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A Study on Variational Monte Carlo of Attractive Hubbard Model

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Abstract

The analysis of the Hubbard model with the wave function of Gutzwiller is proposed to include a variational Monte-Carlo system that combines variational theory with Monte-Carlo method. One, two and three-dimensional models of sites of up to 216 (6×6×6) are applied and arbitrary U/t values (site U and hopping integral t) are applied. In order to accurately measure the expectation values for many multi-body wavefunctions, a series of variational calculations with Monte Carlo better statistics were carried out. Simulations of Quantum Monte Carlo (QMC) are a powerful way of obtaining knowledge on quantum mechanical systems with strong interactions. In this paper, we start by presenting the model of Hubbard and the quantum simulation of Monte Carlo. The Hubbard model is a simple and efficient model that effectively captures several qualitative elements of materials, including metal transition monoxides and superconductors with high temperatures.

Keywords: Monte Carlo, Hubbard Model, Gutzwiller wave function**.**

Introduction:

Knowledge regarding the attractive Hubbard model (AHM) is important particularly with respect to the following points, in order to consider pseudogap phenomena found in cuprate superconductors. I AHM is subject to a crossover in the superconductor process from a BCS to a Bose condensation form as the intensity of the connection increases. ii) It is reasonably straightforward to perform controllable and quantitative calculations. iii) The AHM on standard two-party lattices is connected to the repulsive Hubbard (RHM) — a two-dimensional plausible high-Tc cuprates model (2D) — by a canonic transformation. I and the pseudo-gap are understandable, since an s-wave supraconducting phase prevails in the entire ground phase AHM diagram in higher lattice dimensions, the normal state properties should be studied at low temperature.

It is not easy to research a regular state of T < Tc for QMC methods. Furthermore, reliability worsens, as the frequency of the correlation increases beyond the bandwidth and the device size increases, 10). The above results must therefore be corroborated by complementary methods.

This paper is intended to analyze AHM's normal state properties using a variational Monte Carlo (VMC) method on 2D systems directly. The importance of the VMC method is its application to every intensity of correlation and every electron density, various test wave functions for many bodies and enough grids to verify dependency of systems[1-3].

Model and method:

1. Attractive Hubbard model:

In this paper we study a couple of basic wave functions as normal states of the attractive Hubbard model ($U \leq 0$):

$$\mathcal{H} = \mathcal{H}_t + \mathcal{H}_U = -t \sum_{\langle i,j\rangle\sigma} \left(c^{\dagger}_{i\sigma} c_{j,\sigma} + c^{\dagger}_{j\sigma} c_{i,\sigma} \right) + U \sum_{j} n_{j\uparrow} n_{j\downarrow}, \qquad \text{.....(1)}$$

where $n_{j\sigma} = c^{\dagger}_{j\sigma} c_{j\sigma}$, and the remaining notation is standard. We use t as the unit of energy. In this paper, only bipartite lattices are considered, and the sum of the transfer in Eq. (2·1) is restricted to nearest-neighbor pairs. We focus on a 2D square gate, except in Annex A, which has a significant factor in dependence on the gate dimension. Because of the electron hole symmetry, electron density n (= Ne/N) is confined to n <=1, with Ne and N respectively the electrode numbers and locations. We exclude an outside area here, and thus $N_{\uparrow} = N_{\downarrow} = N_e/2$,

where N_σ is the number of σ-spin electrons. A chemical potential term $\zeta_{j\sigma} n_{j\sigma}$ may be added to adjust the electron density, if necessary.

2. Variational Monte Carlomethod:

A variational Monte Carlo(VMC) variation method is used. [4] However, due to the rapid progress made in computer technology in the last 10 years, the precision of the calculations provided in this paper has been greatly improved. In this paper we consider mainly a 2D

square grid with $N = L \times L$ oscillating sites and consider a 3D simple cubic grid containing $N = L \times L \times L$ in Appendix A for GWF spatial dependence only.To discuss the thermodynamic limit, we carefully check the system-size dependence with systems up to $N = 2 \times N_e = 28 \times 28 = 784$ and $N = N_e = 24 \times 24 = 576$ for 2D and $N = N_e = 10 \times 10 \times 10 = 1000$ for 3D.

All sys-tems we studied with square grid were subject to periodic (P)-Anti-periodic(A) limit conditions. This way, the closed shell structure of systems with arbitrary even values of L for $n = 1$ can be treated. This allows us to monitor system dependency

3. Gutzwiller wavefunction:

As a trial wave function for normal phases of AHM, the celebrated GWF, [5]

$$\Psi_{\mathrm{G}} = \mathcal{P}_{\mathrm{G}}(g)\Phi_{\mathrm{F}} = \prod_j \left[1 - (1-g)n_{j\uparrow}n_{j\downarrow}\right]\Phi_{\mathrm{F}} = \exp\left(\alpha \sum_j n_{j\uparrow}n_{j\downarrow}\right)\Phi_{\mathrm{F}}, \quad \text{..... (2)}$$

Because of its simplicity, it is another useful starting point.In Eq. (2), g or α (= ln g) is the sole variational parameter, which controls the ratio of doubly occupied sites d, and Φ_{F} is the Fermi sea. For AHM, the range of g will be 1 g to enhance d, whereas that for RHM is 0 g 1 to suppress d. The two limiting cases, $g = 0$ and $g =$, Coincide with isolating countries without double occupied sites and without individually occupied sites. The former state is used for the t-J model 18) and is the exact ground condition, particularly for the 1D supersymmetric model with $1/r^2$relation. [19]For$g$=1,GWFisReduced to the case without interaction,Φ_{F}.

To this time, GWF has been extensively studied with RHM to treat itinerant magnetism, the Mott transition, ^{3}He, gravitational waves, etc. Because of the di ﬃculty in measuring the assumption variables with GWF, they had been calculated using a mean-field-type approximation [the Gutzwiller approximation (GA)] after its in- troduction by Gutzwiller itself. [20]

$$|\Psi_G\rangle = g^{\hat{D}} |\mathrm{FG}\rangle \quad \text{.....(3)}$$

$$= \prod_{\boldsymbol{R}_i} [1 - (1 - g)\hat{D}_i] \, |\mathrm{FG}\rangle \, ,$$ ……..**(4)**

whereg^D,with0≤g≤1,isthecorrelationoperatorand|FG)isthegroundstateofthenon- interacting Fermi gas. The correlation operator thus decreases the spin configuration amplitude in |FG) worldwide, with so many places that have double occupied. The g = 1 is the non-interacting case, whereas $g \to 0$ is the $U \to \infty$. the non-interacting cases. In truth, you find for $g \to 0$.

$$g^{\hat{D}}\Big|_{g=0} = \prod_{\boldsymbol{R}_i} [1 - \hat{D}_i] \equiv \hat{P}_G \, .$$ ……..**(5)**

The $\hat{P}_{\boldsymbol{tt}}$ projection operator removes all double occupied site configurations (Projection by Gutzwiller). For the Gutzwiller wave function, the ground state energy is then given

$$E_{\mathrm{G}} = \langle \hat{H} \rangle_G \equiv \frac{\langle \Psi_G | \hat{H} | \Psi_G \rangle}{\langle \Psi_G | \Psi_G \rangle} \, .$$ …….(6)

By replacing |FG), one can also define states with a broken symmetry with a more general starting function; for example, the antiferromagnetic Hartree-Fock wave function (spin wave).

$$|\mathrm{SDW}\rangle = \prod_{\boldsymbol{k},\sigma} [u_{\boldsymbol{k}} \hat{a}^{\dagger}_{\boldsymbol{k}\sigma} + \sigma v_{\boldsymbol{k}} \hat{a}^{\dagger}_{\boldsymbol{k}+\boldsymbol{Q},\sigma}] \, |0\rangle \, ,$$ …….(7)

Where $\boldsymbol{Q}$ is the vacuum and the BCS wave function[6] and where Q is a half reciprocal lattice vector and |0.

$$|\mathrm{BCS}\rangle = \prod_{\boldsymbol{k}} [u_{\boldsymbol{k}} + v_{\boldsymbol{k}} \hat{a}^{\dagger}_{\boldsymbol{k}\uparrow} \hat{a}^{\dagger}_{-\boldsymbol{k}\downarrow}] \, |0\rangle \, ,$$ ……..(8)

This results in a resonant valence bond state (RVB) after projection [7].

Conclusion:

A significant quantitative shift is occurring around an interaction force $U = U_{co}$, much larger than the band width, with the Gutzwiller wave feature. In the region of $U > U_{co}$, the association between the on-site pairing is growing and the effective electrons mass is increasing. However, a transparent surface of Fermi is on both sides of U_{co} and an arousal distance does not exist. Therefore, the shift in GWF is a metal-to-metal overlay, and it is different from the metal-insulator transition between Brinkman and Rice as the U_{co} value is the same as that of U_{BR}.

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