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A Gutzwiller variational scheme for the attractive Hubbard model

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Abstract. A variational wave function to describe the ground-state properties of the attractive Hubbard model is presented. The function is complementary to the Gutzwiller wave function for positive U. The results are in agreement with the canonical transformation which is known to relate the attractive and repulsive Hubbard models for all electronic densities.

The simplest model of systems with local non-retarded electron pairing is the extended Hubbard model with on-site U attractive interaction (for a review see [1]). The model can be considered as generally resulting from a system of narrow band electrons strongly coupled to a bosonic field (phonons, excitons, acoustic plasmons, etc), upon elimination of bosonic degrees of freedom. The parameter U is an effective one and if $U_{\mathrm{eff}} < 0$, the induced local attraction outweighs the on-site repulsion. This is the case of on-site attraction or the negative U Hubbard model.

The concept of local electron pairing is interesting from various points of view and it can be of importance for superconductivity, CDW formation and amorphous semiconductors [1].

The Hamiltonian is given by

$$\hat{H} = t\hat{T}_0 - |U|\,\hat{D}$$

$$\hat{T}_0 = -\sum_{\substack{\langle i,j\rangle \\ \sigma}} c_{i\sigma}^{+} c_{j\sigma} \qquad \hat{D} = \sum_{j} n_{j\uparrow} n_{j\downarrow} \qquad n_{j\sigma} = c_{j\sigma}^{+} c_{j\sigma} \tag{1}$$

where t denotes the transfer integral between nearest neighbours. In this case the model contains three parameters, t, U and $n = N/N_{\mathrm{a}}$, where N is the number of electrons and N_{a} the number of sites.

The model (1) has been intensively studied in the last few years [1] (for exact 1D results see [2]). There exists a canonical transformation (attraction–repulsion transformation) for bipartite lattices:

$$c_{j\downarrow}^{+} = \mathrm{e}^{\mathrm{i}\boldsymbol{Q}\cdot\boldsymbol{R}_j} b_{j\downarrow} \qquad c_{j\uparrow}^{+} = b_{j\uparrow}^{+} \tag{2}$$

with the reciprocal vector $\boldsymbol{Q}$ satisfying the condition $\exp(\mathrm{i}\boldsymbol{Q}\cdot\boldsymbol{R}) = -1$ for any $\boldsymbol{R}$ which

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transforms one sublattice into another, which maps the Hubbard model with on-site attraction and arbitrary electron density ($0 \leqslant n \leqslant 2$) onto the half-filled Hubbard model with on-site Coulomb repulsion in the presence of an appropriate magnetic field [1], [3]. The transformation requires that the magnetisation of the repulsive model has the fixed value along the z direction and being equal to $\frac{1}{2}(n-1)$. Consequently, the magnetic long-range orderings (along the z axis and in the xy plane) in the model with $U>0$ are equivalent to the electronic diagonal (CDW) and off-diagonal (singlet-superconductivity) orderings in the $U<0$ case.

In this paper we extend the Gutzwiller wave function [4] to study the attractive Hubbard model (1) (for previous variational studies of the model see [5], [6]).

We introduce the following *ansatz* for the ground-state of the attractive model, (equation (1))

$$|\psi\rangle = g^{\hat{D}}\,|\psi_0\rangle \qquad g \in (1, \infty) \tag{3a}$$

where g is the variational parameter and $|\psi_0\rangle$ stands for the ground-state of an appropriate single particle effective Hamiltonian. In the simplest case $|\psi_0\rangle$ can be chosen to be the ground state of (1) for $U=0$, i.e. $|\psi_0\rangle \equiv |\mathrm{SL}\rangle$ (where SL is the Slater determinant).

The variational wave function (3a) is nothing but the generalisation for $U<0$ of the Gutzwiller function for $U>0$ [4]

$$|\psi\rangle = g^{\hat{D}}\,|\psi_0\rangle \qquad g \in (0, 1). \tag{3b}$$

We start by comparing the exact ground-state energy expansion derived in reference [7] for the 1D case and $n=1$, with the one obtained from the variational function (3a) for small and intermediate values of $|U|$.

The use of a linked cluster expansion technique ($|U| \leqslant 2zt$, where z is the coordination number) analogously to that for $U>0$ and $|\psi\rangle$ given by (3b) (see references [8–10]), yields for any lattice and $|\psi_0\rangle$ given by the ground-state of $\hat{T}_0$

$$E_0 = t\langle\hat{T}_0\rangle_0 - |U|\langle\hat{D}\rangle_0 - \frac{U^2}{t}\frac{2[\langle D^2\rangle_{0,\mathrm{c}}]^2}{\langle\{\hat{D},\{\hat{D},\hat{T}_0\}\}\rangle_{0,\mathrm{c}}} \tag{4}$$

where $\hat{T}_0$ and $\hat{D}$ are defined in (1). In (4) an average is taken with respect to the uncorrelated state $|\psi_0\rangle$ and $\langle\ldots\rangle_{0,\mathrm{c}}$, means that only connected diagrams are included.

For the 1D case we use Wick's theorem to express the expectation values of the RHS of (4) in terms of the equal-time free propagators

$$P_{ij} = \langle c^{+}_{i\sigma}c_{j\sigma}\rangle_0 = \begin{cases} n/2 & i=j \\ \dfrac{\sin(\pi n m/2)}{\pi m} & i \neq j,\ i-j=m. \end{cases} \tag{5}$$

Following the same procedure as in reference [10] for $U>0$ and after performing the lattice summations we obtain for the ground state energy

$$E_0/N_{\mathrm{a}} = -\frac{4t}{\pi}\sin(\pi n/2) - |U|\frac{n^2}{4} - \frac{U^2}{4t}[(n^2/4)(1-\tfrac{3}{4}n)]^2/\{(n/2)(1-n/2)$$
$$+ [(\sin(\pi n/2)/\pi)]^2\}[(\sin(\pi n/2))/\pi]. \tag{6}$$

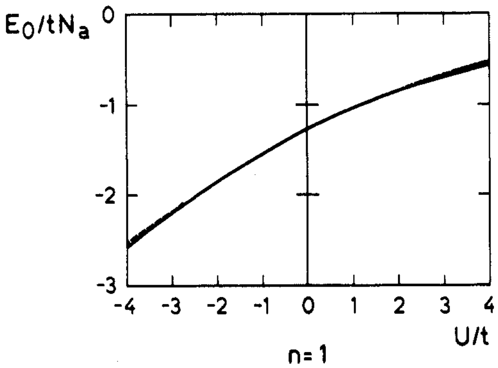

Figure 1. Ground-state energy as a function of U/t in one dimension. Broken curve represents the variational linked cluster energy expansion (present expansion for $U < 0$ and the Gutzwiller expansion of reference [10] for $U > 0$). Full curve represents Woynarovich's exact expansion.

This energy is plotted for $n = 1$ ($U < 0$) in figure 1, together with the corresponding Gutzwiller cluster expansion of reference [10] for $U > 0$. The obtained energy curve is compared with the exact Bethe *ansatz* curve of reference [7].

For $U = -4t$ the energy (6) ($n = 1$) takes account of 98% of the exact result. Like the exact curve, the variational one obtained from the combined use of the linked cluster expansions of functions (3*a*) ($U < 0$) and (3*b*) ($U > 0$), is continuous at $U = 0$.

In the case of a square lattice the equal-time free propagator $P_{ij} = \langle c_{i\sigma}^{+} c_{j\sigma} \rangle_0$ is given by

$$P_{ij} = \begin{cases} n/2 & i = j \\ P_{m'}^{m} = \dfrac{1}{\pi^2} \displaystyle\int_0^{Q_F(o)} \mathrm{d}k \frac{\cos(km)\sin[Q_F(k)m']}{m'} & i \neq j \qquad \boldsymbol{R}_i - \boldsymbol{R}_j \equiv [{}^{m}_{m'}] \end{cases} \tag{7}$$

where

$$Q_F(k) = \cos^{-1}(-\cos k - \varepsilon_F/2t)$$

defines the Fermi surface for $U = 0$ through the equation $k_x = Q_F(ky)$. Inverting the function $n = 2P_{ii}$

$$n(\varepsilon_F) = \frac{2}{\pi^2} \int_0^{Q_F(o)} \mathrm{d}k\, Q_F(k) \tag{9}$$

we get that for $0 \leqslant n \leqslant 1$ ε_F changes continuously from $\varepsilon_F(o) = -4t$ to $\varepsilon_F(1) = 0$.

Following the same steps as in reference [11] for $U > 0$, (4) now leads to

$$E_0/N_a = -8tP_0^1 - |U|\frac{n^2}{4} - \frac{U^2}{4t}\left[\frac{n^2}{4}(1-n) + \sum_{m,m'=-\infty}^{\infty} (P_{m'}^{m})^4\right]^2 \bigg/ \{[n(1-n/2) + 2(P_0^1)^2]\, P_0^1\}. \tag{10}$$

In figure 2 the energy (10) is plotted for $n = 1$ together with the corresponding Gutzwiller cluster expansion of reference [11]. The obtained curve is compared with Monte Carlo results [12].

The energy value in (10) can be improved if the starting ground-state of the RHS of (3*a*), $|\psi_0\rangle$, which in the present calculation was taken to be $|\mathrm{SL}\rangle$, is replaced by the ground-state of an effective Hamiltonian including the appropriate broken symmetries.

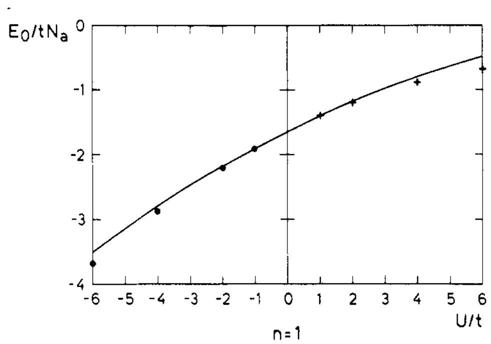

Figure 2. Ground-state energy as a function of U/t for a square lattice. Full curve represents the variational linked cluster expansions. The crosses are QMC results by Hirsch [12]. The full circles were obtained by the $U \to -U$ symmetry.

In fact, contrary to the 1D case, for a square lattice the ground-state is characterised by charge and superconducting long range orders for $U < 0$ (spin long range order for $U > 0$).

So far we have only checked the variational function (3*a*) for small and intermediate values of $|U|$.

Based on the method of reference [13], it is possible to derive the following 1D result for the number of doubly occupied sites, which is exact within the variational function (3*a*)

$$\langle \hat{D} \rangle = N_a\{n(e^{\eta} - 1) - \ln[1 + n(e^{\eta} - 1)]\}/8\sinh^2(\eta/2) \tag{11a}$$

or

$$\langle \hat{D} \rangle = \begin{cases} (N/4)n + \eta(N/4)n(1 - \frac{2}{3}n) + O(\eta^2) & \eta \ll 1 \\ (N/2) - (N_a/2)\,e^{-\eta}[\eta + \ln(n) - n] + O((e^{-\eta})^2) & \eta \gg 1 \end{cases} \tag{11b}$$

where $\eta = 2\ln(g)$. Equations (11*a*, *b*) show that the function (3*a*) leads to the exact values of D for both $U = 0$ and $U \to -\infty$. These limiting values for D can be generalised to any bipartite lattice. We remember that the Gutzwiller wave function also fulfils this condition for $U \to \infty$, i.e. $D = 0$ [13].

An important condition for a good variational wave function is that it reproduces the symmetry properties of the exact ground-state. In the present case, we require that the results obtained with the variational wave functions (3*a*) and (3*b*) transform into each other under the canonical transformation (2).

Our preliminary studies with the wave functions (3*a*) and (3*b*) indicate that this symmetry is fulfilled for all parameter space and any bipartite lattice. In the present paper we check its validity for the 1D lattice to second order in U/t for small and intermediate $|U|$, and to second order in the concentration $\delta = 1 - n$ $(0 \leqslant n \leqslant 1)$. The results for $n > 1$ can be obtained by replacing electrons by holes.

Under the canonical transformation (2), the 1D negative-U Hubbard model (1) is transformed into the repulsive one for the half-filling in an appropriate magnetic field and fixed magnetisation along the z axis equal to $\frac{1}{2}(n - 1)$, [1], [3]

$$\hat{H} = -t\sum_{j,\sigma}[b^{+}_{j\sigma}b_{j+1\sigma} + \text{HC}] + |U|\hat{D} - |U|\sum_{j}\hat{\sigma}^{z}_{j} - \tfrac{1}{2}|U|\sum_{j,\sigma}b^{+}_{j\sigma}b_{j\sigma}$$

$$\frac{1}{N_a}\sum_{j}\langle\hat{\sigma}^{z}_{j}\rangle = s \tag{12}$$

where $\hat{D}$ and $\hat{\sigma}_j^Z$ are expressed in terms of the operators $b_{j\sigma}^+$ and $b_{j\sigma}$. For the ground-state of this Hamiltonian we use the Gutzwiller *ansatz* (3*b*), with $|\psi_0\rangle$ defined as

$$|\psi_0\rangle = \prod_{|k|<K_{F\downarrow}} \tilde{b}_{k,\downarrow}^+ \prod_{|k|<K_{F\uparrow}} \tilde{b}_{k,\uparrow}^+ |0\rangle \qquad \tilde{b}_{k,\sigma}^+ = \mathrm{FT}[b_{j\sigma}^+] \tag{13}$$

and

$$K_{F\sigma} = K_F + \sigma\pi s + O(s^3) \qquad K_F = \pi/2. \tag{14}$$

Our results are valid only to second order in the concentration δ for $U < 0$ because we do not account for the third order term of the RHS of equation (14) (within the canonical transformation $\delta = -2s$).

Besides the Hamiltonian (12), we also consider the one-dimensional corresponding $U < 0$ version of the Hamiltonian (1) for $0 \leqslant n \leqslant 1$ ($0 \leqslant K_F \leqslant \pi/2$). We represent its ground-state by the variational wave function (3*a*) with $|\psi_0\rangle = |\mathrm{SL}\rangle$. If the required symmetry holds, the energy obtained with the Gutzwiller *ansatz* (3*b*) for the Hamiltonian (12), with s replaced by $-\delta/2$, should give the same result as that calculated directly with the use of (3*a*) for the $U < 0$ 1D Hamiltonian.

For $n = 1$, the use of Wick's theorem to express the RHS of (4) in terms of the free propagators

$$P_{ij,\sigma} = \langle b_{i\sigma}^+ b_{j\sigma}\rangle_0 = \begin{cases} \frac{1}{2} + \sigma s & i = j \\ \dfrac{\sin[(\pi/2)(\frac{1}{2} + \sigma s)(i-j)]}{\pi(i-j)} & i \neq j \end{cases} \tag{15}$$

leads to

$$\begin{aligned} E_0/N_a = & -\frac{4t}{\pi}\cos(\pi s) + |U|(\tfrac{1}{4} - s^2) - |U|s - \tfrac{1}{2}|U| \\ & - (U^2/4t)[1/12 - s^2(1 - \tfrac{4}{3}s)]^2/[\tfrac{1}{4} + 1/\pi^2 \\ & - s^2((\sin\pi s)/\pi)^2]((\cos\pi s)/\pi). \end{aligned} \tag{16a}$$

Replacing s by $-\delta/2$ and expanding the correlation term to second order in δ, we finally obtain ($n = 1 - \delta$)

$$\begin{aligned} E_0/N_a = & -\frac{4t}{\pi}\sin(\pi n/2) - |U|\frac{n^2}{4} - \frac{U^2}{4t}\frac{\pi^2}{36(4+\pi^2)} \\ & \times\left[1 - \left(\frac{192 + 28\pi^2 - \pi^4}{32 + 8\pi^2}\right)\delta^2 + O(\delta^3)\right]. \end{aligned} \tag{16b}$$

The use of the variational $U < 0$ wave function (3*a*) in the attractive 1D Hamiltonian leads to the energy (6). Replacing n in the correlation term of the RHS of (6) by $1 - \delta$ and expanding to second order in δ recovers the result (16*b*). The required symmetry is then fulfilled not only for the half-filled band case but for all electronic densities.

The symmetries which relate the ground-states of the 1D $U < 0$ and $U > 0$ models imply that for small U the corresponding U/t expansions of the spin–spin and charge–charge correlation functions of the two models transform into each other by a simple $U \to -U$ transformation. The same is true for the small U expansions of the ground-state energy and other quantities [7]. Moreover, the small U expansions of the spin–spin and charge–charge correlation functions only differ in the sign of U for each of these models. It is then obvious that the interchange of roles which the charge and spin degrees of freedom have in the two models is closely related to the referred symmetry.

Thus the variational wave functions (3*a*, *b*) correctly describe that symmetry.

To close this paper we present preliminary results regarding the superconducting fluctuations of the model (1). This study, which is in progress, uses the variational wave function (3*a*).

Introducing

$$\hat{O}_j = C_{j\uparrow} C_{j\downarrow} \tag{17}$$

we analyse the on-site Cooper pair–Cooper pair correlation function

$$S^s_{ij} = \tfrac{1}{2}\langle\{\hat{O}^+_i, \hat{O}_j\}\rangle \tag{18a}$$

and its Fourier transform $\tilde{S}^s(\boldsymbol{q})$.

Following the same steps as in references [11] and [14], we obtain the linked cluster expansion for the function (18*a*)

$$S^s_{ij} = \tfrac{1}{2}\langle\{\hat{O}^+_i, \hat{O}_j\}\rangle_0 + \frac{2|U|}{t}\frac{\langle D^2\rangle_{0c}\langle\{\hat{D}, \{\hat{O}^+_i, \hat{O}_j\}\}\rangle_{0c}}{\langle\{\hat{D}, \{\hat{D}, \hat{T}_0\}\}\rangle_{0c}} \tag{18b}$$

which holds for any lattice provided that $|\psi_0\rangle$ is the ground-state of $\hat{T}_0$. This is a good choice for the 1D model because the corresponding ground state has no long range orders.

For the one-dimensional case the use of Wick's theorem yields

$$\tilde{S}^s(q) = \begin{cases} \tfrac{1}{2}[1 - |q|/\pi + \eta(n - |q|/\pi)(1 - n/2 - |q|/2\pi)] & 0 \leqslant |q| \leqslant \pi n \\ \tfrac{1}{2}[1 - n/2] & \pi n \leqslant |q| \leqslant \pi \end{cases} \tag{19}$$

where

$$\eta = \frac{|U|}{8t}\frac{n^2(1 - \tfrac{2}{3}n)}{\left[(n/2)(1 - n/2) + \left(\dfrac{\sin(\pi n/2)}{\pi}\right)^2\right]\dfrac{\sin(\pi n/2)}{\pi}}. \tag{20}$$

As expected with increasing $|U|$ the fluctuations for on-site pairing are enhanced, for all electronic densities.

To study superconducting and CDW instabilities for the square lattice one needs to introduce the broken symmetries in the starting ground-state $|\psi_0\rangle$ of the RHS of (3*a*). Such an extension is in progress.

To have an indication about the instability of the paramagnetic state $|\mathrm{SL}\rangle$ towards the superconducting long range order, we have calculated the function (18*b*) for a square lattice. Its Fourier transform $\tilde{S}^s(\boldsymbol{q})$ is largest at $\boldsymbol{q} = 0$. In figure 3 $\tilde{S}^s(\boldsymbol{q})$ is plotted as a function of $|\boldsymbol{q}|$ in the direction defined by the points $(0, 0)$ and $(\pi, 0)$ for various values of U and $n = 0.875$. In figure 4 $\tilde{S}^s(0)$ is plotted as a function of n for various values of U. The fluctuations for on-site Cooper pairing of the paramagnetic state $|\mathrm{SL}\rangle$ increase with increasing $|U|$ for all values of the electronic density. The same result is obtained for the charge fluctuations. On the contrary, the spin fluctuations are reduced with increasing $|U|$. These results are fully consistent with the ones obtained in references [11] and [14] by means of the Gutzwiller function (3*b*) for $U > 0$.

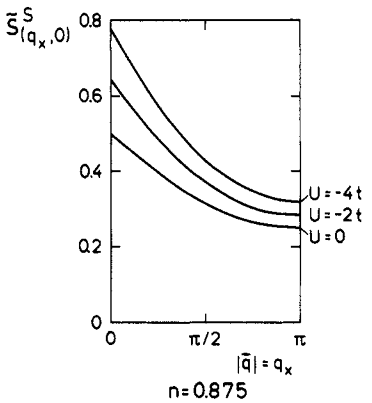

Figure 3. Correlation function $\tilde{S}^s(\boldsymbol{q})$ for a square lattice for $n = 0.875$ and for various values of U as a function of $|\boldsymbol{q}| = q_x$ in the direction defined by the points $[0, 0]$ and $[\pi, 0]$.

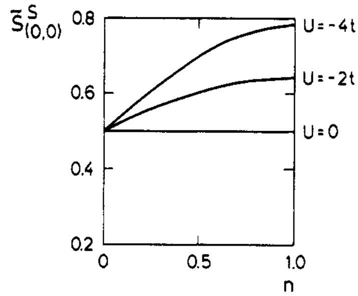

Figure 4. Function $\tilde{S}^s(0)$ for a square lattice as a function of n for various values of U.

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