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Ferromagnetic phase transitions in the single-band Hubbard model

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Abstract. We investigate the zero-temperature phase diagram of the single-band Hubbard model in two and three dimensions, with an emphasis on the region where ferromagnetism occurs. To determine the equilibrium value of the magnetization m, we compute the expectation value of the Hamiltonian using a Gutzwiller variational wavefunction for arbitrary values of m. Analytic calculations are performed using an improved Gutzwiller-type approximation. In two dimensions we predict a first-order transition from a saturated ferromagnetic state to a paramagnetic state. In three dimensions we find both a first-order and a second-order transition depending on the values of the Coulomb repulsion U and the hole concentration δ. We also discuss the possibility that the system phase separates into a region with a large hole concentration and a region with few holes.

1. Introduction

Ferromagnetism in metals has proved very difficult to understand adequately. This is because, on the one hand, the electrons which give rise to the magnetism are also involved in conduction so that one cannot use the relatively simple localized effective Hamiltonians, such as the Heisenberg model, which are good approximations for insulators while, on the other hand, correlations are very important so that the one-electron picture (band theory) is inadequate. It is, however, clearly important to try to learn what are the conditions under which ferromagnetism occurs in metals. In particular, one would like to know whether Hund's rule couplings between different orbitals on the same site, which occur in real magnetic metals and which certainly help ferromagnetism, are *essential* for ferromagnetism to occur or not. This is one of the main reasons for the interest in the one-band Hubbard model [1], which of course does not have such interactions.

The Hamiltonian of the Hubbard model is

$$H = -t \sum_{(i,j),\sigma} c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} \tag{1.1}$$

where (i, j) indicates a nearest-neighbour pair, with both (i, j) and (j, i) being counted separately, $c_{i\sigma}^{\dagger}$ and $c_{i\sigma}$ are the creation and annihilation operators of an electron in the site i, and $n_{i\sigma} = c_{i\sigma}^{\dagger} c_{i\sigma}$. The repulsion of an up spin and a down spin on the same site is represented by the interaction U and the kinetic energy is represented by a tight-binding model with hopping integral t. In the limit that U is much greater than t, the Hubbard

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model can be represented by an effective Hamiltonian, equations (2.1) below, in which doubly occupied sites do not occur explicitly, but virtual states with doubly occupied sites give rise to antiferromagnetic superexchange [2], which does appear explicitly in the Hamiltonian.

It has proved very difficult to demonstrate whether or not this model has a ferromagnetic phase. One approach that has been fairly successful is the use of variational wavefunctions of the type proposed originally by Gutzwiller [3], which include correlation effects due to the on-site repulsion by suppressing doubly occupied sites.

In this paper we investigate the global phase diagram of the Hubbard model in the region for large U where ferromagnetism is expected to occur. We use Gutzwiller-type variational wavefunctions but for the effective Hamiltonian H_{eff} in equation (2.1), rather than for the Hubbard model itself, because we find that this gives more reliable results. We map out the region of the phase diagram where ferromagnetism occurs and also investigate the range of parameters where the system phase separates into a region with a high concentration of holes and an antiferromagnetic region with no holes. We did not investigate the possibility of superconductivity in this model, which has become a fashionable topic [4] since the discovery of high-temperature superconductors. If it occurs at all, superconductivity would appear at larger values of the ratio t/U than studied here.

2. Effective Hamiltonian in the large-U limit

There are two ways of computing the energy of the Hubbard model for large U and arbitrary magnetization m using a Gutzwiller wavefunction. The first is to work in the full Hilbert space of states using the traditional Gutzwiller [3] wavefunction with a variational parameter g which varies the (incomplete) projection of the doubly occupied sites. The second possibility, which we pursue in this paper, consists in working in the subspace of single occupied states with an effective Hamiltonian [5, 6] derived from the original Hubbard Hamiltonian through a unitary transformation. As pointed out by Rice and co-workers [7], this second choice gives more competitive energies at large U even if the wavefunction to be used does not have any variational parameters, because the effective Hamiltonian takes into account in an exact way (to leading order in t/U) the hopping processes in which a doubly occupied site is created in a virtual state. The net effect is that using a Gutzwiller wavefunction in the restricted subspace is the same as working in the full Hilbert space but using a modified wavefunction which contains doubly occupied sites in some optimal sense and, for this reason, gives very competitive energies.

In the limit of large U we can derive an effective Hamiltonian by treating the kinetic term as a perturbation and by going to second order in perturbation theory [5, 6]. One obtains

$$H_{\text{eff}} = H_{\text{kin}} + H_{\text{af}} + H_{\text{pair}} \tag{2.1}$$

where

$$H_{\text{kin}} = P_0 \left(-t \sum_{(i,j),\sigma} c_{i\sigma}^{\dagger} c_{j\sigma} \right) P_0 \tag{2.2}$$

$$H_{\text{af}} = P_0 \left(J \sum_{(i,j)} (S_i \cdot S_j - \tfrac{1}{4} n_i n_j) \right) P_0 \tag{2.3}$$

$$H_{\text{pair}} = P_0 \left(-\frac{J}{4} \sum_{(i,j),(j,l),\sigma}{}' (c_{i\sigma}^{\dagger} c_{j\sigma} c_{j-\sigma}^{\dagger} c_{l-\sigma} + c_{i\sigma}^{\dagger} c_{j-\sigma}^{\dagger} c_{j-\sigma} c_{l\sigma}) \right) P_0. \tag{2.4}$$

In equations (2.2)–(2.4), $P_0 = \Pi_i(1 - n_{i\uparrow} n_{i\downarrow})$ is the projector restricting the action of H_{eff} to the subspace of singly occupied states, $n_i = \Sigma_\sigma n_{i\sigma}$, $S_i^m = \frac{1}{2}\Sigma_{\sigma\sigma'} c_{i\sigma}^{\dagger} \tau_{\sigma\sigma'}^m c_{i\sigma'}$ is the mth component of the spin operator (the $\tau_{\sigma\sigma'}^m$ are elements of the Pauli matrices), $J = 4t^2/U$, and the angular brackets $\langle i, j \rangle$ in equation (2.3) indicate that each distinct nearest-neighbour pair is to be included just once. The prime on the sum in equation (2.4) indicates that terms with $i = l$ have to be omitted since they have already been included in H_{af}. One can recognize H_{af} as the familiar antiferromagnetic interaction due to superexchange, whereas H_{pair} corresponds to the often neglected kinetic energy term associated with the next-nearest-neighbour hopping of holes with and without spin flip. The familiar t–J model is obtained if we neglect H_{pair}.

In this paper we shall use this effective Hamiltonian in conjunction with the Gutzwiller wavefunction

$$|\psi\rangle = P_0 |\psi_0\rangle \tag{2.5}$$

where

$$|\psi_0\rangle = \prod_{k<k_{F\uparrow}} c_{k\uparrow}^{\dagger} \prod_{k<k_{F\downarrow}} c_{k\downarrow}^{\dagger} |0\rangle \tag{2.6}$$

in which $c_{k\sigma}^{\dagger}$ is the operator creating an electron of spin σ in the plane-wave state of crystal momentum k, and $|0\rangle$ is the vacuum state. Note that, in general, we shall be interested in the case in which the up and down bands are not equally populated so that the states $|\psi_0\rangle$ and $|\psi\rangle$ have a net magnetization.

It is important to clarify at this stage that, although variational estimates obtained by using H_{eff} and $|\psi\rangle$ are not, strictly speaking, rigorous bounds on the energy of the Hubbard Hamiltonian described by equation (1.1), these estimates are nevertheless correct to order t/U and are therefore close to being rigorous bounds since our predictions will be for the region where $t/U \ll 1$. A simple way to understand this point is to realize [7] that one can construct a unitary transformation $\exp(iS)$ such that

$$\exp(iS)\, H \exp(-iS) = H_{\text{eff}} + O[(t/U)^2] \tag{2.7}$$

in the subspace of singly occupied states. The operator $\exp(iS)$, which transforms the unperturbed states, which are eigenstates of $U\Sigma_i n_{i\uparrow} n_{i\downarrow}$, into the true eigenstates of the Hubbard Hamiltonian, can be derived by using perturbation theory. To order t/U one finds that

$$S = \frac{i}{U} \left[P_0 \left(-t \sum_{(i,j),\sigma} c_{i\sigma}^{\dagger} c_{j\sigma} \right) P_1 - P_1 \left(-t \sum_{(i,j),\sigma} c_{i\sigma}^{\dagger} c_{j\sigma} \right) P_0 \right] \tag{2.8}$$

where P_1 is the projector on the subspace with one double occupancy: $P_1 = \Sigma_i n_{i\uparrow} n_{i\downarrow} \Pi_{j\neq i} (1 - n_{j\uparrow} n_{j\downarrow})$. From equation (2.7) it is then trivial to show that $\langle\psi|H_{\text{eff}}|\psi\rangle = \langle\tilde{\psi}|H|\tilde{\psi}\rangle + 0[(t/U)^2]$, where $|\tilde{\psi}\rangle = \exp(-iS)|\psi\rangle$. Hence, using $|\psi\rangle$ and H_{eff} is equivalent, to order t/U, to using H and a modified Gutzwiller state containing doubly occupied sites. It is easy to see from equation (2.8) that the net magnetization of the state $|\psi\rangle$ is not modified by this unitary transformation.

Note that in the definition of H_{eff} we keep the pair-hopping kinetic term given by H_{pair}. The reason for doing this is that we are interested in investigating the phase

diagram for all the values of the hole density δ and hence, if δ is not too small, H_{pair} might be comparable with H_{af}, since it is of the same order in t/U. We have explicitly verified, however, that all the qualitative predictions to be made remain unchanged if we neglect H_{pair} and restrict the analysis to the t–J Hamiltonian instead.

3. Improved Gutzwiller approximation

Before explaining how to compute the desired expectation values, let us first introduce some useful notation. We denote by $N_\uparrow$ and $N_\downarrow$ the number of up and down electrons respectively, and by $n_\sigma = N_\sigma/N$ ($\sigma = \downarrow, \uparrow$), the corresponding density, where N is the total number of sites in the system. The density δ of holes is given by $\delta = 1 - n_\downarrow - n_\uparrow$, and the magnetization of the state [8] by $m = n_\uparrow - n_\downarrow$. Given a certain δ, the Gutzwillier state $|\psi\rangle_m$ of magnetization is obtained by choosing $|\psi_0\rangle$ in equation (2.5) so that the lowest $N_\uparrow$ levels in the up and band, and the lowest $N_\downarrow$ levels in the down band are occupied, with $n_\uparrow = (1 + m - \delta)/2$ and $n_\downarrow = (1 - m - \delta)/2$.

We would like to compute the energy of the state with magnetization m which is given by

$$E_\delta(m) \equiv (1/N)(\langle\psi|H_{\text{eff}}|\psi\rangle/\langle\psi|\psi\rangle) \tag{3.1}$$

where the up-spin and down-spin bands in state $|\psi_0\rangle$ in equation (2.5) are filled so as to leave a net magnetization per site of m. The states $|\psi\rangle$ and $|\psi_0\rangle$ have the same magnetization because the Hamiltonian and the projector P_0 conserve the total z-component of the spin. The minimum of $E_\delta(m)$ as a function of m determines the equilibrium magnetization. Note that, because of symmetry, $E_\delta(m)$ is an even function of m and that $|m| \leq 1 - \delta$, with $m = m_{\max} \equiv 1 - \delta$ corresponding to the saturated ferromagnetic state.

Unfortunately, it does not seem possible to perform an analytic calculation of $E_\delta(m)$ for arbitrary values of m, because the presence of the infinite product of site operators which appears in the definition of the Gutzwiller state makes the problem quite untractable. We shall therefore have to make approximations in evaluating the averages in equation (3.1). These will be very similar in spirit to the approximation originally adopted by Gutzwiller [3] and later elucidated further by Ogawa *et al* [9]. Gutzwiller-like approximations have been used very recently [10] to investigate the properties of flux phases in the t-J model, and in that context as well as in the case of the one-dimensional Hubbard model [7] they have been shown to be quantitatively reliable when compared with the exact expectation value computed by numerical techniques. The great advantage of a closed-form expression for $E_\delta(m)$, albeit approximate, is that the parameter space, in both two and three dimensions, can be very thoroughly investigated, making it possible to obtain a rather detailed picture of some of the magnetic phase transitions whose qualitative features, we believe, should persist even if $E_\delta(m)$ were computed exactly from the Gutzwiller wavefunction, e.g. by variational Monte Carlo techniques [11].

We now discuss the approximations that we used. As already stressed, everything could be computed relatively easily if we had to deal with $|\psi_0\rangle$. It is the projector P_0 which makes the problem hard. The idea of our approximation, like that of the other Gutzwiller-like approximations [3, 6, 13], is that we can project away doubly occupied sites in an average sense by using combinatorics, and that the net effect of this projection can be incorporated in a simple renormalization of some matrix elements computed by using the uncorrelated [12] state $|\psi_0\rangle$.

In the Hamiltonian, equation (2.1), both H_{kin} and H_{af} involve only nearest pairs of sites, and we shall firstly discuss how the approximation is used to compute the expectation value of these pair operators. Later we shall describe how it applies to the third term H_{pair} in equation (2.1). Let us therefore consider the expectation value of some pair operator O_{ij}, which is given by

$$\langle O_{ij}\rangle \equiv \langle\psi|O_{ij}|\psi\rangle/\langle\psi|\psi\rangle = \langle\psi_0|P_0O_{ij}P_0|\psi_0\rangle/\langle\psi_0|P_0|\psi_0\rangle. \tag{3.2}$$

The local spin configuration at site i and j is defined by the projector $\hat{p}_i^\alpha\hat{p}_j^\beta$ where the index α denotes either an up or down spin, $\hat{p}_i^\sigma = (1-n_{i-\sigma})n_{i\sigma}$, or an empty site $\hat{p}_i^e = (1-n_{i\uparrow})(1-n_{i\downarrow})$. We therefore approximate the expectation value of O_{ij} as a sum over all allowed configurations of the two sites i and j, weighted by a factor $\eta^{\alpha\beta}$, which is a mean-field estimate of the probability that such a configuration of the two-site cluster actually occurs in the full wavefunction, i.e.

$$\langle\psi_0|P_0O_{ij}P_0|\psi_0\rangle \simeq \sum_{\alpha\beta}\eta^{\alpha\beta}\langle\psi_0|(1-n_{i\uparrow}n_{i\downarrow})(1-n_{j\uparrow}n_{j\downarrow})O_{ij}\hat{p}_i^\alpha\hat{p}_j^\beta|\psi_0\rangle. \tag{3.3}$$

To determine the $\eta^{\alpha\beta}$, consider the spin configurations on the $N-2$ sites different from i and j. Depending on the configuration specified by α and β there will be $N_\uparrow(\alpha,\beta)$ up spins and $N_\downarrow(\alpha,\beta)$ down spins which can be arranged on these $N-2$ sites; for example, if there is an up spin at i, $\alpha\equiv\uparrow$, and an empty site at j, $\beta\equiv$ e, then $N_\uparrow(\alpha,\beta) = N_\uparrow - 1$, $N_\downarrow(\alpha,\beta) = N_\downarrow$. The physical assumption we make is that all configurations of electrons on the remaining $N-2$ sites, with or without double occupancy, give the same contribution to the expectation value in the uncorrelated state $|\Psi_0\rangle$. This means that $\eta^{\alpha\beta}$ is the ratio of the number of configurations of the electrons on these $N-2$ sites satisfying the constraint of no double occupancy, $D=0$, to the total number of configurations including those with double occupancy, i.e.

$$\eta^{\alpha\beta} = M_{D=0}(N-2, N_\uparrow(\alpha,\beta), N_\downarrow(\alpha,\beta))\Big/\sum_D M_D(N-2, N_\uparrow(\alpha,\beta), N_\downarrow(\alpha,\beta)) \tag{3.4a}$$

where

$$M_D(\tilde{N}, N_\uparrow, N_\downarrow) = \tilde{N}!/(N_\uparrow - D)!(N_\downarrow - D)D!(\tilde{N} - N_\uparrow - N_\downarrow + D)! \tag{3.4b}$$

is the number of configurations for $\tilde{N}$ sites, $N_\uparrow$ up spins, $N_\downarrow$ down spins, and D doubly occupied sites. In the limit of large N, $N_\uparrow$ and $N_\downarrow$, one can obtain a simple expression for $\eta^{\alpha\beta}$. We can write

$$M_{D=0}(N-2, N_\uparrow(\alpha,\beta), N_\downarrow(\alpha,\beta)) = M_{D=0}(N, N_\uparrow, N_\downarrow)q_{D=0}^\alpha q_{D=0}^\beta$$

$$\sum_D M_D(N-2, N_\uparrow(\alpha,\beta), N_\downarrow(\alpha,\beta)) = \sum_D M_D(N, N_\uparrow, N_\downarrow)q^\alpha q^\beta$$

where $q_{D=0}^\alpha$ is the probability of finding the configuration α at site i in an ensemble *without* double occupancy (so $q_{D=0}^\sigma = n_\sigma$, $q_{D=0}^e = (1-n_\uparrow - n_\downarrow)$), whereas q^α is the analogous probability without any constraint on the occupancy of the sites (in which case $q^\sigma = (1-n_{-\sigma})n_\sigma$, $q^e = (1-n_\uparrow)(1-n_\downarrow)$). It is then clear that $\eta^{\alpha\beta} = C\eta^\alpha\eta^\beta$, where $\eta^\alpha = q_{D=0}^\alpha/q^\alpha$; so $\eta^\sigma = 1/(1-n_{-\sigma})$, $\eta^e = (1-n_\uparrow - n_\downarrow)/[(1-n_\uparrow)(1-n_\downarrow)]$. The constant C, which is independent of the spin configuration, drops out of the calculation when we compute the ratio of matrix elements in equation (3.2).

If we now sum over the possible local spin configurations α and β, we obtain the desired result

$$\langle O_{ij}\rangle \simeq \langle\psi_0|(1-n_{i\uparrow}n_{i\downarrow})(1-n_{j\uparrow}n_{j\downarrow})O_{ij}\hat{p}_i\hat{p}_j|\psi_0\rangle/\langle\psi_0|\hat{p}_i\hat{p}_j|\psi_0\rangle \tag{3.5a}$$

where

$$\hat{p}_i = \sum_\alpha \hat{p}_i^\alpha \eta^\alpha$$

is given by

$$\hat{p}_i = 1-(n_\uparrow - n_{i\uparrow})(n_\downarrow - n_{i\downarrow})/(1-n_\downarrow)(1-n_\uparrow). \tag{3.5b}$$

Note that $\hat{p}_i$ vanishes for double occupied sites; so the factors of $1-n_{i\uparrow}n_{i\downarrow}$ are unnecessary in the denominator of equation (3.5*a*). The matrix elements on the right-hand side of equation (3.5*a*) can now be evaluated explicitly, for instance by using Wick's theorem.

Note that in the above analysis we have incorporated correlations within the cluster of two sites, i and j, explicitly and treated correlations outside the cluster within a mean-field-like approximation. In order to evaluate the expectation value of a three-site operator, such as H_{pair}, still within a two-site cluster approximation, we select one of the nearest-neighbour pairs in the three-site term, i and j say, and then work out the average precisely as in equation (3.5*a*), i.e.

$$\langle O_{ijl}\rangle \simeq \langle\psi_0|(1-n_{i\uparrow}n_{i\downarrow})(1-n_{j\uparrow}n_{j\downarrow})O_{ijl}\hat{p}_i\hat{p}_j|\psi_0\rangle/\langle\psi_0|\hat{p}_i\hat{p}_j|\psi_0\rangle \tag{3.6}$$

where O_{ijl} denotes the three-site operator. It would clearly be equivalent, once the sites are summed over, to use the other nearest-neighbour pair, (j, l), as the cluster. The original Gutzwiller [3] approximation for the kinetic energy could be obtained by a similar approach, but for a one-site cluster [14]. In our calculations we have taken a two-site cluster because

(i) the evaluation of the matrix elements is still manageable in this case and

(ii) this level of approximation is necessary to get quantitative agreement with the exact expectation value in the only limit in which an exact analytic calculation is possible, namely in the neighbourhood of the saturated ferromagnet, $m \simeq m_{\max}$.

We shall return to this point later on.

Because of the factorization of $\eta^{\alpha\beta}$ noted above, one can also generalize our equations to arbitrarily large clusters. Consider a cluster with m sites, $i_1, i_2, \ldots, i_m$, and an operator which fits entirely into it. To be specific consider a two-site operator O_{jl}, although the generalization to other operators is obvious. We find that

$$\langle O_{jl}\rangle \simeq \langle\psi_0|(1-n_{j\uparrow}n_{j\downarrow})(1-n_{l\uparrow}n_{l\downarrow})O_{jl}\prod_{\alpha=1}^{m}\hat{p}_{i_\alpha}|\psi_0\rangle/\langle\psi_0|\prod_{\alpha=1}^{m}\hat{p}_{i_\alpha}|\psi_0\rangle. \tag{3.7}$$

In fact, our approximation scheme turns out to be equivalent to the cluster factorization procedure described by Razafimandimby [14], and it is worthwhile to discuss this connection in a little more detail. In the limit of very large U, the work of Razifimandimby effectively involves the operator

$$P_i = 1 - n_\uparrow - n_\downarrow + n_\uparrow n_{i\downarrow} + n_\downarrow n_{i\uparrow} - n_{i\uparrow}n_{i\downarrow} \tag{3.8}$$

where, to avoid confusion, we recall that $n\uparrow$ and $n_\downarrow$ are c-numbers, whereas $n_{i\uparrow}$ and

$n_{i\downarrow}$ are operators, and note that $P_i = (1 - n_\uparrow)(1 - n_\downarrow)\hat{p}_i$. It is easy to verify that P_i is non-negative and projects to zero a doubly occupied state at site i. Razafimandimby then considers the state $|\bar{\psi}\rangle = \Pi_i P_i^{1/2}|\psi_0\rangle$, which satisfies the constraint of single occupancy and could also be used as a variational state. Note that $|\bar{\psi}\rangle$ is rather close to the Gutzwiller state. For example, exactly at half-filling and for $m = 0$, it is quite easy to check that $|\bar{\psi}\rangle$ is proportional to the Gutzwiller state. In general, however, the two states are distinct. In Razafimandimby's factorization scheme one writes

$$\overline{\langle O_{jl}\rangle} \equiv \langle\bar{\psi}|O_{ij}|\bar{\psi}\rangle/\langle\bar{\psi}|\bar{\psi}\rangle \simeq \langle\psi_0|\prod_{\alpha=1}^{m}(P_{i_\alpha})^{1/2}O_{jl}\prod_{\alpha=1}^{m}(P_{i_\alpha})^{1/2}|\psi_0\rangle/\langle\psi_0|\prod_{\alpha=1}^{m}P_{i_\alpha}|\psi_0\rangle. \tag{3.9}$$

It is shown in appendix 1 that $\overline{\langle O_{jl}\rangle}$ is equal to [15] $\langle O_{jl}\rangle$ in equation (3.7). Hence, by increasing the cluster size, our method does not converge [16] to the exact expectation value obtained by using the Gutzwiller state, equation (2.5), but rather to that obtained by using the state $|\bar{\psi}\rangle$. Furthermore, the Gutzwiller approximation can be considered as the first expression in a systematic expansion giving expectation values computed with this variational state. The approximation used here then corresponds to the second level of approximation in this scheme.

We now go back to the application of the method. As shown in appendix 2, a somewhat lengthy but straightforward calculation starting from equation (3.5*a*) gives the following expression for the energy:

$$E_\delta(m) = E_\delta^{\text{kin}}(m) + E_\delta^{\text{af}}(m) + E_\delta^{\text{pair}}(m)$$

where

$$E_\delta^{\text{kin}}(m) = z\frac{1 - n_\uparrow - n_\downarrow}{\langle\psi|\psi\rangle_2}\sum_\sigma \mu_\sigma(e_x)[1 - \mu^2_{-\sigma}(e_x)] \tag{3.10a}$$

$$E_\delta^{\text{af}}(m) = -(zJ/2\langle\psi|\psi\rangle_2)\{\mu_\uparrow(e_x)\mu_\downarrow(e_x) + [n_\uparrow + (1 - n_\uparrow)\mu^2_\uparrow(e_x)][n_\downarrow + (1 - n_\downarrow)\mu^2_\downarrow(e_x)]\} \tag{3.10b}$$

$$E_\delta^{\text{pair}}(m) = -\frac{Jz(z-1)(1 - n_\uparrow - n_\downarrow)}{4\langle\psi|\psi\rangle_2}\Bigg[\mu_\uparrow(e_x)\mu_\downarrow(e_x) \times \sum_\sigma\left(1 - \mu_\sigma(e_x + e_y)\frac{z-2}{z-1} - \frac{\mu_\sigma(2e_x)}{z-1}\right) + \sum_\sigma[n_{-\sigma} + (1 - n_{-\sigma})\mu^2_{-\sigma}(e_x)] \times \left(\mu^2_\sigma(e_x) - \mu_\sigma(e_x + e_y)\frac{z-2}{z-1} - \frac{\mu_\sigma(2e_x)}{z-1}\right)\Bigg] \tag{3.10c}$$

where

$$\langle\psi|\psi\rangle_2 = 1 + \mu^2_\uparrow(e_x)\mu^2_\downarrow(e_x) \tag{3.11}$$

$$\mu_\sigma(x) = -\frac{1}{1 - n_\sigma}\frac{1}{N}\sum_{k<k_{F\sigma}}\exp(ik\cdot x) \tag{3.12}$$

and z is the coordination number. We use a square lattice in two dimensions for which $e_x = a(1, 0)$ and $e_y = a(0, 1)$, where a is the lattice spacing, and we have chosen energy

units in which $t = 1$. In three dimensions we use a simple cubic lattice with $e_x = a(1, 0, 0)$ and $e_y = a(0, 1, 0)$. The formulae can easily be generalized to other lattice structures. One should keep in mind that the dependence of the previous expressions on m and δ comes from the factors n_σ, and from the integration region in equation (3.12) which, through $k_{F\sigma}$, also depends on m and δ. We see in this way that the evaluation of $E_\delta(m)$ is reduced to the computation of the integrals in equation (3.12) over the Brillouin zone for arbitrary values of m and δ. The integral over k_z can be performed analytically leaving a $d - 1$-dimensional integral to be evaluated numerically.

Several comments about equations (3.10) are now in order. A trivial check on $E_\delta(m)$ is that it reduces to the correct expression of the energy of a saturated ferromagnet when $m = m_{\max}$. In this limit $n_\downarrow = \mu_\downarrow = 0$ and $E_\delta(m_{\max}) = z\delta\mu_\uparrow(e_x)$ as expected. A more important test can be done if we look at the neighbourhood of $m_{\max}$, where the variational wavefunction corresponds to a saturated ferromagnet with a single spin flip. More specifically one can compute $\Delta E_\delta = E_\delta(1 \text{ spin flip}) - E_\delta^{\text{Nag}}$ where E_δ^{Nag} is the energy of the saturated ferromagnetic state (Nagaoka state). The saturated feromagnetic state is locally stable if this quantity is positive [17]. From our point of view is easy to compute ΔE_δ because

$$\Delta E_\delta = N[E_\delta(m_{\max} - 2/N) - E_\delta(m_{\max})] = -2(\partial E_\delta/\partial m)|_{m_{\max}}. \qquad (3.13)$$

By computing $\partial E_\delta/\partial m|_{m_{\max}}$ and setting it equal to zero we can compute the curve of local stability in the J–δ plane and compare it with the exact calculation performed in the one-spin-flip subspace. It turns out that, because of the structure of our approximation scheme [18], the quantitative agreement is indeed very good, as can be seen in figure 1. In fact, our approximation gives the exact energy for a single spin flip, if H_{pair} can be neglected, which is valid for $\delta \to 0$. The Gutzwiller approximation (which is essentially the one-site cluster approximation) does not have this desirable property.

In order to get a feeling of the validity of the approximation in the opposite limit of zero magnetization, we have compared the value obtained for $E_\delta^{\text{kin}}(m = 0)$ in the one-dimensional case with the exact [19] curve obtained by Rice and co-workers [7] using Monte Carlo techniques. We have found that the quantitative agreement in the case $m = 0$ is very similar to that obtained using the Gutzwiller approximation (which amounts to seting equal to unity the term in parentheses in equation (3.10a)) and is rather good in the whole range of hole densities.

We can now proceed with a discussion of the magnetic phase transitions implied by equations (3.10). Since some of the qualitative features turn out to be different in two and three dimensions, we shall consider these two cases separately.

4. Results in two dimensions

First we shall address the question of the transition between the ferromagnetic and paramagnetic states, and later we shall discuss the possibility of phase separation [20, 21].

The function $E_\delta(m)$ is even in m and therefore the paramagnetic state will be either a local minimum or a local maximum. By considering the curve of local stability we already know that the state with $m = m_{\max}$ is a local minimum in the region of small J and $\delta < 0.49$. Furthermore, because $E_\delta^{\text{af}}(m)$ describes an antiferromagnetic coupling, we know that this term has a global minimum at $m = 0$. This term becomes more

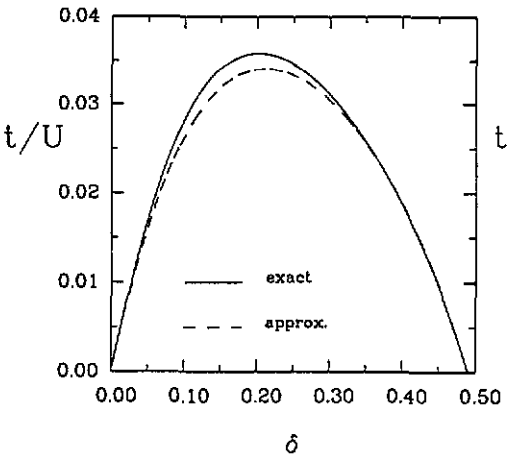

Figure 1. Test of the validity of the two-site cluster approximation in the neighbourhood of $m = m_{max}$. The full curve is the curve above which the Nagaoka state is locally unstable, computed by evaluating $\langle H_{eff} \rangle$ without any approximations in the one-spin-flip subspace. The broken curve is the analogous curve obtained by using the approximate expressions in equations (3.10*a*)–(3.10*c*) and solving the equation $(\partial E_\delta/\partial m)|_{m\,max} = 0$. This shows that the two-site cluster approximation is quite accurate, at least for m close to m_{max}. In fact, as discussed in the text, the only approximation made in the limit of $m \to m_{max}$ is for the pair-hopping term in the effective Hamiltonian, equation (2.4); the treatment of H_{kin} and H_{af} is exact.

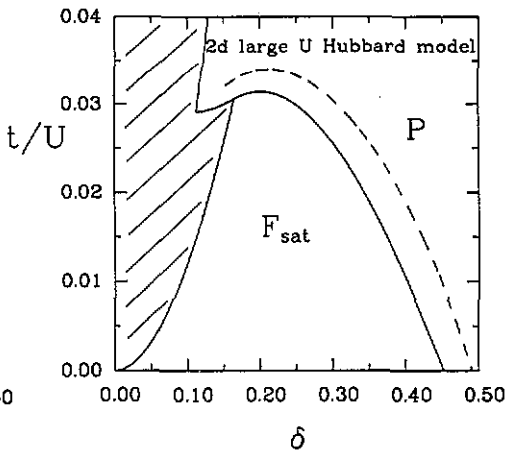

Figure 2. Phase diagram of the two-dimensional Hubbard model at large U obtained by using a Gutzwiller wavefunction to estimate the energy of the different relevant phases. Expectation values have been computed within an improved Gutzwiller-type approximation (see equations (3.10*a*)–(3.10*c*)). In the shaded region the system phase separates into an antiferromagnetic phase without holes and a homogeneous hole-rich phase; the region labelled F_{sat} corresponds to a saturated ferromagnetic phase (Nagaoka state), and that by P to a paramagnetic phase. The broken curve indicates where the Nagaoka state becomes locally unstable against a single spin flip.

important for larger values of J. The competition between these two local minima will determine the nature of the phase transition.

In two dimensions this picture turns out to be rather simple. Let us consider a generic value of δ, say $\delta = 0.2$, and, starting from $J = 0$, slowly increase the value of J. At $J = 0$ the paramagnetic state is a local maximum, and the global minimum is the saturated ferromagnet. As we increase J, $m = 0$ becomes a local minimum but, when this occurs, the state with $m = m_{max}$, is still the global minimum. It is only when J reaches a critical value, $J = J_{cr}(\delta)$, that the paramagnetic state becomes the global minimum and a first-order phase transition, in which m jumps from m_{max} to 0, takes place. This is illustrated in figure 2, where we plot the curve $J_{cr}(\delta)$ at which this transition occurs. For comparison, the broken curve in figure 2 indicates where the saturated ferromagnet becomes *locally* unstable.

However, there is an additional complication, namely the possibility that the system can phase separate [20, 21] into a region rich in holes and an antiferromagnetic region with no holes. The energy of the antiferromagnetic domain can be evaluated very accurately by using the results of numerical simulations [22], whereas the energy of the hole-rich phase can be estimated by using the global minimum of $E_\delta(m)$ at the appropriate value of δ. We omit the derivation of this phase boundary, which is essentially

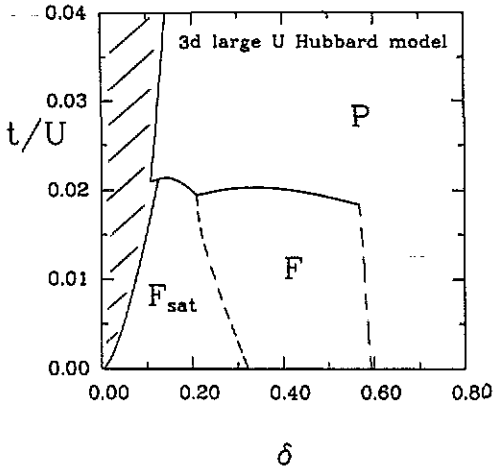

Figure 3. Phase diagram of the three-dimensional Hubbard model at large U obtained by using a Gutzwiller wavefunction to estimate the energy of the different relevant phases. Expectation values have been computed within an improved Gutzwiller-type approximation (see equations (3.10*a*)–(3.10*c*)). In the shaded region the system phase separates into an antiferromagnetic phase without holes and an homogeneous hole-rich phase; F_{sat} corresponds to a saturated ferromagnet, F to a ferromagnet with $0 \leq m \leq m_{max}$, and P to a paramagnet. The broken and full curves correspond to continuous and first-order transitions, respectively.

identical with that given by Emery *et al* [21] and just discuss the results which are plotted in the phase diagram (figure 2).

The shaded region corresponds to phase separation; so values of δ and t/U in this region will not be found in an homogeneous system. The region marked F_{sat} corresponds to a saturated ferromagnet, and the region marked P is a paramagnet. The transition between the saturated ferromagnetic and paramagnetic phases is, of course, first order as noted above. It is worth noting that the ferromagnetic pocket is restricted to very small values of J as other calculations [17, 23] had already pointed out. This justifies our use of H_{eff}, rather than the Hubbard Hamiltonian, when investigating the ferromagnetic region.

5. Results in three dimensions

The structure of the phase diagram is even richer in three dimensions (figure 3). In this case we can distinguish a new region, labelled F, where the globally stable configuration corresponds to a state of partial magnetization, i.e. $0 < m < m_{max}$. The broken curves in figure 3 indicate second-order transitions where m is continuous, while the full curves indicate first-order transitions with a discontinuity in m. Note that, in the saturated ferromagnetic state, $m = m_{max}$ and, in the paramagnetic state, $m = 0$. The transition from the saturated ferromagnetic state to the paramagnetic state is always first order, whereas the transition between the saturated and partially magnetized ferromagnetic states is always continuous. The transition between the partially magnetized state and the paramagnetic state can be first or second order, depending on the path taken in parameter space.

As in two dimensions, phase separation occurs for small δ, and we show the region which cannot exist as a single phase by the shaded region in figure 3. For this calculation, we obtained the energy of the antiferromagnetic state from the spin-wave calculation of Oguchi [24], including the $1/S$ correction. Since the analogous calculation in two dimensions agrees very well with the results of Monte Carlo simulations, e.g. [22], and since we expect the calculation to be more accurate in three dimensions because the coordination number is higher, we estimate that this value for the ground-state energy should be accurate to within about 1%, which is sufficient for our purposes.

We should, however, be quite cautious in taking the precise location of these phase boundaries too serious. In the ferromagnetic region, states of different magnetizations have energies which differ by only of the order of a few per cent, and therefore small errors made in evaluating the energy, either because of the approximations inherent in the wavefunction itself or in the additional approximations made in computing the matrix elements, might change, even qualitatively, the nature of the phase diagram.

6. Conclusions

We have investigated the ferromagnetic region of the phase diagram of the one-band Hubbard model at zero temperature by using a Gutzwiller wavefunction together with a two-site cluster approximation to evaluate the matrix elements. We find that ferromagnetism only occurs for very large values of U/t, as shown in figures 2 and 3. The transition from ferromagnetism to paramagnetism is strongly first order for $d = 2$, while it can be either first or second order for $d = 3$. For very small δ, the system phase separates.

It is important to test, by variational Monte Carlo techniques, the validity of the two-site cluster approximation that we have used in this paper. In future work, we intend to investigate this question, and also to look at better variational wavefunctions.

Acknowledgments

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Appendix 1

In this appendix we show explicitly that the expectation values in equations (3.7) and (3.9) are equal. Although these equations refer to a two-site operator, it should be clear from the following analysis that the same conclusion also applies for an arbitrary local operator satisfying some general conditions to be specified shortly.

First of all note that the operator P_r commutes with O_{jl} if $r \neq j, l$. We can then rewrite equation (3.9) as

$$\langle \bar{O}_{jl} \rangle \simeq \langle \psi_0 | (1 - n_{j\uparrow} n_{j\downarrow})(1 - n_{l\uparrow} n_{l\downarrow})(P_j)^{1/2}(P_l)^{1/2} O_{jl} (P_j)^{1/2}(P_l)^{1/2} \times \prod_{i_\alpha \neq j,l} P_{i_\alpha} |\psi_0\rangle \Big/ \langle \psi_0 | \prod_{\alpha=1}^{m} P_{i_\alpha} |\psi_0\rangle \tag{A1.1}$$

where the factors $1 - n_{j\uparrow} n_{j\downarrow}$ and $1 - n_{l\uparrow} n_{l\downarrow}$ which have been inserted are equal to unity because the operators P_j and P_l suppress states with doubly occupied sites. Consider now the four possible operators acting on site j, namely $c_{j\sigma}^\dagger$, $c_{j\sigma}$, $c_{j\sigma}^\dagger c_{j-\sigma}$ and $c_{j\sigma}^\dagger c_{j\sigma}$. It is a simple matter now to verify the following equalities:

$$(1 - n_{j\uparrow} n_{j\downarrow})(P_j)^{1/2} c_{j\sigma}^\dagger (P_j)^{1/2} = [(1 - n_\sigma)^{1/2}/(1 - n_\uparrow - n_\downarrow)^{1/2}](1 - n_{j\uparrow} n_{j\downarrow}) c_{j\sigma}^\dagger P_j \tag{A1.2}$$

$$(1 - n_{j\uparrow} n_{j\downarrow})(P_j)^{1/2} c_{j\sigma} (P_j)^{1/2} = [(1 - n_\uparrow - n_\downarrow)^{1/2}/(1 - n_\sigma)^{1/2}](1 - n_{j\uparrow} n_{j\downarrow}) c_{j\sigma} P_j \tag{A1.3}$$

$$(P_j)^{1/2} c_{j\sigma}^{\dagger} c_{j-\sigma} (P_j)^{1/2} = [(1-n_\sigma)^{1/2}/(1-n_{-\sigma})^{1/2}] c_{j\sigma}^{\dagger} c_{j-\sigma} P_j \tag{A1.4}$$

and it is obvious that $[(P_j)^{1/2}, n_{j\sigma}] = 0$. Now the local operators that we are interested in conserve separately the total number of up and down electrons. Therefore, whenever in equation (A1.1) there is an operator $c_{j\sigma}^{\dagger}$, there must also be an operator $c_{l\sigma}$ and, analogously, S_j^{+} is necessarily associated with S_l^{-}. Hence we can rewrite equation (A1.1) as

$$\overline{\langle O_{jl} \rangle} = \langle \psi_0 | (1-n_{j\uparrow} n_{j\downarrow})(1-n_{l\uparrow} n_{l\downarrow}) O_{jl} P_j P_l \prod_{\alpha \neq j,l} (P_{i_\alpha}) | \psi_0 \rangle \Big/ \langle \psi_0 | \prod_{\alpha=1}^{m} P_{i_\alpha} | \psi_0 \rangle . \tag{A1.5}$$

The equivalence between equations (3.7) and (3.9) follows directly by noting that $\hat{p}_i$ defined in equation (3.5*b*) is proportional to P_i.

Appendix 2

In this appendix we sketch the calculation leading to equations (3.10*a*)(3.10*c*) and equation (3.11). Let us start with H_{kin}. We have

$$E_\delta^{\text{kin}}(m) = -\frac{z}{\langle \psi | \psi \rangle_2} \sum_\sigma \langle (1-n_{i\uparrow} n_{i\downarrow})(1-n_{j\uparrow} n_{j\downarrow}) c_{i\sigma}^{\dagger} c_{j\sigma} \hat{p}_i \hat{p}_j \rangle \tag{A2.1}$$

where the expectation values in this appendix are always understood to be computed with the uncorrelated state $|\psi_0\rangle$, and the operator $\hat{p}_i$ is given in equation (3.6*b*). Because of the presence of $c_{i\sigma}^{\dagger} c_{j\sigma}$ we can replace $n_{i\sigma}$ to the right (left) of $c_{i\sigma}^{\dagger}$ by zero (one), and $n_{j\sigma}$ to the right (left) of $c_{j\sigma}$ by one (zero). We also use the fact that states of opposite spins are completely uncorrelated in $|\psi_0\rangle$ and rewrite equation (A2.1) as

$$E_\delta^{\text{kin}}(m) = -\frac{z(1-n_\uparrow - n_\downarrow)}{\langle \psi | \psi \rangle_2} \sum_\sigma \frac{\langle c_{i\sigma}^{\dagger} c_{j\sigma} \rangle}{(1-n_\sigma)} \frac{\langle (1-n_{i-\sigma})(1-n_{j-\sigma}) \rangle}{(1-n_{-\sigma})^2} . \tag{A2.2}$$

It is now simple to compute

$$\langle c_{i\sigma}^{\dagger} c_{j\sigma} \rangle / (1-n_\sigma) = -\mu_\sigma(x) \tag{A2.3}$$

$$\langle (1-n_{i\sigma})(1-n_{i+x,\sigma}) \rangle / (1-n_\sigma)^2 = 1 - \mu_\sigma^2(x) \tag{A2.4}$$

where μ_σ is defined in equation (3.12), and to check explicitly that equation (A2.4) reduces to equation (3.10*a*). In a similar way, using $\langle (n_\sigma - n_{i\sigma}) \rangle = 0$, we obtain

$$\langle \psi | \psi \rangle_2 = \langle \hat{p}_i \hat{p}_j \rangle = 1 + \prod_\sigma \frac{\langle (n_\sigma - n_{i\sigma})(n_\sigma - n_{j\sigma}) \rangle}{(1-n_\sigma)^2} . \tag{A2.5}$$

Equation (3.11) now follows immediately because equation (A2.4) implies that

$$\langle (n_\sigma - n_{i\sigma})(n_\sigma - n_{i+x,\sigma}) \rangle / (1-n_\sigma)^2 = -\mu_\sigma^2(x). \tag{A2.6}$$

In order to compute $E_\delta^{\text{af}}(m)$ it is first convenient to rewrite H_{af} in the equivalent way:

$$H_{\text{af}} = \frac{J}{2} \sum_{\langle i,j \rangle} (S_i^{+} S_j^{-} + S_i^{-} S_j^{+} - n_{i\uparrow} n_{j\downarrow} - n_{i\downarrow} n_{j\uparrow}) \tag{A2.7}$$

where $S_i^{+} = c_{i\uparrow}^{\dagger} c_{i\downarrow}$ and $S_i^{-} = c_{i\downarrow}^{\dagger} c_{i\uparrow}$. Following similar manipulations to what we did above for the kinetic energy term, we then obtain

$$\langle \psi | S_i^{+} S_j^{-} | \psi \rangle \simeq \langle c_{i\uparrow}^{\dagger} c_{j\uparrow} \rangle \langle c_{i\downarrow} c_{j\downarrow}^{\dagger} \rangle / (1-n_\uparrow)(1-n_\downarrow) \tag{A2.8}$$

$$\langle \psi | n_{i\uparrow} n_{j\downarrow} | \psi \rangle \simeq \langle n_{i\uparrow} (1-n_{j\uparrow}) \rangle \langle n_{j\downarrow} (1-n_{i\downarrow}) \rangle / (1-n_\uparrow)(1-n_\downarrow). \tag{A2.9}$$

With the help of equations (A2.3) and (A2.4), we then obtain equation (3.10*b*).

Finally we have to consider the contribution from H_{pair}. By going back to equation (2.4) we see we have to compute two terms which can be easily reduced to

$$\sum_{\sigma} \langle\psi|c_{i\sigma}^{\dagger}c_{j\sigma}c_{j-\sigma}^{\dagger}c_{l-\sigma}\rangle\psi\rangle \simeq (1-n_{\uparrow}-n_{\downarrow})\sum_{\sigma}\frac{\langle c_{i\sigma}^{\dagger}c_{j\sigma}\rangle\langle c_{j-\sigma}^{\dagger}c_{l-\sigma}(1-n_{i-\sigma})\rangle}{(1-n_{\sigma})(1-n_{-\sigma})^{2}} \tag{A2.10}$$

$$\sum_{\sigma} \langle\psi|c_{i\sigma}^{\dagger}c_{j-\sigma}^{\dagger}c_{j-\sigma}c_{l\sigma}|\psi\rangle \simeq (1-n_{\uparrow}-n_{\downarrow})\sum_{\sigma}\frac{\langle c_{i\sigma}^{\dagger}c_{l\sigma}(1-n_{j\sigma})\rangle\langle n_{j-\sigma}(1-n_{i-\sigma})\rangle}{(1-n_{\sigma})^{2}(1-n_{-\sigma})}, \tag{A2.11}$$

where (i, j) and (j, l) are nearest-neighbour pairs. These two expressions can now be explicitly evaluated by using equations (A2.3) and (A2.4) together with

$$\langle c_{i\sigma}^{\dagger}c_{i+x,\sigma}(1-n_{i+y,\sigma})\rangle/(1-n_{\sigma})^{2} = \mu_{\sigma}(y)\mu_{\sigma}(y-x) - \mu_{\sigma}(x). \tag{A2.12}$$

In this way we obtain

$$\sum_{\sigma} \langle\psi|c_{i\sigma}^{\dagger}c_{j\sigma}c_{j-\sigma}^{\dagger}c_{l-\sigma}|\psi\rangle \simeq (1-n_{\uparrow}-n_{\downarrow})\sum_{\sigma}\mu_{\sigma}(e_x)\mu_{-\sigma}(e_x)[1-\mu_{-\sigma}(i-l)] \tag{A2.13}$$

$$\sum_{\sigma} \langle\psi|c_{i\sigma}^{\dagger}c_{j-\sigma}^{\dagger}c_{j-\sigma}c_{l\sigma}|\psi\rangle \simeq (1-n_{\uparrow}-n_{\downarrow}) \times \sum_{\sigma}[n_{-\sigma}+(1-n_{-\sigma})\mu_{-\sigma}^{2}(e_x)][\mu_{\sigma}^{2}(e_x)-\mu_{\sigma}(i-l)]. \tag{A2.14}$$

If we now sum over the possible nearest-neighbour pairs (i, j) and (j, l) we finally obtain equation (3.10*c*).

References

[1] Hubbard J 1963 *Proc. R. Soc.* A **276** 238; 1964 *Proc. R. Soc.* A **277** 237; 1964 *Proc. R. Soc.* A **281** 401

[2] Anderson P W 1959 *Phys. Rev.* **115** 2

[3] Gutzwiller M C 1964 *Phys. Rev.* **134** A923; 1965 *Phys. Rev.* **137** A1726

[4] Anderson P W 1987 *Science* **235** 1196

[5] Castellani C, Di Castro C, Feinberg D and Ranninger J 1979 *Phys. Rev. Lett.* **43** 1957

[6] Hirsch J E 1985 *Phys. Rev. Lett.* **54** 1317

[7] Gros C, Joynt R and Rice T M 1987 *Phys. Rev.* B **36** 381

[8] By construction, the states defined in equations (2.5) and (2.6) are eigenstates of the z-component of the total spin of the system. one can easily verify that they are also eigenstates of S^2 by explicitly showing that $S^{+}|\psi_0\rangle = S^{+}|\psi\rangle = 0$, where $S^{+} = \Sigma_i c_{i\uparrow}^{\dagger}c_{i\downarrow}$ is the familiar step-raising angular momentum operator. Hence, these states have the maximum total S^z for a given total spin quantum number.

[9] Ogawa T, Kanda K and Matsubara T 1975 *Prog. Theor. Phys.* **53** 614

[10] Lederer P, Poilblanc D and Rice T M 1989 *Phys. Rev. Lett.* **63** 1519
Poilblanc D, Hasegawa Y and Rice T M 1990 *Phys. Rev.* B **41** 1949

[11] Horsch P and Kaplan T A 1983 *J. Phys. C: Solid State Phys.* **16** L1203
Yokoyama H and Shiba H 1987 *J. Phys. Soc. Japan* **56** 1490
Gros C, Joynt R and Rice T M 1987 *Phys. Rev.* B **36** 381

[12] It is perhaps worthwhile stressing that, because of Fermi statistics, the position of the up spins in $|\psi_0\rangle$ are correlated (and the same is true, of course, for the down spins). When we refer to the state $|\psi_0\rangle$ being uncorrelated we mean that the *only* correlations are those coming from Fermi statistics.

[13] Vollhardt D 1984 *Rev. Mod. Phys.* **56** 99

[14] Razafimandimby H A 1982 *Z. Phys.* B **49** 33

[15] In the case of a generic local operator the equivalence is complete provided that the cluster considered contains all the sites on which the local operator is defined; see appendix 1.

[16] We note that T Hsu (1990 private communication) has shown that, in one dimension, at half-filling and for $m = 0$, the results for the energy obtained by essentially our method with clusters of up to six sites, converge to the exact value for the Gutzwiller wavefunction obtained by variational Monte Carlo simulations. However, we have already commented that, in this case, the Gutzwiller wavefunction and the Razafimandimby wavefunction are equivalent. In general, when this is not the case, the convergence is to the Razafimandimby wavefunction as the cluster size is increased.

[17] Shastry B S, Krishnamurthy H R and Anderson P W 1990 *Phys. Rev.* B **41** 2375

[18] It can be shown rather easily that, if we consider an n-site local operator, the approximate calculation is exact in the one-spin-flip subspace provided that we take the cluster defining our level of approximation to include those n sites. Since we have considered a two-site cluster, it follows that the approximation is exact in this limit for H^{kin} and H^{af}, which are defined in terms of two-site local operators, while it involves only a small error in the case of H^{pair}. If we had used instead the simpler Gutzwiller approximation, which corresponds essentially to a one-site cluster approximation, there would have been an error also for H^{kin} and H^{af}.

[19] Note that when we talk about 'exact' expressions, we always refer to expressions obtained either analytically or numerically, starting with the same Gutzwiller wavefunction but computing the expectation values without further approximations. In this respect, in this paper we are more concerned about our results being a good approximation to the variational expression of $E_\delta(m)$ as given by equation (2.1), rather than to the true ground state in each subspace defined by m. This last problem is much more difficult to decide about, essentially because nothing is known exactly about properties of the ground state of the Hubbard model in two and three dimensions. See, however, [7] for a discussion of the validity of the Gutzwiller variational wavefunction in the one-dimensional case.

[20] Ioffe L B and Larkin A J 1988 *Phys. Rev.* B **37** 5730
Montambaux G, Héritier M and Lederer P 1982 *J. Low Temp. Phys.* **47** 39

[21] Emery V J, Kivelson S A and Lin H Q 1990 *Phys. Rev. Lett.* **64** 475

[22] Reger J and Young A P 1988 *Phys. Rev.* B **37** 5978

[23] Kotliar G and Ruckenstein A 1986 *Phys. Rev. Lett.* **57** 1362

[24] Oguchi T 1960 *Phys. Rev.* **117** 117