Gutzwiller wave function under magnetic field

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Abstract
Magnetization process of the Gutzwiller wave function is studied accurately by a variational Monte Carlo method. We apply it to the one-dimensional (1D) and 2D Hubbard models (HM), and to the 1D periodic Anderson model (PAM) without orbital degeneracy. For the HM, magnetization varies discontinuously to the full moment, as the magnetic field increases. For the PAM, the paramagnetic state is unstable against ferromagnetism, although the energy reduction thereof is small.

keywords
magnetization process, Gutzwiller wave function, Hubbard model, periodic Anderson model

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Recent experiments under strong magnetic field have renewed the interests for heavy-electron systems, such as metamagnetic transitions accompanied by variations of the Fermi surface and the gap vanishing in the Kondo insulators. In this paper, with these in mind, we study properties of the Gutzwiller wave function (GWF)\cite{1} under magnetic field, in particular magnetization process, applying it to the Hubbard model (HM) and the periodic Anderson model (PAM).

The GWF with magnetization $m$ is written as

$$|\Psi_\xi(m)\rangle = \mathcal{P}^\ell(\xi)|\Phi_F(m)\rangle,$$

(1)

where $|\Phi_F(m)\rangle$ is a spin polarized one-body function with $m = (N^\uparrow - N^\downarrow)/N_a$ ($N_\sigma$ and $N_a$ being the numbers of spin $\sigma$ and site, respectively), and $\mathcal{P}^\ell(\xi) = \prod_i \left[1 - (1 - \xi)n_i^\uparrow n_i^\downarrow\right]$, $\ell$ being the orbital index, and $\xi$ a variational parameter which adjusts double occupancy of electrons. Although the GWF is a primary many-body wave function, most variational works so far have resorted to the so-called Gutzwiller approximation (GA)\cite{1, 2, 3, 4} in estimating variational expectation values. Here we use a variational Monte Carlo (VMC) method for exact evaluation, which tells us how to improve the trial wave function.

First, we discuss the single-band HM,

$$\mathcal{H} = -t \sum_{<i,j>,\sigma} \left( c_i^\dagger_{\sigma} c_{j\sigma} + c_j^\dagger_{\sigma} c_{i\sigma} \right) + U \sum_i n_i^\uparrow n_i^\downarrow. $$

(2)

We concentrate on the half-filled band: $n = (N^\uparrow + N^\downarrow)/N_a = 1$, where the magnetic-field effect is the most dominant. The energy due to the applied field $H$ is given by a Zeeman term: $\mathcal{H}_{\text{ext}} = -g\mu_B H \sum_i S_i^z$. For this model, $\Phi_F(m)$ in Eq. (1) becomes a simple Fermi sea, $|\Phi_F(m)\rangle = \prod_\sigma \prod_{k,\xi} c^\dagger_{k\sigma} |0\rangle$, and the effect of magnetic field appears only in magnetization. To obtain a magnetization curve, first, we minimize the energy expectation values for zero field, $E_0(m)$, with respect to the variational parameters ($\xi$ in this case) for each $m$ by VMC calculations. Then, we find the relation between $m$ and $H^*$ by determining $m$ which minimizes $E_{\text{tot}}(H^*, m) = E_0(m) - H^* m$ for a given value of $H^* = g\mu_B H/2$.

Figure 1 shows the magnetization curves in one dimension (1D) thus obtained for some values of $U/t$ with those of two other methods. Under a weak field, these three results agree well. However, at some critical field $H^*_c$, $m$ of the GWF (and the GA) saturates discontinuously in contrast to the exact one. The jump of $m$ becomes large as $U/t$ increases. The origin of this
discontinuity is negative $\partial^2 E_0(m)/\partial m^2$ for $m \sim 1$, which makes $E_{\text{tot}}$ have double minima for $H^* \sim H_c^*$. A similar feature can be seen for large values of $U/t \ (\gtrsim 5)$ in 2D, as shown in Fig. 2. For small $U/t$, however, $m$ increases smoothly. This behavior of $m$ resembles that of the GA[2] except for the existence of the metal-insulator (Brinkman-Rice) transition at $U = U_c$. If one uses half ellipse as the density of state, the discontinuity occurs for $U/U_c > 0.44$.[4]

In addition to the 1D exact result,[3] quantum Monte Carlo calculations in infinite dimension[6] concluded no discontinuity in the magnetization curve. We consider that this discrepancy is attributed to the onsite nature of the correlation factor in the GWF; an intersite correlation factor, spin dependent in this case, will encourage the electron transfer, which becomes more important as $m$ increases.

Incidentally, for the 1D $t$-$J$ model the GWF does not have a jump in the magnetization curve for any value of $J/t$ and well reproduces the exact magnetic properties for the half filling or the supersymmetric case.[7] This is because the intersite correlation effect is introduced through the canonical transformation from the HM to the $t$-$J$ model.[8]

Having restricted $n$ to the half filling, we have confirmed that the tendency mentioned here holds also for $n < 1$.

Next, we consider the 1D periodic Anderson model without f-level degeneracy,

$$
\mathcal{H} = \sum_{k\sigma} \varepsilon_k c_{k\sigma}^\dagger c_{k\sigma} - \sum_{k\sigma} V_k \left( c_{k\sigma}^\dagger f_{k\sigma} + f_{k\sigma}^\dagger c_{k\sigma} \right) + \sum_{k\sigma} \varepsilon_f f_{k\sigma}^\dagger f_{k\sigma} + U \sum_j n_{j\uparrow} n_{j\downarrow}. \tag{3}
$$

For simplicity, we put $\varepsilon_k = -2t \cos k$, $\varepsilon_f$ and $V_k (\equiv V)$ constant, and fix two parameters at typical and convenient values: $V/t = 0.5$ and $U/t = \infty$. Furthermore, as for the Zeeman term we assume $g_c = g_t$.

For this Hamiltonian, we consider the Gutzwiller-projected hybridized band state: Eq. (1) with $\mathcal{P}^f(0)$ and

$$
|\Phi_F(m)\rangle = \prod_{\sigma} \prod_{k \leq \varepsilon_k} \left[ \cos \phi_k c_{k\sigma}^\dagger + \sin \phi_k f_{k\sigma}^\dagger \right] |0\rangle, \tag{4}
$$

where we choose $\phi_k$ as a spin-independent noninteracting form:

$$
\tan \phi_k = \frac{2\tilde{V}}{\varepsilon_f - \varepsilon_k \pm \sqrt{(\varepsilon_f - \varepsilon_k)^2 + 4\tilde{V}^2}} \tag{5}
$$
for the upper (−) and lower (+) bands, respectively. ˜εf and ˜V are variational parameters, which adjust the band form. This wave function is an extension of Yosida’s singlet state for the Kondo problem, and has been extensively studied for the cases without magnetic field.

In Fig. 3 the energy expectation values without field are depicted. We have calculated for metallic (n = 1.6) as well as insulating (n = 2.0) cases. In each case, E0(m)/t varies slightly for small m and then increases abruptly with increasing m. This aspect is similar to the exact-diagonalization results. Meanwhile, the optimized state has finite spin polarization, as well as ∂E0(m)/∂m|m=0 > 0 and ∂2E0(m)/∂m2|m=0 < 0. Also for a finite U (U, V, Ef = 1.0t, 0.5t, −1.0t), we have confirmed that the above derivatives have the same signs with those for infinite U; namely the GWF is unstable against a magnetic order. These aspects agree with the Gutzwiller approximations, but does not with an exact analysis for the symmetric case and a study in infinite dimension, where the ground state is paramagnetic. From these facts we observe that the ground state of the 1D nondegenerate PAM, either paramagnetic or partially ferromagnetic, is rather fragile; actually the energy differences in Fig. 3 are the order of 0.01t. Stable paramagnetism may need f-level degeneracy.

Magnetization curves obtained from Fig. 3 are shown in Fig. 4. There is no sign of metamagnetism. It also remains a future problem how the gap for the insulating case changes as a function of various parameters.

In conclusion, although the VMC results support the GA qualitatively, improvements of the trial function are needed for advanced discussions. To this end, introduction of a spin-dependent one-body part as well as of an intersite (RKKY-like) or off-diagonal correlation factors is important.

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Figure captions

Fig. 1 Magnetization as a function of magnetic field for the 1D Hubbard model. The results of the GWF are shown with those of the GA and the Bethe Ansatz (Exact) for $U/t = 3$. The system used for the GWF has 90 sites with closed-shell condition. For the GA the 1D cosine band is assumed.

Fig. 2 Magnetization as a function of magnetic field of the Hubbard model for the 2D square lattice by the GWF. We use systems of $L \times L$ ($L = 10, 12, 14$) sites with the antiperiodic-antiperiodic boundary condition and closed shell condition.

Fig. 3 Energy expectation values without magnetic field as a function of magnetization for 1D periodic Anderson model. Minimal values for $E_f/t = -1.0$ are plotted by dotted lines as a guide. The system of $N_a = 50$ is used with closed shell condition.

Fig. 4 Magnetization as a function of magnetic field of the 1D periodic Anderson model for some parameter values. For comparison, the data for $U/t = 0, V/t = 0.5$ and $E_f/t = -1.0$ are plotted by dash-dotted lines.