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GUTZWILLER APPROACH TO THE NEGATIVE-U HUBBARD MODEL

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Abstract

The Gutzwiller approach to the repulsive Hubbard model is extended to the negative-U case. The repulsion-attraction transformation of the Hamiltonian is shown to be valid also for this particular mean field approximation. The physical meaning of the results is discussed.

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The discovery of high temperature superconductivity has renewed the interest in the attractive Hubbard model as many proposals involve the concept of negative-U centers[1]:

$$H = -t \sum_{<ij>\sigma} c^{+}_{i\sigma} c_{j\sigma} - U \sum_{i} n_{i\uparrow} n_{i\downarrow} \qquad (1)$$

where the relevant parameters are U/t and the filling of the corresponding band. This apparently simple Hamiltonian contains analogous difficulties as the repulsive one to be solved. In the weak coupling limit, the normal Hartree Fock approximation yields the usual BCS picture. This result can be inferred from the repulsive case, by means of the repulsion-attraction transformation[2] as has been shown by Mertsching.[3] In the opposite strong coupling limit, the fermions form local singlet pairs which behave as hard core bosons and the physics is quite different.[4] The intermediate regime is still strongly discussed, specially in two dimensions,[5] in connection with the superconducting oxides.

Here we use Gutzwiller variational wave function and combinatorial approximation[6,7,8] to solve Eq.(1), at T = 0. Now due to the on-site attraction, simple occupied sites (instead of doubly occupied as in the repulsive case) are reduced. We verify that the repulsion-attraction transformation[2] works also for this mean field approach and we discuss the physical meaning of the results in this case. We conclude that Gutzwiller's approach can be extended to the attractive case, the minimization of the general expression for the energy, yielding g (Gutzwiller's variational parameter) larger or smaller than one depending on the sign of U.

Let L, $N_\uparrow$, $N_\downarrow$, S, D and E be the number of lattice points, up and down spins, single and doubly occupied and empty sites, respectively; $n_\uparrow = N_\uparrow/L$, $n_\downarrow = N_\downarrow/L$, $s = S/L$, $d = D/L$ and $e = E/L$. The projection operator, reducing by a g factor the amplitude of the S sites is defined as:

$$P_i = 1 - (1-g)(n_{i\uparrow} - n_{i\downarrow})^2 \qquad (2)$$

Then the variational wave function for the correlated state results:

$$|\psi> = \prod_i P_i \; |\psi_o> = g^S |\psi_o> \qquad (3)$$

where $|\psi_o>$ is the ground state of the uncorrelated system (U = 0). Taking into account that L and N are fixed quantities:

$$2D + S = N = N_\uparrow + N_\downarrow \qquad (4.a)$$

$$D + E + S = L \qquad (4.b)$$

the ground state energy E_g, which has to be minimized to determine the variational parameter g, can be written:

$$E_g = \frac{<\psi_o|g^{-2D} \sum_{<ij>\sigma} (-tc^{+}_{i\sigma}c_{j\sigma}) g^{-2D}|\psi_o> + <\psi_o|g^{-2D} \sum_i (-Un_{i\uparrow}n_{i\downarrow}) g^{-2D}|\psi_o>}{<\psi_o|g^{-4D}|\psi_o>} \qquad (5)$$

When the spin-configuration dependence of the norm and of the energy expectation values is neglected (the so called Gutzwiller's approximation), the calculation of E_g is reduced to a combinatorial problem, as shown by Ogawa.[9] In the thermodynamic limit, the sums in Eq. (5) can be approximated by their largest term yielding:

$$Eg/L = \sum_\sigma q_\sigma \; (d, n_\uparrow, n_\downarrow) \; \bar{\varepsilon}_\sigma - U d \qquad (6)$$

with

$$q_\sigma = \frac{\left[\sqrt{(n_\sigma - d)(1 - n_\uparrow - n_\downarrow + d)} + \sqrt{(n_{-\sigma} - d)d}\right]}{n_\sigma (1 - n_{-\sigma})} \qquad (7)$$

where $\bar{\varepsilon}_\sigma$ is the average energy of the σ spins in the uncorrelated system. Eqs.(6) and (7) are the same expressions obtained for the repulsive case, they are then valid for all U.

For the paramagnetic half-filled band case: $n_\uparrow = n_\downarrow = 1/2$, as q_σ (Eq. (7)) is an even function of U, there is also a metal-insulator transition (as first remarked by Brinkman and Rice[10] for the repulsive case) for a finite value of the interaction, $U_c = \pm 8|\bar{\varepsilon}_\sigma|$. For an attraction larger than this critical value, all particles form localized pairs, there is no kinetic energy in this approximation, and the ground state energy for $U < U_c$ is $E_g/L = Ud = -|U|/4$. For $U > -8|\bar{\varepsilon}_\sigma|$, $E_g/L = -|\bar{\varepsilon}_\sigma| \; [1 - (U/8|\bar{\varepsilon}_\sigma|)]^2$.

As in the repulsive case, this approximation certainly exagerates the effect of the correlations, and probably in finite dimension there is not a real transition.[11] However, this critical value indicates a change of behavior: from related but not bound particles to singlet boson pairs. For a semielliptical density of states of half-bandwidth B, this critical value:

$$U_c = \pm 8 \; |\bar{\varepsilon}_\sigma| = \pm 8 \times \frac{2}{3\pi} \left[\frac{B}{2}\right] \qquad (8)$$

is ~ 1.7 times larger than the critical interaction needed in an impurity model to split a localized state.[12]

In the U>0 case alternating lattices must be considered to

study the antiferromagnetism of the model,[9,13] the same procedure must be followed for U < 0 to conclude about charge ordering.

In absence of magnetic field, for band filling $n_\uparrow = n_\downarrow = \frac{1}{2} - \frac{\delta}{2}$, Eq. (7) yields

$$q_\uparrow = q_\downarrow = q = \frac{2(1-\delta-2d)}{(1-\delta^2)} \left[\sqrt{\delta+d} + \sqrt{d} \right]^2 \qquad (9)$$

Fig. 1 shows the results for different δ values, assuming for the uncorrelated kinetic energy the following δ-dependence[8]:

$$\bar{\varepsilon}_\sigma(\delta) = (1-\alpha\delta^2)\bar{\varepsilon}_\sigma \ (\delta = 0) \qquad (10)$$

where α is a constant given by the band-shape. For U>0 the abrupt transition disappears, while for U<0 there are no changes with respect to the $\delta = 0$ case. The number of doubly occupied sites, d, saturates at a smaller value, as there are δ less particles, but there still is a change of behavior, at a critical value slightly modified by δ (the variation is in δ^2, due to the denominator in Eq. (9)).

When a magnetic field is applied to the half filled band case, and the spin occupations become: $n_\uparrow = \frac{1}{2} + \frac{m}{2}$; $n_\downarrow = \frac{1}{2} - \frac{m}{2}$, Eq. (9) reads:

$$q_\uparrow = q_\downarrow = q = \frac{4d}{1-m^2} \left(1-2d + \sqrt{(1-2d)^2-m^2}\right) \qquad (11)$$

Fig. 2 shows the results of the minimization of E_g with this q. In this case, d does not saturate for any negative finite U value, it asymptotically approaches the maximum possible value $n_\downarrow$; while q goes to the asymptotic value 2m.

Figs. 1 and 2 show the symmetry of the results, due to the validity of the repulsion-attraction transformation[2] of the Hamiltonian (1):

$$\begin{cases} c^+_{j\downarrow} = e^{i\pi j} b_{j\downarrow} & c_{j\downarrow} = e^{-i\pi j} b_{j\downarrow} & n'_{j\downarrow} = b^+_{j\downarrow} b_{j\downarrow} \\ c^+_{j\uparrow} = b^+_{j\uparrow} & c_{j\uparrow} = b_{j\uparrow} & n'_{j\uparrow} = b^+_{j\uparrow} b_{j\uparrow} \end{cases} \qquad (12)$$

that allows to obtain relations between Hubbard models with repulsive and attractive electron interactions. (This transformation is useful only if the band structure is conserved, e.g. for alternating lattices with nearest-neighbour interactions). Although these relations are strictly valid only for the exact solutions, they must also hold for reasonable approximate solutions. The projection operator (Eq. 2) transforms for U > 0, like:

$$p'_i = 1-(1-g)(n'_{i\uparrow} - 1 + n'_{i\downarrow})^2 \qquad (13)$$

This expression is equivalent to the projector proposed by Gutzwiller for the repulsive case, $p_i = 1-(1-g)n_{i\uparrow}n_{i\downarrow}$, reducing the amplitude of the doubly occupied sites. We choose expression (13) as it explicitly shows the projection of the empty sites (of the $n_{-\sigma}$ sites in the U < 0 case) implicitly included in Gutzwiller's original work,[6] due to relations (4.a) and (4.b).

The same transformation (Eq. (12)) yields to:

$$\begin{aligned} m' &= n'_\downarrow - n'_\uparrow = 1-n_\downarrow - n_\uparrow = \delta \\ \delta' &= 1-n_\uparrow - n'_\downarrow = n_\downarrow - n_\uparrow = m \qquad \text{when } -U \longrightarrow U \\ d' &= \frac{1-m}{2} - d \end{aligned} \qquad (14)$$

which explain the above results.

Thus, within this approximation, also for U < 0 there is a transition from delocalized to localized states for a finite interaction. If $n_\uparrow = n_\downarrow$ all electrons can be paired and localized when the attraction overcomes a critical value. (The pair hopping, being a t^2/U process, is not considered in this approximation). One added σ electron, as it has no $-\sigma$ electron to pair with, will therefore move very easily in the lattice, which has half of the sites empty. This explains the high sensibility of the system to the magnetization in this case; while it is practically unchanged with the difference δ from half-filling. Fig. 2 shows that when these unpaired electrons are added (i.e. $n_\uparrow \neq n_\downarrow$ due to the presence of a magnetic field) some pairs are broken: the number of doubly occupied sites does not saturate at the maximum value (i.e. the smaller n_σ) as the interaction increases. One can speculate that this result is not an artifact of the approximation but that due to the possibility of processes of first order in t when $n_\uparrow \neq n_\downarrow$, the system gains energy allowing the movement of some spins instead of localizing all possible pairs. (The analogous phenomenon occurs for U > 0, but $\delta \neq 0$, see Fig. 1).

Both, the abrupt transition and this extreme sensibility of the system to the magnetization, are certainly a consequence of Gutzwiller approximation, that neglects all t^2/U processes, exagerating the behavior of the system. The critical value must be taken, more cautiously, as an indication of a change of behavior rather than determining a real metal-insulator transition.

To conclude, we have extended the Gutzwiller approach to the Hubbard model to the case of negative-U. Expressions (6) and (7) can be used for both cases and the variational function proposed by Gutzwiller for the repulsive case:

$$|\psi> = 1 - (1-g)n_{i\uparrow} n_{i\downarrow} |\psi_o>$$

can also be used for U < 0. The parameter g, obtained from the minimization of the energy, will be larger (favouring doubly occupied states) or smaller than one (favouring single occupied states) depending on the sign of U. We have shown that the Gutzwiller approach verifies the repulsion-attraction transformation of the Hubbard Hamiltonian.

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Figure Captions

Fig. 1: Paramagnetic case, $n_\uparrow = n_\downarrow$. Curve a) number of doubly occupied sites, b) reduction of the uncorrelated kinetic energy and c) ground state energy, vs. the interaction in units of the critical value; for different band fillings: —— δ=0, ---δ=0.1, ...δ=0.2.

Fig. 2: Same as Fig. 1 but for the half-filled magnetized case, $m=n_\downarrow-n_\uparrow$; —— m=0, --- m=0.1, ... m=0.2.

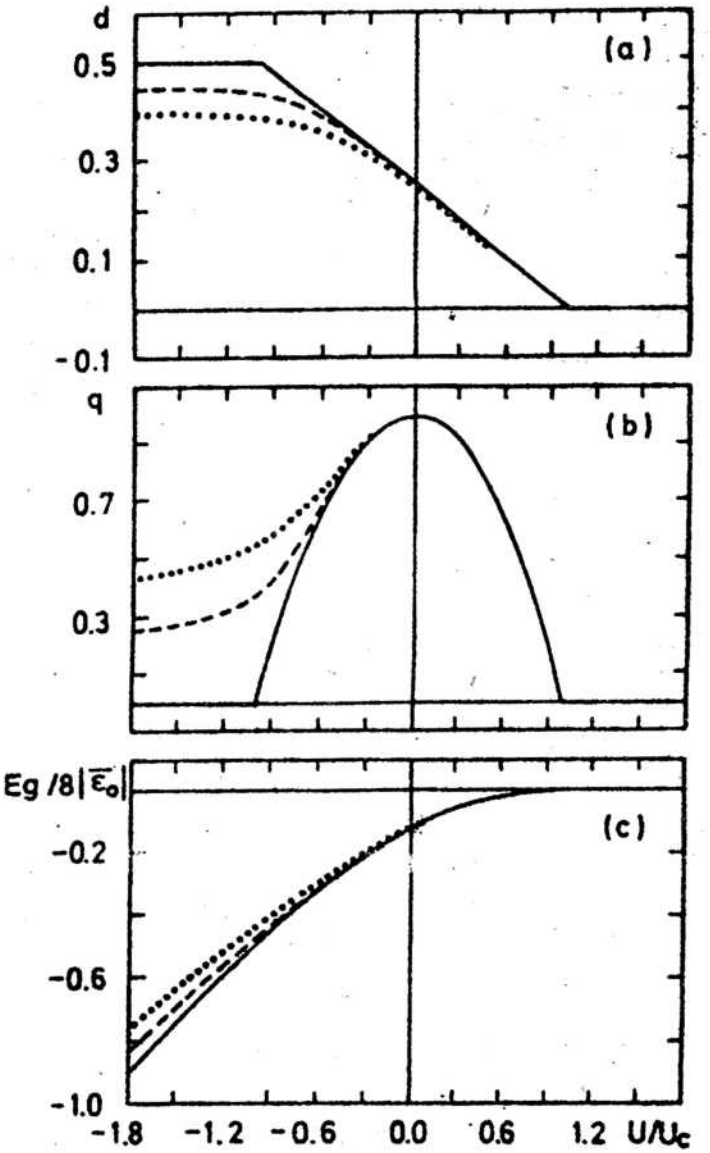

Fig. 2

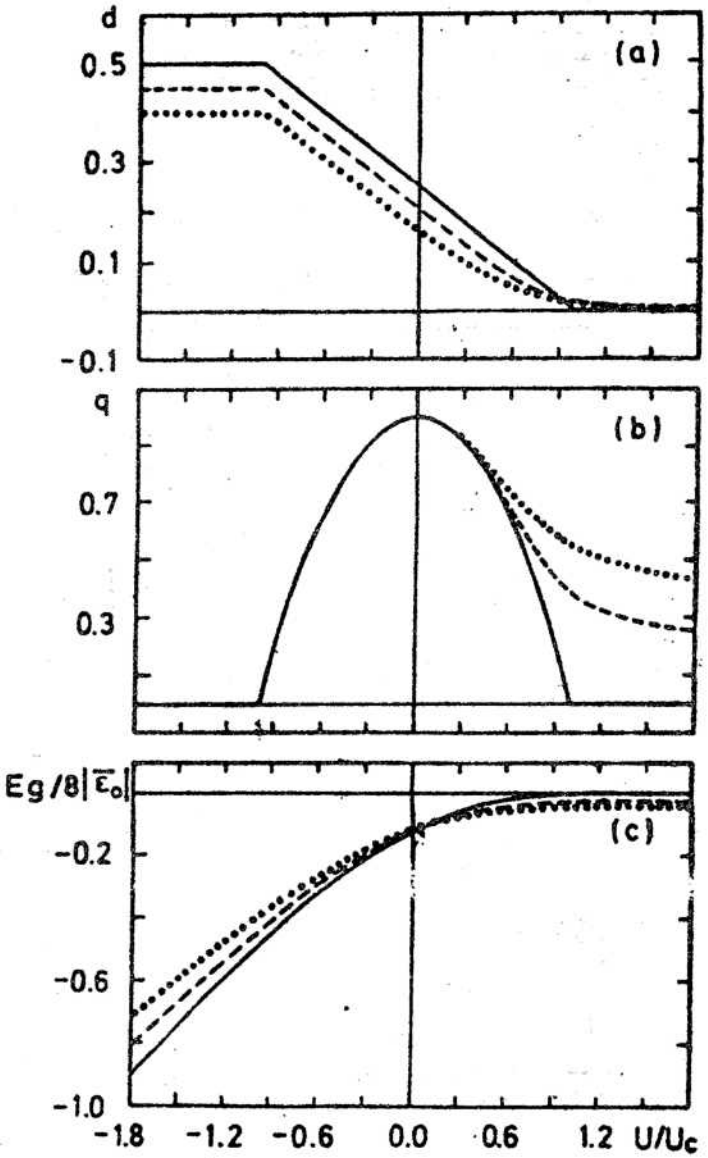

Fig. 1