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1991 J. Phys.: Condens. Matter 3 9843

(http://iopscience.iop.org/0953-8984/3/49/002)

J. Phys.: Condens. Matter 3 (1991) 9843–9857. Printed in the UK

On the Fermi liquid behaviour in doped antiferromagnetic correlated systems

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Received 25 March 1991, in final form 28 August 1991

Abstract. A reformulation of the Gutzwiller-type approximation for so-called correlated ferrimagnetic states is developed to obtain an analytical expression for the ground-state energies. The physical properties of two-dimensional antiferromagnetic states in the doped regime, such as the longitudinal spin susceptibility and the charge compressibility, are calculated from this formalism. We have estimated the Landau parameters in Fermi liquid theory near the critical doping concentration for antiferromagnetism and we show the fundamental difference of these correlated antiferromagnetic systems with liquid ^{3}He. In particular, we suggest the possibility of singlet superconductivity in the intermediate regime for the repulsive electron interaction ($U \sim W$) due to antiferromagnetic correlation.

1. Introduction

The most remarkable differences in the observed properties of the high-T_c copper oxide superconductors from the conventional superconductors are in magnetic properties. It is now widely believed that they arise from strong two-dimensional (2D) antiferromagnetic (AF) correlation between the spins of copper d holes in the insulating phase of these materials. Recently, the existence of strong spin correlations in the superconducting phase has also been reported from neutron scattering experiments performed in $La_{2-x}Sr_xCuO_4$ [1] and $YBa_2Cu_3O_{7-y}$ [2]. Naturally, this fact raises the question of a possible link between the superconducting state, through doping with the magnetic insulator parent. From a theoretical point of view, there have been two limiting ways to approach the 2D antiferromagnetic insulating state based on the single-band Hubbard model. The first, advanced by Schrieffer *et al* [3, 4], is the weak-coupling or 'itinerant electron' treatments in which the on-site repulsion U is assumed to be smaller than the bandwidth W ($=8t$). In this approach, the half-filled reference state is characterized by the spin-density-wave (SDW) state, which occurs due to the perfect Fermi-surface nesting. It causes an energy gap $2\Delta_{SDW}$ at the Fermi surface for the undoped material, leading to an insulator. An essential point is the existence of the antiferromagnetic order, which presumably extends to the superconducting phase although it becomes short-range ordering. The latter leads to an electronic pseudo-gap, which is slowly varying temporally as well as spatially. In the neighbourhood of the introduced mobile holes, the pseudo-gap is locally suppressed and that produces an effective potential or a bag inside which

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0953-8984/91/499843 + 15 $03.50

the hole is trapped self-consistently. As a result one finds that an entity comprising the quasi-hole surrounded by a local distortion of SDW background moves with charge $+e$ and spin $1/2$, which is referred to as a 'spin bag'. It has been considered that two spin bags attract each other to form a Cooper pair with the result that the two holes tend to share one common bag to lower their total energy. Quantitatively, the proper random-phase approximation (RPA) approaches [3, 5, 6] for fluctuations of a Landau–Fermi liquid have shown that these induce an attraction between the quasi-holes through exchanging the longitudinal magnetization fluctuations of the antiferromagnetic background. Since materials such as La_2CuO_4 have been found to be in the borderline situation $U \simeq W$ [7], it seems very important to understand the validity of RPA calculations in the large-U limit [8–10]. From this point of view it is interesting to note the result of Weng *et al* [8], who study the motion of a spin bag in the SDW background by using a variational method. Although the p-wave- and d-wave-like attractive potential is still obtained, its behaviour as a function of U is quite different from the simple RPA approach. For example, while the d-wave component of the attractive potential obtained in RPA reaches a maximum around $U \sim 3t$ and decreases as $1/U^3$ with increase of U, the result of [8] shows that the total attractive interaction is much reduced in the weak-coupling regime ($U < W$) and its maximum is pushed into the large-U regime (around $U \sim 10t$). The alternative way is from the strong-coupling, localized limit ($U > W$) where one gets a Mott insulator in the half-filled case with one electron per Cu site, described by the antiferromagnetic Heisenberg Hamiltonian [11]. In this limit, where the basis of most theoretical work is the t–J model ($J = t^2/U$), a theory of superconducting depends on the manner in which the quasi-particles can be described in the different ground states upon doping [11–13]. While the ultimate goal remains the understanding of the antiferromagnetism at relatively high doping level (~15%), it has so far proven elusive. In the limit of a very low doping concentration ($\delta \to 0$), where the Fermi liquid theory is expected to break down, there has been some progress including the studies of a single hole in an antiferromagnetic background [14]. For doping in the proximity of the critical concentration where AF states disappear, the Fermi liquid picture is not clear. Recently, a phenomenological model, in which the leading role is played by antiferromagnetic correlation, has been proposed to give a quantitative description of NMR measurements of high-T_c copper oxide superconductor [15].

The purpose of this paper is to study the behaviour of a doped antiferromagnetic state in a region close to the Mott transition ($U \simeq W$). For this, the antiferromagnetic Gutzwiller-type analytical approximation based on the slave-boson functional-integral approach is employed to calculate static properties of the system. Our calculation is a natural generalization of the formalism developed by Vollhardt [16] for liquid ^{3}He considered as a nearly localized Fermi liquid in which the Brinkmann–Rice metal–insulator transition (when $U = U_c \simeq \frac{8}{3}W$) can be understood. One of us was the first to remark on the fundamental difference with ^{3}He in heavy-fermion systems if antiferromagnetic correlations occur [17]. He found that the estimated value of F_0^a which characterizes the renormalization of the static spin susceptibility is likely to be small in comparison with those of ^{3}He. The consequence is that singlet superconductivity is possible in heavy-fermion compounds. Here we want to show that this idea is realized in the two-dimensional Hubbard model where strong magnetic correlations are important. The organization of this paper is the following. In section 2 we reformulate the Gutzwiller variational approach in order to obtain explicitly an expression for the ground-state energy in the antiferromagnetic state in analogy with Vollhardt's one for liquid ^{3}He. This may be called the correlated ferrimagnetic state. Then we first estimate analytically

the Landau parameter F_0^a by using a constant density of states (DOS) for the uncorrelated system. This result, valid for the interesting case $U \sim W$, allows us to compare with an expression of F_0^a in the case when the magnetic correlation is neglected [18, 19]. An analytical minimization of the ground-state energy with respect to the probability of doubly occupied sites d by expanding in a Taylor series in $d - d_{HF}$, where d_{HF} is the same probability in the Hartree–Fock approximation (HFA), is derived in section 3. This approximation not only gives good agreement with the numerical calculation for all the doping region but also describes qualitative behaviour in the weak and strong limit of U. In the proximity of the critical concentration, the longitudinal spin susceptibility and the charge compressibility are calculated in section 4. In particular, we show that the correlation effect can decrease the stability domain of ferrimagnetism for intermediate values of U in comparison with the HFA. For this regime of concentration where the long-range antiferromagnetic order is not present, the Landau parameters are estimated, in section 5, with a correction due to the contribution of the transverse spin susceptibility. These parameters determine the average 'molecular field' that arises from spin fluctuation effects. Assuming the forward scattering sum rule for $l < 2$, we discuss the singlet superconductor in this system. Finally, section 6 discusses the results and possible improvements in relation with other works.

2. Formulation

Let us start by considering the two-dimensional Hubbard model on a square lattice:

$$H = -t \sum_{\langle i,j \rangle} (C_{i\sigma}^{+} C_{j\sigma} + \text{HC}) + U \sum_{i} C_{i\uparrow}^{+} C_{i\uparrow} C_{i\downarrow}^{+} C_{i\downarrow} \tag{1}$$

where $C_{i\sigma}^{+}(C_{i\sigma})$ is a creation (annihilation) operator of an electron with spin σ at site i; $-t$ is the nearest-neighbour hopping integral; and U is the on-site electron interaction. By using the Gutzwiller-type analytical approximation based on the slave-boson functional-integral approach [20], the ground-state energy is given by [21]:

$$E = \sum_{i} \left((Ud_i + \xi_i m_i + \gamma_i n_i) + \int \mathrm{d}\varepsilon f(\varepsilon) \varepsilon \sum_{\sigma} \rho_{i\sigma}(\varepsilon) \right). \tag{2}$$

In equation (2), d_i is the density of doubly occupied sites; ξ_i and γ_i denote the exchange and charge fields, respectively; $f(\varepsilon)$ is the Fermi distribution function; and $\rho_{i\sigma}(\varepsilon)$ is the local density of states of σ spin and site i. In order to treat the antiferromagnetic states, one divides the crystal into two sublattices, A and B. Then in the alloy analogy approximation [22] $\rho_{i\sigma}(\varepsilon)$ can be determined from the local Green function. They have the following forms:

$$\rho_{A\sigma}(\varepsilon) = [X_{B\sigma}(\varepsilon)/X_{A\sigma}(\varepsilon)]^{1/2} \rho^0\{[X_{A\sigma}(\varepsilon)X_{B\sigma}(\varepsilon)]^{1/2}\} \tag{3a}$$

$$\rho_{B\sigma}(\varepsilon) = [X_{A\sigma}(\varepsilon)/X_{B\sigma}(\varepsilon)]^{1/2} \rho^0\{[X_{A\sigma}(\varepsilon)X_{B\sigma}(\varepsilon)]^{1/2}\} \tag{3b}$$

with $\rho^0(\varepsilon)$ being the unperturbed DOS of electrons of either spin. The locators $X_{i\sigma}$ are given by:

$$X_{i\sigma}(\varepsilon) = (\varepsilon - \gamma_i + \sigma\xi_i)/q_{i\sigma}. \tag{4}$$

The band-narrowing factor $q_{i\sigma}$ in general, is a function of n_i, m_i and d_i:

$$q_{i\sigma}(n_i, m_i, d_i) = \frac{2\{[(n_i + \sigma m_i - 2d_i)(1 - n_i + d_i)]^{1/2} + [d_i(n_i - \sigma m_i - 2d_i)]^{1/2}\}^2}{(n_i + \sigma m_i)(2 - n_i - \sigma m_i)}. \tag{5}$$

The expressions given by equations (2) and (5) include the original Gutzwiller

approximation (GA) and antiferromagnetic Hartree–Fock approximation (AFHFA) as a special case. The former is realized when $\xi_i = m_i = 0$ and the latter when $q_{i\sigma} = 1$ and $d_i^{HF} = (n_i^2 - m_i^2)/4$. In order to obtain a more transparent form for the energy expectation value as a function of the physical quantities $q_{i\sigma}$ and d_i following Vollhardt in the case of liquid ^{3}He, it is necessary for us to derive the expression of the kinetic energy in HFA. From equation (2) it is not difficult to identify this expression (for $T = 0$ K):

$$E_c^{HF} = \sum_i \left((\xi_i^{HF} m_i - \chi_i^{HF} n_i) + \int d\varepsilon\, \varepsilon \sum_\sigma \rho_{i\sigma}^{HF}(\varepsilon) \right) \tag{6}$$

with

$$\xi_i^{HF} = (U/2)m_i \qquad \gamma_i^{HF} = (U/2)n_i. \tag{7}$$

The related expressions for locator $X_{i\sigma}^{HF}$ may be written as

$$X_{i\sigma}^{HF}(\varepsilon) = \varepsilon - \Delta_{i\sigma} \tag{8}$$

with

$$\Delta_{i\sigma} = U n_{i-\sigma}. \tag{9}$$

When an infinitesimal longitudinal magnetic field is applied to our system, the sublattice magnetic moment m_i can be defined as

$$m_A = m_0 + m \qquad m_B = -m_0 + m \tag{10}$$

where m_0 is the staggered magnetization in AF states and m is the magnetic moment created by the external field. If the total electron number at a site is supposed to be independent of the field, as has been done by Penn [23], $n_i = n$, we have the following expressions for $n_{i\sigma}$:

$$n_{A\sigma} = [n + \sigma(m_0 + m)]/2 = [1 - \delta + \sigma(m_0 + m)]/2 \tag{11a}$$

$$n_{B\sigma} = [n + \sigma(-m_0 + m)]/2 = [1 - \delta + \sigma(-m_0 + m)]/2 \tag{11b}$$

where we denote δ as the doping concentration. Instead of (9) we use the new 'ferrimagnetic order parameters':

$$\Delta_{0\sigma} = (\Delta_{A\sigma} + \Delta_{B\sigma})/2 = U(n \pm m)/2 \tag{12a}$$

and

$$\Delta_{Q\sigma} = (\Delta_{A\sigma} - \Delta_{B\sigma})/2 = \pm U m_0/2. \tag{12b}$$

The upper (lower) sign in expression (12) corresponds to $\sigma = 1\,(-1)$. From the definition of the Fermi level $\varepsilon_{F\sigma}$:

$$n_\sigma = \tfrac{1}{2} \int^{\varepsilon_{F\sigma}} [\rho_{A\sigma}(\varepsilon) + \rho_{B\sigma}(\varepsilon)]\, d\varepsilon \tag{13}$$

we can obtain exactly the general relation for ferrimagnetic states in HFA [23]:

$$\Delta_{0\sigma} = U n_{-\sigma} \tag{14}$$

and

$$\Delta_{Q\sigma} = U\Delta_{-\sigma} \int^{\varepsilon_{F\sigma}} \frac{\rho_0(\varepsilon)\, d\varepsilon}{[\pm(\varepsilon^2 + \Delta^2)^{1/2}]}. \tag{15}$$

The plus sign of (15) is chosen when $\varepsilon > 0$. With the definitions (14) and (15) we obtain the following expression for the kinetic energy per site:

$$\varepsilon_c^{HF} = \frac{E_c^{HF}}{N} = \sum_\sigma \varepsilon_\sigma^{HF} - \frac{2}{U}(\Delta_{0\uparrow}\Delta_{0\downarrow} + \Delta_{Q\uparrow}\Delta_{Q\downarrow}) = \sum_\sigma \varepsilon_{c\sigma}^{HF} \tag{16}$$

with

$$\varepsilon_\sigma^{HF} = \int^{\varepsilon_{F\sigma}} [\Delta_{0\sigma} \pm (\Delta_{Q\sigma}^2 + \varepsilon^2)^{1/2}]\, \rho_0(\varepsilon)\, d\varepsilon \tag{17a}$$

and

$$\varepsilon_{c\sigma}^{HF} = \int^{\varepsilon_{F\sigma}} \frac{\varepsilon^2 \rho_0(\varepsilon)\, d\varepsilon}{[\pm(\varepsilon^2 + \Delta_{Q\sigma}^2)^{1/2}]}. \tag{17b}$$

By using (17*b*) we can rewrite the energy expectation value (equation (2)) in the presence of correlation in the form:

$$\varepsilon_g = \sum_\sigma q_\sigma \varepsilon_{c\sigma}^{HF}(\Delta_{Q\sigma}) + \frac{1}{N}\sum_i U d_i \tag{18}$$

with $\varepsilon_{c\sigma}^{HF}(\Delta_{Q\sigma})$ has the same form as (17) but $\Delta_{Q\sigma}$ must be considered as a variational parameter determined from minimization of (18). The renormalization factor q_σ is given by

$$q_\sigma = (q_{A\sigma} q_{B\sigma})^{1/2}. \tag{19}$$

Expression (18) can be considered as the ground-state energy of the so-called correlated 'ferrimagnetic' state. In the particular case when $m = 0$ we have $n_{A\sigma} = n_{B-\sigma}$ and therefore $q_\sigma = q = (q_{A\sigma} q_{A-\sigma})^{1/2}$. The expression (18) is then identical to a well known result for the ground-state energy of the antiferromagnetic state in the Gutzwiller approximation (AFGA) [24, 25]. Obviously, for $m_0 = 0$, one finds from (18) the ground-state energy of the original GA, which has been analysed by Vollhardt for liquid ^{3}He [16].

Before deriving an analytical minimization of ε_g with respect to d, we want to indicate that there is a possibility to calculate the spin susceptibility form (18) in a particularly interesting case $U \sim W$ if we use the constant DOS to evaluate ε_g. At this point it is necessary to emphasize that although expression (18) has a similar form in comparison with those of original GA, there is an important difference. If the ground state of the paramagnetic state is spin rotationally invariant, this property no longer holds in the AF state. In particular, owing to the spin broken symmetry we have $\chi_s^L \neq \chi_s^T$, where χ_s^L and χ_s^T are longitudinal and transverse susceptibility, respectively. However, we will show in section 5 that in the doped antiferromagnetic regime the ratio $r_{LT} = \chi_s^T/\chi_s^L$ is approximately equal to 1. So we think that one can use the value χ_s^L instead of an average value $\bar{\chi}$ to evaluate, for example, the Landau parameter F_0^s in the proximity of the critical doping concentration for antiferromagnetism.

Using a constant DOS of width $\Delta = W/2$, the expression (17*b*) for $\varepsilon_{c\sigma}^{HF}(\Delta_Q)$ is greatly simplified:

$$\varepsilon_{c\sigma}^{HF} = [1/(4\Delta)][\varepsilon_{F\sigma}(\Delta_{Q\sigma}^2 + \varepsilon_{F\sigma}^2)^{1/2} - \Delta(\Delta_{Q\sigma}^2 + \Delta^2)^{1/2}] - \Delta_{Q\sigma}\Delta_{Q-\sigma}/(2U) \tag{20}$$

with

$$\varepsilon_{F\sigma} \simeq \Delta(-\delta + \sigma m). \tag{21}$$

Near the critical doping concentration we can assume that $\Delta_{Q\sigma} < W, \varepsilon_{F\sigma}$. Then for $U = W$ the expression (20) in conjunction with (12*b*) yields

$$\varepsilon_{c\sigma}^{HF} \simeq -(\Delta/2)[1 - m_0^2 - (\delta - \sigma m)^2]. \tag{22}$$

The square brackets in (22) can be compensated by the denominator of renormalization factor q_σ (equation (19)) in the same doping regime. Equation (18) then reduces to

$$\varepsilon_g = -\frac{\Delta}{2}\sum_\sigma f_\sigma + \frac{U}{N}\sum_i d_i. \tag{23}$$

with $f_\sigma = (f_{A\sigma} f_{B\sigma})^{1/2}$ the numerator of q_σ. From the minimization with respect to d_i,

$(\partial\varepsilon_g/\partial d)|_{m=0} = 0$, it is not difficult to show that the dependence of ε_g on m gives the following first correction:

$$\delta\varepsilon_g \sim (\delta d)^2 \sim m^4. \tag{24}$$

Then the spin susceptibility χ_s, given by

$$\chi_s^{-1} = (1/\mu_0^2)(\partial^2\varepsilon_g/\partial m^2)|_{m=0} \tag{25}$$

where μ_0 is the Bohr magneton, is found from the first term of the RHS of (23) as

$$\frac{\chi_0}{\chi_s} = \frac{2d^{1/2}(\delta + d)^{1/2}(1 - \delta - 2d)}{(1 - \delta - 2d)^2 - m_0^2} + \frac{(\delta + 2d)m_0^2}{[(1 - \delta - 2d)^2 - m_0^2]^{3/2}}. \tag{26}$$

The second term of (26) gives a new contribution to the spin susceptibility from the antiferromagnetic state with respect to the first one, which can be obtained in the original GA when $m_0 = 0$ [18, 19]. This contribution is always positive, so the value of F_0^a must be reduced in comparison with the paramagnetic state if antiferromagnetic correlations occur.

3. Ground-state energy

The minimization of (18) with respect to d may be performed numerically for the AF state for the half-filled case [20] and has been done recently for all doping concentrations [26]. But it is difficult to study other physical properties like spin susceptibility from these calculations. On the other hand, one notes that the antiferromagnetic state in HFA leads to energies that are in good agreement with the AFGA in the weak- and strong-coupling limits. This leads us to find the ground-state energy of 'ferrimagnetic state' by expanding ε_g in $d_i - d_i^{HF}$. So the change of this factor can be written as

$$q_\sigma = 1 + \tfrac{1}{2}\sum_{ij} \frac{\partial^2 q_\sigma}{\partial d_i\, \partial d_j}\bigg|_{d_{i(j)} = d^{HF}_{i(j)}} (d_i - d_i^{HF})(d_j - d_j^{HF}) + O((d - d^{HF})^3) \tag{27}$$

with

$$(\partial^2 q_\sigma/\partial d_i\, \partial d_j)|_{d_{i(j)} = d^{HF}_{i(j)}} < 0. \tag{28}$$

By limiting the expansion up to second order in $d_i - d_i^{HF}$, it is not difficult to find that

$$\varepsilon_g = \varepsilon_T^{HF} - \tfrac{1}{8}U^2(1/a + 1/b) \tag{29}$$

where ε_T^{HF} is the total energy of system in the HFA. It can be written as

$$\varepsilon_T^{HF} = \sum_\sigma \varepsilon_{c\sigma}^{HF} + \frac{1}{U}(\Delta_{0\uparrow}\Delta_{0\downarrow} + \Delta_{Q\uparrow}\Delta_{Q\downarrow}) = \sum_\sigma \varepsilon_{c\sigma}^{HF} + \frac{U}{4}[(1 - \delta)^2 - m^2 - m_0^2]. \tag{30}$$

The expressions a and b in (29) are found to be

$$a = \varepsilon_{c\uparrow}^{HF}\, \partial^2 q_\uparrow/\partial d_A^2 + \varepsilon_{c\downarrow}^{HF}(\partial^2 q_\downarrow/\partial d_A^2)|_{d_A = d_A^{HF}} \tag{31a}$$

$$b = \varepsilon_{c\uparrow}^{HF}\, \partial^2 q_\uparrow/\partial d_B^2 + \varepsilon_{c\downarrow}^{HF}(\partial^2 q_\downarrow/\partial d_B^2)|_{d_B = d_B^{HF}}. \tag{31b}$$

The second term on the RHS of (29) is then always negative and gives a correction to the ground-state energy with respect to the HFA. If we denote

$$a_\sigma = (n_A + \sigma m_A)(2 - n_A + \sigma m_A) \tag{32a}$$

$$b_\sigma = (n_B + \sigma m_B)(2 - n_B + \sigma m_B) \tag{32b}$$

then we obtain the simple expressions for a and b:

$$a^{-1} = -(a_\uparrow a_\downarrow)^2/[16(\varepsilon_{c\uparrow}^{HF} a_\downarrow + \varepsilon_{c\downarrow}^{HF} a_\uparrow)] \tag{33a}$$

$$b^{-1} = -(b_\uparrow b_\downarrow)^2/[16(\varepsilon_{c\uparrow}^{HF} b_\downarrow + \varepsilon_{c\downarrow}^{HF} b_\uparrow)]. \tag{33b}$$

When $m = 0$, we have the ground-state energy for the AF case:

$$\varepsilon_g^{AF} = \varepsilon_T^{HF} - (U^2/64|\varepsilon_c(\delta, m_0)|)\{[(1+\delta)^2 - m_0^2][(1-\delta)^2 - m_0^2]\}^2/(1 - \delta^2 - m_0^2). \tag{34}$$

The corresponding expressions for q^{AF} and d^{AF} are

$$q^{AF} = 1 - (U^2/64|\varepsilon_c(\delta, m_0)|)\{[(1+\delta)^2 - m_0^2][(1-\delta)^2 - m_0^2]\}^2/(1 - \delta^2 - m_0^2) \tag{35}$$

and

$$d^{AF} = d^{HF} - (U/32|\varepsilon_c(\delta, m_0)|)\{[(1+\delta)^2 - m_0^2][(1-\delta)^2 - m_0^2]\}^2/(1 - \delta^2 - m_0^2) \tag{36}$$

with

$$d^{HF} = (n^2 - m_0^2)/4.$$

The results (34)–(36) allow us to discuss various limits. First, we remark that in the weak-coupling limit $U < W$ they give a useful correction in comparison with HFA. For the half-filled case, where $\delta = 0$, we have

$$\varepsilon_g^{AF} = \varepsilon_T^{HF} - (U^2/64|\varepsilon_c|)(1 - m_0^2)^3. \tag{37}$$

In the strong-interaction region, $U \to \infty$, one finds $1 - m_0 \to 1/U^2$ and $|\varepsilon| \to t^2/U$. So we have a correction to the ground-state energy of order $1/U^3 \to 0$, which is in good agreement with recent numerical calculation [21]. Finally, for $m_0 = 0$, from (34) we obtain

$$\varepsilon_g = \varepsilon_T^{HF} - (U^2/64|\varepsilon_0|)(1 - \delta^2)^3. \tag{38}$$

When $\delta = 0$, we have $\varepsilon_T^{HF} = -|\varepsilon_0| + U/4$, so ground-state energy (38) gives exactly the Brinkman–Rice metal–insulator transition at $U = U_c = 8|\varepsilon_0|$, i.e. localization occurs at a finite interaction strength.

In order to verify quantitatively, we compare our analytical results (34)–(36) with the numerical ones from AFGA [26]. The ground-state energies ε_g calculated in the AFGA, AFHFA, GA and paramagnetic Hartree–Fock approximation (PHFA) by both methods are shown in figure 1, for various doping concentrations at $U = 8t = W$. We note that, in all the cases investigated, the analytical expressions (34)–(36) give a good approximation to the results of the numerical calculations. Figures 2 and 3 show the ground-state energy correction of GA in comparison with HFA as a function of sublattice magnetization for different doping. The quantity is always a decreasing function of the magnetization for all values of doping concentration. This result seems natural since in the presence of a magnetic moment the spin up and spin down tend to avoid each other and we can expect that the introduction of correlation has a smaller effect when the magnetic moment is increased. As a consequence, the energy of the paramagnetic phase is lowered more

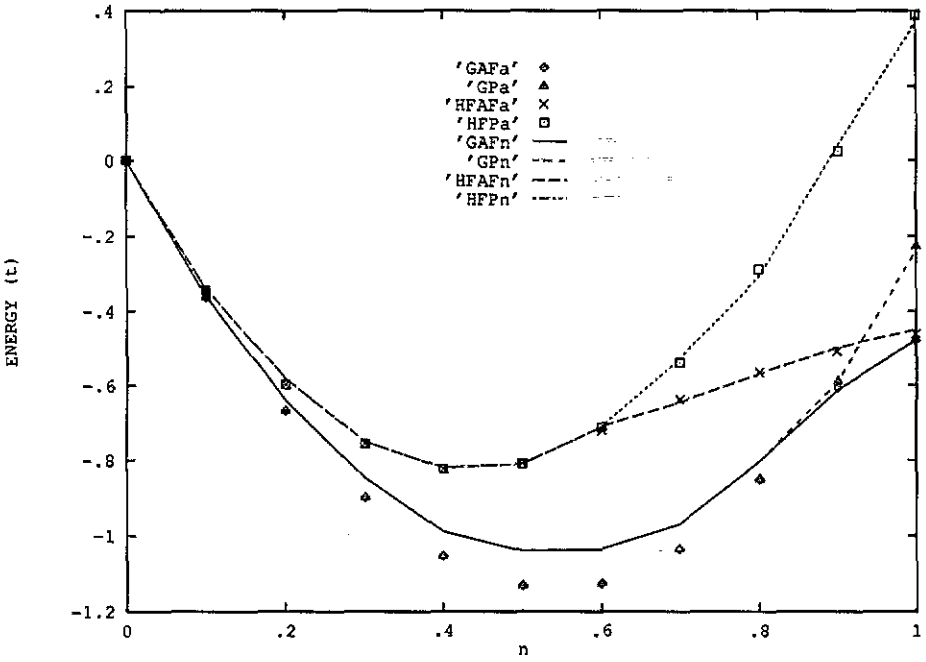

Figure 1. The ground-state energy as a function of the number of holes per site calculated by different approximations. The suffixes a and n mean analytical and numerical results, respectively. Energies are measured in units of the hopping matrix element.

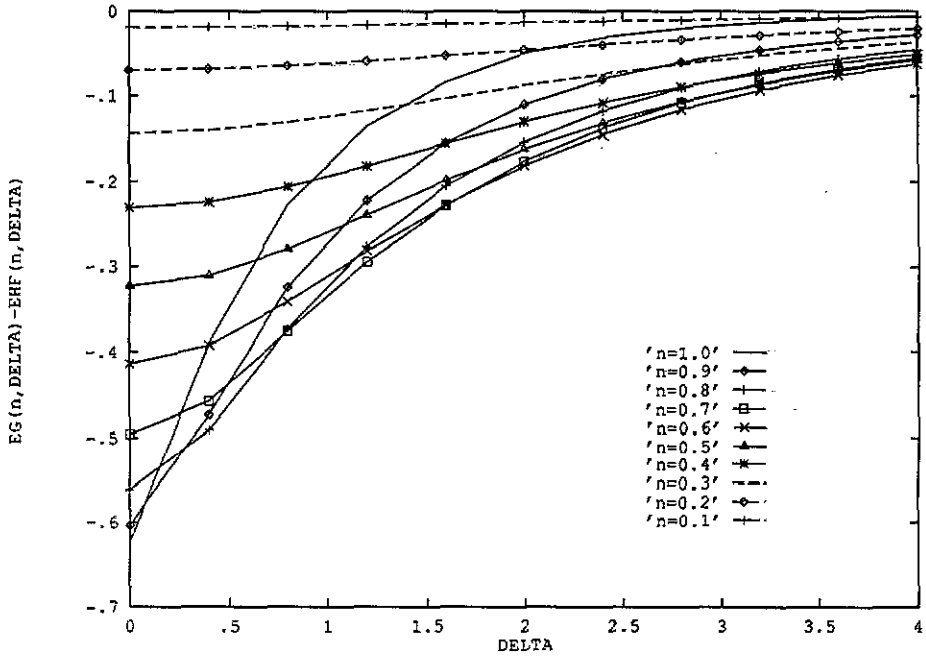

Figure 2. The energy correction with respect to Hartree–Fock approximation as a function of the variational parameter Δ with different number of holes per site for $U = 8t$.

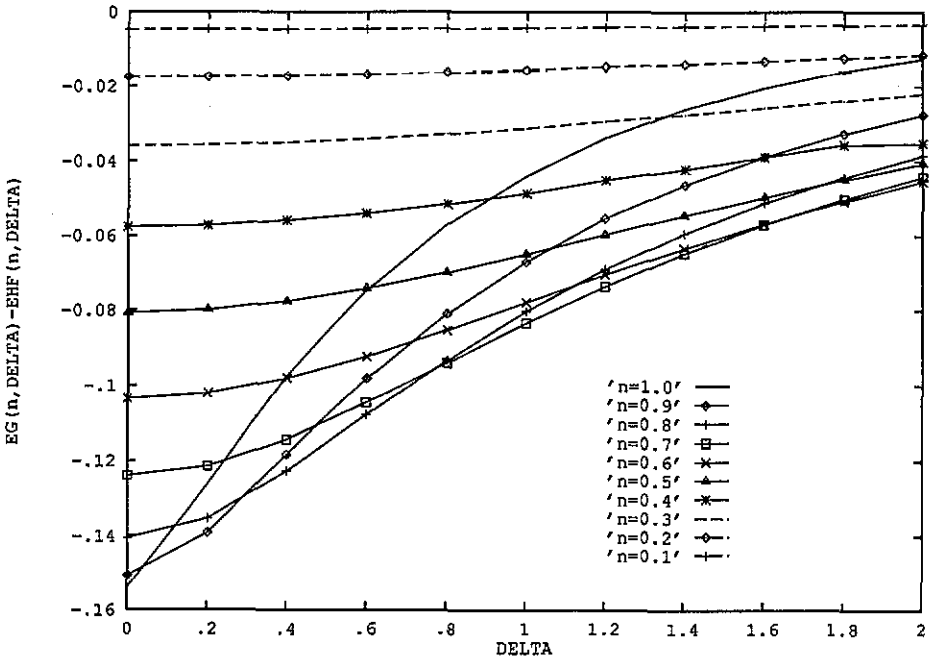

Figure 3. The same functions as in figure 2 for $U = 4t$.

than that of the antiferromagnetic phase when correlations are taken into account. An important conclusion is that the doping range for antiferromagnetism in this case is smaller compared to that of HFA.

4. Properties of the solution

We now want to show that our Gutzwiller's results for the ground-state energy (equations (29)–(33)) can be used to extract two important physical quantities of the system: the longitudinal spin susceptibility and the charge compressibility in doped AF state. From definitions we have the following two expressions, respectively:

$$1/\chi_s^L = (1/\mu_0^2)(\partial^2 \varepsilon_g/\partial m^2)|_{m=0} = (1/\mu_0^2)[2\varepsilon_c^{(2,m)} - U/2 - (U^2/4)(\partial^2(a^{-1})/\partial m^2)|_{m=0}] \tag{39}$$

and

$$1/k = (\partial^2 \varepsilon_g/\partial \delta^2)|_{\delta=\delta_c} = 2\varepsilon_c^{(2,\delta)} + U/2 - (U^2/4)(\partial^2(a^{-1})/\partial \delta^2)|_{\delta=\delta_c} \tag{40}$$

where one denotes δ_c as a critical concentration. The second derivative values in (39) and (40) are obtained from equations (17*b*) and (29) in conjunction with (13). They have the following forms:

$$\left.\frac{\partial^2(a^{-1})}{\partial m^2}\right|_{m=0} = \sum_{i=0}^{2} A_m^i \tag{41}$$

and

$$\left.\frac{\partial^2(a^{-1})}{\partial \delta^2}\right|_{\delta=\delta_c} = \sum_{i=0}^{2} A_\delta^i \tag{42}$$

where $A^{L}_{m(\delta)}$ are the contributions of 'correlation terms' (third terms of equations (39) and (40) respectively) and $\varepsilon_c^{(n,m(\delta))}$ are the nth derivative of the kinetic energy with respect to m and δ. Their expressions are given in the appendix. The first two terms of (39) and (40) represent the Hartree–Fock contributions to $(\chi_s^L)^{-1}$ and $(k)^{-1}$ respectively. They have opposite sign for the first quantity and the same sign (positive) for the second one. The numerical calculations for increased values of U (see section 5) show that this contribution decreases continuously to zero for $(\chi_s^L)^{-1}$ whereas it increases greatly for $(k)^{-1}$. The third terms of these equations give the 'correlation contributions' and they always have a positive sign. For the large-U regime, the latter contribution becomes an important correction with respect to the Hartree–Fock one. This will decrease the stability domain of ferrimagnetism as compared to the phase diagram obtained by Penn in HFA [23].

5. Landau parameters

In this section we want to apply the Fermi liquid theory to the doped antiferromagnetic system where the properties with average spin fluctuations can be evaluated from preceding calculations. This has been done by Vollhardt [15] for liquid ^{3}He considered as a nearly localized Fermi liquid and by Valls and Tesanovic [27] for heavy fermions. Contrary to these authors, we show that if superconductivity can occur, it is likely to be singlet. The presence of antiferromagnetic correlations seems to be responsible for this difference. It is well known that by introducing the concept of quasi-particles the Landau theory of a Fermi liquid gives the possibility to understand the physical properties of the system. Here the quasi-particles are characterized by an effective mass m^* and an effective interaction. The latter can be parametrized by means of an infinite set of 'molecular fields' quantified by the Landau parameters $F_l^{s(a)}$ [28]. For example, the spin susceptibility χ_s, the compressibility k and the effective mass m^* can be related to the first usual Landau parameters F_0^s, F_0^a, F_1^s by the following equations:

$$F_0^s = -1 + m^* k^{(0)}/mk \tag{43}$$

$$F_0^a = -1 + m^* \chi^{(0)}/m\chi_s \tag{44}$$

$$m^*/m = 1 + F_1^s/3. \tag{45}$$

It is obvious that the 'Fermi liquid' term (i.e. the molecular fields) will in general affect the response to external fields. So if we want to apply the expressions (43)–(45) to the system with antiferromagnetic correlation, it is necessary to clarify the value χ_s in equation (44). Since in the AF phase the ground state defined by spin-density wavefunction breaks the continuous spin rotation invariance, we have in general $\chi_s^L \neq \chi_s^T$, where L and T denote the longitudinal and transverse components. So we want to evaluate the relation

$$r_{LT} = \chi_s^T/\chi_s^L \tag{46}$$

in the proximity of the critical doping concentration δ_c. For a general AFGA wavefunction, one can extract this relation from the nearest-neighbour spin–spin correlation functions [25]. The latter may be calculated exactly only for the limit $d \to \infty$ where one reproduces the results of the Kotliar–Ruckenstein path integral approach to the Hubbard model in finite dimension. Their results can be written as

$$\langle S_i^z S_{i+\tau}^z \rangle = -m_0^2/4 + g_{s^z s^z} C^{s^z s^z}(g = 1) \tag{47}$$

$$\langle S_i^+ S_{i+\tau}^- \rangle = g_{s^+ s^-} C^{s^+ s^-}(g = 1) \tag{48}$$

where $g_{s^zs^z}$ ($g_{s^+s^-}$) and $C^{s^zs^z}(g=1)$ ($C^{s^+s^-}(g=1)$) are the longitudinal (transverse) of renormalization factor for the spin–spin correlation function (SSCF) and the SSCF values calculated from non-correlated spin-density wavefunction, respectively. Note that, owing to the broken symmetry, we have in general $g_{s^+s^-} \neq g_{s^zs^z}$:

$$g_{s^zs^z} = 4[(n-2d-m_0^2)^2 - (1-n)^2m_0^2]/(n^2-m_0^2)[(2-n)^2-m_0^2] \tag{49}$$

and

$$g_{s^+s^-} = 4[(n-2d)^2 - m_0^2]/(n^2-m_0^2)[(2-n)^2-m_0^2]. \tag{50}$$

In the paramagnetic case, $m_0 = 0$, we have

$$g_{s^zs^z} = g_{s^+s^-} = 4(n-2d)^2/n^2(2-n)^2. \tag{51}$$

Expressions (50) and (51) can be deduced from the simple matrix-density representation for Gutzwiller approximation [17]. Unfortunately, this is not the case for (49) because this method assumes that the correlation between the sites is neglected. The presence of the factor 4 in equations (49)–(51) can be explained by the fact that the probability for the spin–spin interaction process occurs only when both sites are singly occupied. We have used (47) and (48) to evaluate the value r_{LT}. Instead of $C^{s^zs^z}(g=1)$ we calculate the longitudinal and transverse spin susceptibility in HFA from the linear response of an AF to an external magnetic field [22]. It is not difficult to show that

$$\chi_L^{HF}(g=1) = -2\mu_0^2 \lim \Gamma_\uparrow(q)|_{q\to 0} \tag{52}$$

with

$$\Gamma_\uparrow(q) = \sum_k \frac{f(E_{k+q,\uparrow}) - f(E_{k,\uparrow})}{E_{k+q,\uparrow} - E_{k,\uparrow}} \tag{53}$$

and

$$\chi_T^{HF}(g=1) = -2\mu_0^2 \lim \Gamma_{\uparrow\downarrow}(q)|_{q\to 0} \tag{54}$$

with

$$\Gamma_{\uparrow\downarrow}(q) = \sum_k \frac{f(E_{k+q,\uparrow}) - f(E_{k,\downarrow})}{E_{k+q,\uparrow} - E_{k,\downarrow}} \tag{55}$$

where $f(\varepsilon)$ is the Fermi distribution function and $E_{k,\sigma}$ is the AF eigenstate in HFA. The expressions (52)–(55) in conjunction with (47) and (48) allow us to calculate r_{LT}, which in turn is used to estimate the average susceptibility of the system:

$$\bar{\chi} \simeq \tfrac{1}{3}\chi_s^L(1+2r_{LT}). \tag{56}$$

We use equation (56) to estimate the Landau parameter F_0^a with the value of χ_s^L determined from the ground-state energy calculation (see equation (39)). The calculations are carried out by using the exact square lattice DOS $\rho^0(\varepsilon)$. Two other Landau parameters F_0^s and F_1^s can be obtained from equations (40) and (35), respectively. The latter quantity (q_{AF}) can be identified as the discontinuity of the momentum distribution at the Fermi surface and determines the mass renormalization, i.e.

$$q_{AF} = (m^*/m)^{-1}. \tag{57}$$

If we define

$$A_l^{s(a)} = F_l^{s(a)}/\{1 + [F_l^{s(a)}/(2l+1)]\} \tag{58}$$

which determines the spin singlet (triplet) quasi-particle scattering amplitude in the

Table 1. Physical properties and Landau parameters calculated in the doped antiferromagnetic state for different values of U.

U	$4t$	$6t$	$8t$
δ	0.125	0.125	0.140
m_0	0.049	0.073	0.167
d	0.117	0.080	0.042
q	0.908	0.794	0.656
$q_{s^z s^z}$	1.692	2.099	2.472
$q_{s^+ s^-}$	1.695	2.109	2.538
r_{LT}	1.011	1.033	1.109
χ_s^L	0.312	0.361	0.449
k	0.141	0.116	0.096
F_0^a	−0.253	−0.274	−0.351
F_0^s	0.665	1.309	2.248
F_1^s	0.304	0.777	1.573
g_0	0.033	−0.333	−0.565
g_1	0.010	0.031	0.025

particle–hole channels $T^{s(a)}(\theta, \varphi = 0)$, we can study the existence of superconductivity from the Fermi liquid theory [29]. It has been observed by Patton and Zaringhalam [30] that if the scattering amplitude is chosen to contain only $l = 0$ and $l = 1$ partial waves in the scattering angle φ (s–p approximation), then the effective interaction $g_j (j = 0, 1)$ can be derived from the spin singlet and triplet amplitudes $T_{s,t}(\theta, \varphi)$ in the particle–particle channels. They have the following expressions in term of the Landau parameters:

$$g_0 = \sum_l (-1)^l (A_l^s - 3A_l^a)/4 \tag{59}$$

and

$$g_1 = \sum_l (-1)^l (A_l^s + A_l^a)/12. \tag{60}$$

If g_j is negative, the $j = 0\,(1)$ indicates pairing in a singlet (triplet) state. Here we assume that $A_l^{s(a)} = 0$ for $l \geqslant 2$ and use the sum rule $\Sigma_l (A_l^s + A_l^a) = 0$ to estimate the value of A_l^a. The results of our calculation are presented in table 1 for three different values of U ($U = 4t$, $6t$, $8t$). Numerical error for the estimated values in this table is 10^{-3}. The following points can be deduced from this table:

(i) The magnitude of the renormalization factor is generally reduced in the $U \leqslant W$ regime for doped AF phase. This tendency, which is in agreement with those of the half-filled case [21], leads to an increase in the Landau parameter F_1^s for effective-mass relation.

(ii) The contribution of 'correlation term' (third term of equation (39)) for magnitude of $(\chi_s^L)^{-1}$ with respect to Hartree–Fock terms becomes dominating when $U \rightarrow W$ (first two terms have opposite sign).

(iii) In doped antiferromagnetic regime, the ratio r_{LT} increases with U, so the transverse magnetization fluctuations may be important in the large-U limit [10]. However, for moderate magnitude of U, the value of r_{LT} is not very different from 1. This property concerns not only χ_s^T/χ_s^L but also the relation between their renormalization factors $g_{s^+s^-}/g_{s^zs^z}$. So the Landau parameter F_0^a is then determined principally by the value of χ_s^L. The magnitude of F_0^a is greatly reduced in comparison with those for liquid ^{3}He

where $F_0^a \sim -0.75$. From our calculations this reduction corresponds not only to increasing effective masses but also to a new contribution in the spin susceptibility relation χ_0/χ_s from antiferromagnetic state in the proximity of the critical concentration, as has been explained in the case of expression (26). We have mentioned that this is a fundamental property of the system when antiferromagnetic correlations occur.

(iv) The 'correlation term' of inverse compressibility (k^{-1}) (equation (40)) also increases with U but there is no compensation between the first two terms of this equation. So the Landau parameter F_0^s is very large. The same conclusion is obtained by Kotliar *et al* [31] in their Fermi liquid description of $La_{2-x}Sr_xCuO_4$.

(v) Finally, from our calculation we came to a very interesting conclusion with respect to superconducting properties of the system. Singlet superconductivity can occur in the antiferromagnetic doped phase. But this effect appears only for $U > 4t$ when the antiferromagnetic correlations become important. Our conclusion seems to be in agreement with the dependence of the attractive interaction as a function of U obtained by Weng *et al* [8] from a variational approach for the 'spin bag' model. Recently Monte-Carlo simulations [32] have been performed in the two-dimensional Hubbard model to study a quasi-particle attraction. Here the authors did not find evidence for long-range pairing correlation in a very small sample (4×4 and 6×6 for $U/t = 4$ and 4×4 for $U/t = 10$). We do not consider that these calculations can really prove that the ground state of the Hubbard model cannot be superconducting, especially for $U \sim W$.

6. Conclusions

In the present paper we have studied the properties of 2D antiferromagnetic doped phase in the Hubbard model. The Gutzwiller approximation for this case is reformulated in order to obtain useful expressions for the ground-state energy. The latter, in fact, is the energy of the 'ferrimagnetic correlated state'. We have derived analytically the minimized expressions (with respect to d) for this state, which allow us to study some essential properties of the longitudinal magnetization fluctuations. We have found that the longitudinal and transverse spin susceptibilities have comparable magnitude at or near the critical concentration for moderate regime of U.

The Landau parameter estimated for this system with non-long-range AF order has three principal properties:

(i) In the intermediate range for U ($U \leqslant W$) the bandwidth renormalization factor q increases with U.

(ii) The reduced value of Landau parameter F_0^a with respect to the paramagnetic Fermi liquid case shows the important effect of the presence of antiferromagnetic fluctuations.

(iii) There is a very large value of F_0^s.

All these properties lead to a possible existence of singlet superconductivity in the system for $U > 4t$. The natural way to extend our results is to study the behaviour of Landau parameters in a more realistic model for a high-T_c superconductor, for example, the two-band model [33]. In this model, one can predict strong two-dimensional antiferromagnetic fluctuations for doping much above the critical doping obtained from the single Hubbard model [34]. This fact confirms that superconductivity can exist in the presence of relatively strong antiferromagnetic correlations.

Acknowledgments

One of us (D Nguyen Manh) is extremely grateful for the support of the Université Joseph Fourier de Grenoble and in particular to F Cyrot-Lackmann for her hospitality at LEPES (CNRS).

Appendix

The following expressions for $A^i_{m(\delta)}$ are obtained:

$$A^0_m = -[4m_0^2(1+\delta^2-m_0^2)^2 - (a_\uparrow a_\downarrow)_0(1+\delta^2-3m_0^2)]/2\varepsilon_c^{(0)}(a_\uparrow + a_\downarrow)_0 \tag{A1}$$

$$A^1_m = 4m_0^2(a_\uparrow a_\downarrow)_0(1+\delta^2-m_0^2)(\varepsilon_c^{(1,m)}\delta + \varepsilon_c^{(0)})/[\varepsilon_c^{(0)}(a_\uparrow + a_\downarrow)_0]^2 \tag{A2}$$

$$A^2_m = \frac{(a_\uparrow a_\downarrow)_0^2}{8}\left(\frac{\varepsilon_c^{(2,m)}(1-\delta^2-m_0^2) - 2\varepsilon_c^{(0)} - 4\varepsilon_c^{(1,m)}\delta}{[\varepsilon_c^{(0)}(a_\uparrow + a_\downarrow)_0]^2} - \frac{16m_0^2(\varepsilon_c^{(1,m)}\delta + \varepsilon_c^{(0)})^2}{[\varepsilon_c^{(0)}(a_\uparrow + a_\downarrow)_0]^3}\right) \tag{A3}$$

and

$$A^0_\delta = -[4\delta^2(1-\delta^2+m_0^2)^2 - (a_\uparrow a_\downarrow)_0(1-3\delta^2+m_0^2)]/2\varepsilon_c^{(0)}(a_\uparrow + a_\downarrow)_0 \tag{A4}$$

$$A^1_\delta = 2\delta(1-\delta^2+m_0^2)(a_\uparrow a_\downarrow)_0[2\varepsilon_c^{(0)}\delta - (1-\delta^2-m_0^2)\varepsilon_c^{(1,\delta)}]/[\varepsilon_c^{(0)}(a_\uparrow + a_\downarrow)_0]^2 \tag{A5}$$

$$A^2_\delta = \frac{(a_\uparrow a_\downarrow)_0^2}{8}\left(\frac{\varepsilon_c^{(2,\delta)}(1-\delta^2-m_0^2) - 2\varepsilon_c^{(0)} - 4\delta\varepsilon_c^{(1,\delta)}}{[\varepsilon_c^{(0)}(a_\uparrow + a_\downarrow)_0]^2} - \frac{4[\varepsilon_c^{(0)}\delta - (1-\delta^2-m_0^2)\varepsilon_c^{(1,\delta)}]}{[\varepsilon_c^{(0)}(a_\uparrow + a_\downarrow)_0]^3}\right) \tag{A6}$$

where $(a_\uparrow a_\downarrow)_0$ and $(a_\uparrow + a_\downarrow)_0$ are their values at $m = 0$ and $\delta = \delta_c$.

The nth derivatives of the kinetic energy $\varepsilon_c^{(n,m(\delta))}$ with respect to m (δ) have the forms

$$\varepsilon_c^{(0)} = -\int^{\varepsilon_F} \frac{\varepsilon^2\rho(\varepsilon)\,d\varepsilon}{(\varepsilon^2+\Delta_Q^2)^{1/2}} \tag{A7}$$

$$\varepsilon_c^{(1,m)} = E_0^{(1)} + E_1^{(1)} \qquad \varepsilon_c^{(1,\delta)} = E_0^{(1)} - E_1^{(1)} \tag{A8}$$

where

$$E_0^{(1)} = U\Delta_Q^2 I_{31}/2(1+UI_{31})(\varepsilon_F^2+\Delta_Q^2)^{1/2} \tag{A9a}$$

$$E_1^{(1)} = \varepsilon_F^2/2(1+UI_{31})(\varepsilon_F^2+\Delta_Q^2)^{1/2} \tag{A9b}$$

and the forms

$$\varepsilon_c^{(2,m)} = -E_0^{(2)} + E_1^{(2)} + E_2^{(2)} + E_3^{(2)} + E_4^{(2)} - E_5^{(2)} \tag{A10a}$$

$$\varepsilon_c^{(2,\delta)} = E_0^{(2)} + E_1^{(2)} + E_2^{(2)} + E_3^{(2)} - E_4^{(2)} - E_5^{(2)} \tag{A10b}$$

where

$$E_0^{(2)} = U^2\varepsilon_F^2\Delta_Q^2 I_{31}/2(1+UI_{31})^2(\varepsilon_F^2+\Delta_Q^2)^2 \tag{A11a}$$

$$E_1^{(2)} = 3U^3\Delta_Q^2 I_{31}I_{53}/4(1+UI_{31})^3(\varepsilon_F^2+\Delta_Q^2) \tag{A11b}$$

$$E_2^{(2)} = U\varepsilon_F\Delta_Q^2 I_{31}/4\rho_0(\varepsilon_F)(1+UI_{31})(\varepsilon_F^2+\Delta_Q^2)^{3/2} \tag{A11c}$$

$$E_3^{(2)} = U^2\Delta_Q^2 I_{51}/4(1+UI_{31})^2(\varepsilon_F^2+\Delta_Q^2) \tag{A11d}$$

$$E_4^{(2)} = U^2\varepsilon_F^2\Delta_Q^2/4(1+UI_{31})(\varepsilon_F^2+\Delta_Q^2)^2 \tag{A11e}$$

$$E_5^{(2)} = \varepsilon_F(\varepsilon_F^2+2\Delta_Q^2)/4\rho_0(\varepsilon_F)(\varepsilon_F^2+\Delta_Q^2)^{3/2}. \tag{A11f}$$

The integrals are defined as

$$I_{31} = -\int^{\varepsilon_F} \frac{\varepsilon^2\rho_0(\varepsilon)\,d\varepsilon}{(\varepsilon^2+\Delta_Q^2)^{3/2}} \tag{A12a}$$

$$I_{53} = -\int^{\varepsilon_F} \frac{\varepsilon^2\rho_0(\varepsilon)\,d\varepsilon}{(\varepsilon^2+\Delta_Q^2)^{5/2}} \tag{A12b}$$

$$I_{51} = -\int^{\varepsilon_F} \frac{\varepsilon^2(\varepsilon^2 - 2\Delta_Q^2)\rho_0(\varepsilon)\,d\varepsilon}{(\varepsilon^2 + \Delta_Q^2)^{5/2}} \tag{A12c}$$

The value of parameter Δ_Q in expressions (A7)–(A12) can be determined from minimization of ground-state energy with respect to m_0. When $\Delta_Q = 0$, it is evident that the second derivative of ε_c yields the spin susceptibility and the charge compressibility in PHFA.

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