行政院國家科學委員會專題研究計畫　成果報告

二維哈巴特模型自洽場微擾理論計算及進階研究

計畫類別：個別型計畫
計畫編號：NSC93-2112-M-032-019-
執行期間：93 年 08 月 01 日至 94 年 07 月 31 日
執行單位：淡江大學物理學系

計畫主持人：楊棨
共同主持人：蔣幼齡
計畫參與人員：陳凌硯

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中　華　民　國 94 年 7 月 29 日

行政院國家科學委員會補助專題研究計畫
成果報告

二維哈巴特模型自洽場微擾理論計算及進階研究

Investigation of 2d Hubbard Models With Use of Self-Consistent Field Perturbation Theory

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計畫主持人：楊棨

共同主持人：蔣幼齡　中國文化大學物理系

計畫參與人員： A. N. Kocharian　California State University, U.S.A.

陳凌硯　淡江大學物理系

成果報告類型(依經費核定清單規定繳交)：*精簡報告

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中　華　民　國　94　年　7　月　28　日

一、摘要

本計劃中預定之各項研究已全部完成。

用廣義自洽場 （GSCF）及 Bethe-ansatz 精確解方法(一維)進一步研究了在任意磁場 h 下一維及二維排斥性哈巴特模型的各項基態與熱力學性質及相圖。相互作用強度 U、電子濃度 n 及磁場 h 為任意 ($0 \leq U < \infty$ ， $0 \leq n \leq 1$, $h/t \geqq 0$)。分析了橫向自旋（磁化強度）、雙佔有結點濃度 D、動能、化學勢等物理量在不同 n, U/t 及 h 下之變化。我們發現，當 n 及 U/t 變化時，磁序參數之波試射矢 $\boldsymbol{q}$ 會從一個位置躍遷到另一個位置。這是一種新的磁過渡相變。

本計劃研究成果發表於國際學術期刊 [1-2]，並在中華民國物理學會年會上宣讀 [3-4]。

關鍵詞：低維度哈巴特模型、基態性質、相圖、磁過渡相變，廣義自洽場近似、電子關聯

Abstract

The ground state and thermodynamic properties and phase diagram of the 1d and 2d repulsive Hubbard models are investigated numerically within the generalized self-consistent field (GSCF) and exact Bethe-ansatz approach (for 1d) over a wide range of interaction strength U/t, electron concentration n, and magnetic field h ($0 \leq U < \infty$, $0 \leq n \leq 1$, $h/t \geqq 0$) . A new efficient converging perturbation technique in terms of interacting quasi-particles about GSCF solution valid for arbitrary interaction strength U/t and electron concentration n is applied. The wave vector $\boldsymbol{q}$ for the magnetic order parameter shows a crossover from one position into another as U/t or n change.
Our results are published in [1-2] and reported at [3-4].

Key words: low-dimensional Hubbard model, thermodynamic properties, phase diagrams, magnetic crossover, generalized self-consistent field approximation, electron correlation

二、主要成果

The study of strongly correlated electrons becomes in the last decade one of the most active fields in condensed matter physics. However, despite remarkable efforts the understanding of electron correlations is still far from complete. The Hubbard model has been solved exactly only in one dimension. Among different methods, insufficient attention was given to the detailed analysis of the standard mean field approximation or so called generalized self-consistent field (GSCF) approach, which often allows to formulate a problem in physically transparent way and get analytical solution in any spatial dimension. Indeed, even in 1d,the GSCF theory in terms of non-interacting quasi-particles correctly describes the ground state properties in wide range of U>0 and U<0. Moreover in the limiting cases U/t \to 0 and U/t\to \infty for all h \geq 0 and 0 \leq n \leq 1 the GSCF ground state energy is exact, which is necessary for formulation of converging perturbation procedure about the GSCF solution in the entire parameter space.

We studied the dynamic many body effects of strongly correlated electrons in the periodic lattices by including the second order perturbation fluctuations around the self-consistent field solution.

From the perturbation standpoint it is a first attempt to develop a regular perturbation method for studying the intermediate range of interaction, where there is no small parameter.

We initially test the developed perturbational approach up to the second order around GSCF theory for the repulsive Hubbard model and numerical results in one dimensions (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.

Then the GSCF theory is applied to the 2d case.

The GSCF ground state at arbitrary wave vector $\boldsymbol{q}$ ($0 \le q_x, q_y < \pi$) for the spin order parameter (antiferromagnetism corresponds $q_x = \pi$ or/and $q_y = \pi$) and U>0 is

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

where $\alpha^{+}_{kq\lambda}$ is the qusi-particle operator, $\boldsymbol{k}$ 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 ($\Delta^{(+)}_{\boldsymbol{q}}$) and longitudinal (s) spin order parameters and the chemical potential $\mu^{(+)}$. The eigenvalue of the GSCF Hamiltonian in the ground state is

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

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 (for 1d) 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.

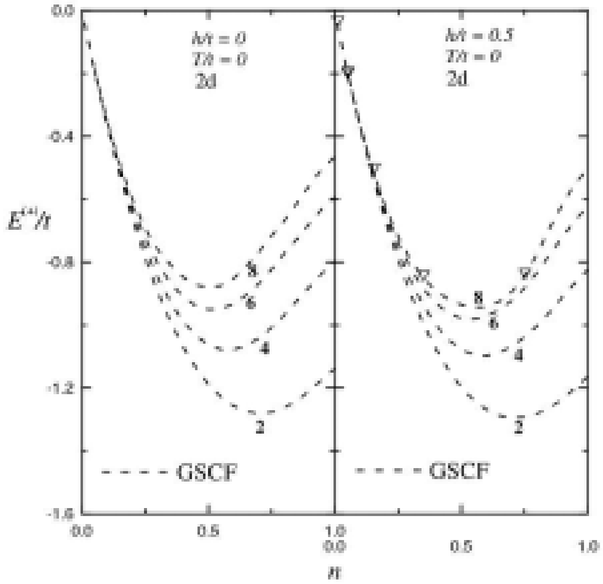

Fig. 1. The 2d ground state energy $E^{(+)}/t$ as a function of n for various U/t in the GSCF approach (dashed curves).

The GSCF theory does not account for the strong dynamic fluctuations around the average values.

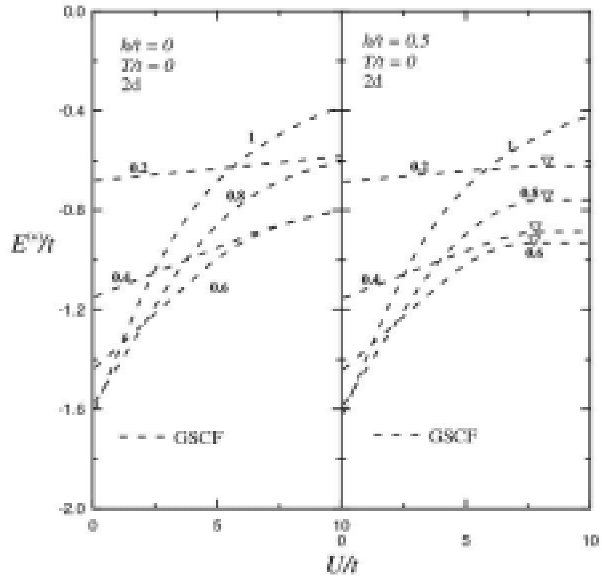

Fig. 2. The 2d ground state energy $E^{(+)}/t$ as a function of U/t for various n in the GSCF approach (dashed curves).

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]

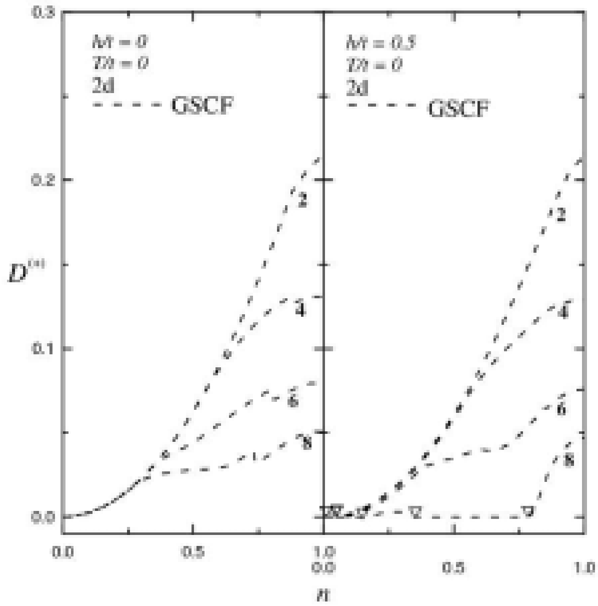

Fig. 3. The 2d ground state density of double occupied sites $D^{(+)}$ as a function of n for various U/t in the GSCF approach (dashed curves).

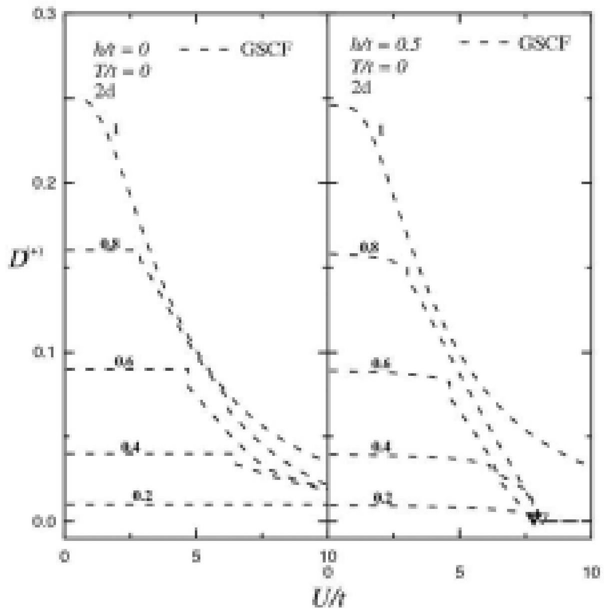

Fig. 4. The 2d ground state density of double occupied sites $D^{(+)}$ as a function of U/t for various n in the GSCF approach (dashed curves).

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 $D^{(+)}$ are shown in Figs.1-5. In the case of n=1 we got good agreement with the Quantum Monte-Carlo (QMC) and Hartree-Fock (HF) results.

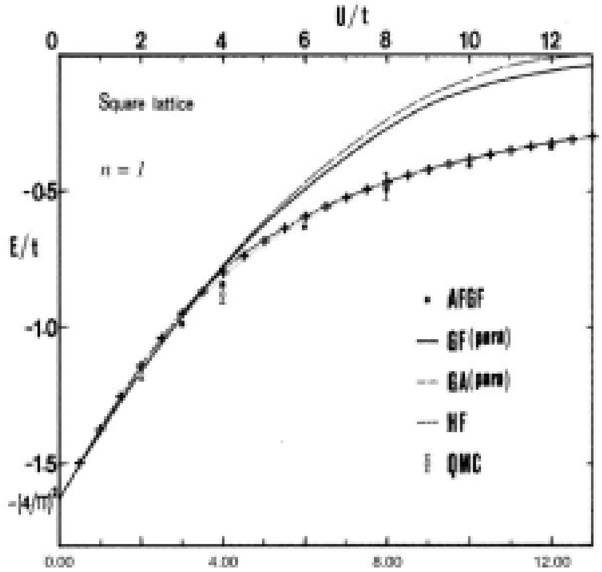

Fig. 5. The 2d ground state energy E/t as function of U/t for $n=1$ in GSCF (+), quantum Monte-Carlo (QMC), Hartree-Fock (HF) and some other approaches.

We found that the 2d wave vector $\boldsymbol{q}$ for the magnetic order parameter shows a crossover from one position in the $\boldsymbol{k}$-space into another as U/t or n changes.

三、計劃成果自評

In this work we carried out the investigation of ground state and thermodymamic properties of 2d repulsive Hubbard model and 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. The PertB is a reasonable interpolation scheme between the weak and strong interaction.

The 1d 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. We applied the same technique in 2d, where, however, exact solutions are unavailable. We found that the 2d wave vector $\boldsymbol{q}$ for the magnetic order parameter shows a crossover from one position in the $\boldsymbol{k}$-space into another as *U/t* or *n* changes. We think that our non-traditional approach is more accurate in 2d, 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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