行政院國家科學委員會補助專題研究計畫

成果報告

在磁場中哈巴特模型之非傳統自洽場微擾理論研究

Investigation of Hubbard Models in Magnetic Fields With Use of Untraditional Self-Consistent Field Perturbation Theory

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一、摘要

本計劃中預定之各項研究已全部完成。

我們用解析及數值方法研究了哈巴特模型中強關連電子系統的電子能帶結構及基態物理性質。相互作用強度 U、電子濃度 n 及磁場 h 為任意（$0 \le U < \infty$, $0 \le n \le 1$, $h/t \ge 0$）。傳統的微擾理論是把無交互作用(理想電子) 哈密頓量作為零級近似，僅適合於 $U/t << 1$ 情形。我們發展了一種非傳統的微擾理論：把廣義自洽場 （GSCF）哈密頓量 H_{GSCF} 作為零級近似，而精確哈密頓量 H_{exact} 與 H_{GSCF} 之差作為微擾。這種非傳統微擾理論在 $U/t \to 0$ 及 $U/t \to \infty$ 時 (磁場 $h \ge 0$ 及電子濃度 $0 \le n \le 1$ 為任意) 都給出精確結果，而在二者之間比傳統微擾理論及廣義自洽場都更靠近精確結果，是一種相當不錯的內推方法。

本計劃研究成果發表於國際學術期刊 [9-11]，並在國內及國際學術會議上宣讀 [5-8]，[12]。

關鍵詞：哈巴特模型、微擾理論、廣義自洽場近似、電子關聯

Abstract

The accurate analytical and numerical calculations of the electronic band structure and ground state properties of strongly correlated electrons within the Hubbard model are performed for general interaction strength U/t, magnetic field h ($h/t \ge 0$) and electron concentration n. We test the developed untraditional perturbation approach about generalized self-consistent field (GSCF) solution in the extreme conditions of one dimensionality for entire parameter space of $0 \le U < \infty$ and $0 \le n \le 1$. The developed many-body perturbation formalism up two second order about GSCF Hamiltonian differs significantly from the standard perturbation theory by incorporating systematically the effect of the random-phase-type perturbation techniques and controlled expansion of the energy functional for general U/t and n. The second order perturbation correction vanishes at small and large U/t limit and performed calculations of the ground state energy show a next to the perfect numerical agreement with the Bethe-ansatz results.

Our results are published in [9-11] and reported at [5-8], [12].

Key words: Hubbard model, perturbation theory; generalized self-consistent field approach, correlated electrons

二、主要成果

The analytical theory for the interacting electron gas was first developed by Gell-Mann and Bruckner, now known as random phase approximation (RPA), gives the exact values for the correlation energy in the high density-weak coupling regime. However, this method runs into difficulties due to the insufficient treatment of fluctuations. Starting from the weak coupling regime Schrieffer, Wen and Zhang examined the fluctuations around the SDW mean field solution for repulsive Hubbard model using the RPA. This fact gave a rise the hope that the RPA fluctuations might be able to interpolate between the large and small coupling limits. However, the low-energy physics is still not properly treated within the traditional mean field with corresponding RPA extensions.

We study the dynamic many body effects of strongly correlated electrons in the periodic lattices by including the effect of fluctuations around the GSCF solution. It is a combination of the self-consistent approach with systematic use of the effect of the random-phase-type perturbation techniques applied in entire space of electron concentration, magnetic field and U/t for calculation of the ground state properties by comparison with the rigorous results in one and in two dimensions.[1-4],[11]

We initially test the developed perturbational approach up to the second order around so called linearized generalized self-consistent field (GSCF) theory for the repulsive Hubbard model and numerical results in one dimension (1d) are compared with the Bethe-ansatz solution. At large limit U/t the result of second order perturbation converges to the GSCF solutions and in small and intermediate U/t range our approximation gives rather good agreement with the Bethe-ansatz result.

The GSCF theory for attractive and repulsive interaction has been successfully used in calculating of the ground state properties and electronic structure of many body systems.

The GSCF ground state at arbitrary wave vector q ($0 \le q < \pi$) for the spin order parameter (antiferromagnetism corresponds $q = \pi$) and $U>0$ is [11]

$$|0_{\mathrm{GSCF}}\rangle = \prod_{k} \alpha^{+}_{kq\lambda} |0\rangle ,$$

where $\alpha^{+}_{kq\lambda}$ is the qusi-particle operator, k is inside the Fermi-region (``Fermi-sea''), the quasi-particle energy spectrum is determined by

$$\mathcal{E}^{(+)}_{k\lambda}(q) = \frac{\epsilon_k + \epsilon_{k+q} + nU - \lambda\sqrt{(\epsilon_k - \epsilon_{k+q} - 2Us - h)^2 + \left(\Delta^{(+)}_q\right)^2}}{2},$$

λ=1 ↑or -1 ↓ with transverse ($\Delta^{(+)}_q$) and longitudinal (s) spin order parameters and the chemical potential $\mu^{(+)}$. The eigenvalue of the GSCF Hamiltonian in the ground state is

$$E^{(+)(0)}_{\mathrm{GSCF}} = \frac{1}{N_{\mathrm{latt}}} \sum_{k,\lambda} \mathcal{E}^{(+)}_{k\lambda}(\mathbf{q}) n^{(+)(0)}_{kq\lambda} + \frac{(\Delta^{(+)}_q)^2}{4U} - \frac{n^2 U}{4} + s^2 U,$$

where $n^{(+)(0)}_{kq\lambda}$ means occupation numbers of quasi-particle states. The GSCF eigenvalue provides for energy a simple interpolation scheme between the weak and strong interaction in entire range of U/t, h and all $0 \le n \le 1$. The GSCF and exact results coincide in extreme limits of weak and strong interaction. However, instead of a common belief that the mean field approximation is a valid starting point at weak interaction limit, the GSCF numerical results clearly demonstrate qualitative discrepancy for all $n \le 1$ in prediction of behavior for double occupancy $D^{(+)}$ and kinetic energy E_{kin} at $U/t \ll 1$. The exact and the GSCF limiting values of $D^{(+)}$ are the same, although the GSCF result barely changes at weak interaction $|U|/t \ll 1$, while the exact result gives a linear dependence. The GSCF theory also fails in description of the chemical potential $\mu^{(+)}$ at intermediate and strong interaction limit, especially at n=1. In fact the GSCF solution for $\mu^{(+)}$ *versus* n unstable and has a tendency toward the phase separation, while the exact $\mu^{(+)}$ is everywhere monotonous function on n.

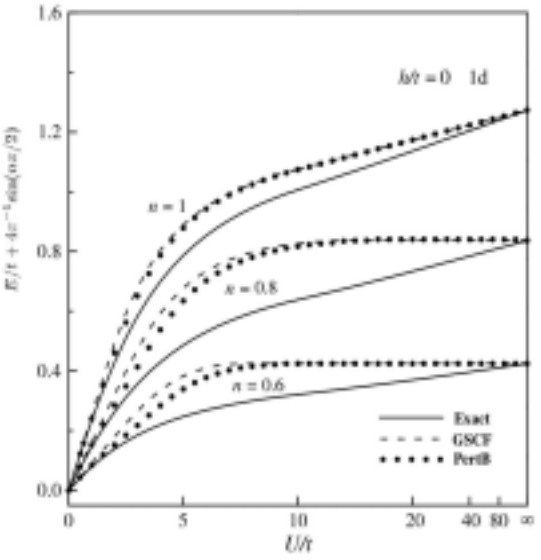

Fig. 1. The ground state energy $E^{(+)}/t$ as a function of U/t for various n in the Bethe-ansatz solution (solid curve), the GSCF approach (dashed curve) and II order perturbation result (dark bullets).

The GSCF theory does not account for the strong dynamic fluctuations around the average values. In traditional perturbation theory the expansion in U/t includes the perturbation term about non-interacting Hamiltonian and therefore there is no perturbational expansion at large U/t. One can naively think that because U/t can be the largest energy scale for systems of interest, such straightforward expansion of fluctuations about zero order mean field Hamiltonian do not necessary vanish.

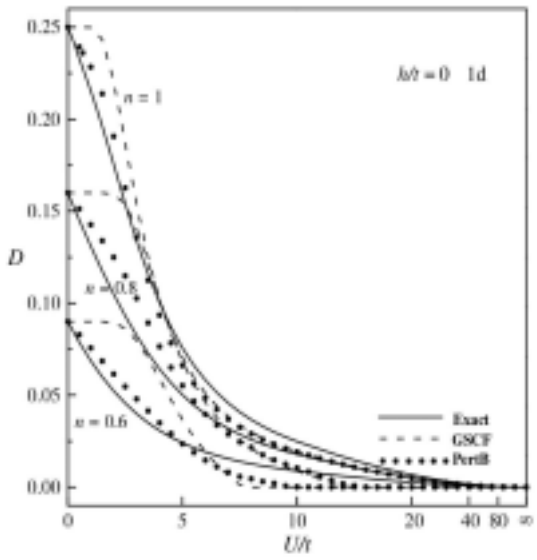

Fig. 2. The ground state density of double occupied sites $D^{(+)}$ as a function of U/t for various n in the Bethe-ansatz solution (solid curve), the GSCF approach (dashed curve) and II order perturbation result (dark bullets).

We suggest here perturbation approach beyond the standard linear approximation, using the Bogolyubov-type transformation to the new quasi-particles. The problem can be reduced simply to carefully resorting the contribution of different terms in transformed the GSCF and exact Hubbard models by calculating of corresponding matrix elements. We consider the GSCF Hamiltonian H_{GSCF} as a zero order term and take the difference H_{exact}- H_{GSCF} as a perturbation. [8,10] In equilibrium the GSCF self-consistent equations are satisfied and the I order correction is identical to zero, $E^{(+)(1)}= 0$. The next correction to the GSCF result $E^{(+)(0)}{}_{GSCF}$ for the ground state energy is II order perturbation term, $E^{(+)(2)}$.

The performed numerical calculations of the ground state energy $E^{(+)}/t$ and ground state density of double occupied sites $D^{(+)}$ (Fig.1 and Fig.2) demonstrate the good numerical agreement with the Bethe-*ansatz* results at weak and intermediate range of U/t. However the results at large U/t differ from Bethe-ansatz ones. It also should be kept in mind that the comparison with the exact result in 1d is probably a "worst-case" scenario for most approximation theories due to strong quantum fluctuations. We expect that this approach will be more accurate in higher dimensions, where corresponding fluctuations are suppressed.

三、計劃成果自評

In this work we demonstrated a non-standard second order perturbation PertB approach for interacting quasi-particles about exactly solvable single-particle GSCF Hamiltonian. The variational GSCF ground state energy is exact in limiting cases $U/t\rightarrow 0$ and $U/t \rightarrow \infty$ for arbitrary $h \geq 0$ and all $0\leq n\leq 1$. We constructed a converging second order perturbation theory, valid for arbitrary interaction strength, by choosing the single-particle GSCF Hamiltonian for quasi-particles as a zero order approximation.

The problem was shown been reduced to calculation of corresponding matrix elements for the difference between the transformed GSCF and exact Hamiltonian. The performed PertB technique gives the first two terms of the non-standard perturbation expansion series. The calculated PertB theory for the ground state energy converges to PertA at small U/t limit and approaches asymptotically to the GSCF result at large U/t.

We analyzed the ground-state properties from the standpoint of both traditional and non-traditional perturbational approaches about non-interacting electrons (PertA) and GSCF quasi-particles (PertB) respectively. In one dimension we checked the accuracy of different approaches by comparison with the Bethe-*ansatz* calculations. Numerical simulations in PertB at relatively small

electron concentrations show quite good agreement with the Bethe-*ansatz* result in the intermediate region of *U/t*. The ground-state properties with magnetic field become closer to the corresponding exact results. The PertB approach gives better agreement with the exact solution in intermediate range of U/t, when *n* is small or *h* is large enough. Thus the PertB is a reasonable interpolation scheme between the weak and strong interaction. However, at large *U/t* the result for the chemical potential at half-filling case differs from Bethe-*ansatz*.

The GSCF stable long-range spiral phases at $n \neq 1$ is still well described by second order perturbation theory, while exact solution in one dimension is a singlet with short-range correlations. One can also apply the same technique in higher dimensions, where, however, exact solutions are unavailable. We expect that this non-traditional approach will be even more accurate in higher dimensions, where corresponding fluctuations are suppressed.

The developed PertB about the GSCF solution can be applied to more complicated many body problems. Although the construction of the linear non-perturbed zero order Hamiltonian in general is far from simple, we can formulate the procedure for obtaining a convergent series for arbitrary perturbation parameter. A zero order approximation Hamiltonian can be constructed in mean field approximation manner necessary to reproduce exact features at infinity large and zero interaction limit, small electron concentration and strong magnetic field close to saturation.

The GSCF solution for non-interacting quasi-particles at small *U/t* follows the first order standard perturbation approximation.

However, the GSCF theory has advantage over the traditional first order perturbation theory, since it describes the system at arbitrary *U/t* values. Thus one can consider the linear GSCF theory as a self consistent first order perturbation approach applied for general *U/t*, *h* and *n*.

We can see now the relationship between the second order perturbation theory and the variational principle. Thus the basic shortcoming of the PertB is that it is not variational by nature.

The work currently in progress is aimed to apply second order perturbation theory for development of non-linear self-consistent theory, based on the PertB theory for quasi-particles.

These obtained results are important because they provide a reliable and firm base for the further investigation of Hubbard models in two- and three-dimensional cases and at finite temperatures. Some preliminary calculations and analysis in these directions are being carried out.

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