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Hartree theory for the negative-U extended Hubbard model: Ground state

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We have investigated the ground-state properties of the negative-U extended Hubbard model in the weak-coupling regime with the Hartree theory formulated in terms of the Bogoliubov variational approach. While the pure phases of charge order (CO), singlet superconducting (SS), and nonordered can be solved analytically with a model density of states, the mixed phase of CO and SS requires numerical computation. The ground-state phase diagram is derived, and the order parameters and the chemical potential of the ground state are analyzed. The characteristic difference between the behaviors of the SS and the CO order parameters at very weak coupling suggests a complicated competition between various interactions. Present results are compared with those derived earlier for the strong-coupling regime.

I. INTRODUCTION

Extensive investigations on the Hubbard model[1] point out the fact that the model Hamiltonian including only the electron-transfer integral and the intra-atomic Coulomb repulsion U is inadequate to describe realistic systems. One generalization is to take into account the exchange and correlation between electrons located on different atoms (the extended Hubbard model). We then face the problem of what should be the proper values of these interaction energies which are screened to various extents. Even for the simple Hubbard model there is no answer to the correct value of the screened effective U. However, estimates suggested the possible existence of the novel situation of an effective intra-atomic attraction (negative U) due to the coupling between electrons and intramolecular vibrations or electronic excited states,[2–5] or between electrons in different bands in a chemical complex.[6]

Anderson,[7] Street and Mott,[8] and Adler and Yoffa[9] could explain the electrical, magnetic, and optical properties of amorphous materials with such a Hubbard model with attractive intra-atomic interaction (AII). Ionova *et al.*[6,10] suggested the use of this model with AII to tackle the alternating-valence ordering in some inorganic compounds. The negative-U states have recently been connected to the silicon vacancies[11] and the defects in glasses.[12] Since it is difficult to determine accurately the values of U in different materials, the qualitative features of the AII Hubbard model have been studied by many authors[13–23] taking U as a varying parameter.

If the effective U is negative, it favors the formation of pairs of antiparallel spin electrons on same atom. Therefore, the ground state of the AII Hubbard model exhibits no magnetic ordering. For the case of one electron per atom, the mean-field approximation[24,25] and the solution derived from the functional integral method[26,27] as well as the variational treatment[28] predict a charge-ordered ground state in the large-$|U|$ limit.

On the other hand, there is only a little work on the AII extended Hubbard model including the interatomic electron interactions. The existing papers[17–19,29] have drawn interesting conclusions mainly for the strong correlation limit. In this paper we will investigate the ground-state properties of the AII extended Hubbard model for weak correlation with the Hartree approximation (HA). From the study of the ordinary Hubbard model, the HA gives rather reliable results at $T=0$. For example, HA predicts the existence of an energy gap in the single-particle excitation spectrum and gives the ground-state energy in

good agreement with the exact solution of Lieb and Wu[30] in a large range of the value of U.[31] Also, at the zero-bandwidth limit the HA calculation for the half-filled extended Hubbard model (positive U) gives the exact ground-state energy and the correct condition for the existence of the charge-ordered state.[22]

In Sec. II we present the Hartree theory for the AII extended Hubbard model. It is possible to derive analytical solutions for some special cases as we will see in Sec. III. Section IV is devoted to the numerical solutions for the ground-state phase diagram, the chemical potential, and the order parameters. A short discussion follows in Sec. V.

II. HARTREE THEORY

Consider the AII extended Hubbard Hamiltonian

$$H=\sum_{ij\sigma}{}' t_{ij}c_{i\sigma}^{\dagger}c_{j\sigma}+\frac{1}{2}U\sum_{i\sigma}n_{i\sigma}n_{i-\sigma}+\frac{1}{2}\sum_{ij\sigma\sigma'}{}' W_{ij}n_{i\sigma}n_{j\sigma'}-\mu\sum_{i\sigma}n_{i\sigma}\ , \tag{2.1}$$

where $c_{i\sigma}^{\dagger}$, $c_{i\sigma}$, and $n_{i\sigma}$ are, respectively, the creation, the destruction, and the number operators associated with the localized orbital at site i. t_{ij} is the hopping integral and $U<0$ is the intra-atomic attraction energy. The interatomic interaction energy W_{ij} is assumed in this paper to be spin independent for simplicity. μ is the chemical potential. In the Bloch representation we have

$$H=\sum_{k\sigma}(\epsilon_k-\mu)c_{k\sigma}^{\dagger}c_{k\sigma}+\frac{1}{2N}\sum_{kk'q\sigma\sigma'}(W_q+U\delta_{\sigma-\sigma'})\times c_{k+q\sigma}^{\dagger}c_{k\sigma}c_{k'-q\sigma'}^{\dagger}C_{k'\sigma'}\ , \tag{2.2}$$

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

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 approach,[32] an upper bound of the free energy can be obtained as

$$F_0=-\frac{1}{\beta}\ln\{Tr[\exp(-\beta H_0)]\}+\langle H-H_0\rangle_0+\mu N_e\ , \tag{2.3}$$

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.

The first term in the Hamiltonian (2.1) is of the Bloch-electron character and so will not yield any magnetic ordering. No magnetic ordering can be introduced by the third term in H since it is spin independent. The second term in Eq. (2.1) favors the formation of pairs of antiparallel spin electrons on various atoms. Therefore, the ground state of H exhibits no magnetic ordering. We then only need to introduce a charge order parameter Δ and a singlet-superconducting order parameter $X_{\sigma-\sigma}$ to construct the trial Hamiltonian

$$H_0=\sum_{k\sigma}(\epsilon_k-\mu-A_0)c_{k\sigma}^{\dagger}c_{k\sigma}-\frac{1}{2}\sum_{k\sigma}(\Delta c_{k\sigma}^{\dagger}c_{k+Q\sigma}+\text{H.c.})+\frac{1}{2}\sum_{k\sigma}(X_{\sigma-\sigma}c_{k\sigma}^{\dagger}c_{-k-\sigma}^{\dagger}+\text{H.c.})\ . \tag{2.4}$$

Here A_0, Δ, and $X_{\sigma-\sigma}$ are variational parameters to minimize F_0. Comparing Eqs. (2.2) and (2.4), we see that this approach is essentially the Hartree approximation, though some authors[33–36] called it the Hartree-Fock approximation in their treatments of the ordinary extended Hubbard model with positive U. H_0 is also similar in mathematical structure to Eq. (2.5) of Levin *et al.*[37] where they named it the mean-field effective Hamiltonian. We will return to this point for discussion in Sec. V.

H_0 can be easily diagonalized with either the Green's-function or the equation-of-motion approach. The energy spectrum of H_0 consists of four branches

$$A_k^{\pm}=[(E_k\pm\bar{\mu})^2+|X|^2]^{1/2}\ . \tag{2.5}$$

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

$$F_0/N=(A_0+\mu)(n-1)+\Delta n_Q+Xx_0^*+X^*x_0+\frac{1}{4}U(n^2+n_Q^2+4|x_0|^2)+\frac{1}{2}ZW(n^2-n_Q^2)-\frac{1}{\beta N}\sum_k\left[\ln\left(2\cosh\frac{\beta A_k^+}{2}\right)+\ln\left(2\cosh\frac{\beta A_k^-}{2}\right)\right]\ , \tag{2.6}$$

where

$$n_Q=\frac{1}{N}\sum_{k\sigma}\langle c_{k+Q\sigma}^{\dagger}c_{k\sigma}\rangle_0=\frac{\Delta}{2N}\sum_k\left[\left(1+\frac{\bar{\mu}}{E_k}\right)B_k^+-\left(1-\frac{\bar{\mu}}{E_k}\right)B_k^-\right]\ , \tag{2.7}$$

$$n=\frac{1}{N}\sum_{k\sigma}\langle c_{k\sigma}^{\dagger}c_{k\sigma}\rangle_0=1+\frac{1}{2N}\sum_k[(E_k+\bar{\mu})B_k^+-(E_k-\bar{\mu})B_k^-]\ , \tag{2.8}$$

$$x_0=\frac{X}{4N}\sum_k(B_k^+-B_k^-)\ , \tag{2.9}$$

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

The next step is to minimize F_0 with respect to Δ, X, and A_0 to obtain the optimum values of these parameters as

$$\Delta=(2ZW-U)n_Q/2 \ , \tag{2.10}$$

$$X=-Ux_0 \ , \tag{2.11}$$

and

$$A_0=-(2ZW+U)n/2 \ . \tag{2.12}$$

We should point out here that Δ and X are gap parameters and n_Q and x are order parameters of the charge-ordered and the singlet-superconducting states, respectively. Substituting these relations into Eq. (2.6), we have the minimum free energy

$$F_0/N=\bar{\mu}(n-1)+\frac{(U+2ZW)n^2}{4}-\frac{\Delta^2}{(U-2ZW)}-\frac{|X|^2}{U}-\frac{1}{\beta N}\sum_k\left[\ln\left(2\cosh\frac{\beta A_k^+}{2}\right)+\ln\left(2\cosh\frac{\beta A_k^-}{2}\right)\right] \ . \tag{2.13}$$

The ground-state energy is then simply

$$\frac{E_0}{N}=\lim_{\beta\to\infty}\left(\frac{F_0}{N}\right)=\bar{\mu}(n-1)+\frac{(U+2ZW)n^2}{4}-\frac{\Delta^2}{U-2ZW}-\frac{|X|^2}{U}-\frac{1}{2N}\sum_k(A_k^+ + A_k^-) \ . \tag{2.14}$$

For given values of U, W, n, and the band structure ϵ_k, we can substitute Eqs. (2.10) and (2.11) into Eqs. (2.7) and (2.9) and then solve the three coupled equations (2.7)–(2.9) numerically for Δ, X, and the chemical potential $\bar{\mu}$. There are in general four branches of solutions for different phases: (1) $\Delta\neq 0$ and $X=0$ for the charge-ordered (CO) state, (2) $\Delta=0$ and $X\neq 0$ for the singlet-superconducting (SS) state, (3) $\Delta\neq 0$ and $X\neq 0$ for the mixed (M) state of CO and SS, and (4) $\Delta=X=0$ for the nonordered (NO) state. The energy of each state is then calculated from Eq. (2.14) using the corresponding solutions of Δ, X, and $\bar{\mu}$ as well as the value of A_0 given by Eq. (2.12). Comparing the energies of various states, we can determine the ground-state structure.

III. SOME ANALYTICAL SOLUTIONS

Before presenting the numerical solution we will first derive the analytical expressions for a few cases. Such analytical results can be used to check the accuracy of the self-consistent numerical computation. Since a model square density of states is used for the numerical calculation in the next section, the analysis in this section will also be restricted to this density of states if necessary.

A. Mixed phase

We first examine the condition for the existence of the M phase. If the M phase exists, i.e., if $\Delta\neq 0$ and $X\neq 0$, then subtracting Eq. (2.9) from Eq. (2.7) yields

$$Q\equiv 8ZW/U(2ZW-U)=\frac{\bar{\mu}}{N}\sum_k\frac{1}{E_k}\left[\frac{\tanh\frac{1}{2}\beta[(E_k+\bar{\mu})^2+|X|^2]^{1/2}}{[(E_k+\bar{\mu})^2+|X|^2]^{1/2}}-\frac{\tanh\frac{1}{2}\beta[(E_k-\bar{\mu})^2+|X|^2]^{1/2}}{[(E_k-\bar{\mu})^2+|X|^2]^{1/2}}\right] \ . \tag{3.1}$$

For $n\neq 1$, it is clear from Eq. (2.8) that $\bar{\mu}\neq 0$. Since Q is an even function of $\bar{\mu}$, we need only to examine the region $\bar{\mu}>0$. As a function of temperature, Q behaves as

$$Q=\begin{cases}0, & \text{for } \beta=0\\ -\frac{4}{N}\sum_k\frac{\bar{\mu}^2}{[(E_k+\bar{\mu})^2+|X|^2]^{1/2}[(E_k-\bar{\mu})^2+|X|^2]^{1/2}}<0 \ , & \text{for } \beta=\infty\end{cases}$$

and for all values of β

$$\frac{dQ}{d\beta}=-\frac{\bar{\mu}}{2N}\sum_k\frac{1}{E_k}\left[\tanh^2\frac{\beta}{2}[(E_k+\bar{\mu})^2+|X|^2]^{1/2}-\tanh^2\frac{\beta}{2}[(E_k-\bar{\mu})^2+|X|^2]^{1/2}\right]<0 \ .$$

Therefore, if we ignore the unphysical case of infinite temperature, we always have $Q\equiv 8ZW/U(2ZW-U)<0$ if $\Delta\neq 0$ and $X\neq 0$. Since $U<0$, if $n\neq 1$ the necessary condition for the possible existence of the M phase is either $W>0$ or $2ZW<U$. However, both the gap parameter Δ and the order parameter n_Q must be positive for the M phase. From Eq. (2.10) we then obtain $2ZW-U=2\Delta/n_Q>0$ if the M phase exists. Consequently, the M phase may exist only if $W>0$.

B. Pure phases

If we use a model square density of states, analytical results can be derived for the pure phases. For the NO phase, since $\Delta = X = 0$, we only need to solve Eq. (2.8) which becomes

$$n-1=\frac{1}{2N}\sum_k\left[\tanh\frac{\beta}{2}(\epsilon_k+\bar{\mu})-\tanh\frac{\beta}{2}(\epsilon_k-\bar{\mu})\right] . \tag{3.2}$$

For a square density of states

$$\rho(E)=\begin{cases}\dfrac{1}{2D}, & \text{for } |E|<D\\ 0, & \text{otherwise},\end{cases} \tag{3.3}$$

it is easy to see from Eqs. (3.2) and (2.14) that at $T=0$

$$\bar{\mu}(T=0)=(n-1)D \tag{3.4}$$

and

$$E_0(\mathrm{NO})/N=Dn(n-2)/2+(2ZW+U)n^2/4 . \tag{3.5}$$

Next we consider the SS phase for which $\Delta=0$. For $T=0$ with the square density of states, Eqs. (2.8), (2.9), and (2.14) can be reduced to the simple forms

$$\bar{\mu}(T=0)=-(n-1)D\coth\frac{2D}{U} , \tag{3.6}$$

$$X=-\sqrt{n(2-n)}D/\sinh\frac{2D}{U} , \tag{3.7}$$

and

$$\frac{E_0(\mathrm{SS})}{N}=\tfrac{1}{2}Dn(n-2)\coth\frac{2D}{U}+\frac{(2ZW+U)n^2}{4} . \tag{3.8}$$

Finally, we examine Eqs. (2.7), (2.8), and (2.14) with $X=0$ for the CO phase. Again for $T=0$ and the square density of states, analytical expressions are derived as

$$\bar{\mu}(T=0)=D\left[1-|n-1|\cosh\frac{2D}{2ZW-U}\right]\Big/\sinh\frac{2D}{2ZW-U} , \tag{3.9}$$

$$\Delta^2=\bar{\mu}(T=0)^2-(n-1)^2D^2 , \tag{3.10}$$

and

$$E_0(\mathrm{CO})/N=D\left[|n-1|/\sinh\frac{2D}{2ZW-U}-\tfrac{1}{2}[1+(n-1)^2]\coth\frac{2D}{2ZW-U}\right]+\frac{(2ZW+U)n^2}{4} . \tag{3.11}$$

Since $\Delta^2\geq 0$, from Eqs. (3.9) and (3.10) we conclude that at $T=0$ the CO phase exists only if $2D/(2ZW-U)\leq -\ln|n-1|$.

C. Phase boundaries

Since there is no M-phase solution for $n\neq 1$ and $W\leq 0$, the ground state can be easily determined by comparing the energies $E_0(\mathrm{NO})$, $E_0(\mathrm{SS})$, and $E_0(\mathrm{CO})$. We found the ground state always singlet superconducting.

For $n=1$, we see from Eq. (2.8) that $\bar{\mu}=0$. Therefore, Eqs. (2.7) and (2.9) become

$$\frac{\Delta}{2ZW-U}=\frac{\Delta}{4N}\sum_k(B_k^+ + B_k^-) \tag{3.12}$$

and

$$-\frac{X}{U}=\frac{X}{4N}\sum_k(B_k^+ + B_k^-) . \tag{3.13}$$

Again we see no M-phase solution if $W\neq 0$. In this case the ground-state energy is the lowest value of $E_0(\mathrm{NO})$, $E_0(\mathrm{SS})$, and $E_0(\mathrm{CO})$. We found a SS ground state if $W<0$ and a CO ground state if $W>0$. If $W=0$, Eqs. (3.12) and (3.13) are identical except for the factors Δ and X. Consequently, we solve the same equation

$$-\frac{1}{U}=\frac{1}{2N}\sum_k(\epsilon_k^2+\alpha^2)^{-1/2}\tanh\frac{\beta}{2}(\epsilon_k^2+\alpha^2)^{1/2} \tag{3.14}$$

for the CO phase ($\alpha=\Delta$), the SS phase ($\alpha=X$), and the M phase ($\alpha^2=\Delta^2+X^2$). Also, the energies $E_0(\mathrm{CO})$, $E_0(\mathrm{SS})$, and $E_0(\mathrm{M})$ can be expressed as

$$\frac{E_0}{N}=\frac{U}{4}-\frac{\alpha^2}{U}-\frac{1}{N}\sum_k(\epsilon_k^2+\alpha^2)^{1/2} \tag{3.15}$$

for the CO phase ($\alpha=\Delta$), the SS phase ($\alpha=X$), and the M phase ($\alpha^2=\Delta^2+X^2$). Hence, in this case ($n=1$ and $W=0$) the three CO, SS, and M phases are degenerate. Comparing with the energy $E_0(\mathrm{NO})$, in this case we found the ground state to be degenerate in SS, CO, and M phases.

The numerical solution for $n\neq 1$ and $W>0$, as will be shown in the next section, indicates a second-order transition between the SS and the M phases. The phase boundary between the two phases

can be analytically derived as follows. We start from the M-phase solutions (2.7) and (2.9). These two equations can be combined as

$$\frac{1}{2ZW-U}=-\frac{1}{U}+\frac{\bar{\mu}}{4N}\sum_k\frac{1}{E_k}(B_k^+-B_k^-) \quad . \tag{3.16}$$

Approaching the phase boundary from the M phase, we have $\Delta\to 0$. For a model square density of states, along the boundary we substitute $\bar{\mu}$ and X from Eqs. (3.6) and (3.7) into Eq. (3.16) to obtain

$$\frac{1}{2ZW-U}$$

$$=-\frac{1}{U}+\frac{\eta}{4D\xi}\ln\left[\frac{1-\eta\xi^{-2}+[1+(1-2\eta)\xi^{-2}]^{1/2}}{1+\eta\xi^{-2}+[1+(1+2\eta)\xi^{-2}]^{1/2}}\right] , \tag{3.17}$$

where

$$\xi^2=(n-1)^2+\mathrm{csch}^2\frac{2D}{U} \tag{3.18}$$

and

$$\eta=-(n-1)\coth\frac{2D}{U} \quad . \tag{3.19}$$

In the next section, we can use this analytical phase boundary to check the accuracy of the self-consistent numerical solutions.

IV. GROUND-STATE PROPERTIES

As we mentioned before, for $n\neq 1$ and $W>0$ the M phase must be solved numerically. Using a square density of states (3.3), we solve numerically for all the four phases and whenever possible check with the analytical results derived in the previous section. Our self-consistent solutions are found to be accurate within 0.1%. Since the Hartree approximation is not reliable for large values of the correlation strength, we have restricted ourselves to $-U/D\leq 2$ and $ZW/D\leq 1$.

Within this range of U/D and W/D, the NO and the CO phases are unstable against the SS and the M phases. In Fig. 1 we show the phase boundaries between the M and the SS phases for various values

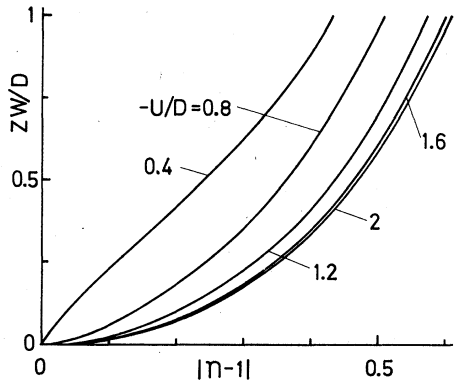

FIG. 1. Ground-state phase diagrams for various values of U/D.

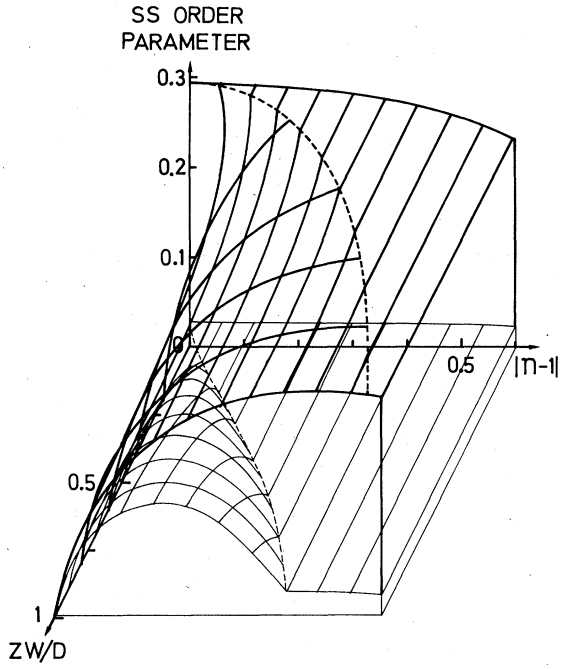

FIG. 2. SS order parameter for $-U/D=0.4$ (thin curves) and for $-U/D=1.2$ (heavy curves).

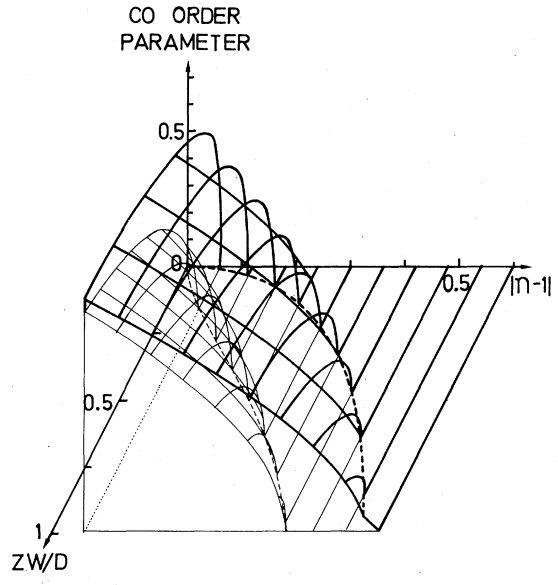

FIG. 3. CO order parameter for $-U/D=0.4$ (thin curves) and for $-U/D=1.2$ (heavy curves).

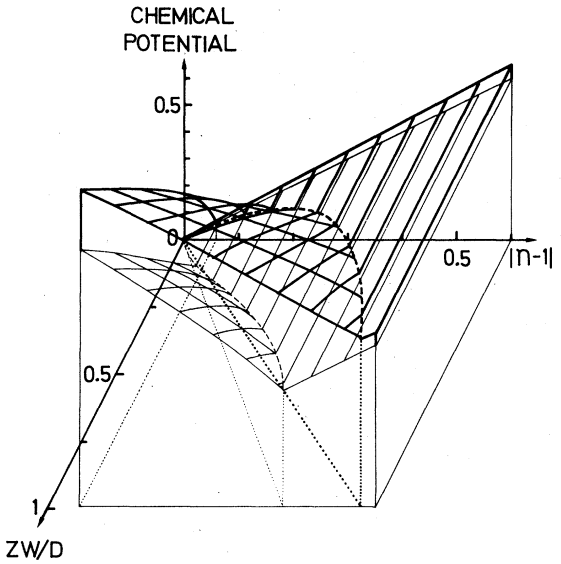

FIG. 4. Chemical potential for $-U/D=0.4$ (thin curves) and for $-U/D=1.2$ (heavy curves).

of $-U/D$. The boundary has the same characteristic feature as the one for the strong-coupling limit derived by us earlier.[29]

The ground-state SS and CO order parameters are shown in Figs. 2 and 3, respectively. Approaching the phase boundary from the M phase, while the CO order parameter decreases monotonically, the SS order parameter increases monotonically only if $-U/D$ is not very small. For very small value of $-U/D$, say $-U/D=0.4$, we see the enhancement of the SS order parameter in the M phase as compared to its value in the pure SS phase. Consequently, the competing interactions for various ordered phases become more complicated as the intra-atomic attraction gets weaker.

In Fig. 4 we show the chemical potential. As predicted by Eq. (3.6), in the SS phase $\bar{\mu}$ is linear in $|n-1|$ but independent of W. It is important to point out that the stable phase always has the largest chemical potential. Therefore, along the phase boundary, two sheets of chemical potential join with a cusp pointing downward.

V. DISCUSSION

In this paper we have used the (broken symmetry) Hartree approximation to investigate the Hamiltonian (2.1). A complete Hartree-Fock decoupling on the interatomic interaction $W_{ij}n_{i\sigma}n_{j\sigma'}$ should consist of the Hartree terms

$$W_{ij}(\langle n_{i\sigma}\rangle n_{j\sigma'}+\langle n_{j\sigma'}\rangle n_{i\sigma}-\langle n_{i\sigma}\rangle\langle n_{j\sigma'}\rangle) \ ,$$

the "normal" Fock terms

$$-W_{ij}(\langle c_{i\sigma}^{\dagger}c_{j\sigma}\rangle c_{j\sigma}^{\dagger}c_{i\sigma}+\langle c_{j\sigma}^{\dagger}c_{i\sigma}\rangle c_{i\sigma}^{\dagger}c_{j\sigma}-\langle c_{i\sigma}^{\dagger}c_{j\sigma}\rangle\langle c_{j\sigma}^{\dagger}c_{i\sigma}\rangle) \ ,$$

and the "anomalous" Fock terms

$$W_{ij}(\langle c_{i\sigma}^{\dagger}c_{j-\sigma}^{\dagger}\rangle c_{j-\sigma}c_{i\sigma}+\langle c_{j-\sigma}c_{i\sigma}\rangle c_{i\sigma}^{\dagger}c_{j-\sigma}^{\dagger}-\langle c_{i\sigma}^{\dagger}c_{j-\sigma}^{\dagger}\rangle\langle c_{j-\sigma}c_{i\sigma}\rangle) \ .$$

For the case $W>0$, the Fock terms only play a secondary role,[38] especially at $T=0$. The effect of the normal Fock terms appears as a renormalization of the band energy $\epsilon_k\rightarrow\epsilon_k-2W_k\langle c_{i\sigma}^{\dagger}c_{j\sigma}\rangle$. Such renormalization does not have strong influence on the phase stability at $T=0$, since the transitions are second order. The anomalous Fock terms are of even less significance for $W>0$ as far as the phase boundary is concerned. However, for $W<0$ the Fock terms may stabilize another type of superconducting phase. This problem will be treated in detail in a subsequent paper.

In an earlier paper[29] we have shown that for an alternating lattice, the negative-U extended Hubbard Hamiltonian for arbitrary electron density n can be exactly mapped onto the positive-U extended Hubbard Hamiltonian of $n^*=1$ with an Ising-type interatomic exchange interaction in an effective magnetic field. The effective magnetic field is not constant but has to be determined from the self-consistent condition that the magnetization of the transformed system along the z axis has a fixed value $n-1$. Since the effective magnetic field is n dependent, in the strong-coupling regime the phase diagram at $T=0$ exhibits only the SS and the M phases whereas the CO phase is unstable with respect to the SS and the M phases for any $n\neq 1$. This conclusion is entirely different from what one would expect from the analogous behavior of the anisotropic antiferromagnet in an external field. In this paper we found that a similar property is preserved in the weak-coupling regime, i.e., in the ground state the CO phase is unstable with respect to the SS and the M phases. Such behavior is again related to the fact that in the present case the chemical potential has to be determined self-consistently. It remains to be proved whether this feature is a consequence of the symmetry requirement in the entire range of the coupling strength.

It is interesting to notice some other features com-

mon to both the weak- and the strong-coupling regimes. From Eqs. (2.12) and (3.6), the true chemical potential in the SS phase at $T=0$ can be expressed as

$$\mu_{SS}(T=0)=\tfrac{1}{2}n(2ZW+U)-(n-1)D\coth(2D/U) \quad . \tag{5.1}$$

In the limit $D/|U|\to 0$, it becomes

$$\mu_{SS}(T=0)\simeq U/2+nZW-2D^2(n-1)/3U \quad . \tag{5.2}$$

Though Eq. (5.1) is valid only for weak intra-atomic attraction, Eq. (5.2) is qualitatively correct since from Ref. 29 we have the chemical potential at the strong intra-atomic attraction as

$$\mu_{SS}(T=0)=U/2+nZW-D^2(n-1)/2ZU \quad . \tag{5.3}$$

In this limit of strong coupling, from Eq. (3.7) we see the SS order parameter turns out to be $x_0=\sqrt{n(2-n)}$ if we naively extend the validity of Eq. (3.7) to a large value of $-U/D$. Yet accidentally, this is just the correct result derived previously for the strong-coupling limit.[29]

Finnaly, we must emphasize that the numerical results in this work are based on the model square density of states. A realistic density of states may change the phase diagram even qualitatively. We are performing such a calculation and the results will be reported in the near future.

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