SOME REMARKS ON THE GUTZWILLER WAVE FUNCTION

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The Gutzwiller variational wave function for the Hubbard model has seen a recent upsurge of interest(1,2,3,4). In this preliminary report, we present some analytical results for the variational energy. In Sec (A) we present the calculation of the energy in the ladder approximation, which is expected be exact for low particle density. Sec (B) contains an approximation equivalent to the Gutzwiller approximation (GA) to the calculation of the expectation value of the Hamiltonian with the help of a density matrix scheme, which appears to be the most streamlined rederivation available, and brings out the local nature of the approximation. In Sec (C) we focus on the 1/2 filled case and examine the possibility of a metal-insulator transition within the wave function. Sec (D) contains a simple exactly solvable model for which both the exact answer, and the variational calculation a la Gutzwiller are possible, and may shed some light on the possible singularities of the energy for the original problem.

A) Low density limit-linked cluster expansion

We wish to calculate the Gutzwiller variational energy for the Hubbard model

$$E_V(\alpha) = \langle\phi|e^{\alpha/2V} H\, e^{\alpha/2V}|\phi\rangle/\langle\phi|e^{\alpha V}|\phi\rangle \tag{1}$$

where $|\phi\rangle$ is the free Fermi wavefunction, and $V = \sum n_{i\uparrow}n_{i\downarrow}$, $H = T + UV$ with $T = \sum \varepsilon_k\, C^+_{k\sigma}C_{k\sigma}$. The linked cluster expansion follows most simply by considering the generating function

$$\exp\{NG(\alpha,\beta,\gamma)\} \equiv \langle\phi|e^{\alpha/2V}e^{\gamma/2V(\beta)}|\phi\rangle/\langle\phi|e^{\alpha/2V}|\phi\rangle \tag{2}$$

with $V(\beta) = e^{\beta T}Ve^{-\beta T}$. The function G is expected to be or order 1 and has a representation in terms of connected diagrams obtained by expanding in powers of γ. It follows that

$$E_V(\alpha) = E_o + \frac{\partial}{\partial\beta} G(\alpha,\beta,\alpha)/\beta{=}0 + 2U \frac{\partial}{\partial\gamma} G(o,o,\gamma)/\gamma{=}2 \qquad (3)$$

One meaningful expansion can be carried out to infinite order in the parameters α and γ, corresponding to particle-particle multiple scattering ladders (this should be exact within the Gutzwiller scheme for a low particle density) and yields with $\bar{f}_k = 1-f_k$, f_k the usual fermi step function, the angular brackets signifying an average over all wave vectors and $S(Q) \equiv \langle \bar{f}_{\frac{Q}{2}+k_\uparrow} \bar{f}_{\frac{Q}{2}-k_\downarrow} \rangle$,

$$E_V^L(\alpha)/N = e_o + \langle (\varepsilon_{k+Q} + \varepsilon_{p-Q} - \varepsilon_k - \varepsilon_p) f_{k_\uparrow} f_{p_\downarrow} \bar{f}_{k+Q_\uparrow} \bar{f}_{r-Q_\downarrow} ((e^{\alpha/2S(k+p)}-1)/ S(k+p))^2 \rangle + U \langle f_{k_\uparrow} f_{p_\downarrow} e^{\alpha S(k+p)} \rangle \qquad (4)$$

The single particle momentum distribution function $\langle\langle n_k \rangle\rangle = \delta E_v/\delta\varepsilon_k$ can be also worked out from (4). We may note that this scheme breaks down for increasing particle density – at half-filling the energy should be zero for $U \to \infty$, $\alpha \to -\infty$ but overshoots somewhat, and also the Migdal discontunity in $\langle\langle n_k \rangle\rangle$ exceeds unity. For low density, however, this scheme is appealing since it is presumably exact, and also exhibits a sensitivity to the band structure.

(B) The Gutzwiller approximation using a density matrix

In this section we present what appears to be the most concise "derivation" of the Gutzwiller approximation (GA) to the problem of evaluating $E_v(\alpha)$ (1), in the hope that the nature of the approximation would be clarified. Consider the variational density matrix $\rho_G = \rho_o\, e^{\alpha/2V} e^{-\beta T} e^{\alpha/2V}$ with $\rho_o = \exp \beta \sum_{i\sigma} \mu_\sigma n_{i\sigma}$. By virtue of the Peierls-Feynman argument, the expectation value $\mathrm{tr}\rho_G H/\mathrm{tr}\rho_G$, in the limit $\beta \to \infty$ tends to E_v, which is an upper bound to the true energy. The GA for the potential energy, or equivalently $d_i \equiv n_{i_\uparrow} n_{i_\downarrow}$, is obtained by considering $d = \mathrm{tr}(\rho_o e^{\alpha V} e^{-\beta T} d)/\mathrm{tr}(\rho_o e^{\alpha V} e^{-\beta T})$, expanding $e^{-\beta T}$ formally as a power series in β, and retaining the first nonzero term in the numerator and denominator. For d, it is sufficient to set $e^{-\beta T} \sim 1$, which gives the approximation a highly local character (since propagation arises through T!). We find $d = x_\uparrow x_\downarrow e^\alpha/\mathcal{D}$, $\rho_\uparrow = (x_\uparrow + x_\uparrow x_\downarrow e^\alpha)/\mathcal{D}$ where $\rho_\uparrow = N_\uparrow/N$ and $x_\sigma = \exp\beta\mu_\sigma$ and $\mathcal{D} = 1 + x_\uparrow + x_\downarrow + x_\uparrow x_\downarrow e^\alpha$. The two unknowns $x_\uparrow$ and $x_\downarrow$ can be eliminated in favour of $\rho_\uparrow$ and $\rho_\downarrow$ and this leads to the famous relation $e^\alpha = d(1-\rho+d)/(\rho_\uparrow-d)(\rho_\downarrow-d)$. In the paramagnetic 1/2 filled case we find $d = \frac{1}{4}[1+\tanh(\alpha/4)]$. In order to calculate the kinetic energy, we need for i neighbour of j, $\langle\langle C^+_{i_\uparrow} C_{j_\downarrow} \rangle\rangle$ $\mathrm{tr}(\rho_a C^+_{i_\uparrow} C_{j_\uparrow})/\mathrm{tr}\,\rho_G$. For this quantity the numerator requires a single hop from T whereas the denominator does not, and hence a sensible approximation can be made by forming the ratio $q_\uparrow = \langle\langle C^+_{i_\uparrow} C_{j_\downarrow} \rangle\rangle / [\mathrm{tr}(\rho_o e^{-\beta T} C^+_{i_\uparrow} C_{j_\uparrow})/\mathrm{tr}\rho_o e^{-\beta T}]$.

Within the same spirit we can expand $e^{-\beta T}$ in both numerator and denominator and a straightforward calculation gives $q_\uparrow = \frac{1}{\rho_\uparrow(1-\rho_\uparrow)} x_\uparrow[1+2x_\downarrow e^{\alpha/2}+x_\downarrow^2 e^\alpha]/D^2$, which is the usual answer. For 1/2 filling we find $q = \mathrm{Sech}^2(\alpha/4)$. Note that $d-1/4$ is an odd function of α within this scheme, which is actually a reflection of the symmetry of the system (p-h conjugation of one species), and is difficult to preserve in a perturbative expansion in α as in sec. A.

C. 1/2-filled large U limit

Within the GA, Brinkman and Rice noted(2) that a metal insulator transition follows for $U > U_c$, with the minimizing value of α tending to $-\infty$. This happens because both the potential energy (Ud) and kinetic energy ($= qe_o$) behave as $e^{-|\alpha|/2}$ as $\alpha \to -\infty$ (see above). This transition is characterized by d vanishing for $U > U_c$. This vanishing of d is not borne out by the recent finite chain or Monte Carlo simulations(3,4) and has been argued to be unreasonable within the Gutzwiller wave function(3). The crux of the argument is that the Gutzwiller wave function $e^{-|\alpha|/2}|\phi>$ can be expanded in the complete set of eigenfunctions of $\bar{V}$ (which has a trivial spectrum 0,1,2,...) in the form $|\chi_0> + e^{-|\alpha|/2}|\chi_1> + \ldots$. Here $|\chi_0> = \sum_\nu |<\nu|\phi>|^2|\nu>$ and $|\chi_1> = \sum_\mu |<\mu|\phi>|^2|\mu>$, with $|\nu>$ as a basis in the manifold of 2^N singly occupied states, and $|\mu>$ in the manifold of $2^{N-2}\ NC_2$ states. It is expected than that $d \sim e^{-|\alpha|}$ and $<<K.E.>> \sim e^{-|\alpha|/2}$ (since the latter connects $|\chi_0>$ and $|\chi_1>$). This argument is, however, not totally convincing in view of the large number of states in the manifold of states with d=1 relative to d=0. The key question is whether or not there is some correlation within the Fermi wave function between a doubly occupied site and a partner hole. (The GA sets all determinants as unity thereby making the weight of $|\chi_1>$ as $O(N^2)$ relative to $|\chi_0>$ thereby leading to $d \sim e^{-|\alpha|/2}$). The following simple calculation sheds some light on this issue. Consider a configuration of down spins frozen on one sublattice of the s.c. lattice and allow the up spins to be mobile. The Fermi wave function is written for up spin fermions and a straightforward calcula ion of d can be performed yielding $d = \frac{1}{4}(1 + \mathrm{th}(\alpha/2))$. (Similarly if we carry out an annealed average over down spins, the same expression for d results). This supports the expectation that the correct asymptotic form of d should be $\sim e^{-|\alpha|}$, as suggested by the simple argument, thereby ruling out the vanishing of d for any U. In fact it seems most likely that the Gutzwiller wave function describes a metallic state, for any value of U, other than $U = \infty$.

As an amusing extension of this argument, consider the variational wave function $|\psi> = \exp[\frac{\alpha}{2}\sum_i (n_{i\uparrow}\nu_i + n_{i\downarrow}(1-\nu_i))]|\phi>$, where $\nu_i = (1 + \exp i(Q.r_i))/2$, with Q as the AFM ordering wave vector $\pi/2(1,1,1)$ for the s.c. lattice. For large α, the prefactor pushes the up and down electrons to different sublattices thereby reducing double occupation. The variational calculation can be performed exactly and we find $e_v = -|e_o|/\mathrm{ch}(\alpha/2) + U/(4\mathrm{ch}^2(\alpha/2))$ leading to a metal to antiferromagnetic insulator transition for $U > U_c$. There exists a gap in the excitation spectrum for adding an extra particle. However, the momentum space distribution $\langle\langle C_k^+ C_k \rangle\rangle$ for the original k's, continues to show a Migdal jump ($Z_k = \mathrm{sech}(\alpha/2)$) and the signal of the transition is only found by examining the behaviour of $\partial d/\partial U$, which has a jump discontinuity at U_c.

D. A solvable mean field model

We present here a simplified version of the Hubbard model on a s.c. lattice which breaks rotation and translation invariance, for which (at half filling) the exact answer and a Gutzwiller like variational calculation can both be performed analytically. Consider $H = T + \frac{U}{N} \rho_{Q_\uparrow} \rho_{Q_\downarrow}$ where Q = AFM ordering vector and ρ_Q in the usual charge density operator (summing over Q would give the Hubbard model). The exact solution proceeds by writing H in terms of particle and hole operators, followed by utilizing the Schwinger coupled fermion representation of spins, to write $H = \sum_k |\varepsilon_k| [\sigma_k^z + \tau_k^z] - U/N \sum_k \sigma_k^x \sum_k \tau_k^x + U/N$, where the summation extends over half the zone. This problem is familiar from Anderson's treatment of the BCS Hamiltonian, and the solution corresponds to an antiferromagnetic insulator for all non zero values of U. Consider now a Gutzwiller like wave function $|\psi_v\rangle = \exp((\alpha/N) \rho_{Q_\uparrow} \rho_{Q_\downarrow})|\phi\rangle$. The variational calculation can be performed exactly and turns out to be rather non trivial. We find that $\langle\langle K.E.\rangle\rangle = e_o \, \mathrm{sech}(\alpha/2 \tanh(\alpha y_o/2))$ and $\langle\langle P.E.\rangle\rangle = U/4(1 + y_o \tanh(\alpha y_o/2))$, where $y_o = \tanh(\alpha/2 \tanh(\alpha y_o/2))$. The solution exhibits a metal insulator transition for $U = U_c$, which is again characterized by a jump discontinuity in $\partial(P.E.)/\partial U$. Note that y_o is non vanishing only for $|\alpha| > 2$, and the nontrivial insulating phase cannot be reached from the metallic one by "perturbation theory" in α.

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