\alpha\sigma})(\omega-\epsilon_{\beta\sigma})\gamma_{\beta,\alpha;\sigma} + t(\omega-\epsilon_{\alpha\sigma})=0 \ . \tag{9}$$

From this equation, we see that there is a gap in the local density of states given by

$$\Delta = \epsilon_{\beta\sigma} - \epsilon_{\alpha\sigma} \ . \tag{10}$$

This is a consequence of the periodicity of the magnetic moments and disappears in the ferromagnetic phase where $\mu_\alpha = \mu_\beta$.

The values for μ_ν are obtained in a self-consistent manner; this is done by requiring that

$$\mu_\nu = \int_{-\infty}^{\epsilon_F} (\rho_{\nu\uparrow} - \rho_{\nu\downarrow}) d\omega \ ; \quad \rho_{\nu\sigma} = -\frac{1}{\pi} \mathrm{Im} G^{\nu}_{0,0;\sigma} \tag{11}$$

and those used in Eq. (6) are equal. The Fermi energy is obtained from the equation

$$\tfrac{1}{2}(n_\alpha + n_\beta) = n \ . \tag{12}$$

The number of electrons on the two sublattices n_α and n_β are equal for the paramagnetic, ferromagnetic, short-range order, and antiferromagnetic arrangements. This is not the case of ferrimagnetic solutions where charge transfer between atoms in different sublattices exists.

The above formalism holds for ordered arrangements of magnetic moments. To obtain the electronic structure in the short-range-order (SRO) phase, pair probabilities have to be explicitly included[2] in Eqs. (4) and (5).

The degree of local order is given by the short-range-order parameter ξ defined by[6]

$$\xi = 1 - 2(p^{+-} + p^{-+}) \ , \tag{13}$$

where p^{+-} denotes the probability of finding a pair of magnetic moments pointing in opposite directions. This parameter takes the values of -1, 0, and 1 for the antiferromagnetic, completely random, and ferromagnetic situations.

In order to obtain the most stable state for a given Coulomb integral and a given number of electrons, we calculate all the different self-consistent solutions of our Hamiltonian and then we keep the one with the lowest energy. Our results are shown in Fig. 1, where we display the different phases in the $[U/2t(Z-1)^{1/2}]$ vs n parameter space. Five different phases were found. The ferromagnetic state is stable for large values of U and n. The boundary between this state and the paramagnetic phase is given by the Stoner condition:

$$U\rho(\epsilon_F) = 1 \ . \tag{14}$$

For values of n near the half-filled band, the energy is lowered by opening a gap in the local density of states (LDS) and forming an antiferromagnetic arrangement. Between the ferromagnetic and antiferromagnetic phases we find that the ferrimagnetic state has the lowest energy over a large region of the

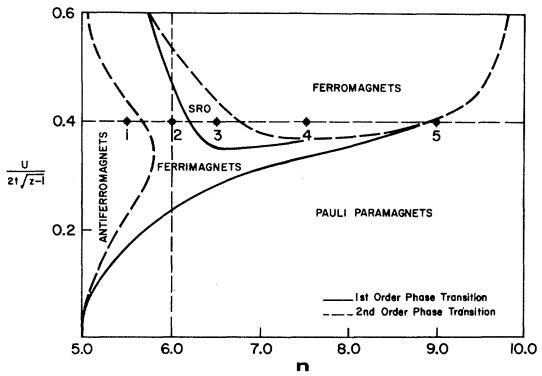

FIG. 1. Phase diagram in $[U/2t(Z-1)^{1/2}, n]$ parameter space, showing the different ground-state solutions to the Hubbard Hamiltonian in the Hartree-Fock approximation. Solid and broken lines correspond to first- and second-order phase transitions, respectively.

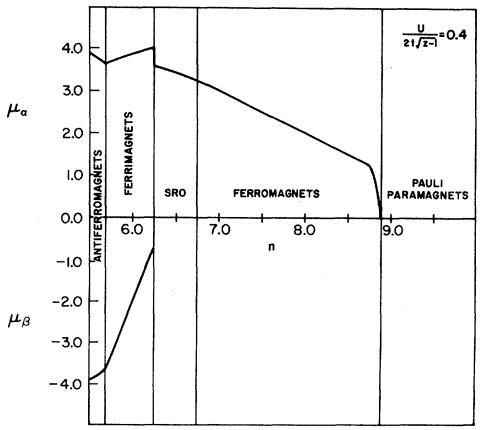

FIG. 2. Magnetic moments at the two sublattices μ_α and μ_β as a function of the number of electrons and for $U/2t(Z-1)^{1/2}=0.4$. The different magnetic phases are shown.

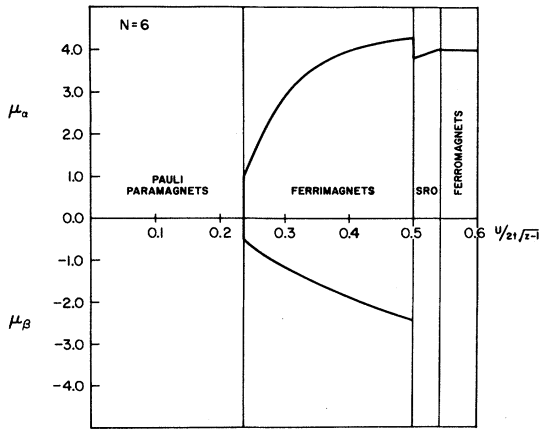

FIG. 3. Magnetic moments at the two sublattices, μ_α and μ_β as a function of the normalized Coulomb integral $U/2t(Z-1)^{1/2}$ and for $n=6.0$ electrons. The different magnetic phases are shown.

parameter space. We found also that there is a small section where the lowest energy corresponds to the short-range-order situation. Previous studies[1–4] did not consider ferrimagnetic solutions and reported only the short-range-order phase. We believe that if other more complex ordered states were considered, the SRO phase would eventually disappear. We show also in Fig. 1 that the phase transition between paramagnets-ferromagnets, ferromagnets-SRO, antiferromagnets-ferrimagnets, and ferromagnets-ferrimagnets is of second order and that the phase transition between paramagnets-ferrimagnets and ferrimagnets–short-range-order is of first order.

In Fig. 2 we show how the magnetic moments change as a function of n for $U/2t(Z-1)^{1/2}=0.4$. This line is shown in Fig. 1. A similar sequence is shown in Fig. 3 but in this case we fixed $n=6.0$ and plotted μ_α and μ_β as a function of the Coulomb integral. In these two figures the order of the phase transitions is clearly displayed.

As a final comment, we can say that within a simple method of solution we have found a richer phase diagram than those previously reported. Penn[7] has also shown, for a simple-cubic crystal and by using a more complicated method of solution, that other more complex ordered solutions with lower energy may exist.

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