行政院國家科學委員會專題研究計畫　成果報告

在磁場中低維度有限尺度哈巴特模型之物理性質

計畫類別：個別型計畫
計畫編號：NSC91-2112-M-032-016-
執行期間：91 年 08 月 01 日至 92 年 07 月 31 日
執行單位：淡江大學物理系

計畫主持人：楊棨

計畫參與人員：A. N. Kocharian （California State University, U.S.A.），蔣幼齡 （中國文化大學物理系），陳凌硯（ 淡江大學物理系）

報告類型：精簡報告

處理方式：本計畫可公開查詢

中　華　民　國 92 年 10 月 27 日

行政院國家科學委員會補助專題研究計畫

成果報告

在磁場中低維度有限尺度哈巴特模型之物理性質

Physical Properties of Low-dimensional Finite Size Hubbard Models in Magnetic Fields

計畫類別：*個別型計畫
計畫編號：NSC 91－2112－M －032－016－
執行期間： 2002 年 08 月 01 日至 2003 年 07 月 31 日

計畫主持人：楊棨

共同主持人：無

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

蔣幼齡 中國文化大學物理系

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

執行單位：淡江大學物理系

中 華 民 國 92 年 10 月 17 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 精確解方法進一步研究了在不同溫度 T 及任意磁場 h 下一維排斥性的有限尺度哈巴特模型的各項熱力學性質及相圖。相互作用強度 U、電子濃度 n 及磁場 h 為任意（$0 \le U < \infty$, $0 \le n \le 1$, $h/t \ge 0$）。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 下之溫度變化。我們發現，當溫度上昇時，磁序參數之波數 q 在半填充附近的金屬相中有磁過渡現象:從非公度磁相 $(0 \le q < \pi)$ 到強反鐵磁關連態 $(q = \pi)$ 的過渡。GSCF 自洽場及 Bethe-ansatz 精確解的計算結果在不同溫度及各參數的廣泛範圍內定性及定量都符合頗佳。

本計劃研究成果發表於國際學術期刊 [1-4]，並在國內及國際學術會議上宣讀 [5-8]。

關鍵詞：低維度哈巴特模型、熱力學性質、相圖、磁過渡，廣義自洽場近似、電子關聯，高溫超導

Abstract

The phase diagram and thermodynamic properties of the repulsive Hubbard model of finite sizes in one dimension are investigated numerically within the generalized self-consistent field (GSCF) and exact Bethe-ansatz approach over a wide range of temperature T, magnetic field h, interaction strength U/t and electron concentration n （$0 \le U < \infty$, $0 \le n \le 1$, $h/t \ge 0$）. The temperature variation of the transverse magnetization, double occupied sites and chemical potential at various n, U/t and h is also analyzed. The wave vector q for the magnetic order parameter in the vicinity of the half-filling in the metallic phase shows a crossover from incommensurate magnetic phase $(0 \le q < \pi)$ into the state with strong antifferomagnetic correlations $(q = \pi)$ as temperature is increased. Overall our numerical results in the approximate theory finite temperatures are in good quantitative and qualitative agreement with the Bethe-ansatz results.
Our results are published in [1-4] and reported at [5-8].

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

二、主要成果

We studied the phase diagram and behavior of the transverse magnetization and the chemical potential of the one-dimensional Hubbard model of finite sizes with magnetic field h in wide range of temperature. Our generalized self-consistent field (GSCF) approach is a straightforward extension of the existing mean-field solutions for incommensurate spiral phase with the wave number $0 \le q \le \pi$ for general U/t, h, $0 \le n \le 1$ and all temperatures T.

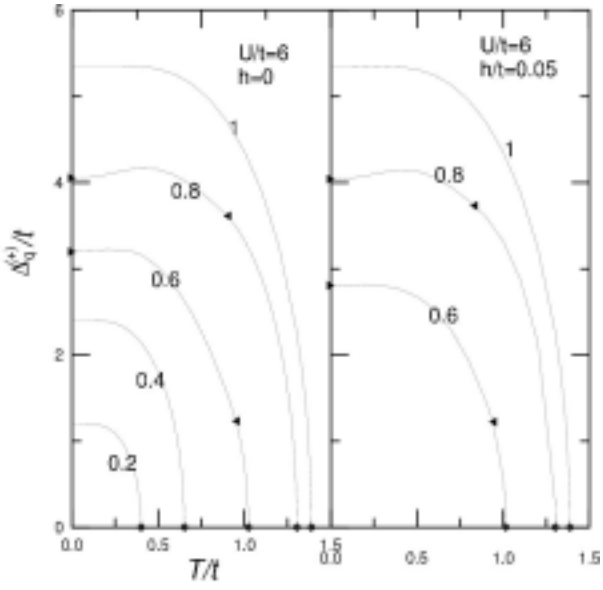

Fig. 1

We obtained the variation of the order parameter $\Delta^{(+)}_q \equiv 2U \Sigma_k \langle c^+_{q-k\downarrow} c_{k\uparrow} \rangle / N_{latt}$ *versus* temperature for $U/t = 6$ and $h = 0$ (Fig. 1). At $n = 1$ $q = \pi$ and $\Delta^{(+)}_\pi$ is equal to the energy gap. At middle $n \neq 1$ there is an incommensurate phase $0 < q < \pi$ (between the triangles in Fig. 1). At small n we have $q = 0$ at $\Delta^{(+)}_q \neq 0$. At $n \neq 1$ $\Delta^{(+)}_q$ *versus* T/t shows slightly non-monotonic behavior. At all n the order parameter $\Delta^{(+)}_q$ vanishes at some critical temperatures T_c depending on n and h/t.

The state with strong antiferromagntic correlations ($q = \pi$) becomes stable in some range of temperatures and magnetic field. Away from $n = 1$ the GSCF theory provides a smooth transition in the absence and presence of magnetic field h from the incommensurate state with the order parameter $\Delta^{(+)}_q \neq 0$ for wave number $0 < q < \pi$ into antiferromagnetic state with $q = \pi$.

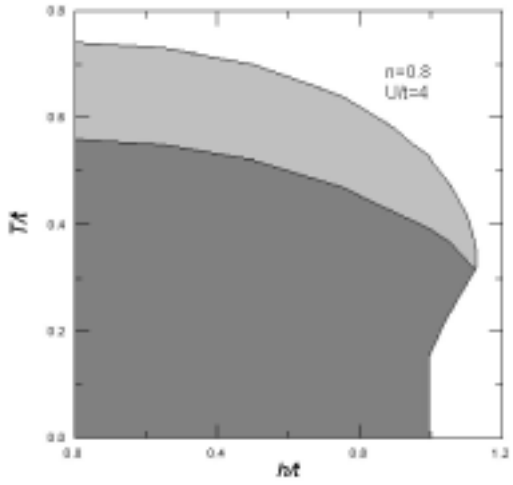

Fig. 2

We investigated the phase T-h diagram in the presence of magnetic field (*e.g.* for $U/t = 4$ and $n = 0.8$ see Fig. 2). In general, relatively large doping ($n \leq 0.8$) results in a phase diagram of the metallic state, which consists of three different phases. The white area indicates the normal phase with $\Delta^{(+)}_q = 0$ and arbitrary q. This phase is stable at relatively large h/t or high temperatures. The separation boundary T_c *versus* h/t between the dark and light shaded areas describes the smooth transition from the normal metallic state into antiferromagnetic phase. There is also a narrow range of h where incommensurate phase one can reach from the normal phase in strong magnetic field by increasing the temperature. Further increase of temperature results in development of the antiferromagnetic correlations.

We compared the dependence of the GSCF chemical potential $\mu^{(+)}$ *versus* electron concentration and the Bethe-ansatz result for fixed U/t and h/t. The GSCF results qualitatively well reproduce the exact Bethe-ansatz except in close vicinity of half-filling. In contrast to the exact theory, the GSCF chemical potential *versus* n in metallic phase is a non-monotonous function in the ground state and at very low temperatures. At finite temperatures it becomes monotonous.

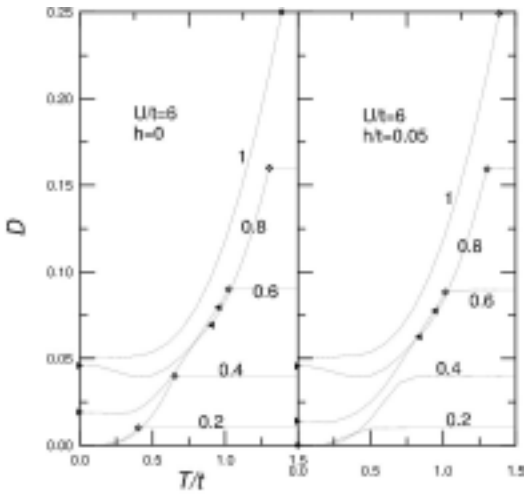

Fig. 3

We obtained also the variation of double occupied sites $D^{(+)}$ under the variation of temperature for $h = 0$ and $h/t = 0.05$ (Fig. 3). In general $D^{(+)}$ increases with temperature as in exact theory.

The Hubbard model with $U > 0$ in the

presence of magnetic field $h \geq 0$ ($s \geq 0$) can be reinterpreted in terms of the electron-hole pairs for the attractive Hubbard model, using the exact mapping between the repulsive and attractive Hubbard models. Earlier we found the stability for inhomogeneous superconducting phase with finite magnetization $s \neq 0$ and $\Delta_q \neq 0$ and $q \neq 0$. Based on this analogy we have for $U > 0$ the transition close to the half-filling case under the variation of n from antiferromagnetic dielectric with $q=\pi$ into incommensurate metallic state with $q \neq \pi$.

We studied the dynamic many body effects of strongly correlated electrons in the periodic lattices by including the effect of fluctuations around the self-consistent 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.

We initially tested the developed perturbational approach up to the second order around GSCF theory for the Hubbard model and numerical results in one dimension 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 numerical results clearly demonstrate qualitative discrepancy for all $n \leq 1$ in prediction of behavior for double occupancy $D^{(+)}$ and kinetic energy $E_{\rm kin}$ 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.

We suggested perturbation approach beyond the standard linear approximation, using the Bogolyubov-type transformation to the new quasi-particles. We consider the GSCF Hamiltonian $H^{(+)}_{\rm GSCF}$ as a zero order term and take the difference $H_{\rm exact} - H^{(+)}_{\rm GSCF}$ as a perturbation. 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 $E^{(+)(0)}_{\rm GSCF}$ for the ground state energy is II order perturbation term, $E^{(+)(2)}$.

Using the analogy between $U>0$ and $U<0$ Hubbard models we showed the correspondence (mapping) between the xy ferromagnetism in the vicinity of half-filling and superconductivity of polarized electrons near the empty band in higher dimensions $d>1$. Below we establish the strict mapping between $U>0$ and $U<0$ Hubbard models, using the exact Bethe-ansatz calculations along with the developed GSCF results in one dimesion.

Under this transformation the spin-up spectrum of the Hubbard model ($U>0$) is replaced by $\epsilon_k \rightarrow -\epsilon_k$. The wave vector is reduced to $q \rightarrow \pi - q$, and correspondingly $n \rightarrow 1-2s$ and $s \rightarrow (1-n)/2$. There is a simple relation $\Delta^{(+)}_{\mathbf{q}} \rightarrow \Delta^{(-)}_{\pi - \mathbf{q}}$.

We found the mapping between $U>0$ and $U<0$ models in the GSCF approach along with exact solution are shown for the kinetic energy as well as the energy E ($U>0$) and $E-nU/2$ ($U<0$) at half-filling ($U>0$) and in the

presence of magnetic field (U<0) in the entire space of 1-2s and n respectively (Fig. 4, 5).

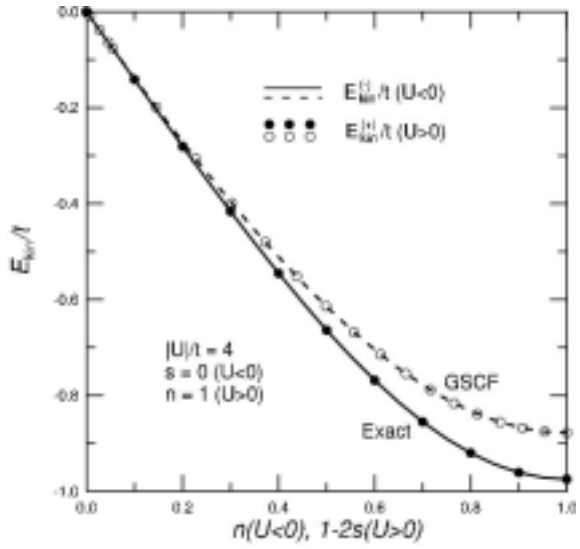

Fig. 4

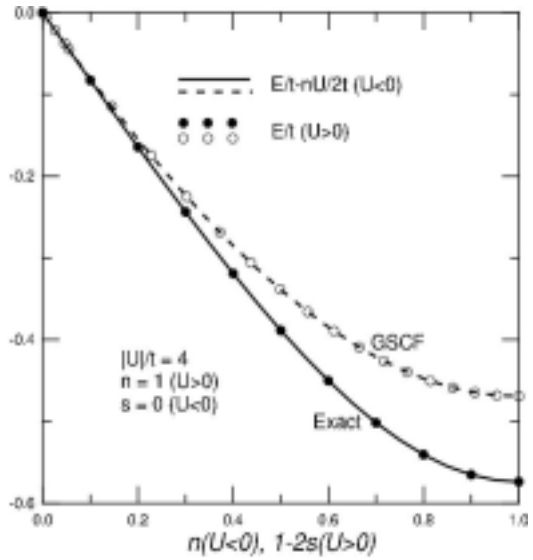

Fig. 5

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 and electron concentration. We test the developed perturbation approach about mean field solution in the extreme conditions of one dimensionality for entire parameter space of electron interaction U/t and electron concentration n. The developed many-body perturbation formalism up two second order about generalized self-consistent field (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.

三、計劃成果自評

In summary, the GSCF theory in the ground state and at finite temperatures reproduces qualitatively and sometimes quantitatively the general features of the Bethe-ansatz solution. The GSCF theory predicts the enhancement of antiferromagnetic correlations with temperature in metallic state and properly describes observed instability in behavior of $\mu^{(+)}$ for PES and ARPES data in $Nd_{2-x}Ce_xCuO_4$.

We demonstrated within the Bethe-ansatz and the GSCF approaches an exact mapping and equivalency between U<0 and U>0 Hubbard models in entire space of n and s for bipartite lattices in 1d case. The excellent agreement between U<0 and U>0 Hubbard models for the GSCF approach in 1d case puts the exact mapping within this approach on a firmer basis also in higher dimensions, where fluctuations are weaker.

We have carried out the investigation of one-dimensional Hubbard models of finite sizes in the presence and absence of external magnetic field by using of both the Bethe-*ansatz* equations and the generalized self-consistent field (GSCF) approach. We continued the detailed analysis of the ground state properties and phase diagrams in a wide

range of the coupling strength ($-\infty<U<\infty$), electron concentration ($0 \le n \le 1$) and magnetic field ($h \ge 0$). We investigated the crossover in both the attractive and the repulsive models.

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.

四、參考文獻

[1] C. Yang (楊棨), A. N. Kocharian, Y. L. Chiang, 2002, "Phase diagram and magnetic correlations in one-dimensional repulsive Hubbard model with magnetic field", Journal of the Physical Society of Japan, v. 71 Supplement pp.193-195. (SCI)

[2] A. N. Kocharian, C. Yang (楊棨), Y. L. Chiang, 2002, "Superconductivity, magnetism and mapping in entire parameter space between the attractive and repulsive Hubbard models", Journal of the Physical Society of Japan, v. 71 Supplement pp.223-224. (SCI)

[3] C. Yang (楊棨), A. N. Kocharian, Y. L. Chiang, 2003, "Thermodynamic Properties of One-Dimensional Hubbard Model at Finite Temperatures" (有限溫度下一維哈伯模型之熱力學性質), *Intern Journal of Modern Physics* B, vol. 17, NN. 18, pp. 3354-3358. (SCI)

[4] A. N. Kocharian, C. Yang (楊棨), Y. L. Chiang, 2003, "Perturbation Theory About Self-Consistent Field Solution in One-Dimensional Hubbard Model" (一維哈伯模型自洽場解之微擾理論), *Intern Journal of Modern Physics* B, vol. 17, NN. 18, pp. 3363-3366. (SCI)

[5] L. Y. Chen, Y. L. Chiang, T. Y. Chou, C. Yang (楊棨), A. N. Kocharian, 2003 九十二年中華民國物理學會年會, 物理雙月刊, v. 25, no. 1, pp. 141-142. Thermodynamic Properties and the phase diagram of the Hubbard Model in one-dimension

[6] Y. L. Chiang, T. Y. Chou, C. Yang (楊棨), A. N. Kocharian, 2003 九十二年中華民國物理學會年會, 物理雙月刊, v. 25, no. 1, pp. 142.

[7] C. Yang (楊棨), A. N. Kocharian, Y. L. Chiang, 2003, "Thermodynamic properties of one dimensional Hubbard model at finite temperatures ", International Conference on New Theories, Discoveries, and Applications of Superconductors and Related Materials (New^{3}SC-4), Jan. 16 - 21, 2003, San Diego, California, USA.

[8] A. N. Kocharian, C. Yang (楊棨), Y. L. Chiang, 2003, "Perturbation theory about self-consistent solution in one dimension", International Conference on New Theories, Discoveries, and Applications of Superconductors and Related Materials (New^{3}SC-4), Jan. 16 - 21, 2003, San Diego, California, USA.