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GROUND STATE PHASE DIAGRAM OF EXTENDED ATTRACTIVE HUBBARD MODEL †

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ABSTRACT

The ground state phase diagram of the extended Hubbard model with intraatomic attraction has been derived in the Hartree-Fock approximation formulated in terms of the Bogoliubov variational approach. For a given value of electron density, the nature of the ordered ground state depends essentially on the sign and the strength of the nearest neighbor coupling.

Due to the coupling between electrons and intra-molecular vibration or electronic excited states (Little 1964, Beni et al 1974) the effective intraatomic electronic interaction may become attractive. A modified Hubbard model has been used by many authors to investigate this problem (Takahashi 1969, Shiba 1972, Emery 1976, Efetov and Larkin 1976, Mertsching 1977, Robaszkiewicz 1979, Chao et al 1979). In particular, Anderson (1975), Street and Mott (1975) and Adler and Yoffe (1976) have applied the Hubbard model with attractive intraatomic interaction to the interpretation of the measured electrical, magnetic and optical properties of amorphous materials.

To be more general and to certain extent more realistic, recently the extended Hubbard model (including the nearest neighbor interactions) with intraatomic attraction has been studied. In this letter we will present its ground state phase diagram.

We start from the extended Hubbard Hamiltonian in Wannier representation

$$H = \sum_{ij\sigma}{}' t_{ij} a^{\dagger}_{i\sigma} a_{j\sigma} + \frac{U}{2}\sum_{i\sigma} n_{i\sigma} n_{i-\sigma} + \frac{1}{2}\sum_{ij\sigma\sigma'}{}' W_{ij} n_{i\sigma} n_{j\sigma'} - \mu \sum_{i\sigma} n_{i\sigma} \qquad (1)$$

Where $U<0$ and μ is the chemical poteneial. The primed sums exclude the terms with $i=j$. In Bloch representation, it becomes

$$H = \sum_{k\sigma} (\epsilon_k - \mu) c^{\dagger}_{k\sigma} c_{k\sigma} + \frac{1}{2N}\sum_{kk'q\sigma\sigma'} (W_q + U\delta_{\sigma-\sigma'}) c^{\dagger}_{k+q\sigma} c_{k\sigma} c^{\dagger}_{k'-q\sigma'} c_{k'\sigma'} \quad , \qquad (2)$$

where N is tha number of sites and ϵ_k and W_k are, respectively, the Fourier transforms of t_{ij} and W_{ij}.

Since t_{ij} and W_{ij} are spin independent, they can not cause any magnetic ordering. The intraatomic attraction favors the formation of singlet electron pair on each site. Consequently, the ground state of H is nonmagnetic and the only possible ordered-states are the charge-ordered and the singlet superconducting states.

Let N_e be the number of electrons. We consider the general situation that the electron density N_e/N has an arbitrary value between 0 and 2. However, we restrict ourselves to systems which can be divided into two interpenetrating sublattices A and B. That is, there exists a vector $\vec{Q}$ such that $\exp(i\vec{Q}\cdot\vec{R})=1$ if $\vec{R}$ belongs to A and $\exp(i\vec{Q}\cdot\vec{R})=-1$ if $\vec{R}$ belongs to B.

Following the Bogoliubov variational approach (Tyablikov 1967), an upper bound of the free energy can be obtained as

$$F_0 = -\frac{1}{\beta}\ln\{\mathrm{Tr}\{\exp(-\beta H_0)\}\} + \langle H-H_0\rangle_0 + \mu N_e \quad , \tag{3}$$

where $\beta=1/k_BT$, H_0 is a trial Hamiltonian, and $\langle\cdots\rangle_0$ is the thermal average with respect to H_0. Since the ground state of H is nonmagnetic, we only need to introduce a charge order parameter Δ and a superconducting order parameter $X_{\sigma-\sigma}$ to construct the trial Hamiltonian

$$H_0 = \sum_{k\sigma}(\epsilon_k-\mu-A_0)c^\dagger_{k\sigma}c_{k\sigma} - \frac{1}{2}\sum_{k\sigma}(\Delta c^\dagger_{k\sigma}c_{k+Q\sigma} + \mathrm{h.c.}) + \frac{1}{2}\sum_{k\sigma}(X_{\sigma-\sigma}c^\dagger_{k\sigma}c^\dagger_{-k-\sigma} + \mathrm{h.c.}) \ . \tag{4}$$

Here A_0, Δ and $X_{\sigma-\sigma}$ are variational parameters to minimize F_0. This approach is essentially the Hartree-Fock approximation.

With standard procedure, H can be easily diagonalized to yield four branches of eigenenergies $\pm A_k^\pm$:

$$A_k^\pm = \{(E_k \pm \bar{\mu})^2 + |X|^2\}^{1/2} \quad , \tag{5}$$

where $E_k=(\epsilon_k^2+\Delta^2)^{1/2}$, $\bar{\mu}=\mu+A_0$, $X=X_{\uparrow\downarrow}$ and k is restricted to the inner half of the first Brillouin zone. In terms of the eigenstates of H_0, F_0 can be readily calculated as

$$F_0/N = (A_0+\mu)(n-1) + \Delta n_Q + Xx_0^* + X^*x_0 + \frac{1}{4}U(n^2+n_Q^2+4|x_0|^2) + \frac{1}{2}ZW(n^2-n_Q^2)$$
$$- \frac{1}{\beta N}\sum_k\{\ln(2\cosh\beta A_k^+/2) + \ln(2\cosh\beta A_k^-/2)\} \quad , \tag{6}$$

where

$$n_Q = \frac{1}{N}\sum_{k\sigma}\langle c^\dagger_{k+Q\sigma}c_{k\sigma}\rangle_0 = \frac{\Delta}{2N}\sum_k\{(1+\frac{\bar{\mu}}{E_k})B_k^+ + (1-\frac{\bar{\mu}}{E_k})B_k^-\} \quad , \tag{7}$$

$$n = \frac{1}{N}\sum_{k\sigma}\langle c^\dagger_{k\sigma}c_{k\sigma}\rangle_0 = 1 + \frac{1}{2N}\sum_k\{(E_k+\bar{\mu})B_k^+ - (E_k-\bar{\mu})B_k^-\} \quad , \tag{8}$$

$$x_0 = \frac{X}{4N}\sum_k(B_k^+ + B_k^-) \quad , \tag{9}$$

with $B_k^\pm=(A_k^\pm)^{-1}\tanh(\beta A_k^\pm/2)$ and $ZW=-W_Q$. Here Z is the coordination number.

Now we can minimize F_0 with respect to Δ, X and A_0. The optimum values of these parameters are

$$\Delta = \frac{1}{2}(2ZW-U)n_Q \quad , \tag{10}$$

$$X = -Ux_0 \quad , \tag{11}$$

$$A_0 = -\frac{1}{2}(2ZW+U)n \quad . \tag{12}$$

The minimum free energy then turns out to be

$$F_0/N = \bar{\mu}(n-1) + \frac{1}{4}(U+2ZW)n^2 - \Delta^2/(U-2ZW) - |X|^2/U$$
$$- \frac{1}{\beta N}\sum_k\{\ln(2\cosh\beta A_k^+/2) + \ln(2\cosh\beta A_k^-/2)\} \quad . \tag{13}$$

The ground state energy is readily obtained as

$$E_0/N = \lim_{\beta\to\infty}(F_0/N) = \bar{\mu}(n-1) + \frac{1}{4}(U+2ZW)n^2 - \Delta^2/(U-2ZW) - |X|^2/U - \frac{1}{2N}\sum_k(A_k^+ + A_k^-) \ . \tag{14}$$

For given values of U, W, n and the band structure ϵ_k, we solve for Δ, X, A_0 and the chemical potential μ from Eqs. (7)-(12). There are four branches of solutions for four different phases: (i) $\Delta\neq0$ and X=0 for the charge-ordered (CO) state, (ii) $\Delta=0$ and $X\neq0$ for the singlet-superconducting (SS) state, (iii) $\Delta\neq0$ and $X\neq0$ for the mixed (M) state of CO and SS, and (iv) $\Delta=X=0$ for the non-ordered (NO) state. We then compare the energies of various solutions, using Eq. (14) to determine the ground state structure. To get the explicit results, we have assumed a square density of states with bandwidth 2D.

For $W\leq0$ we found no M-phase solution and for the other three phases the coupled equations can be solved analytically. The ground state is SS for all values of n if W<0. However, if W=0 the ground state remains SS for $n\neq1$ but becomes degenerate in SS, M and CO for n=1. This phase diagram is very simple compared to the phase diagram of the ordinary Hubbard model (W=0 and U>0), as shown in Fig. 1.

The coupled equations can still be solved analytically for the CO, the SS and the NO phases even if W>0. However, for the M phase one must solve the problem numerically. Furthermore, due to the technical difficulty, reliable solution can be derived only in the weak coupling regime. That is, (2ZW-U)/2D should not be too large. In Fig. 2 we show the phase boundaries separating the M and the SS phases for various values of |U|/2D=0.25, 0.5 and 1. On the vertical axis, i.e., for n=1 the ground state is charge-ordered. The limitting positions of the phase boundaries as $ZW/D \to \infty$ are marked on the horizontal axis by arrows. However, we should point our that such limitting positions may not be accurate because the numerical solution for the M phase contains error when (2ZW-U)/2D gets too large. All the transitions across the phase boundaries are second order.

To finish up this letter, we would like to emphasize that although the detail structure of the phase diagram depends on the density of states used, the following feature is characteristic to the model Hamiltonian itself. The CO phase is not stable and the ground state is always SS for all values of |U|/2D and n if W<0. The CO phase begins to appear together with the SS and the M phases as the degenerate ground state when W=0 and n=1. It becomes the only stable phase as the nondegenerate ground state when W>0 and n=1. With increasing |U|/2D and W, the region of |n-1| in which the M phase is stable grows at the expense of the region of the stable SS phase.

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FIGURE CAPTIONS

Fig. 1. The left side is the phase diagram of the extended attractive Hubbard model ($W\leq 0$ and $U<0$) and the right side is that of the ordinary Hubbard model ($W=0$ and $U>0$). On the vertical line with n=1, the SS, the M and the CO phases are degenerate for $U<0$ and $W=0$, while the AF is the stable one for $U>0$ and $W=0$.

Fig. 2. The phase diagrams for $W>0$ and $U<0$ with the values of $|U|/2D$ marked next to the phase boundaries which separate the SS and the M phases. Heavy arrows indicate the limitting positions of the phase boundaries as $ZW/D \to \infty$. The vertical axis with n=1 is the region of stable CO phase.

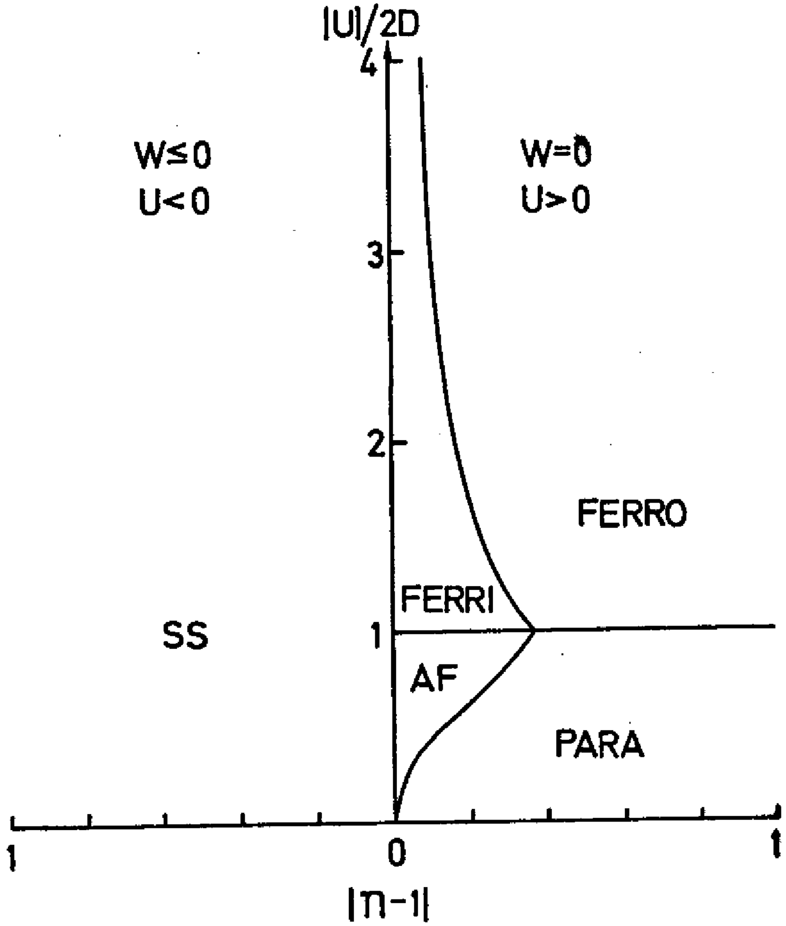

FIG. 1

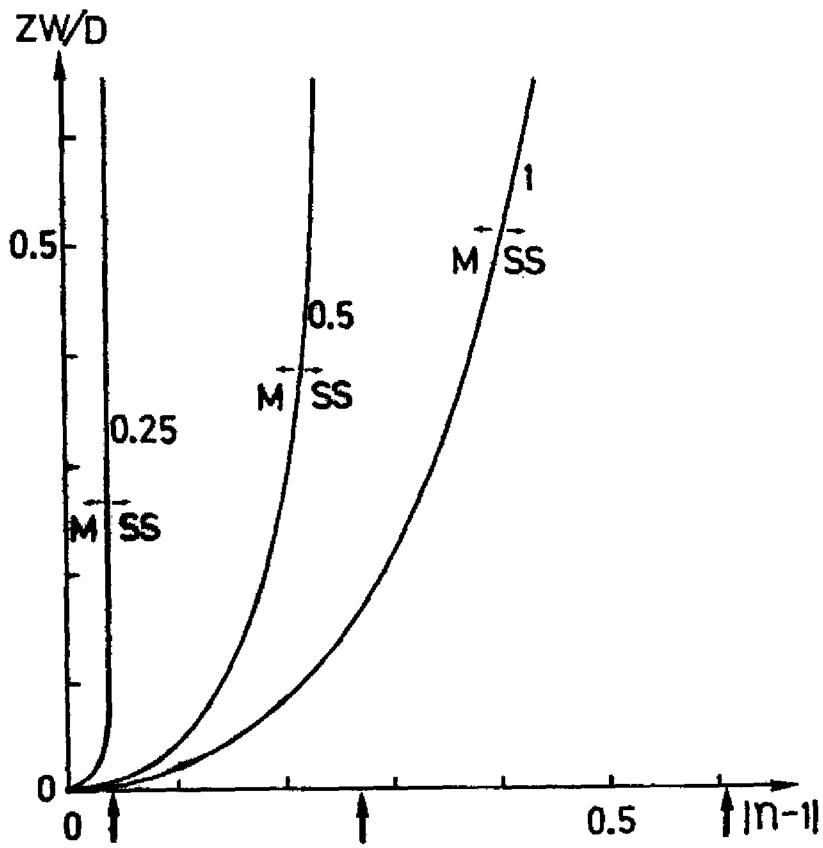

FIG.2

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