Onsager reaction terms for quantum many-body systems: Application to antiferromagnetic and superconducting order in the Hubbard model

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We demonstrate that an expansion in powers of the strength of the interaction, of the free energy at *fixed* order parameter, can be used to generate and correct mean-field theories for interacting quantum many-body systems. The first two terms in the expansion generally yield ordinary Hartree-Fock mean-field theory and the next term gives an "Onsager reaction field" correction to Hartree-Fock theory. This method can be used to directly generate expansions for *inverse* susceptibilities. We illustrate the method for the one- and two-dimensional Hubbard model, for which we consider corrections to mean-field theories of antiferromagnetism for the repulsive-U half-filled case and superconductivity in the attractive-U case. These corrections give a quantitative account superior to that of the random-phase approximation (RPA) for the correlation energy at small and intermediate values of U. For susceptibilities, we recover from the first two terms in the expansion the usual RPA results, while higher-order terms give systematic corrections to the RPA susceptibilities. For the case of superconductivity in the repulsive-U Hubbard model, we show that the higher-order terms in the expansion must be considered to determine whether or not an instability exists. We find that there is no superconducting instability in the repulsive-U case, at least towards ordinary singlet or triplet pairing. We also find no evidence for a superconducting instability driven by a coexisting antiferromagnetic order.

I. INTRODUCTION

In this paper we present a new and very simple method to derive mean-field theories and corrections to those theories for interacting quantum many-body systems which exhibit some kind of long-range order. The method is an expansion in powers of the strength of the interaction of the free energy $A(m)$ considered at a fixed order parameter m. The first two terms in the expansion will generally reproduce the ordinary Hartree-Fock approximation, and higher-order terms can be used to derive corrections in a simple and systematic way. The technique can actually be applied to any Hamiltonian which can be decomposed into a part which can be diagonalized plus a remainder. In this paper, we consider as an example the popular Hubbard model,[1] and although the method is easily generalized to finite temperature T, we will restrict ourselves to $T=0$.

Our method of deriving a mean-field theory and its corrections is very useful for at least two kinds of situations.

(i) For low-dimensional systems where fluctuations are large. For example, the ordinary Hartree-Fock mean-field theory of antiferromagnetism in the Hubbard model[2] predicts that half-filled one-dimensional chains will exhibit antiferromagnetic long-range order, in contradiction with known results. When we calculate the corrections to Hartree-Fock mean-field theory using our technique, we find that, indeed, fluctuations destroy the long-range order in one dimension, while in two or more dimensions, the corrections merely weaken the long-range order.

(ii) When there is no sensible Hartree-Fock mean-field theory because (in our language) one of the first two terms of the expansion of the free energy does not depend on the order parameter (usually for some symmetry reason). Such a situation actually arises for the case of superconductivity in the repulsive-U Hubbard model. For these cases, it is crucial to consider the higher-order terms in the expansion in order to assess the possible existence of the relevant order parameter.

Our technique can also be used to calculate any desired susceptibilities. The fact that we work at a fixed order parameter means that we effectively resum infinitely many ordinary Feynman diagrams, as is demonstrated by the fact that the susceptibilities that we obtain from just the first two terms of our expansion are identical for the Hubbard model to the ordinary random-phase approximation (RPA) susceptibilities.[3] However, our technique has the advantage that it will work even for models for which an RPA resummation is impossible. In fact, it actually provides a direct systematic expansion for *inverse* susceptibilities.

The outline of this paper is as follows. In Sec. II, we illustrate our method for the case of the half-filled, repulsive-U Hubbard model where antiferromagnetic order is expected in two or more dimensions. We use our corrections to the Hartree-Fock mean-field theory to calculate the "correlation energy" in this case. In Sec. III, we apply our technique to generate and correct mean-field theories of superconductivity in the attractive-U Hubbard model, while in Secs. IV, and V, we consider the

possibility of superconductivity in the repulsive-U Hubbard model, either with or without coexisting antiferromagnetic order.

II. ANTIFERROMAGNETISM IN THE HALF-FILLED REPULSIVE-U HUBBARD MODEL

The Hamiltonian for the Hubbard model is

$$H=-t\sum_{(i,j)\sigma}(c_{i\sigma}^{\dagger}c_{j\sigma}+c_{j\sigma}^{\dagger}c_{i\sigma})+U\sum_{i}n_{i\uparrow}n_{i\downarrow}\ , \tag{1}$$

where i and j are nearest-neighbor sites on a lattice, $n_{i\sigma}\equiv c_{i\sigma}^{\dagger}c_{i\sigma}$, and the $c_{i\sigma}^{\dagger}$ are creation operators for electrons with spin σ. We will choose our units so that $t=1$. Fourier transforming, we have

$$H=\sum_{k,\sigma}\varepsilon_k c_{k\sigma}^{\dagger}c_{k\sigma}+\frac{U}{N}\sum_{k,k',p}c_{k\uparrow}^{\dagger}c_{k+p\uparrow}c_{k'\downarrow}^{\dagger}c_{k'-p\downarrow}\ , \tag{2}$$

where N is the number of lattice sites, $\varepsilon_K=-2\cos(k)$ in one dimension, and

$$\varepsilon_k=-2[\cos(k_x)+\cos(k_y)]$$

on the square lattice.

We are interested in the case where $U>0$ and the density of electrons per lattice site $n=1$. Now we could simply expand the energy in powers of U around the free case, but if we do that without imposing a staggered magnetization, we would be neglecting a possible phase transition (that presumably indeed occurs in more than one dimension) to an antiferromagnetic state. Instead, we will use a Lagrange multiplier to fix the staggered magnetization, and then expand the free energy at constant staggered magnetization and density. Then we can truncate our expansion at some power of U and minimize the resulting free energy as a function of the staggered magnetization. The free energy truncated at $O(U)$ is identical to the Hartree-Fock free energy, while if one truncates at $O(U^2)$, one obtains corrections which we identify as "Onsager reaction terms."

The following description of our technique may, at first sight, appear excessively pedantic, and, indeed, the Hartree-Fock theory can be derived in simpler ways, but actually one must proceed very carefully in order to obtain the higher-order corrections correctly. To work at fixed density n and staggered magnetization m, we introduce Lagrange multipliers $\mu(U)$ and $h(U)$. We will work with a staggered magnetization in the x direction but, of course, spin-rotation symmetry ensures that equivalent results are found when working with a magnetization in the y or z directions. Thus, we consider the free-energy operator $\hat{A}(U,n,m)$ which, at zero temperature, is

$$\begin{aligned}\hat{A}(U,n,m)=&-\sum_{(i,j)\sigma}(c_{i\sigma}^{\dagger}c_{j\sigma}+c_{j\sigma}^{\dagger}c_{i\sigma})\\&+\mu(U)\left[Nn-\sum_{i,\sigma}c_{i\sigma}^{\dagger}c_{i\sigma}\right]\\&+h(U)\left[Nm-\sum_{i}(-1)^i c_{i\uparrow}^{\dagger}c_{i\downarrow}\right]\\&+U\sum_{i}c_{i\uparrow}^{\dagger}c_{i\uparrow}c_{i\downarrow}^{\dagger}c_{i\downarrow}\end{aligned} \tag{3}$$

[for the square lattice, $(-1)^i=+1$ on the A sublattice, and $(-1)^i=-1$ on the B sublattice] or when Fourier transformed is

$$\begin{aligned}\hat{A}(U,n,m)=&\sum_{k,\sigma}\varepsilon_k c_{k\sigma}^{\dagger}c_{k\sigma}+\mu(U)\left[Nn-\sum_{k,\sigma}c_{k\sigma}^{\dagger}c_{k\sigma}\right]\\&+h(U)\left[Nm-\sum_{k}(c_{k\uparrow}^{\dagger}c_{k-Q\downarrow}+c_{k-Q\downarrow}^{\dagger}c_{k\uparrow})\right]\\&+\frac{U}{N}\sum_{k,k',p}c_{k\uparrow}^{\dagger}c_{k+p\uparrow}c_{k'\downarrow}^{\dagger}c_{k'-p\downarrow}\ .\end{aligned} \tag{4}$$

Q equals π in one dimension and the vector (π,π) in two dimensions. $\mu(U)$ and $h(U)$ are functions of U and vary in order to keep n and m fixed:

$$n=\langle\Omega_U|\hat{n}|\Omega_U\rangle=\left\langle\Omega_U\left|\frac{1}{N}\sum_{k,\sigma}c_{k\sigma}^{\dagger}c_{k\sigma}\right|\Omega_U\right\rangle \tag{5}$$

and

$$\begin{aligned}m&=\langle\Omega_U|\hat{m}|\Omega_U\rangle\\&=\left\langle\Omega_U\left|\frac{1}{N}\sum_{k}(c_{k\uparrow}^{\dagger}c_{k-Q\downarrow}+c_{k-Q\downarrow}^{\dagger}c_{k\uparrow})\right|\Omega_U\right\rangle\ ,\end{aligned} \tag{6}$$

where $|\Omega_U\rangle$ is the true ground state of the system.

We now perform a Taylor expansion of A in powers of U around $U=0$. At zeroth order, we must diagonalize $\hat{A}(U=0)$, remembering that $\mu(U)$ and $h(U)$ are set at their $U=0$ values (which we denote by μ_0 and h_0). $\hat{A}(U=0)$ is diagonalized by a transformation to the fermionic operators b_k and d_k defined by

$$\begin{aligned}b_k&=\alpha_k c_{k\uparrow}-\beta_k c_{k-Q\downarrow}\ ,\\d_k&=\beta_k c_{k\uparrow}+\alpha_k c_{k-Q\downarrow}\ ,\end{aligned} \tag{7}$$

with

$$\begin{aligned}\alpha_k^2&=\frac{1}{2}\left[1+\frac{\varepsilon_k}{E_k}\right]\ ,\\\beta_k^2&=\frac{1}{2}\left[1-\frac{\varepsilon_k}{E_k}\right]\ ,\end{aligned} \tag{8}$$

where the quasiparticle energy E_k is $E_k=(\varepsilon_k^2+h_0^2)^{1/2}$. The diagonal form of $\hat{A}(U=0)$ is

$$\hat{A}(U=0)=\sum_{k}(\tilde{E}_k^{+}b_k^{\dagger}b_k+\tilde{E}_k^{-}d_k^{\dagger}d_k)+Nh_0m+N\mu_0 n\ , \tag{9}$$

where $\tilde{E}_k^{\pm}=\pm E_k-\mu_0$. All our sums over k should be taken over the full original Brillouin zone.

Equations (5) and (6) hold for any value of U, including $U=0$. We find from Eq. (5) that

$$\begin{aligned}n&=\left\langle\Omega_0\left|\frac{1}{N}\sum_{k}(b_k^{\dagger}b_k+d_k^{\dagger}d_k)\right|\Omega_0\right\rangle\\&=\frac{1}{N}\sum_{k}[\Theta(-\tilde{E}_k^{+})+\Theta(-\tilde{E}_k^{-})]\ ,\end{aligned} \tag{10}$$

where $|\Omega_0\rangle$ now represents the ground state of $\hat{A}(U=0)$.

The ground state of $\hat{A}(U=0)$ at density $n=1$ will clearly have $\mu_0=0$ and will fill up all the d levels while leaving the b levels empty, so that

$$b_k|\Omega_0\rangle=d_k^\dagger|\Omega_0\rangle=0 \ .$$

We find from Eq. (6) that

$$m=\frac{1}{N}\sum_k \frac{h_0}{E_k}[\Theta(-\tilde{E}_k^-)-\Theta(-\tilde{E}_k^+)]\underset{n\to 1}{=}\frac{1}{N}\sum_k \frac{h_0}{E_k} \ , \tag{11}$$

so that the free energy A at $U=0$ and $n=1$ is

$$A(U=0)=\langle\Omega_0|\hat{A}(U=0)|\Omega_0\rangle=\sum_k \frac{\varepsilon_k^2}{E_k} \ . \tag{12}$$

Equation (11), relating m and h_0, will not be modified at higher order as it only depends on definitions which hold at $U=0$.

To compute A to $O(U)$, we need

$$\left.\frac{\partial\hat{A}}{\partial U}\right|_{U=0}=\frac{1}{N}\sum_{k,k',p} c_{k\uparrow}^\dagger c_{k+p\uparrow}c_{k'\downarrow}^\dagger c_{k'-p\downarrow} +N\left.\frac{\partial\mu}{\partial U}\right|_{U=0}(n-\hat{n})+N\left.\frac{\partial h}{\partial U}\right|_{U=0}(m-\hat{m}) \ . \tag{13}$$

We find, after a short computation, that

$$\begin{aligned} U\left.\frac{\partial A}{\partial U}\right|_{U=0} &= U\langle\Omega_0|(\partial A/\partial U)_{U=0}|\Omega_0\rangle \\ &= \frac{U}{N}\left\langle\Omega_0\left|\sum_{k,k',p} c_{k\uparrow}^\dagger c_{k+p\uparrow}c_{k'\downarrow}^\dagger c_{k'-p\downarrow}\right|\Omega_0\right\rangle \\ &= \frac{UN}{4}(n^2-m^2) \ , \end{aligned} \tag{14}$$

where we have substituted in the b_k and d_k quasiparticles and used our previous results for m and n.

To recap, we have found that, for the half-filled Hubbard model,

$$\frac{1}{N}A(U,n=1,m)=\frac{-1}{N}\sum_k \frac{\varepsilon_k^2}{E_k}+\frac{U}{4}(n^2-m^2)+O(U^2) \ , \tag{15}$$

where m and h_0 are related by Eq. (11). μ_0 is kept equal to zero to maintain the constraint $n=1$. If we truncate the free energy at this order, we recover ordinary Hartree-Fock theory.[2,4] Note that the $O(U^0)$ term acts as a kind of "quantum entropy" or zero-point motion which suppresses the staggered magnetization, while the $O(U^1)$ term favors a staggered magnetization. Minimizing the truncated free energy over m, the usual self-consistent equation for m is found:

$$1=\frac{1}{N}\sum_k \frac{U}{(4\varepsilon_k^2+U^2m^2)^{1/2}} \ . \tag{16}$$

This equation has a nonzero solution for m in one or more dimensions. Note that the solution of the self-consistent equation will have a form that is not perturbative in U (i.e., $m\sim e^{-2\pi/U}$ in one dimension and $m\sim e^{-2\pi/\sqrt{U}}$ on the square lattice), even though we originally made a perturbative expansion for A.

Because we expand at fixed order parameter m rather than fixed field h, we actually obtain a direct expansion for the *inverse* susceptibility. In fact, the inverse antiferromagnetic susceptibility χ^{-1} is given by

$$\chi^{-1}=\frac{1}{N}\frac{\partial^2 A}{\partial m^2} \ , \tag{17}$$

so we find immediately from Eq. (15) that

$$\chi^{-1}=\chi_0^{-1}-\frac{U}{2}+O(U^2) \ , \tag{18}$$

where χ_0^{-1} is the inverse susceptibility of the free system.[5] Equation (18) is the standard RPA formula for the inverse susceptibility,[6] so it is clear that working at fixed order parameter effectively resums an infinite number of diagrams calculated at fixed field.

The $O(U^2)$ correction to A is, in principle, obtained from two parts: one that comes from the second-order correction to $\hat{A}$ inserted into a first-order perturbation formula, plus a part that comes from the first-order correction to $\hat{A}$ inserted into a second-order perturbation formula:

$$U^2\left[\left\langle\Omega_0\left|\left[\frac{\partial^2\hat{A}}{\partial U^2}\right]_{U=0}\right|\Omega_0\right\rangle+\left\langle\Omega_0\left|\left[\frac{\partial\hat{A}}{\partial U}\right]_{U=0}\frac{1-|\Omega_0\rangle\langle\Omega_0|}{A(0)-\hat{A}(0)}\left[\frac{\partial\hat{A}}{\partial U}\right]_{U=0}\right|\Omega_0\right\rangle\right] \ . \tag{19}$$

The term that comes from the second derivative of $\hat{A}$ actually vanishes identically because of the definitions of m and n. To compute the other term, we need to use Eq. (13) and the Maxwell relations

$$\left.\frac{\partial\mu}{\partial U}\right|_{U=0}=\frac{1}{N}\left.\frac{\partial^2 A}{\partial n\partial U}\right|_{U=0}=\frac{n}{2} \tag{20}$$

and

$$\left.\frac{\partial h}{\partial U}\right|_{U=0}=\frac{1}{N}\left.\frac{\partial^2 A}{\partial m\partial U}\right|_{U=0}=-\frac{m}{2} \ . \tag{21}$$

Substituting in the quasiparticle operators d_k and b_k for the electron operators c_k, we find after a tedious but straightforward computation the free energy to $O(U^2)$:

$$\frac{1}{N}A(U,n=1,m)=\frac{-1}{N}\sum_k\frac{\varepsilon_k^2}{E_k}+\frac{U}{4}(1-m^2)$$
$$-U^2\frac{1}{N^3}\sum_{k,k',p}\frac{(\alpha_k^2\alpha_{k'}^2-\alpha_k\beta_k\alpha_{k'}\beta_{k'})(\beta_{k+p}^2\beta_{k'-p}^2-\alpha_{k+p}\beta_{k+p}\alpha_{k'-p}\beta_{k'-p})}{E_k+E_{k'}+E_{k+p}+E_{k'-p}}+O(U^3)\ . \tag{22}$$

The equations given above relating m and n to h_0 and μ_0 are still valid. If we set $m=0$, we recover the ordinary perturbative expansion in U of the energy of the Hubbard model.[7]

The $O(U^2)$ correction has a form that is very reminiscent of the form of the TAP-Onsager term in the theory of spin glasses,[8] and indeed the Thouless-Anderson-Palmer (TAP) free energy for a spin-glass model can be derived in an entirely analogous way through an expansion in powers of β (the inverse temperature) at a fixed site-dependent order parameter.[9,10]

In contrast to the Hartree-Fock theory, we find that in one dimension the minimum of the corrected free energy given in Eq. (22) is always at $m=0$. This agrees with the fact that there is, indeed, no long-range antiferromagnetic order in one dimension. On the square lattice, we do find a minimum with $m>0$. We tabulate our $m(U)$ and compare it with the result of the Hartree-Fock theory in Table I.[11] Note that the staggered magnetization is reduced from its Hartree-Fock value, although in our approximation m still approaches 1 as $U\to\infty$. The large-U behavior is, of course, wrong, but because our approach is ultimately based on a small-U expansion, it can only really be expected to be reliable for relatively small U. The $O(U^2)$ correction to the inverse antiferromagnetic susceptibility can be straightforwardly computed from Eq. (22), but since the expression is long and not particularly enlightening, we do not write it down here.[5]

Using our method, we have also computed the correlation energy (defined as the difference between the energy and the Hartree-Fock energy $\Delta E_c=A-A_{\rm HF}$.) In one dimension, since our equilibrium magnetization is zero, our result is the same as that of an ordinary-second order perturbation theory, and the comparison with the exact result has already been made in Ref. 7, where it was noted that the error in the correlation energy is less than 10% even for intermediate values of U ($U\le 10$). In Table I, we give our result for the two-dimensional case, and compare it with the RPA estimate[12] and numerical results using the antiferromagnetic Gutzwiller variational wave function.[13] For small U, both our result and the RPA result give the exact U^2 coefficient. For large U, our correlation energy vanishes as it should, while the RPA result approaches an unphysical negative-constant value. We believe our result to be accurate for small and intermediate values of U—in particular, the maximum as a function of U is most likely a real feature.[12]

III. SUPERCONDUCTIVITY IN THE ATTRACTIVE-U HUBBARD MODEL

For the Hubbard model with $U<0$, one expects an instability towards a BCS-like singlet superconductivity[14] with a nonzero order parameter

$$\psi(k)=\langle\Omega_U|c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger+c_{-k\downarrow}c_{k\uparrow}|\Omega_U\rangle\ .$$

Therefore, we apply a Lagrange multiplier $\Delta(k,U)$ which fixes $\psi(k)$ to its equilibrium value. We proceed in a very similar way to the antiferromagnetic case discussed in the previous section. $\hat{A}(U=0)$ is diagonalized by the Bogoliubov transformation:

$$\begin{aligned}c_{k\uparrow}&=u_k^*b_k+v_kd_k^\dagger\ ,\\ c_{-k\downarrow}^\dagger&=-v_k^*b_k+u_kd_k^\dagger\ ,\end{aligned} \tag{23}$$

with

$$\begin{aligned}|v_k^2|&=\frac{1}{2}\left[1-\frac{\xi_k}{E_k}\right]\ ,\\ |u_k^2|&=\frac{1}{2}\left[1+\frac{\xi_k}{E_k}\right]\ ,\end{aligned} \tag{24}$$

where $\xi_k=\varepsilon_k-\mu_0$ and

$$E_k=(\xi_k^2+|\Delta_0(k)|^2)^{1/2}\ .$$

TABLE I. The staggered magnetization m and correlation energy ΔE_c using our method to $O(U^2)$ for the repulsive-U Hubbard model at half-filling. We compare with the staggered magnetization of the Hartree-Fock theory and the correlation energy using either RPA or variational antiferromagnetic Gutzwiller wave functions (AFGWF).

U/t	1	2	3	4	5	6	8	12
m	0.09	0.24	0.42	0.57	0.69	0.78	0.87	0.94
$m_{\rm HF}$	0.12	0.38	0.57	0.69	0.77	0.83	0.89	0.95
ΔE_c	−0.012	−0.035	−0.045	−0.042	−0.033	−0.025	−0.013	−0.006
ΔE_c (RPA)	−0.012	−0.043	−0.072	−0.093	−0.106	−0.115	−0.124	−0.130
ΔE_c (AFGWF)		−0.039	−0.044		−0.036	−0.027	−0.013	

In terms of the fermionic quasiparticles b_k and d_k, $\hat{A}(U=0)$ can be written

$$\hat{A}(U=0)=\sum_k(\xi_k-E_k)+\sum_k E_k(b_k^\dagger b_k+d_k^\dagger d_k) +N\mu_0 n+\tfrac{1}{2}\sum_k[\Delta_0(k)\psi(k) +\Delta_0^*(k)\psi^*(k)] . \quad (25)$$

(The sums over k should again be taken over the full original Brillouin zone.) The ground state $|\Omega_0\rangle$ of $\hat{A}(U=0)$ will have no b or d states occupied:

$$b_k|\Omega_0\rangle=d_k|\Omega_0\rangle=0 .$$

Again we derive relations which are true to all orders connecting n and ψ_k to μ_0 and $\Delta_0(k)$ (the chemical potential and conjugate field at $U=0$):

$$n=\frac{2}{N}\sum_k|v_k|^2 \quad (26)$$

and

$$\psi(k)=\frac{\Delta_0(k)}{E_k} . \quad (27)$$

This last relation makes clear why it is legitimate to treat the "gap" $\Delta_0(k)$ as the order parameter instead of $\psi(k)$, as is usually done in discussions of BCS theory, However, $\Delta_0(k)$ should not be confused with the conjugate field $\Delta(k)$.

Repeating the steps of Sec. II, we find that the free energy to $O(U^2)$ is given by

$$A[U,n,\Delta_0(k)]=2\sum_k\varepsilon_k|v_k|^2+\frac{NU}{4}\left[n^2+\left|\frac{1}{N}\sum_k\frac{\Delta_0(k)}{E_k}\right|^2\right] -\frac{U^2}{N^2}\sum_{k,k',p}\frac{(|v_k|^2|u_{k'-p}|^2-u_k v_k^* u_{k'-p}^* v_{k'-p})(|v_{k'}|^2|u_{k+p}|^2-u_{k'}v_{k'}^* u_{k+p}^* v_{k+p})}{E_k+E_{k'}+E_{k+p}+E_{k'-p}}+O(U^3) . \quad (28)$$

To $O(U)$, this has the familiar BCS form[14] and yields for $\Delta_0(k)=\Delta_0$ constant, the gap equation

$$1+\frac{U}{2N}\sum_k\frac{1}{E_k}=0 . \quad (29)$$

The $O(U^2)$ terms can be used to obtain corrections to the gap equation[15] (for any density) just as was done for the antiferromagnetic order parameter in Sec. II. Note that when $n=1$, the gap equation is identical to the self-consistent equation for the staggered magnetization for the repulsive-U case, as can be expected based on the mapping between the models with $U<0$ and $U>0$ at $n=1$,[16] and therefore Table I also gives the corrected superconducting order parameter for $n=1$ and $U<0$.

IV. SUPERCONDUCTIVITY IN THE REPULSIVE-U HUBBARD MODEL

The current revival of interest in the Hubbard model has, in large part, been motivated by Anderson's suggestion that the two-dimensional repulsive-U model provides a good description of the copper-oxygen planes of the high-temperature cuprate superconductors.[17] Numerous works have since been devoted to this model, but the phase diagram remains largely unknown. Even the weak-coupling situation is not yet clarified, in particular, concerning the possible existence of superconducting order. Some work[18] done previous to the discovery of the high-T_c superconductors and based on RPA approximations for various coupling channels did suggest the existence of superconductivity based on the enhancement of the d-wave singlet channels close to half-filling. More recent work using the renormalization-group[19] or "conserving approximations"[20] basically agree with this picture. Quantum Monte Carlo calculations on the other hand, seem to indicate that no superconducting long-range order is present in the ground state,[21] although they do find some enhancement of the singlet d-wave pairing channel near half-filling.[22]

In this section, we use our method to investigate the possibility of ordinary singlet or triplet pairing in the $U>0$ Hubbard model. Because, in this section, superconducting order alone is considered, our approach is valid provided no other phase boundary is crossed before reaching the possible superconducting phase. The region of the U-n phase diagram which we have in mind is depicted very schematically in Fig. 1. Another obvious restriction of our results is that only "conventional" pairing between electrons of opposite momenta is considered [although with an arbitrary k dependence for the gap $\Delta_0(k)$].

For singlet pairing, with order parameter

$$\psi(k)=\langle\Omega_U|c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger+c_{-k\downarrow}c_{k\uparrow}|\Omega_0\rangle$$

we can, of course, simply take over the formulas from the previous section and apply them for $U>0$. Examining the free energy in Eq. (28), we note that, as usual, the $O(U^0)$ term suppresses superconductivity. The $O(U^1)$ term also cannot favor superconductivity, as it is positive definite. On the other hand, the $O(U^1)$ term can be set equal to zero by choosing an appropriate symmetry for $\Delta_0(k)$: indeed, any angular-momentum $l>0$ symmetry will do, as well as appropriate extended s-wave gap functions. These channels are therefore favored. Given that the $O(U^0)$ term suppresses superconductivity and the $O(U^1)$ term can be set equal to zero, we must go on and consider the $O(U^2)$ term, which could, in principle, favor superconductivity and give us an equilibrium order pa-

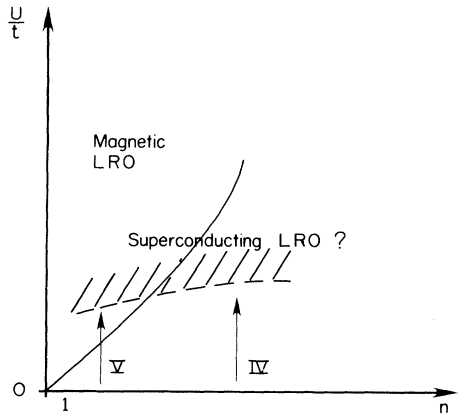

FIG. 1. A schematic drawing of the U-n phase diagram of the repulsive-U Hubbard model, and where one might hope superconductivity would occur, either with coexisting magnetic order (Sec. V) or without (Sec. IV). The arrows represent the fact that we are searching for a phase transition from the small-U side.

rameter. We have numerically evaluated the momentum sums in the $O(U^2)$ term, and searched for a possible gap function $\Delta_0(k)$ which would lower the $O(U^2)$ term below its value at $\Delta_0(k)=0$. We first considered an explicit form with $d_{x^2-y^2}$ symmetry like

$$\Delta_0(k)=\Delta(\cos[k_x]-\cos[k_y])$$

and concluded that the minimum value of the $O(U^2)$ term is always at $\Delta=0$. We then tried much more general forms, including discretizing the Brillouin zone and using general minimization algorithms, but never succeeded in lowering the $O(U^2)$ term below its value at $\Delta_0(k)=0$. Of course, the zero-point motion represented by the $O(U^0)$ term further acts to suppress any superconductivity. We therefore conclude that, at least to this order, there is no indication of ordinary singlet superconductivity for the weak-coupling repulsive-U Hubbard model. This conclusion is subject to some caveats which we will discuss later.

The conclusions are the same for triplet superconductivity. For example, consider the pairing of up spins of opposite momenta, with order parameter

$$\psi_k=\langle\Omega_U|c^\dagger_{k\uparrow}c^\dagger_{-k\uparrow}+c_{-k\uparrow}c_{k\uparrow}|\Omega_U\rangle\ .$$

We can compute the free energy in this case exactly the same way as before, and we find

$$A[U,n,\Delta_0(k)]=\sum_k\varepsilon_k v_k^2+\sum_k\varepsilon_k n_k^0+\frac{UN}{4}n^2-\frac{U^2}{N^2}\sum_{k,k',p}\frac{n^0_{k'}(1-n^0_{k'-p})(u^2_{k+p}v^2_k-u_kv_ku_{k+p}v_{k+p})}{E_k+E_{k+p}+|\xi_{k'}|+|\xi_{k'+p}|}+O(U^3), \tag{30}$$

where $\xi_k=\varepsilon_k-\mu_0$,

$$E_k=[\xi_k^2+\Delta_0(k)^2]^{1/2}\ ,$$

n_k^0 is the distribution function of the noninteracting system,

$$\frac{n}{2}=\frac{1}{N}\sum_k v_k^2=\frac{1}{N}\sum_k n_k^0 \tag{31}$$

and

$$u_k^2=\frac{1}{2}\left[1+\frac{\xi_k}{E_k}\right],\qquad v_k^2=\frac{1}{2}\left[1-\frac{\xi_k}{E_k}\right]. \tag{32}$$

Again, the $O(U^0)$ term suppresses superconductivity; now the $O(U^1)$ term is always unimportant as expected, but again the $O(U^2)$ term appears to suppress superconductivity.

At this point, we want to stress that, in order to obtain sensible results from a Hartree-Fock (or RPA) theory, it is important that one works at fixed density n as we have done, rather than at fixed chemical potential μ. For example, if we consider an expansion of the potential $\Omega(U,\mu,\psi_k)$ in powers of U, we find

$$\Omega[U,\mu,\psi_k]=\sum_k\left[\xi_k-\frac{\xi_k^2}{E_k}\right]+\frac{U}{4}\left[n^2+\left|\sum_k\frac{\Delta_0(k)}{E_k}\right|^2\right]+O(U^2) \tag{33}$$

with the same definitions as we had for singlet superconductivity except that any μ_0 is replaced with a μ and n is now given by $n=-d\Omega/d\mu$. The point is that $\psi_k=0$ is no longer a minimum of the potential Ω, which rather prefers to have some superconductivity to decrease N and thereby reduce the Coulomb repulsion from the $Un^2/4$ term.

Of course, if we had available the true free energy $A(U,n,\psi_k)$ and the true potential $\Omega(U,\mu,\psi_k)$, it would not matter, in principle, which one we used—the problem comes from the fact that we must truncate our expansion for these quantities at some power of U. Working at fixed n at each order is apparently important, in practice, to ensure that we do not have any spurious effects.

V. SUPERCONDUCTIVITY DRIVEN BY ANTIFERROMAGNETIC FLUCTUATIONS

In this section, we consider the possibility that a superconducting instability which is driven by antiferromagnetic fluctuations might exist in the Hubbard model. On the mean-field level, the antiferromagnetic order will be long ranged, although it is possible that only short-ranged antiferromagnetic order actually exists away from half-filling. The region of the phase diagram that we have in mind in this section is again drawn very schematically in Fig. 1.

In the "spin bag" mechanism of superconductivity,[23] one considers the possible pairing of antiferromagnetic quasiparticles. Pairing can increase the local magnetic order, and thereby lower the energy. In Ref. 23, an effective Hamiltonian for the quasiparticle interactions was calculated within the RPA, and it was demonstrated that attractive channels exist because of this effect. Nevertheless, one might wonder whether the effects of quantum zero-point motion, which always acts to suppress any kind of order, would be stronger or weaker than the attractive channels which favor superconductivity. In the following development, we directly address this issue by constructing a mean-field theory with antiferromagnetic order and pairing between antiferromagnetic quasiparticles. In contrast to the results in the other sections, our calculation is only done to $O(U)$, but given the correspondence already noted between our scheme and the RPA, the calculation can be considered a direct RPA calculation of the pairing susceptibility for antiferromagnetic quasiparticles. As shall be seen, we do find terms in the free energy which favor pairing between quasiparticles (which would not exist without the antiferromagnetic background), but the zero-point motion dominates so that superconductivity does not occur.

As was done in Ref. 23, we will only consider commensurate antiferromagnetic order, even though it is now known[24] that, at the mean-field level, incommensurate order is expected away from half-filling. Unfortunately, the exact nature of the incommensurate order is still not fully understood. Whether or not an incommensurate spin background would significantly affect the possibility of superconductivity is an interesting issue.

We begin by introducing, as in Sec. II, a Lagrange multiplier $h(U)$ which fixes the staggered magnetization m. We transform to antiferromagnetic quasiparticles b_k and d_k which are defined as in Sec. II, by Eqs. (7) and (8). We work at less than half-filling so that the b_k band is empty and the chemical potential cuts through the d_k band. As was done in Ref. 23, we study a pairing between d_k quasiparticles symmetrically placed around the antiferromagnetic gap. In other words, we consider a possible superconducting order parameter

$$\psi(k)=\langle d_k^\dagger d_{Q-k}^\dagger + \text{H.c.}\rangle ,$$

where, again, Q is the momentum vector (π,π). As the d_k's are spinless fermions, we now make the Bogoliubov transformation

$$d_k = u_k f_k + v_k f_{-k}^\dagger , \tag{34}$$

where

$$\begin{aligned} u_k^2 &= \frac{1}{2}\left[1+\frac{\tilde{E}_k^-}{F_k}\right], \\ v_k^2 &= \frac{1}{2}\left[1-\frac{\tilde{E}_k^-}{F_k}\right], \\ F_k &= [(\tilde{E}_k^-)^2+\Delta_0(k)^2]^{1/2} , \end{aligned} \tag{35}$$

and where the other quantities in these equations are defined as in Sec. II. Suppressing the upper band of quasiparticles, we can write the free-energy operator at $U=0$ in terms of the f_k quasiparticles as

$$\begin{aligned} \hat{A}(U=0) = &\tfrac{1}{2}\sum_k(\tilde{E}_k^- - F_k)+\sum_k F_k f_k^\dagger f_k \\ &+N\mu_0 n + N h_0 m \\ &+\tfrac{1}{4}\sum_k[\Delta_0(k)\psi(k)+\Delta_0^*(k)\psi^*(k)] . \end{aligned} \tag{36}$$

Again, we can relate the density and magnetization to the value of the Lagrange multipliers when $U=0$:

$$n=\frac{1}{N}\sum_k v_k^2, \quad m=\frac{h_0}{N}\sum_k \frac{v_k^2}{(\varepsilon_k^2+h_0^2)^{1/2}} . \tag{37}$$

We can compute the $O(U)$ term as usual by expressing the c_k operators in the interaction term in terms of the b_k and f_k operators and using the fact that the ground state at $U=0$ contains no b_k or f_k quasiparticles:

$$b_k|\Omega_0\rangle = f_k|\Omega_0\rangle = 0 .$$

Finally, we find the free energy to $O(U)$:

$$\begin{aligned} \frac{A}{N} = &-\frac{1}{N}\sum_k E_k v_k^2 + h_0 m \\ &+\frac{U}{4}\left[n^2-m^2+\frac{4}{N}\left[\sum_k \beta_k^2 u_k v_k\right]^2\right] . \end{aligned} \tag{38}$$

This free energy should be minimized over m and $\Delta_0(k)$ at fixed n. It reduces to the free energy for antiferromagnetism considered in Sec. II when $\Delta_0(k)=0$, and to the free energy for singlet superconductivity considered in Sec. IV when $m=0$. The last term in the free energy is positive definite, so it cannot possibly favor superconductivity. As in Sec. IV, it can be set equal to zero by choosing an appropriate symmetry for the superconducting gap.

From Eq. (37) for the staggered magnetization, we see that a superconducting gap function which alters v_k so that more of the density is located near the antiferromagnetic gap will increase the staggered magnetization, and from the free energy we see that this would indeed lower the $O(U)$ part of the energy as envisioned in the "spin bag" scenario. Such an effect does not exist without the background antiferromagnetic order. However, numerical and analytical[25] study of the free energy given above for many values of U and n convincingly shows that the increase to the energy that a nonzero superconducting gap causes through the $O(U^0)$ term always far outweighs the gain in the $O(U)$ term. In a physical description, the zero-point motion will destroy any tendency to pairing.

VI. DISCUSSION AND COMMENTS

Some comments about our results are in order. First, our conclusions illustrate an advantage of our method, which is that it symmetrically generates *all* terms of the same order, so that the competition between them can be fairly assessed. It also allows one to work directly at a fixed density, which can be important, in practice, as emphasized at the end of Sec. IV.

A second comment is that, while our results seem consistent with recent conclusions based on quantum Monte Carlo calculations,[21] we, by no means, have ruled out the possibility of superconductivity in the repulsive-U Hubbard model. One possibility is that superconductivity only occurs for larger U, while our approach is based on a weak-coupling expansion. Our normal paramagnetic state is always a Fermi liquid, so mechanisms in which superconductivity results because Fermi-liquid theory breaks down in the normal state might be difficult to understand within our method. (On the other hand small-U expansions do give quantitatively reasonable results for short-ranged quantities like the energy in one dimension, when the Hubbard model is certainly not a Fermi liquid.) Weak coupling in the third dimension might be a crucial ingredient.[26] Another possibility is that the superconducting order parameter is more complicated than those based on the pairing between electrons of opposite momenta that we have considered. Finally, it is possible that one should consider *incommensurate* magnetic and superconducting order simultaneously in order to obtain a superconducting instability, particularly for small doping.

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