行政院國家科學委員會補助專題研究計畫成果報告

※※※※※※※※※※※※※※※※※※※※※※※※※※

※※ 吸引性及排斥性哈巴特模型的相變及熱力學磁性質

※※ Phase Transitions and Magnetic Thermodynamic ※※ Properties of Attractive and Repulsive Hubbard Models ※※

※※※※※※※※※※※※※※※※※※※※※※※※※※※

計畫類別：*個別型計畫　□整合型計畫

計畫編號：NSC　90-2112-M-032-014

執行期間：90 年 08 月 01 日至 91 年 07 月 31 日

計畫主持人：楊棨

共同主持人：

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

魯崇磊　淡江大學物理系

本成果報告包括以下應繳交之附件：

□赴國外出差或研習心得報告一份

□赴大陸地區出差或研習心得報告一份

□出席國際學術會議心得報告及發表之論文各一份

□國際合作研究計畫國外研究報告書一份

執行單位：淡江大學物理系

中　華　民　國　九十一　年　十　月　十六　日

行政院國家科學委員會專題研究計畫成果報告

吸引性及排斥性哈巴特模型的相變及熱力學磁性質

Phase Transitions and Magnetic Thermodynamic Properties of Attractive and Repulsive Hubbard Models

計畫編號：NSC 90-2112-M-032-014

執行期限：90 年 08 月 01 日至 91 年 07 月 31 日

主持人：楊榮　執行機關：淡江大學物理系

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

魯崇磊　淡江大學物理系

一、摘要

本計劃中預定之各項研究已全部完成。

用自洽場 （GSCF）及精確解方法進一步研究了在任意磁場h下一維吸引性及排斥性的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（$-\infty < U < \infty$,$0 \leq n \leq 1$, $h/t \geqq 0$）。計算了基態能量、平均自旋(磁化強度)、雙佔有結點濃度D、動能、化學勢、磁化率及電荷壓縮率等物理量。自洽場及精確解的計算結果在n, h及U的廣泛範圍內符合頗佳。我們發現，在排斥性模型中序參數$|\ddot{A}_q^{(+)}|/2U$即為橫自旋，其變化與縱自旋s之變化有一定關連。在排斥性模型中分析了相圖及鐵磁，反鐵磁及渦磁結構的穩定條件。在排斥性模型中探討了從電子電洞對偶（$|k_F| = ®$）轉成波色凝聚（$k_F = 0$）的磁過渡並與在吸引性模型中的 BCS-波色凝聚（$s = 0$）的過渡比較。

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]。

在執行本計劃的過程中，一位碩士生(魯崇磊)寫成學位論文[9]並高分通過答辯。

關鍵詞：低維度哈巴特模型、基態特性、相圖、磁過渡，廣義自洽場近似、電子關聯，高溫超導

Abstract

The phase transitions and magnetic thermodynamic properties of one-dimensional Hubbard models within the generalized self-consistent field (GSCF) approach are compared with the Bethe-*ansatz* results in an entire parameter space of interaction strength U, magnetic field h 0 and electron concentration 0 n 1. The phase diagrams are derived and the criteria are found for the stability of ferro-, antiferro- and incommensurate magnetic structure (U/t 0) at n 1 with the wave number q ð. The GSCF theory is exact in the limiting cases $U/t \rightarrow 0$ and $U/t \rightarrow \infty$ for all h 0 and 0 n 1. For all n and h the GSCF concentration of the double occupied sites $D^{(+)}$ underestimates electron correlations at weak and intermediate U/t values. In contrast at large U/t, $D^{(+)}$ strongly overestimates correlations and vanishes at some critical U_{homog}/t at all n 1 for transition into saturated "transverse ferromagnetism" with q=0 ($S_{\perp}$ =n/2), while the exact result for $D^{(+)}$ approaches to zero gradually as $U/t \rightarrow \infty$. The GSCF chemical potential $\grave{\imath}^{(+)}$ *versus* n is non-monotonous and displays the instability toward the phase separation in the vicinity of n=1. At half-filling, $\grave{\imath}^{(+)}$ *versus* U/t is non-monotonous and differs significantly from the exact solution at strong interaction. The evolution of the energy gap $E^{(+)}_{gap}$ with h and U/t in the momentum space at n=1 describes magnetic crossover from *itinerant* magnetism of weakly bound electron-hole pairs into the *localized* magnetic regime, with the Bose condensation of local electron-hole pairs. The spectrum of quasi-particles is calculated and total "volume" of electrons in occupied Fermi region is found the same independent on U/t and h/t, consistent with the Luttinger theorem. The relationship for general n between the GSCF wave number q in incommensurate phase and corresponding momentum of the spin-spin correlation function in the exact theory is discussed.

Keywords: Hubbard models, ground state properties, phase diagrams, magnetic crossover, generalized self-consistent field approach, electron correlation, high T_c superconductivity

二、主要成果

There are direct relationships between the expectation values for the local spin components < $_{jx}$ >, < $_{jy}$ >, < $_{jz}$ > and the parameters n^{c}, $n_{\downarrow}^{c}$, $\ddot{A}_{j}^{(+)}$ in the repulsive Hubbard model. In the common case *s* and $|\ddot{A}_q^{(+)}|/2U$ both are continuous functions of *U/t*, *n*, and *h* (Fig.1). At *h*=0 the longitudinal spin is always zero (*s*=0), while $|\ddot{A}_q^{(+)}|/2U$ increases monotonously with *U/t* and becomes saturated (if *n*<1) as *U* exceeds some critical value U_{homog} (marked by rhombuses), depending on *n*. At *h*=0 and *n*=1 the parameter $|\ddot{A}_q^{(+)}|/2U$ approaches asymptotically to the limiting value 1/2 at *U/t* $\to \infty$. In the presence of magnetic field (*h*>0) the longitudinal spin s increases with *U/t* and becomes saturated at all n as *U* exceeds the critical value U_{sat} (marked by downward-pointing triangles), which depends on *n* and *h/t*, while $|\ddot{A}_q^{(+)}|/2U$ vanishes at *U* U_{sat}.

U/t

U/t

U/t

Fig. 1 The ground-state longitudinal (*s*) and the local transverse ($|\ddot{A}_q^{(+)}|/2U$) spin components in dependence on *U/t* for various *n* (figures label the curves) and *h* in the GSCF approach (dashed curves) along with the one-dimensional Bethe-*ansatz* result for *n*=1 and *n*=0.6 (solid curves). The triangles and rhombuses mark the longitudinal and local transverse spin saturation correspondingly.

The transverse spin $|\ddot{A}_q^{(+)}|/2U$ is a non-monotonous function of *U/t*, while at given *U/t* the spin *s* increases with *h* and becomes saturated (*s*=*n*/2) as *h* exceeds some critical value h_{sat}. The GSCF results (dashed curves) agree with the exact results (solid curves) at least qualitatively under the suppression of fluctuations at large *U/t* and strong field h. Our calculations show also that the total spin monotonously increases with *U/t* and *h*.

The Bethe-*ansatz* ground state at *h*=0 is a singlet irrespective of *n*, while the GSCF theory at large *U/t* shows the tendency toward the Nagaoka-like transverse ferromagnetism (spatial homogeneous phase) for all *n*   1 and *h*=0.

In the spiral phase at 0   *h* h_{sat} we have non-saturated longitudinal spin (*s*<*n*/2). However, at sufficiently large *U* U_{sat}, the system at *h*   0 in Fig. 1 undergoes a transition into *s*=*n*/2 and $s_{j\perp}=|\ddot{A}_q^{(+)}|/2U=0$ with q arbitrary (degenerate).

The critical parameter U_{sat} depends on *n* and *h/t*.

The *U*-*n* phase diagram at given *h/t* is shown in Fig. 2. The thick dotted curve (*h*=0) divides the entire *U*-*n* plane on two parts with *q*>0 (the left upper part) and *q*=0 (the right lower part). At *h*=0, the GSCF energies of the states with *s*=0, *q*=0, $s_{j\perp}=n/2$ and with *s*=*n*/2, $s_{j\perp}=0$ (*q* is arbitrary) are equal to the same value at *h*=0. This degeneracy results in a sharp transition (*i.e.* spin reorientation) from saturated transverse into fully polarized longitudinal phase in the presence of infinitesimal magnetic field.

From self-consistent equations at *h*=0 and $q \to 0$ we find in *U*-*n* plane the equation of the phase boundary curve $U_{homog}(n)$ between the spiral and homogeneous (ferromagnetic) phases.

Below the curve U_{homog} *versus* *n* we have the homogeneous (transverse ferromagnetic) state (at *h*=0) or saturated longitudinal spin state (at *h*   0). The spatial homogeneity (transverse ferromagnetism) at *h*=0 prevails at large *U/t* and small *n*, while the spiral phase dominates at weak interaction and in close vicinity of *n*=1 (Fig. 3).

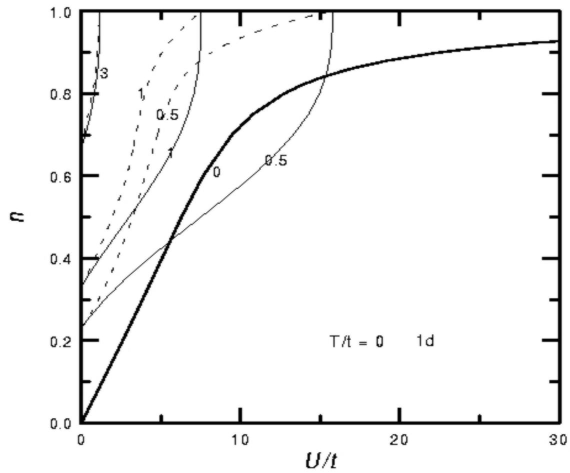

Fig. 2 The phase diagram in the *U-n* plan for various *h/t* (figures label the curves) in the Bethe-*ansatz* (the solid curves) and GSCF (the thin dashed curves) approaches. On the right of these curves we have the saturated "longitudinal ferromagnetic" phase with $s=n/2$ (q is arbitrary) at the corresponding *h/t*, on the left we have the "transverse spiral incommensurate" phase with q 0, $s<n/2$. The thick dashed curve corresponds the boundary between the "transverse spiral incommensurate" phase with $s=0$ and the spatially homogeneous "transverse ferromagnetic" phase (on the right of the curve) with $\ddot{A}_q^{(+)}/2U=Un$, $q=0$, $s=0$ in the GSCF approach. At infinitesimal *h/t* the thin dashed curve coincides with the thick dashed one.

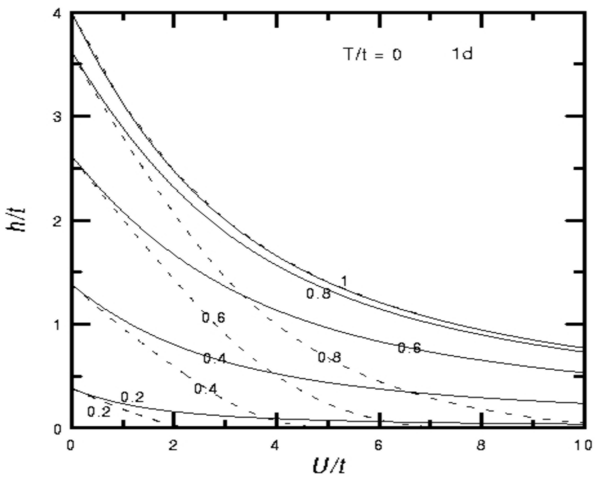

Fig. 3 The ground state phase diagram in the *U-h* plan for various n (figures label the curves) in the Bethe-*ansatz* (the solid curves) and GSCF (the dashed curves) approaches.

At half-filling the lower branch of the two quasi-particle energy sub-bands is fully occupied and the higher one is empty. Thus the two energy bands for arbitrary h and U 0 are separated by the finite energy gap.

At sufficiently large *U/t* and $h>0$ we have the state of saturated longitudinal spin. The maximal energy of quasi-particles in the occupied band occurs at $k=\pm$ð(or $k_{F2}=-k_{F1}=$ ð).

The critical magnetic field h_{sat} or corresponding critical interaction strength is coincides with the exact one \cite{Kore,Sebo}. Particularly, if h $4t$ the longitudinal spin is always saturated independently of *U/t*. Above h_{sat} or U_{sat}, the energy gap $E^{(+)}_{gap}=U+h-4t$ increases linearly with h and *U/t* (Fig. 4).

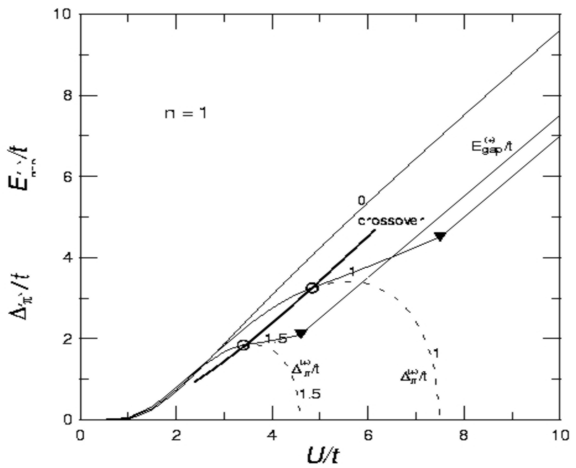

Fig. 4 The GSCF ground state energy gap $E^{(+)}_{gap}/t$ (the thin solid curves) and the order parameter $\Delta_\pi^{(+)}/t$ (the thin dashed curves) *versus U/t* for $n=1$ and various *h/t* (figures label the curves). The thick solid curve and the circles correspond the spin (magnetic) crossover. The triangles mark the longitudinal spin saturation.

The total spin introduced in section~\ref{ComC} (equation (\ref{totsp})) is also the root of the expectation value of the square local spin components (see (\ref{ssquar})) averaged over all the lattice sites (see (\ref{3}) and (\ref{Doub})) or the root-mean-square local spin.

Evidently for $n=1$ the maximal value of S_{tot} is 1/2 and the minimal value is $2^{-3/2}$ 0.35355 (at $U/t=h/t=0$, $D^{(+)}=1/4$).

In Fig. 5 the GSCF average spin s (magnetization) and S_{tot} both relatively close follow the exact result. The GSCF results for s and S_{tot} *versus U/t* increase monotonously and intersect the corresponding bold curves for the boundary of the magnetic crossover. The system is in the regime of itinerant magnetism or localized magnetism below and above these curves respectively. The upper bold curve describes the magnetic crossover for S_{tot} and in a wide range of U/t this curve is located in close vicinity to the saturation limit with S_{tot}=0.5. Even though the spin above the upper curve is well developed the average spin s is still far from its saturation limit (1/2). Thus magnetic crossover within the GSCF approach displays the changes in the local (short-range) characteristics such as the local magnetic moment rather than the long-range magnetic ordering (magnetization).

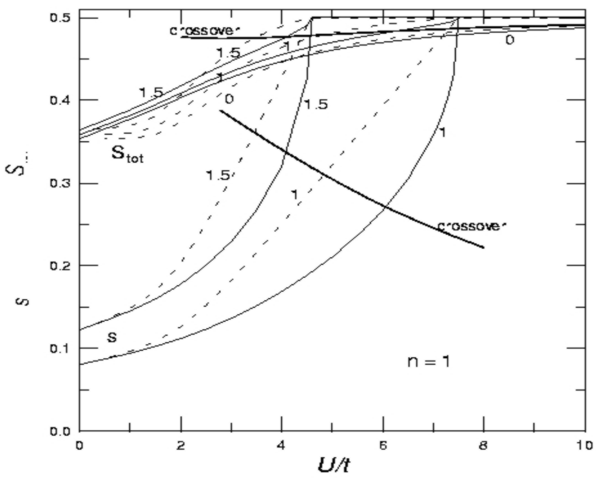

Fig. 5 The ground state total spin (or the root-mean-square local spin) S_{tot} and longitudinal spin s for n=1 as a function of U/t at various h/t (figures label the curves) in the Bethe-*ansatz* (the thin solid curves) and the GSCF (the dashed curves) approaches. The thick solid curve marks the spin crossover.

The total spin S_{tot} *versus* U/t never intersects the bold curve at h=0 and therefore there is no magnetic crossover from localized to itinerant magnetism in the absence of magnetic field no matter how strong is U/t. We conclude that the ordering of the well-developed local magnetic moment is apparently different from a band-like moment, usually characterized by relatively small moment.

三、計劃成果自評

We have continued the investigation of attractive and repulsive Hubbard models 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 have 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] **Ñ. Yang**, A. N. Kocharian, Y. L. Chiang, 2001, "Induced magnetization and inhomogeneous superconductivity in presence of external magnetic field" (在外磁場下之感應磁化及不均勻超導性), *Physica* C, v. 364-365, pp.155-157. (SCI)

[2] A. N. Kocharian, **C. Yang**, Y. L. Chiang, 2001, "Phase diagram and BCS-Bose condensation crossover in 1D and 2D Hubbard models" (一維及二維哈伯模型中之相圖及 BCS-玻色凝聚過渡), *Physica* C, v. 364-365, pp.131-133. (SCI)

[3] **C. Yang**, 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)

[4] A. N. Kocharian, **C. Yan**g, 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)

[5] Y. L. Chiang, T. Y. Chou, C. Yang, A. N. Kocharian, 2002 "Magnetic ground state properties and magnetic phase of one-dimensional repulsive Hubbard Model", 九十一年中華民國物理學會年會, 物理雙月刊, v. 24, no. 1, pp. 160-161.

[6] **C. Yang**, A. N. Kocharian, Y. L. Chiang, 2002, "Exact and Self-Consistent Studies of the Ground State Properties for 1D and 2D Hubbard Models in Entire Parameter Space", 2002 Gordon Research Conference on Correlated Electron Systems, June 29 - July 3, 2002, Colby College, Waterville, ME, USA.

[7] A. N. Kocharian, **C. Yang**, Y. L. Chiang, 2002, "Inhomogeneous Superconductivity and BCS-Bose Condensation Crossover in Attractive One-Dimensional Hubbard Model", 2002 Gordon Research Conference on Correlated Electron Systems, June 29 - July 3, 2002, Colby College, Waterville, ME, USA.

[8] A. N. Kocharian, **C. Yang**, Y. L. Chiang, 2002, "Exact and Self-consistent Perturbation Calculations of Thermodynamic Properties in Half-metallic Magnetic Materials", ICCE/9 Conference, July 1-6, 2002, San Diego, California, USA

[9] 魯崇磊 (Chung-Lei Lu) 2002, "Generalized Self-consistent Field Results of One-dimensional Hubbard models and Perturbation Corrections" (一維哈伯模型廣義自洽場結果及其微擾修正) 淡江大學物理學系碩士論文. 台灣, 淡水.