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Abstract. We investigate the half-filled Hubbard model in one and two dimensions using approximations to the energy expressed as functionals of the momentum distribution. The functionals are calculated using the Hartree–Fock approximation and density functional theory in the local-spin-density and self-interaction-corrected (SIC) local-spin-density approximations (LSDA) by expressing the ground-state spin densities as a variational *ansatz* in which the momentum distribution enters as a variational quantity. We calculate the momentum distribution, energy and local moment, as well as our *ansatz* orbitals, in all three approximations and find that the SIC always improves upon the LSDA.

1. Introduction

The theoretical study of high-temperature superconductivity has been an area of intense investigation for the past few years now, since the discovery of the ceramic superconductors in late 1986 [1], with research being carried out on both real materials and model Hamiltonians. While many different approaches are taken towards the latter, the former problem may be best studied using density functional theory (DFT) [2–4].

DFT provides a formally exact approach; the energy for an interacting system of electrons, say, whether in an external field or not, is expressible as a functional of the electronic density and is minimized at the ground-state density, with the Kohn–Sham scheme [3] providing a method of determining the ground-state energy and density. However, the exact functional is unknown and so it has to be approximated. This may be achieved by splitting up the energy into three functionals of the spin densities, $n_\sigma(x)$: $T[n_\uparrow, n_\downarrow]$, the kinetic energy for a non-interacting set of electrons, $U[n_\uparrow, n_\downarrow]$, the Hartree electrostatic energy and $E_{XC}[n_\uparrow, n_\downarrow]$, the exchange and correlation (XC) energy. A fourth term arises if external fields are considered, but since none will be present, we shall ignore it. In this manner T and U are relatively straightforward to calculate, while E_{XC} is unknown and must be approximated. One approach is the local-spin-density approximation (LSDA), which is quantitatively successful in many cases, but fails where strong electron correlation effects, leading to localized states, are present. The high-T_c materials provide suitable examples, where LSDA calculations fail to give antiferromagnetic insulating ground states, e.g. for La_2CuO_4 [5–9] and $YBa_2Cu_3O_6$ [9].

In order to deal with these failures of the LSDA and to improve upon it, the use of a self-interaction-corrected (SIC) LSDA was proposed [10]. In the Kohn–Sham scheme [4] the electrons occupy fictitious single-particle states, with wavefunctions $\phi_{i\sigma}(x)$ (i denoting all the quantum numbers of the state, other than the spin, σ), related to the true ground-state spin densities, $n_\sigma(x)$, by

$$n_\sigma(x) = \sum_{occ} |\phi_{i\sigma}(x)|^2 \qquad (1)$$

where the sum is over the occupied orbitals with spin σ. However, in the LSDA each state has a spurious electrostatic self-interaction, which increases as they localize. The SIC-LSDA is then defined to be the LSDA with the self-interaction for each individual occupied state subtracted, i.e.

$$E_{XC}^{SIC} = E_{XC}^{LSDA}[n_\uparrow, n_\downarrow] - \sum_\sigma \sum_i^{occ} (U[n_{i\sigma}] + E_{XC}^{LSDA}[n_{i\sigma}]) \tag{2}$$

$$E_{XC}^{SIC} = E_{XC}^{LSDA}[n_\uparrow, n_\downarrow] - \Delta\, E_{XC}^{SIC}[\{n_{i\sigma}\}] \tag{3}$$

where $n_{i\sigma}(x)$ is the density due to $\phi_{i\sigma}(x)$ and the braces indicate that the functional takes as arguments the densities of all the occupied states. The SIC introduces an orbital-dependent potential and the eigenstates of the effective Hamiltonian are therefore not automatically orthogonal, so the expectation value of this Hamiltonian is not invariant under a unitary change of states. The Hamiltonian can now exhibit a broken symmetry between extended and localized states, which is lacking in the LSDA, but the implementation of the SIC-LSDA is more complicated. However, Svane and Gunnarsson have described a method [11] that they claim is only slightly more difficult to implement than the LSDA and have applied it to the transition metal oxides, obtaining the correct nature of the ground states. Furthermore, Svane [12] has recently studied La_2CuO_4 using this scheme and again the SIC-LSDA leads to the correct ground state, with a moment on the Cu in good agreement with experiment.

The more difficult nature of the SIC-LSDA led first Svane and Gunnarsson [13,14] then Ishii and Terakura [15] and later Miyazaki, Ishii and Terakura [16] to use the Hubbard model as a test of their algorithms; the first two papers dealt with the one- and two-dimensional models, while the last two only considered the one-dimensional model, but both employed a discrete DFT (DDFT) [17] extended to the SIC-LSDA. Svane and Gunnarsson [14] and Miyazaki *et al* [16] have also investigated the two-dimensional dp model using DDFT, while Majewski and Vogl [18, 19] have similarly examined the one and two-dimensional Hubbard–Peierls models. In this paper we return to the Hubbard model, employing an *ad hoc*, but much simpler method, by which we are able to express the energy, in the Hartree–Fock (HF), LSD and SIC-LSD approximations, as a functional of the momentum distribution. In section 2 we describe our method and in section 3 we present our results, which expand upon those previously published.

2. Method

Our method is to construct a set of localized states, in which the momentum distribution, $n(k)$, enters as a variational quantity, from which the spin densities may be calculated, assuming a Néel ordered antiferromagnetic spin arrangement. The expectation values of the site occupation operators are then given by functionals of the momentum distribution and hence the energy, which we shall evaluate in the HF, LSD and SIC-LSD approximations, is given as a functional of the momentum distribution too.

Since it will prove to be convenient, we write the Hubbard model, taken to be on a d-dimensional square lattice (with lattice constant $a = 1$ and d equal to 1 or 2), as

$$\hat{H} = t \sum_\sigma \sum_{\langle n,n' \rangle} \hat{W}_\sigma^\dagger(n)\hat{W}_\sigma(n') + U \sum_n \hat{n}_\uparrow(n)\hat{n}_\downarrow(n) \tag{4}$$

where $\hat{W}_\sigma^\dagger(n)$ is the creation operator (CO) for an electron in the Wannier state centred on the lattice site at $n = (n_1, \ldots, n_d)$ with spin σ, so $\hat{n}_\sigma(n) = \hat{W}_\sigma^\dagger(n)\hat{W}_\sigma(n)$ and $\langle , \rangle$ indicates

that the sum is to be taken over all ordered pairs of nearest neighbours. The n sums are assumed to be over a d-square region of the lattice containing N sites (where N is even; see the appendix), with periodic boundary conditions applied, which shall be called the fundamental domain (FD).

Letting $\hat{B}_\sigma^\dagger(k)$ be the CO for the Bloch state with wavenumber k and spin σ, we define our localized *ansatz* state centred on the lattice site n with spin σ to have CO $\hat{c}_\sigma^\dagger(n)$ given by

$$\hat{c}_\sigma^\dagger(n) = \sum_k \left(\frac{2n(k)}{N}\right)^{1/2} e^{-ik\cdot n} \hat{B}_\sigma^\dagger(k) \tag{5}$$

$$\hat{c}_\sigma^\dagger(n) = \sum_{n'} w(n' - n) \hat{W}_\sigma^\dagger(n') \tag{6}$$

where $n(k)$ is the momentum distribution of either spin (i.e. $n(k) = n_\sigma(k)$), assumed to be an even function of k,

$$w(n) = \frac{1}{N} \sum_k [2n(k)]^{1/2} e^{ik\cdot n} \tag{7}$$

and the k-sums are over the first Brillouin zone (1BZ).

Since we are at half-filling we may write

$$n(k) = \frac{1}{2} + \sum_{n\neq 0} A(n) e^{ik\cdot n} \tag{8}$$

that is

$$n(k) = \frac{1}{2} + g(k) \tag{9}$$

and then

$$[\hat{c}_\sigma(n), \hat{c}_{\sigma'}^\dagger(n')]_+ = \delta_{\sigma\sigma'} \sum_{n''\neq 0} A(n'')\delta_{n'',n'-n}. \tag{10}$$

States in different sublattices are orthogonal by virtue of being in different spin states, but if states in the same sublattice are to be orthogonal then $A(n) = 0$ for n lying in the sublattice, i.e. if $\sum_{i=1}^d n_i$ is even. It follows that $g(k + \tilde{K}) = -g(k)$ for $\tilde{K}$ a vector in the reciprocal lattice to the sublattice that does not also lie in the reciprocal lattice to the full lattice. Thus, $g(k)$ is an odd function about the points $\tilde{K}/2$ and so, with the evenness of $g(k)$, if $g(k)$ is known over a sub-sector, K_d say, of the d-dimensional 1BZ then it is given over the whole 1BZ. These symmetries are then constraints upon the function, but may be effectively removed if we consider variations of it only over K_d. Therefore, we shall almost invariably take reciprocal space sums and integrals to be over these regions, with expressions for the former implicitly including the different multiplicities for different points in passing from the 1BZ to K_d. Furthermore, being at half-filling, the Fermi zone (FZ) for the non-interacting model is the same as the 1BZ of the reciprocal lattice to the sublattice (which we shall denote by $\widetilde{\text{1BZ}}$).

Writing $n_\sigma(n)$ for the discrete spin density and using the Kohn–Sham *ansatz*, it is given by

$$n_\sigma(n) = \sum_{n^{(\sigma)}} |w(n^{(\sigma)} - n)|^2 \tag{11}$$

where $n^{(\sigma)}$ indicates that the sum is to be taken over the sites on which spin σ are centred; this holds in the HF approximation (HFA) too. From equations (7), (A6) and (A7) it therefore follows that

$$n_\sigma(n) = \frac{1}{2} + \frac{2\sigma(-1)^{\sum_i n_i}}{N} \sum_{K_d} [1 - 4g(k)^2]^{1/2} \tag{12}$$

or

$$n_\sigma(n) = \frac{1}{2} + 2\sigma(-1)^{\sum_i n_i} \left(\frac{1}{2\pi}\right)^d \int_{K_d} [1 - 4g(k)^2]^{1/2} \, \mathrm{d}^d k \tag{13}$$

where the first equation holds when N is finite, the second when N is taken to infinity.

Having found expressions for the $n_\sigma(n)$s we are now ready to discuss the approximations we shall use to calculate the energy, by which we shall always mean the energy *per* electron. Let $|\Psi_{HF}\rangle$ be the HF wavefunction, taken to be

$$|\Psi_{HF}\rangle = \prod_\sigma \left(\prod_{n^{(\sigma)}} \hat{c}_\sigma^\dagger(n^{(\sigma)}) \right) |0\rangle \tag{14}$$

with $n^{(\sigma)}$ as above, so the energy in the HFA is $\langle \Psi_{HF} | \hat{H} | \Psi_{HF} \rangle / N$, which is the functional

$$E_d^{HF}[g] = 8 \left(\frac{1}{2\pi}\right)^d \int_{K_d} \epsilon_d(k) g(k) \, \mathrm{d}^d k + U \left[\frac{1}{4} - \left(\frac{2}{(2\pi)^d} \int_{K_d} [1 - 4g(k)^2]^{1/2} \, \mathrm{d}^d k \right)^2 \right] \tag{15}$$

where we have taken the infinite-FD limit and $\epsilon_d(k) = 2t \sum_{i=1}^d \cos(k_i)$, the nearest-neighbour tight-binding band for the Hubbard model. $E^{HF}[g]$ is stationary, as $g(k)$ is varied, when

$$g(k) = \pm \frac{\epsilon_d(k)}{2U} \frac{1}{[I_d[g]^2 + (\epsilon_d(k)/U)^2]^{1/2}} \tag{16}$$

with the minimum given by the negative root, $\epsilon_d(k)$ satisfying the symmetries required of g, and

$$I_d[g] = 2 \left(\frac{1}{2\pi}\right)^d \int_{K_d} [1 - 4g(k)^2]^{1/2} \, \mathrm{d}^d k. \tag{17}$$

Combining equations (16) and (17) gives

$$2 \left(\frac{1}{2\pi}\right)^d \int_{K_d} \frac{1}{[I_d[g]^2 + (\epsilon_d(k)/U)^2]^{1/2}} \, \mathrm{d}^d k = 1 \tag{18}$$

so I_d and therefore g and E^{HF}/U are functions of t/U, the latter of which we shall write as $\epsilon^{HF}(t/U)$. The integral equation (18) is solved numerically to determine $I_d(t/U)$ and hence $\epsilon^{HF}(t/U)$, since

$$\epsilon_d^{HF}(t/U) = -4 \left(\frac{1}{2\pi}\right)^d \int_{K_d} \frac{(\epsilon_d(k)/U)^2}{[I_d(t/U)^2 + (\epsilon_d(k)/U)^2]^{1/2}} \, \mathrm{d}^d k + \frac{1}{4} - I_d(t/U)^2. \tag{19}$$

The integrand of (18) is too complicated to be written in terms of simple functions, but we may simplify it by the use of elliptic integrals. In one dimension the integral is expressible

as a simple function involving a complete elliptic integral of the first kind, while in two dimensions the double integral can be reduced to a single integral with an incomplete elliptic integral appearing in the integrand. Equation (18) is the same as that derived by Penn [20], with $I_d = \Delta/U$, where Δ is the band gap.

For the LSDA we use the functional proposed by Svane and Gunnarsson [13], and also used by Ishii and Terakura [15], in which the energy is given as a function of the $n_\sigma(n)$s by

$$E^{\text{LSDA}} = T(n_\uparrow, n_\downarrow) + U(n_\uparrow, n_\downarrow) + E_{\text{XC}}^{\text{LSDA}}(n_\uparrow, n_\downarrow), \qquad (20)$$

where T, the 'kinetic' energy term, is

$$T(n_\uparrow, n_\downarrow) = \frac{t}{N} \sum_{\langle n, n' \rangle} w^*(n) w(n') \qquad (21)$$

U is the Hartree energy, i.e.

$$U(n_\uparrow, n_\downarrow) = \frac{U}{2N} \sum_n (n_\uparrow(n) + n_\downarrow(n))^2 \qquad (22)$$

and $E_{\text{XC}}^{\text{LSDA}}$ is the exchange–correlation energy, approximated by

$$E_{\text{XC}}^{\text{LSDA}}(n_\uparrow, n_\downarrow) = \frac{U}{N} \sum_n \left\{ [n_\uparrow(n) + n_\downarrow(n)]^{4/3} \right.$$

$$\left. \times \left[-\alpha - \frac{\beta}{\gamma}([1 + \zeta(n)]^{4/3} + [1 - \zeta(n)]^{4/3} - 2) \right] \right\} \qquad (23)$$

with $\gamma = 2^{4/3} - 2$ and $\zeta(n)$ the spin-polarization, i.e. $\zeta = (n_\uparrow - n_\downarrow)/(n_\uparrow + n_\downarrow)$. The parameters α and β are taken to be 0.3840 and 0.0705, respectively, so the given functional reproduces the LSDA results for atomic hydrogen. Writing the kinetic energy term in k-space and using $n_\uparrow(n) + n_\downarrow(n) = 1$ permits us to express E^{LSDA} as the functional of g, $E^{\text{LSDA}}[g]$, where

$$E_d^{\text{LSDA}}[g] = 8 \left(\frac{1}{2\pi} \right)^d \int_{K_d} \epsilon_d(k) g(k) \, \mathrm{d}^d k + U \left(\frac{1}{2} - \alpha + \frac{2\beta}{\gamma} - \frac{\beta}{\gamma} \sum_\sigma (1 + \sigma \zeta[g])^{4/3} \right) \qquad (24)$$

and $\zeta[g] = 2I_d[g]$, the infinite-N limit having been taken once again. $E^{\text{LSDA}}[g]$ is stationary with respect to variation of $g(k)$ when

$$g(k) = \pm \frac{\epsilon_d(k)}{2U} \frac{1}{[J_d[g]^2 + (\epsilon_d(k)/U)^2]^{1/2}}. \qquad (25)$$

where

$$J_d[g] = \frac{4\beta}{3\gamma} \sum_\sigma \sigma (1 + 2\sigma I_d[g])^{1/3} \qquad (26)$$

so we may replace $J_d[g]$ by $J(I_d[g])$, and the minimum of the energy is again given by the negative root. Combining (25) and (26), while noting that I_d must be a function of t/U, gives

$$I_d(t/U) = 2 \left(\frac{1}{2\pi} \right)^d \int_{K_d} \frac{J(I_d(t/U))}{[J(I_d(t/U))^2 + (\epsilon_d(k)/U)^2]^{1/2}} \, \mathrm{d}^d k \qquad (27)$$

providing a self-consistent equation to solve for I_d and hence $J(I_d)$, from which the energy $\epsilon^{\text{LSDA}}(t/U) = E^{\text{LSDA}}[g]/U$, is calculated, where

$$\epsilon_d^{\text{LSDA}}(t/U) = -4 \left(\frac{1}{2\pi} \right)^d \int_{K_d} \frac{(\epsilon_d(k)/U)^2}{[J(I_d(t/U))^2 + (\epsilon_d(k)/U)^2]^{1/2}} \, \mathrm{d}^d k$$

$$+ \frac{1}{2} - \alpha + \frac{2\beta}{\gamma} - \frac{\beta}{\gamma} \sum_\sigma (1 + 2\sigma I_d(t/U))^{4/3}. \tag{28}$$

The LSDA therefore leads to a simple set of equations of the same form as those found in the HF approximation. Furthermore, we have reduced the problem to simple quadrature, avoiding the partial-differential equations, or rather the analogues that appear in the discrete case, that arise in the Kohn–Sham scheme.

The SIC-LSDA is more complicated than the LSDA and requires a little extra explanation. The *ansatz* state centred on the lattice site at n has an occupation $|w(n' - n)|^2$ on the site at n', using (6). So, from the definition of the SIC given by (3), the SIC per electron is

$$\Delta E^{\text{SIC}} = U \sum_n \left\{ \frac{1}{2} (|w(n)|^2)^2 - (\alpha + \beta)(|w(n)|^2)^{4/3} \right\}. \tag{29}$$

Since a lattice sum is present, for ease of calculation we shall use a finite value of N, so that instead of functionals of g, we have functions which take as arguments $g(k)$ for all the discrete k in the region K_d, consistent with the FD, which for a kernel f, say, we shall denote by $f(\{g\})$. Therefore, $w(n) = w(n; \{g\})$, where

$$w(n; \{g\}) = \frac{2}{N} \sum_{K_d} \left\{ \left([1 + 2g(k)]^{1/2} + (-1)^{\sum_i n_i} [1 - 2g(k)]^{1/2} \right) \cos(k \cdot n) \right\}. \tag{30}$$

It is useful to rewrite (30) using the identity

$$[1 + x]^{1/2} \pm [1 - x]^{1/2} = 2^{1/2} [1 \pm (1 - x^2)^{1/2}]^{1/2} \qquad 0 \leqslant x \leqslant 1 \tag{31}$$

as

$$w(n; \{g\}) = \frac{2}{N} \sum_{K_d} \left\{ 2^{1/2} \left[1 + (-1)^{\sum_i n_i} (1 - 4g(k)^2)^{1/2} \right]^{1/2} \cos(k \cdot n) \right\} \tag{32}$$

since by doing so we are able to find an expression for $g(k)$ similar to those arising in the HF and LSD approximations. If we define

$$I_d(\{g\}) = \frac{2}{N} \sum_{K_d} [1 - 4g(k)^2]^{1/2} \tag{33}$$

then the energy in the SIC-LSDA is

$$E_d^{\text{SIC}}(\{g\}) = \frac{8}{N} \sum_{K_d} \epsilon_d(k) g(k)$$

$$+ U \left(\frac{1}{2} - \alpha + \frac{2\beta}{\gamma} - \frac{\beta}{\gamma} \sum_\sigma \left[1 + 2\sigma \, I_d(\{g\}) \right]^{4/3} \right) - \Delta E^{\text{SIC}}(\{g\})/N. \tag{34}$$

We make this stationary by solving $\partial E_d^{\text{SIC}}(\{g\})/\partial g(k) = 0$ for all the ks in K_d. The solutions are

$$g(k) = \pm \frac{\epsilon_d(k)}{2U} \frac{1}{[(J(l_d) + H_d(k))^2 + (\epsilon_d(k)/U)^2]^{1/2}} \tag{35}$$

where

$$H_d(k) = \sum_n \left\{ \left(\frac{2}{3} w(n)(w(n)^2)^{1/3} - \frac{1}{2} w(n)^3 \right) \right.$$
$$\left. \times \frac{2^{1/2}(-1)^{1+\sum_i R_i} \cos(k \cdot n)}{[1 + (-1)^{\sum_i R_i}[1 - 4g(k)^2]^{1/2}]^{1/2}} S_n(k) \right\} \tag{36}$$

and

$$S_n(k) = \begin{cases} 1 & \text{if } k \text{ is in } \widetilde{\text{IBZ}} \\ (-1)^{\sum_i R_i} & \text{otherwise.} \end{cases} \tag{37}$$

The negative root again corresponds to the minimum of the energy and (35) also displays the correct symmetries. Unlike in the previous two approximations, we are unable to reduce the problem to determining just one quantity self-consistently; instead the full function g must be calculated so. We perform this calculation by taking, for given t/U, the LSDA result as our first iteration for $g(k)$ and then iterate towards a consistent answer. The form of g, while like that obtained for the other two approximations, differs in that we now have a k-dependent 'gap', a consequence of the non-local nature of the SIC.

Inspection of (36) reveals that $H_d(k)$ is undefined when $g(k) = 0$. This is not a serious problem since, by using (30) for $w(n)$ when extremizing the energy, we may obtain an equation for g, valid when $g = 0$. Using this equation we may show that starting from a g that is zero on the Fermi surface, which holds for g in the LSDA, all subsequent iterations of g are zero on the Fermi surface too. Since g is also zero on the Fermi surface in the HF approximation, then all three approximations yield a state that is an antiferromagnetic insulator. In one dimension the Hubbard model, while an insulator at half-filling [21], is not an antiferromagnetic state, but in higher dimensions this may well be the case [24,25].

While the SIC-LSDA equations are more complicated than those for the other approximations, and we have to be careful when $g(k) = 0$, using our method we have not employed the Kohn–Sham scheme and hence we have been able to ignore the extra difficulty the SIC-LSDA introduces by way of the orbitals no longer being orthogonal.

We have thus found the energy in the three approximations of interest and in each case the energy has the form $E = \sum_\sigma \sum_k \epsilon(k)n(k) + F[n]$, where we have used n instead of k, the k-sum is over the entire IBZ and the spin sum is shown explicitly. From the Feynman–Hellmann theorem, if we regard the band-structure as a variable, then the momentum distribution follows from the exact energy, $\mathcal{E}$, via $n(k) = \delta\mathcal{E}/\delta\epsilon(k)$, which provides a method of calculating the approximate $n(k)$, if we use E instead. Therefore, using E we can obtain

$$\frac{\delta E}{\delta \epsilon(k)} = n(k) + \sum_{k'} \frac{\delta n(k')}{\delta \epsilon(k)} \left[\epsilon(k') + \frac{\delta F}{\delta n(k)} \right] \tag{38}$$

so when E is stationary, i.e. the term in square brackets is zero, $\delta E/\delta n(k) = n(k)$ which means that the $n(k)$ appearing is indeed an approximation to the momentum distribution.

With our method we may also calculate the local moment, L_0, defined by Shiba to be

$$L_0 = \frac{1}{N} \sum_n \langle \Psi_0 | \hat{S}(n)^2 | \Psi_0 \rangle \qquad (39)$$

that is

$$L_0 = \frac{3}{4N} \sum_n \langle \Psi_0 | \left(\hat{n}_\uparrow(n) + \hat{n}_\downarrow(n) - 2\hat{n}_\uparrow(n)\hat{n}_\downarrow(n) \right) | \Psi_0 \rangle \qquad (40)$$

where $|\Psi_0\rangle$ is the exact ground state. Using the Feynman–Hellmann theorem again, it follows that

$$\frac{1}{N} \frac{\partial \langle \Psi_0 | \hat{H} | \Psi_0 \rangle}{\partial U} = \frac{1}{N} \sum_n \langle \Psi_0 | \hat{n}_\uparrow(n)\hat{n}_\downarrow(n) | \Psi_0 \rangle \qquad (41)$$

and therefore

$$L_0 = \frac{3}{4} + \frac{3}{2} \frac{t^2}{U^2} \frac{\mathrm{d}(U\epsilon(t/U)/t)}{\mathrm{d}(t/U)} \qquad (42)$$

where $\epsilon(t/U) = \langle \Psi_0 | \hat{H} | \Psi_0 \rangle / UN$, from which we calculate L_0.

Finally, before proceeding to the results, we should comment on the value of the approximations used. The LSD and SIC-LSD approximations used here both employ a rather arbitrary functional derived from calculations on the homogeneous electron liquid. The HFA, however, is simply the expectation value of the Hamiltonian in the HF state, so there can be no doubt about form of the functional. Furthermore, as it is the only strictly variational approximation to the energy, it provides the only upper bound to the exact energy. However, the main thrust of the paper is to investigate the improvement effected by the SIC on the LSD and to demonstrate the simplicity of the momentum density functional approach for a one-band antiferromagnetic insulator.

3. Results

Since all the approximations used are devised to calculate the energy, we shall discuss this first. In the limit $t/U \ll 1$, expressions can be found for the limiting forms of the energy. Since $g = O(t/U)$, then $g \ll 1$ too, and so it follows, from (17) that

$$I_d = \frac{1}{2} - 4 \left(\frac{1}{2\pi} \right)^d \int_{K_d} g(k)^2 \, \mathrm{d}^d k + O(g^4). \qquad (43)$$

Using this we can proceed to minimize the energy in the HFA and LSDA analytically and doing so we find that for the HFA, $E_d^{\mathrm{HF}} \approx -2dt^2/U$, while for the LSDA we obtain $E_d^{\mathrm{LSDA}} \approx U(1/2 - \alpha - \beta) - d\left(3\gamma/2^{1/3}4\beta\right)t^2/U = 0.0455U - 4.3894dt^2/U$. For the SIC-LSDA we also need to determine $w(n)$ in this limit, which is readily done by expanding the square root in (7), giving

$$w(n) = \delta_{n,0} + \frac{1}{N} \sum_k g(k)\mathrm{e}^{\mathrm{i}k \cdot n} - \frac{1}{2N} \sum_k g(k)^2 \mathrm{e}^{\mathrm{i}k \cdot n} + O(g^3) \qquad (44)$$

where the infinite-N limit has been taken. We are now able to minimize the energy analytically once again, giving $E_d^{SIC} \approx -2dt^2/AU$, where $A = 1-4(\alpha+\beta)/3+2^{4/3}4\beta/3\gamma$, so $2/A = 2.3539$.

In the opposite limit, $t/U \gg 1$, the electrons are only weakly interacting and so the momentum distribution may be approximated by the filled FZ, i.e.

$$g(k) = \begin{cases} \dfrac{1}{2} & \text{if } k \text{ is in the FZ} \\ -\dfrac{1}{2} & \text{otherwise} \end{cases} \tag{45}$$

so $I_d \approx 0$. The kinetic energy, T_d say, is the same in all three approximations, being

$$T_d \approx \begin{cases} 4t/\pi & d = 1 \\ (4t/\pi)^2 & d = 2. \end{cases} \tag{46}$$

So in the limit $t/U \gg 1$ we have $E_d^{HF} \approx T_d + U/4$ and $E_d^{LSDA} \approx T_d + (\frac{1}{2} - \alpha)U$. For the SIC-LSDA we must calculate the $w(n)$ using (45) and then perform the lattice sums appearing in the SIC; the results are shown in table 1.

Table 1. Limiting forms of the energy.

| | Limiting form of the energy | | | |
| | $t/U \ll 1$ | | $t/U \gg 1$ | |
Calculation	1D	2D	1D	2D
Exact	$-2.77t^2/U$	$-4.69t^2/U$	$(4/\pi)t + U/4$	$(4/\pi)^2t + U/4$
HF	$-2t^2/U$	$-4t^2/U$	$(4/\pi)t + U/4$	$(4/\pi)^2t + U/4$
LSDA	$-4.389t^2/U + 0.0455U$	$-8.779t^2/U + 0.0455U$	$(4/\pi)t + 0.116U$	$(4/\pi)^2t + 0.116U$
SIC-LSDA	$-2.354t^2/U$	$-4.71t^2/U$	$(4/\pi)t + 0.247U$	$(4/\pi)^2t + 0.233U$

In table 1, for one and two dimensions, we array the limiting forms of the energy in the three approximations used for comparison with the exact results: the analytic result of Lieb and Wu [21] in one dimension and in two dimensions numerical results for the spin-$\frac{1}{2}$ Heisenberg antiferromagnet [29], which is an effective Hamiltonian derivable from the Hubbard Hamiltonian in the limit $t/U \ll 1$ and the perturbation result for $t/U \gg 1$. At half-filling and $t/U \gg 1$, $\langle \hat{n}_\sigma(n) \rangle \approx \frac{1}{2}$ and $\langle \hat{n}_\uparrow(n)\hat{n}_\downarrow(n) \rangle \approx \frac{1}{4}$, from which the last results follow. Our limits for the energy in the LSD and SIC-LSD approximations in one dimension agree with those of Svane and Gunnarsson [13]. We can see that the HFA is reasonable in the limit $t/U \ll 1$ and is exact in the opposite limit. The LSDA is fairly poor in both limits and both dimensions, while the SIC-LSDA is generally good and exceptional for $t/U \ll 1$ in two dimensions. The SIC-LSDA is also better than the LSDA when $t/U \gg 1$, when the orbitals are most extended. For a totally delocalized Bloch state the SIC is $O(N^{1/3})$ and so vanishes as $N \to \infty$. However, the *ansatz* states used here do not tend to such a delocalized state as a Bloch state since the SIC remains non-zero.

We have also calculated for the three approximations the energy in one and two dimensions for a wide range of t/U, which we display in figures 1 and 2, as functions of $U/4t$ and U/t, respectively, following Svane and Gunnarsson [13, 14]. In these and all the other calculations of the SIC-LSDA, we have taken a chain of 258 sites and a grid of

64×64 sites in one and two dimensions, respectively, unless otherwise noted. For such lattice sizes, the results are practically unchanged by increasing the size further, except in the case we shall detail below. For comparison we include Lieb and Wu's exact result for one dimension [21] and the quantum Monte Carlo (QMC) results of Hirsch [24] and Moreo *et al* [25] in two dimensions. Our results are in good agreement with the few numerical values given in [15] (differing by at most 0.001) and also appear to agree with those in [13, 14].
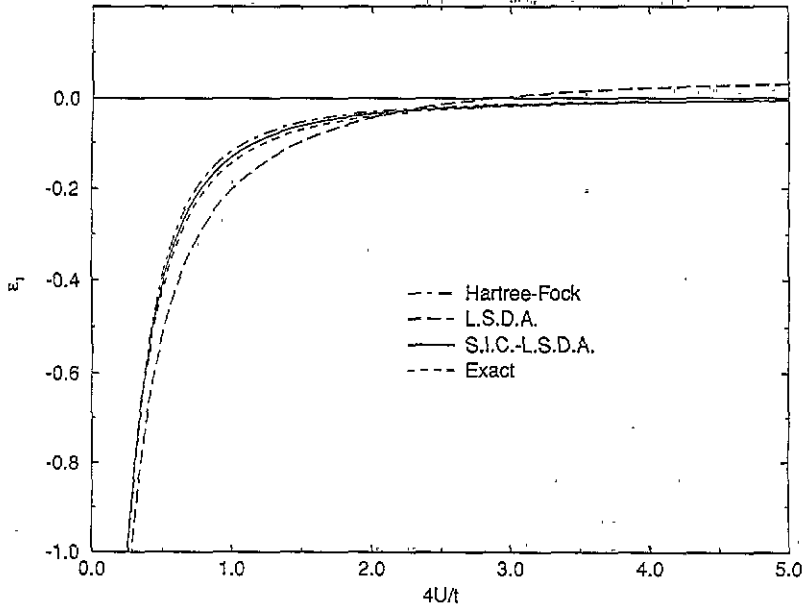
Figure 1. Plot of the total energy per site divided by U, for the half-filled Hubbard model in one dimension, $\epsilon_1 (t/U)$, against $4U/t$, in the Hartree–Fock, LSD and SIC-LSD approximations. The exact result of Lieb and Wu [21] is included for comparison.

The results for the momentum distribution in one dimension are plotted over the IBZ in figure 3 for $t/U = 0.1$. For reference we include Takahashi's [27] solution for $n(k)$, correct to second order in t/U. In two dimensions we plot our solutions for $n(k)$, along the line X–Γ–M, in figure 4, again for $t/U = 0.1$. Takahashi's [27] result for a spin-wave approximation is included for comparison. We find that in the LSDA the momentum distribution tends most quickly to that given by (45) showing that the LSDA leads to the most delocalized solutions.

This may be seen more directly by determining the coefficients $w(n)$, which give the weight of the single-particle state on other sites. The results are displayed in figures 5 and 6 for one and two dimensions respectively with $t/U = 0.1$ and similarly in figures 7 and 8 for $t/U = 1.0$. In two dimensions we display $w(n, 0)$. The greater delocalization of the LSDA compared with the HF and SIC-LSD approximations is readily noted.

The results for the local moment are displayed in figures 9 and 10 for one and two dimensions respectively, with the two dimensional QMC results of White *et al* [26] included too. We see that once again the SIC-LSDA is generally better than the HFA, except as $t/U \to \infty$, when the HFA becomes exact. However, the LSDA is plainly wrong for all values of t/U, whereas Svane and Gunnarsson [13, 14] appeared to obtain more reasonable
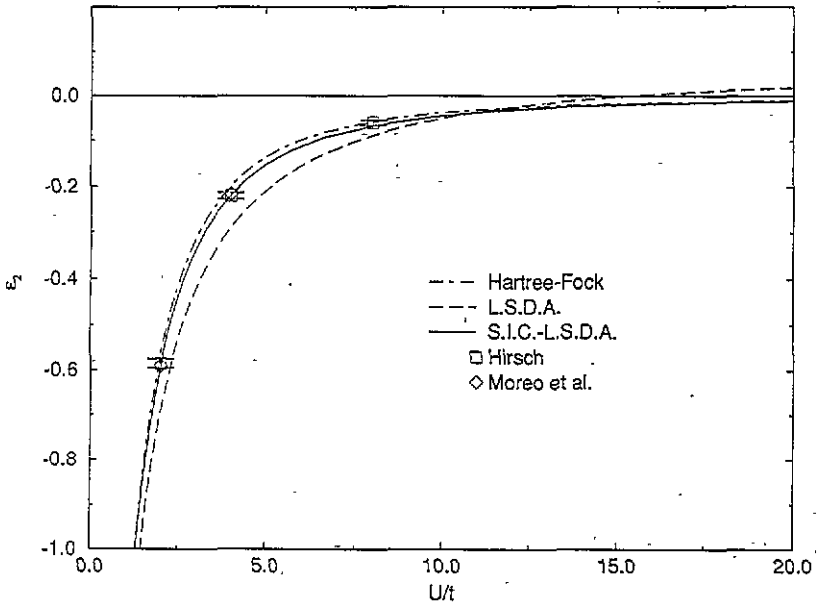
Figure 2. Plot of the total energy per site divided by U, for the half-filled Hubbard model in two dimensions, $\epsilon_2(t/U)$, against U/t, in the Hartree–Fock, LSD and SIC-LSD approximations. The QMC results of Hirsch [24] and Moreo *et al* [25] on grids of 8×8 and 12×12 sites respectively. Quoted error bars are included for the former.
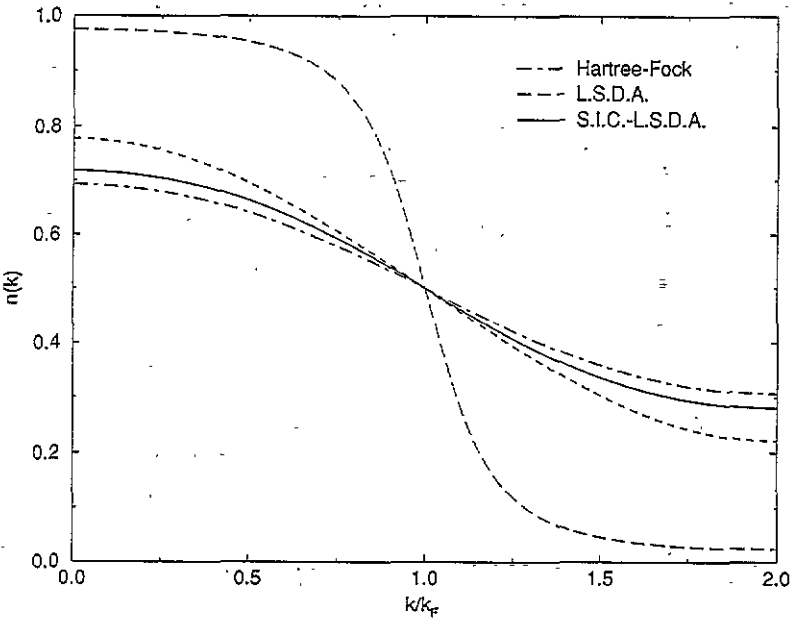

Figure 3. Plot of the momentum distribution, n(k), for the half-filled Hubbard model in one dimension, with $t/U = 0.1$, in the HF, LSD and SIC-LSD approximations. The dotted line is the exact result of Takahashi [27].
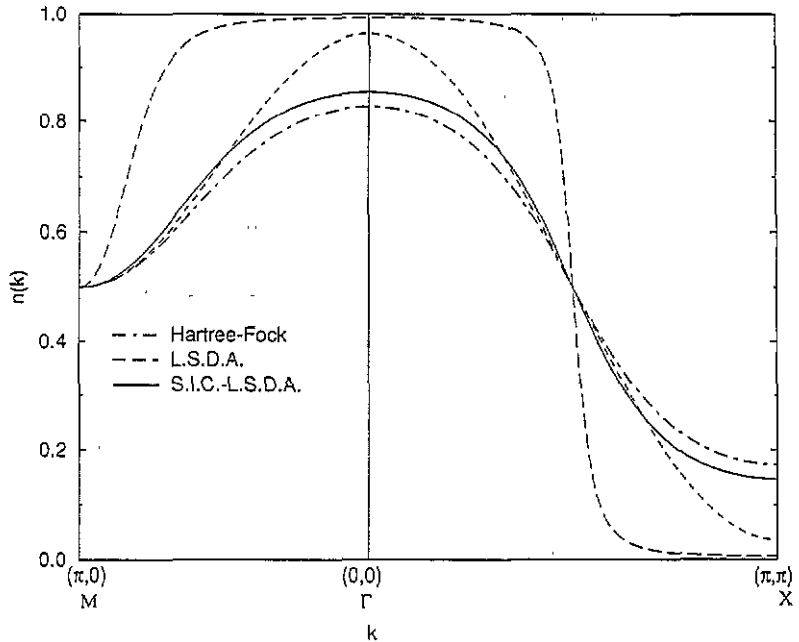
Figure 4. Plot of the momentum distribution, n(k), for the half-filled Hubbard model in two dimensions, with $t/U = 0.1$, along the M–Γ–X line, in the HF, LSD and SIC-LSD approximations. The dotted line is Takahashi's result in the spin-wave approximation.
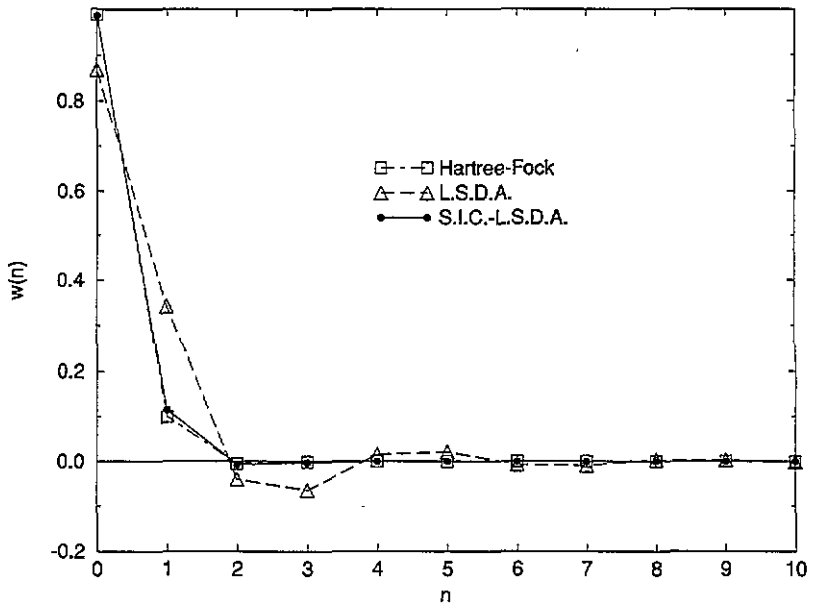

Figure 5. Plot of $w(n)$ in one dimension for $t/U = 0.1$.

results. The explanation of this discrepancy is as follows; Svane and Gunnarsson appear to have used the result of the HFA, $L_0 = 3(1 - 2\langle n_\uparrow\rangle\langle n_\downarrow\rangle)/4$, which, is incorrect for the LSDA and SIC-LSDA. Thus, while in the LSDA the orbitals are the most delocalized, the energy
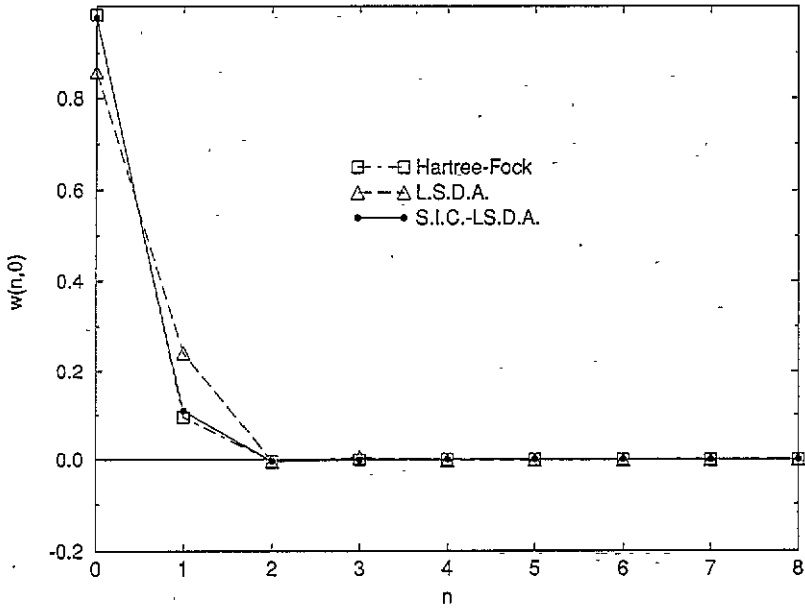
Figure 6. Plot of $w(n)$ in two dimensions for $t/U = 0.1$.
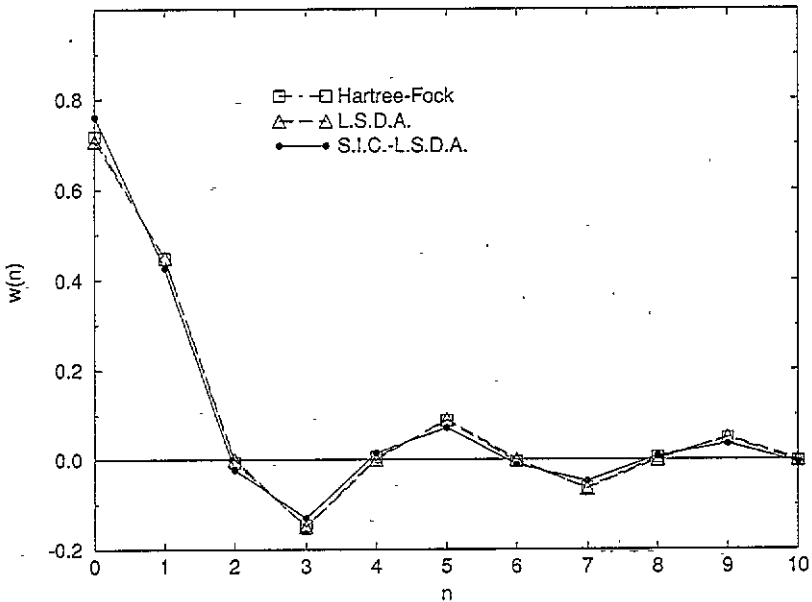

Figure 7. Plot of $w(n)$ in one dimensions for $t/U = 1.0$.

functional used is an exceedingly poor approximation to the correlation energy.

We have also calculated the sublattice magnetization $m = |n_\uparrow - n_\downarrow|$, which is shown in figures 11 and 12. Note that for the SIC-LSDA in two dimensions, m remains finite as $U \to 0$, which is a finite-size effect. Instead, $m = (4\nu - 1)/2\nu^2$ if the number of sites $N = (4\nu)^2$, which arises because when $U = 0^+$, the summand of I_2 is zero for all points
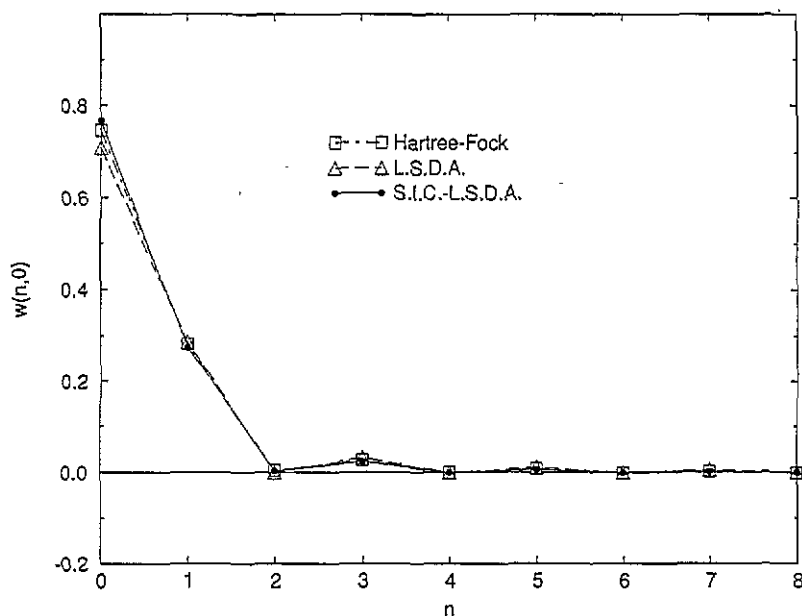
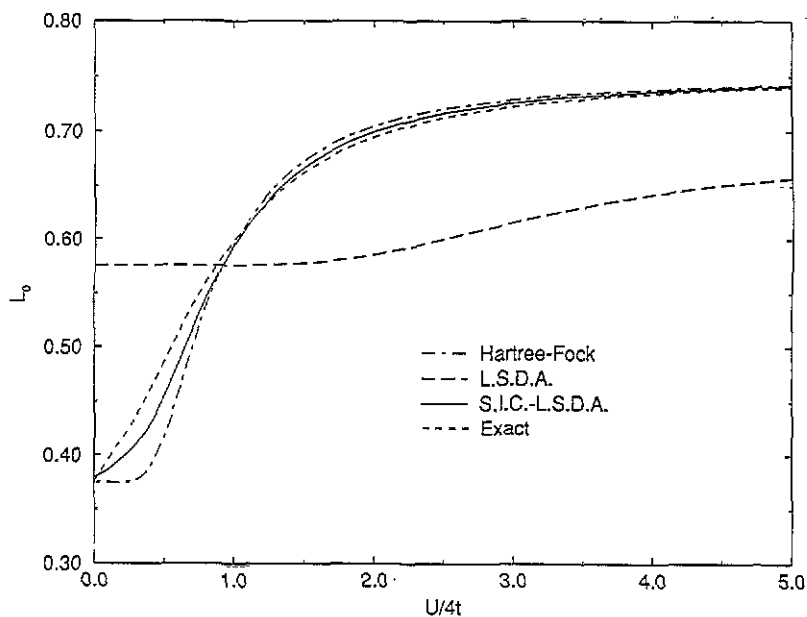**Figure 8.** Plot of $w(n)$ in two dimensions for $t/U = 1.0$.

Figure 9. Plot of the local moment, L_0, in one dimension for the three approximations considered, along with the exact result from Lieb and Wu.

in K_2, except for the points on the Fermi surface, where it equals 1. Thus, because I_2 is a sum, these points have a finite weight and so m is finite too, but it does tend to the correct limit, $m = 0$, as $N \rightarrow \infty$. Similarly, in one dimension, the summand of I_1 is also only non-zero, being equal to 1, on the Fermi surface, which is now just the two points
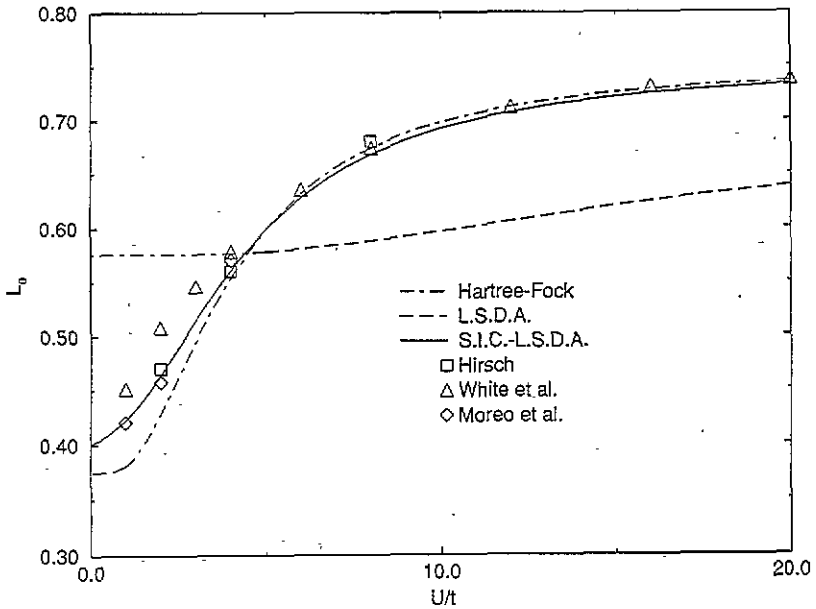
Figure 10. Plot of the local moment, L_0, in two dimensions for the three approximations considered, along with the QMC results of Hirsch [24], White *et al* [26] and Moreo *et al* [25], on grids of 6×6, 4×4 and 12×12 sites, respectively.

$k = \pm\pi$. However, if we take $N = 2(2\nu + 1)$, these points are not included in the k-sum and so we obtain the correct limit with no finite-size problems, which is in contrast to the two-dimensional case where no such judicious choice of N exists. Finally, we compared our results with those of Miyazaki *et al* [16], using $N = 256$ for the SIC-LSDA, and found that our results differed by no more than 0.001. (The results published in [15] for $n_\uparrow - n_\downarrow$ are erroneous and have been corrected in [16].)

Finally, before passing onto the conclusions we should like to explain that the choice of a finite system in calculating the SIC-LSDA was prompted by the requirement of having to find the function g self-consistently, which can only be achieved numerically by so calculating the unknown function at a finite set of points. Thus, a finite system is quite attractive as not only do we have a finite set of points, but these points are not arbitrarily chosen, but are fixed by the choice of system size and boundary condition. However, a calculation for an infinite system is not ruled out, since any k-integral present will numerically be written as a sum and so we once again have g only over a finite set of points, but now a set that is somewhat more arbitrary than before. We have tried just such a calculation, using the Cunningham points [28] for the square Fermi-zone for performing the k-integrals, which has the advantage of not including those points at which the integrand of I_2 would have non-zero values for $U = 0$ and so ensuring the correct limit for m. Furthermore, we deal with the n sum in $H_2(k)$ by summing it to convergence for each k-point. Unfortunately, this method was found to be numerically stable only for certain values of t/U, so we have not presented the results here. However, we mention this scheme to indicate that treating the infinite case is, at least in principle, possible.
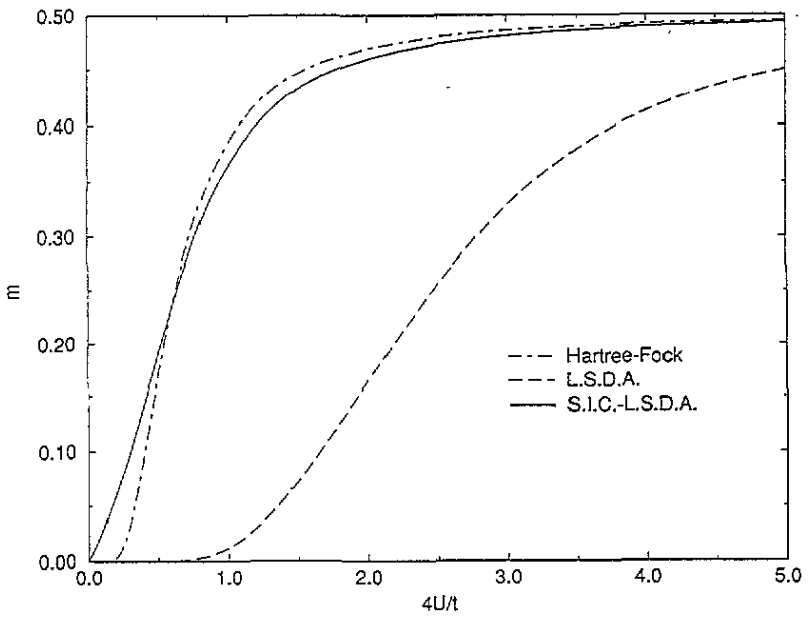
Figure 11. Plot of the sublattice magnetization, m, in one dimension, calculated in the three approximations considered.
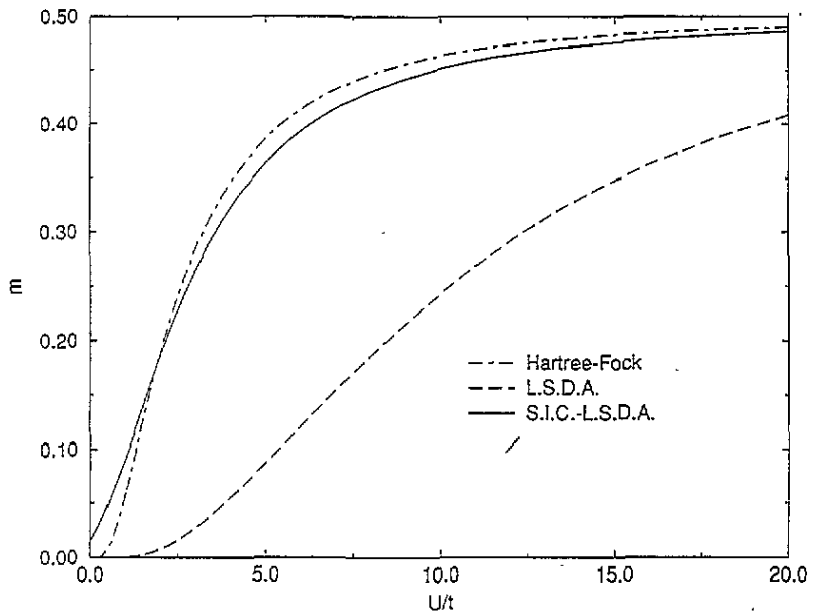

Figure 12. Plot of the sublattice magnetization, m, in two dimensions, calculated in the three approximations considered.

4. Conclusions

By constructing a set of *ansatz* orbitals for the ground state of a d-dimensional Hubbard

model on a square lattice and at half-filling we have been able to obtain energy functionals of the momentum distribution in the HF, LSD and SIC-LSD approximations. We have calculated the energy in these approximations by minimizing with respect to the momentum distribution and have been able to obtain expressions for the limiting forms of the energy. All calculations have been at worst quadrature as our method avoids having to solve finite-difference equations. Our implementation also avoids the problem of non-orthogonal orbitals in the SIC-LSDA. Our results are in generally good agreement with those already published [13–16] and those obtained by other methods [24, 25], except where noted above.

The HFA is reasonable across the whole range of t/U, while the LSDA is always fairly poor. The addition of a SIC to the LSDA leads to a great improvement for all values of t/U, with the SIC-LSDA being the best approximation of the three when $t/U \ll 1$. This improvement is most readily seen in the results for the local moment where, despite the LSDA calculation being so very poor, the SIC almost totally corrects it. We may therefore conclude that the SIC-LSDA is an improvement upon the LSDA in all the examples considered. What is more, even though the latter employed a somewhat arbitrary functional for the XC energy and could lead to results that were clearly in error, e.g. the energy as $t/U \to 0$, the SIC-LSDA corrected these errors almost totally.

The method described in this paper assumes a system with one electron per site and just such a system is the low-density state of the electron liquid which we shall discuss elsewhere [29].

Acknowledgments

Appendix. Sub-lattice sums

As we have a Néel state present we are naturally led to consider sums over the sublattices of terms like $e^{ik \cdot n}$. Let us assume that we have a d-dimensional cubic lattice, with lattice constant a, and apply periodic boundary conditions to a section containing N unit cells and of volume V, which we shall refer to as the fundamental domain (FD). Now partition the sites between two interpenetrating sublattices, labelled $+$ and $-$, and consider

$$S(k, x) = \sum_{n^+} e^{ik \cdot (x - n^+)} \tag{A1}$$

where the sum is over all the sites in the $+$ sublattice, assumed to include the origin. $S(k, x)$ is a periodic function of x, with the periodicity of the sublattice, if in the FD along any line of sites, parallel to a primitive lattice vector, there are as many $+$ as $-$ sites. Given this then N must be an even number. The periodicity of S permits us to write it as

$$S(k, x) = \sum_{\bar{k}} s_{\bar{k}}(k) e^{i\bar{k} \cdot x} \tag{A2}$$

with

$$s_{\bar{k}} = \frac{1}{\tilde{v}} \int_{\widetilde{UC}} S(k, x) e^{-i\bar{k} \cdot x} \, d^d x \tag{A3}$$

where $\bar{k}$ is a reciprocal sublattice vector and $\tilde{v}$ is the volume of the sublattice unit cell, which is the region of integration, denoted by $\widetilde{UC}$. From (A1) and (A3) we obtain

$$s_{\bar{k}}(k) = \frac{V}{\tilde{v}} \delta_{k,\bar{k}}.$$
(A4)

Since $\tilde{v} = 2v$ it follows that

$$S(k, x) = \frac{N}{2} \sum_{\bar{k}} \delta_{k,\bar{k}} e^{ik \cdot x}$$
(A5)

and therefore

$$\sum_{n^+} e^{-ik \cdot n^+} = \frac{N}{2} \sum_{\bar{k}} \delta_{k,\bar{k}}$$
(A6)

Since for all the $-$ sites, $n^- = n + a$ holds, if $a = a(1, 0, \ldots, 0)$, then from (A1) and (A6)

$$\sum_{n^-} e^{-ik \cdot n^-} = \frac{N}{2} \sum_{\bar{k}} \delta_{k,\bar{k}} e^{ik \cdot a}$$
(A7)

follows.

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