行政院國家科學委員會專題研究計畫成果報告

磁場作用下低維度哈伯特模型的熱力學性質(1/2，2/2)

Thermodynamic Properties of Low-Dimensional Hubbard Models In External Magnetic Fields

計畫編號：NSC 89-2112-M-032-010
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一、摘要

本計劃中預定之各項研究已全部完成。

用自洽場（GSCF）及精確解方法研究了在任意磁場h下低維度吸引性及排斥性的哈伯特模型的各項熱力學性質及相圖。所格點相互作用強度U及電子濃度n為任意（$-\infty<U<\infty$，$0\leq n\leq 1$）。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，在半填滿情形下電子自旋磁化率當U趨近於零時為不連續及非解析。精確理論表示，對任意電子濃度，在$U\leq 0$時無電荷能隙存在；此理論提供在半填滿能帶及空能帶中化學勢之上限及下限。在弱耦合極限及強耦合逼近展開下所得的解析結果和數值計算結果完全符合。GSCF基態能量及雙佔有結點濃度和精確解結果也有很好的符合。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。在吸引性模型中探討了從電子電洞對偶（$|k_{\mathrm{F}}|=\pi$）轉成波色凝聚（$k_{\mathrm{F}}=0$）的磁過渡。

本計劃研究成果發表於國際學術期刊[1-9]，並在國內及國際學術會議上宣讀[10-19]。

在執行本計劃的過程中，一位博士生（蔣約齡）及一位碩士生（曹庭瑜）寫成學位論文[20-21]並高分通過答辯。

關鍵詞：低維度哈伯特模型、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 thermodynamic properties and phase diagrams, both exact (Bethe-ansatz) and in the generalized self-consistent field (GSCF) approach, of the low-dimensional attractive and repulsive Hubbard models in the presence of an arbitrary magnetic field for various electron concentrations n and on-site interaction strengths $U<0$ or $U>0$ are calculated and investigated. The ground-state properties, namely, the ground-state energy, the average spin (magnetization), the concentration of the double occupied sites, the kinetic energy, the chemical potential, the spin (magnetic) susceptibility and the charge compressibility are calculated and examined in a wide range of interaction strengths U for various h and n. It is found that the spin susceptibility at half-filling is non-analytic and changes discontinuously as $U\to 0$. The exact theory shows the absence of charge energy gap at $U\leq 0$ region for all n and provides for the chemical potential the rigorous upper and lower bounds at half-filled and empty band respectively. The derived analytical results in the weak coupling limit and asymptotic expansions at strong coupling are in full agreement with the numerical calculations. The GSCF ground state energy and the GSCF concentration of double occupied sites are also in perfect agreement with the exact results. The phase diagrams are derived and the criteria are found for the stability of ferro-, antiferro- and spiral magnetic structures in the repulsive model. The GSCF chemical potential displays the instability toward the phase separation in the vicinity of half-filling. As in the exact theory the GSCF result for k_{F} at $n=1$ and $h=0$, is unrenormalized by U/t, $k_{\mathrm{F}}=\pi/2$ ($q=\pi$), while the evolution of the gap at $h\neq 0$ describes a magnetic crossover from *itinerant* magnetism of weakly bound electron-hole pairs with $|k_{\mathrm{F}}|=\pi$ to the *localized* magnetic regime, with the Bose condensation of local pairs ($k_{\mathrm{F}}=0$).

Keywords: low-dimensional 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

The low-dimensional attractive Hubbard models with the coupling strength U, both attractive ($U<0$) and repulsive ($U>0$), in the presence of magnetic field h are studied in a wide range of U, temperature T and electron concentration (band filling) n by using the generalized self-consistent field (GSCF) approach with renormalized chemical potential. Pairing, the smooth crossover from the BCS regime into the Bose condensation state and the inhomogeneous superconductivity with the non-uniform order parameter are investigated. The excitation spectrum, the momentum distribution function and thermodynamic properties, including the concentration of double occupied sites D, the kinetic energy E_{kin}, and the chemical potential μ are calculated. The numerical calculations are found in a good agreement with the Bethe-ansatz results and quantum Monte-Carlo calculations in a wide range of system parameters U, n and h. The concentration of double occupied sites and the bound electron pairs n_{pair} are calculated and we found a simple relationship between the order parameter and n_{pair}, valid for the arbitrary U and all n (see Figs.1 and 2). The GSCF theory correctly displays the separation of the energy gap from the order parameter (crossover) as n or U decrease (see Figs.3 and 4).

The developed GSCF approach in magnetic field suggests a smooth transition (thick solid curves in Figs. 1-3) into the inhomogeneous superconducting state.

The ground-state phase diagram and the critical behavior of the one-dimensional Hubbard model, both attractive and repulsive, are investigated numerically in the entire parameter space of electron concentration n, interaction strength U and magnetic field h. The magnetic ground-state properties, including the spin and charge susceptibilities, and the spin and charge energy gaps are calculated as functions of U, h and n. It is found that the spin (magnetic) susceptibility at half-filling changes discontinuously as $U \to 0$ and is enhanced by electron repulsion in comparison with that of the non-interacting case. The compressibility decreases with n at $U < 0$ and shows non-monotonous behavior with dramatic increase while $U > 0$. The critical behavior near the onset of magnetization and magnetic saturation is also analyzed. Our numerical results are in full agreement with calculated analytical expressions at strong magnetic field near the saturation, empty band filling, strong and weak interaction limits, the previous numerical studies for $h = 0$ and provide a solid ground for the evaluation of the different self-consistent theories.

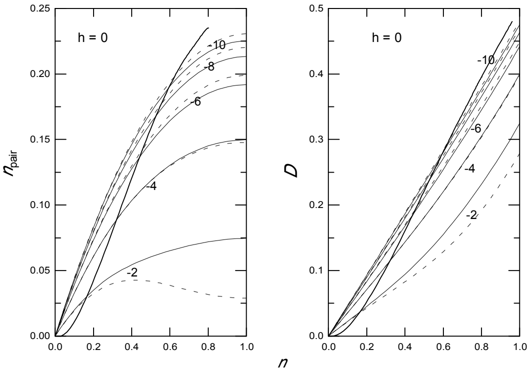

Fig. 1 The number of bound electron pairs n_{pair} the concentration of double occupied sites D in dependence of electron concentration n in the attractive model without external magnetic field for exact (thin solid curves) and GSCF (dashed curves) results. The thick solid curves mark crossover. The figures at the curves mean the values of U/t.

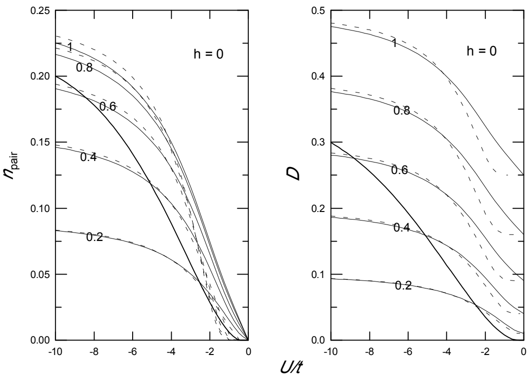

Fig. 2 The number of bound electron pairs n_{pair} the concentration of double occupied sites D in dependence of coupling strength U/t in the attractive model without external magnetic field for exact (thin solid curves) and GSCF (dashed curves) results. The thick solid curves mark crossover. The figures at the curves mean the values of n.

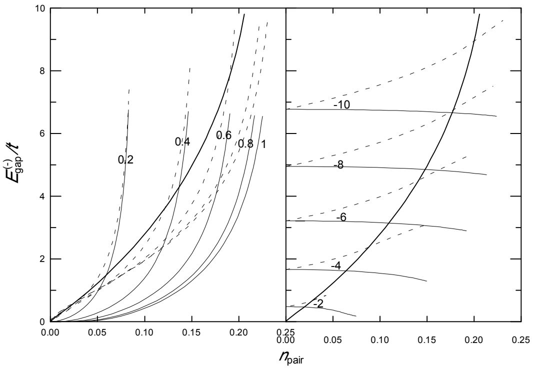

Fig. 3 The spin energy gap (at zero magnetic field h/t = 0) in the attractive model $E_{\rm gap}^{(-)}/t$ in dependence of the number of bound electron pairs $n_{\rm pair}$ at given n (the left curves) and at given U/t (the right curves) for exact (thin solid curves) and GSCF (dashed curves) results. The thick solid curves mark crossover. The figures at the curves mean the values of n or U/t respectively.

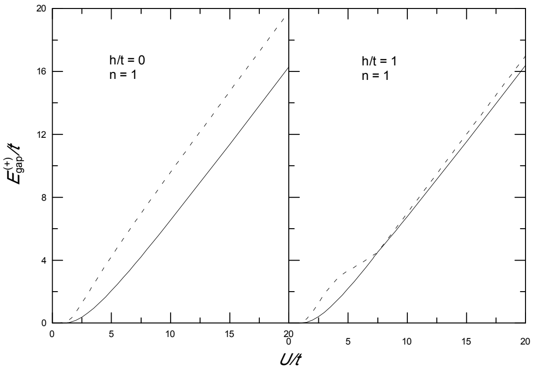

Fig. 4 The charge energy gap (at half-filling n = 1) in the repulsive model $E_{\rm gap}^{(+)}/t$ in dependence of the coupling strength U/t at h/t = 0 (the left curves) and at h/t = 1 (the right curves) for exact (thin solid curves) and GSCF (dashed curves) results.

The analysis of the thermodynamic phase diagram in the attractive model for various magnetic fields shows the presence of three different phases (see Fig. 5): 1. normal phase with $\Delta_q^{(-)}$ = 0 and q is arbitrary (unshaded area), 2. homogenous phase with q = 0 and $\Delta_q^{(-)} \neq 0$ (light shaded area), 3. inhomogeneous phase with $q \neq 0$ and $\Delta_q^{(-)} \neq 0$ (dark shaded area). The normal phase 1 is stable in some range of h/t also in the ground state (T = 0). At low temperatures ($T/t << 1$) spin onset is a sharp transition. Our calculations show that this transition occurs at the boundary of the phase 2 (light shaded area): s = 0 inside the phase 2 and $s \neq 0$ outside. In the inhomogeneous phase (dark shaded area) the spin (magnetization) is finite.

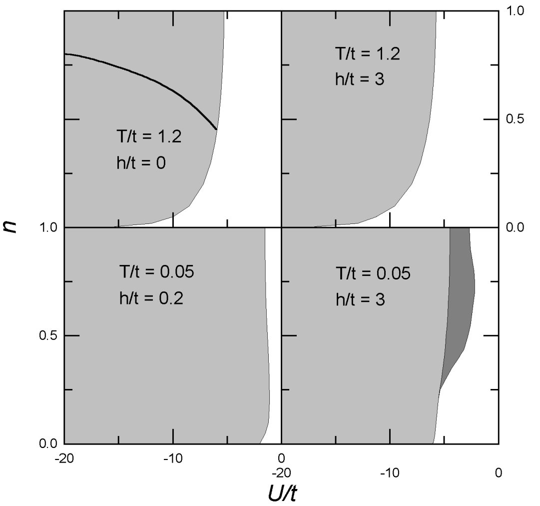

Fig. 5 The GSCF phase diagram in the n-U plane of the one-dimensional attractive Hubbard model at finite magnetic field h and temperature T. The unshaded, light shaded and dark shaded areas correspond the normal phase with $\Delta_q^{(-)} = 0$ and q is arbitrary, the homogenous phase with q = 0 and $\Delta_q^{(-)} \neq 0$ and the inhomogeneous phase with $q \neq 0$ and $\Delta_q^{(-)} \neq 0$.

In the ground state (T = 0) and at h = 0 the crossover from the itinerant pairing (BCS) regime of weakly bound electron pairs with momentum $k_F \neq 0$ into the Bose-Einstein condensation (BC) regime of local pairs with momentum $k_F = 0$ starts from infinitesimal small $|U|/t$ ($n_{\rm cross} \to 0$ at $|U|/t \to 0$), while it starts from finite $n_{\rm cross}$ (or $U_{\rm cross}$) whenever $T \neq 0$ and corresponding normal phase dramatically increases with the temperature and magnetic field h/t. The boundary curve between these two regimes is getting shorter with the increase of temperature, although, in general, its rest part remains temperature independent. In addition at relatively weak coupling we found a stable solution with $s \neq 0$, $q \neq 0$ and $\Delta_q^{(-)} \neq 0$ (dark shaded area).

The phase diagram in the h-T plane shows the dependence of the critical temperature T_c upon h for various U and n

describing the phase transition from the superconducting state with $\Delta_q^{(-)} \neq 0$ (phase 2 or 3, shaded area) into the normal paramagnetic state with $\Delta_q^{(-)} = 0$ (phase 1, unshaded area).

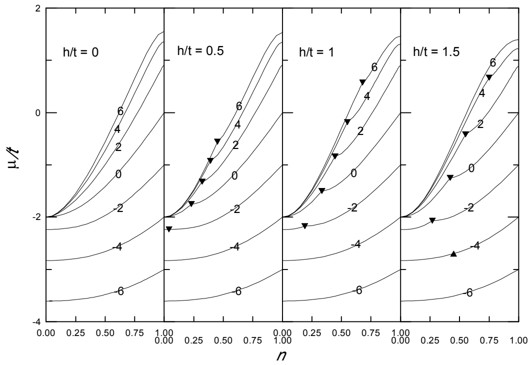

Fig. 6 The chemical potential μ in the attractive and repulsive Hubbard models in dependence of electron concentration n in the presence of external magnetic field h for exact (thin solid curves) and GSCF (dashed curves) results. The thick solid curves mark crossover. The figures at the curves mean the values of U/t. The downward triangles denote the spin (magnetic) saturation.

The critical temperature T_c monotonously decreases with increasing of h/t. Close to the half-filling case or in intermediate region of $|U|/t$ we found the stability for inhomogeneous superconducting state with finite spin with $q \neq 0$ and $\Delta_q^{(-)} \neq 0$ (phase 3, dark shaded area).

For both attractive and repulsive models the chemical potential μ monotonously increases in the entire range of n (see Fig. 6). In the presence of magnetic field there is a sharp transition (the downward triangles in Fig. 6) into the fully saturated spin phase ($s = n/2$).

For $n \neq 1$ the chemical potential μ increases monotonously in the entire range of U/t. In the attractive case for $0 < n < 1$ the chemical potential μ increases with h until the average spin s reaches the saturation and it is field independent in the fully saturated spin phase ($s = n/2$). In the repulsive case for $n = 1$ the chemical potential μ decreases with h in the unsaturated spin phase ($s < n/2$). The monotonous behavior of μ with U, n and h provides the upper and lower bounds for μ in the entire parameter space. The chemical potential μ is not an analytical function and exhibits sharp transitions (kinks) at the onset of magnetization and spin (magnetic) saturation.

The compressibility κ_{ch} (charge susceptibility) in both attractive and repulsive models for all $0 < n < 1$ is finite (see Fig. 7) because there is no energy gap in the charge excitation spectrum. Electrons are incompressible ($\kappa_{ch} = 0$) in an empty band ($n = 0$) for arbitrary U. Then κ_{ch} monotonously increases with n at $U < 0$. For $U > 0$ electrons become again incompressible exactly at half-filling and κ_{ch} is a non-monotonous function of n with one maximum (if $h = 0$) or more (if $h \neq 0$). Both for $h = 0$ and $h \neq 0$ the function κ_{ch} *versus* U is continuous everywhere including the vicinity $U = 0$ at $n \neq 1$, while at $n = 1$ it shows discontinuity (jump) at U/t → 0. In fully saturated phase κ_{ch} has the same value for n and $1 - n$.

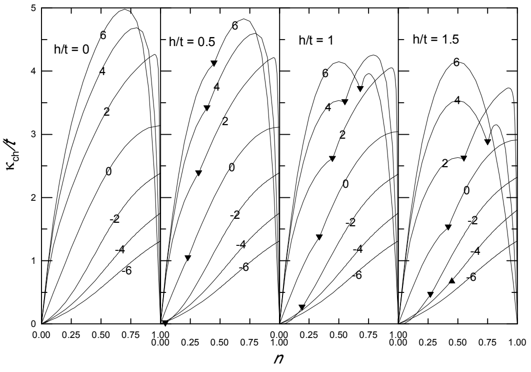

Fig. 7 The compressibility κ_{ch} in dependence on n at $h/t = 0, 0.5, 1, 1.5$ for various U/t (figures at the curves). The upward and downward triangles denote the spin onset and spin saturation correspondingly.

In the zero spin phase ($s = 0$) or in the saturated spin phase ($s = n/2$) average spin is field independent, the spin susceptibility χ equals to zero and χ^{-1} exists only in the intermediate phase with finite spin $0 < s < n/2$ (see Fig. 8). The behavior of χ as a function of U in the presence of h diverges in the critical point of spin saturation at $n = 1$

and is finite at any $n \neq 1$. The function of χ^{-1} on U is continuous for all n in the presence of finite magnetic field, but in an infinitesimal field this function shows discontinuity (jump) at $U/t \to 0$ for all n.

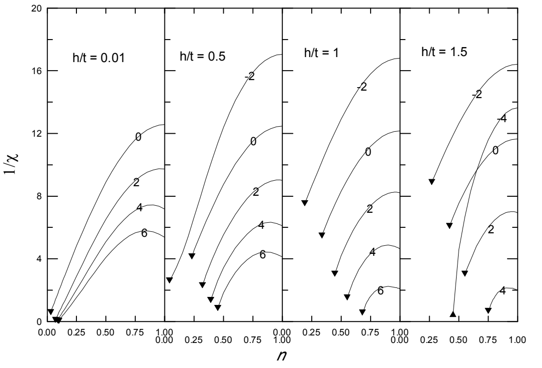

Fig. 8 The spin (magnetic) susceptibility χ in dependence on n at h/t = 0.01, 0.5, 1, 1.5 for various U/t (figures at the curves). The upward and downward triangles denote the spin onset and spin saturation correspondingly.

The dependence of χ^{-1} on n in the intermediate phase with finite spin (to the right of downward triangles in Fig. 8) for $U>0$ is in general a non-monotonous function with one maximum at n close to 1. For $U<0$, in contrast, χ^{-1} increases monotonously with n and approaches to its maximum value at $n = 1$.

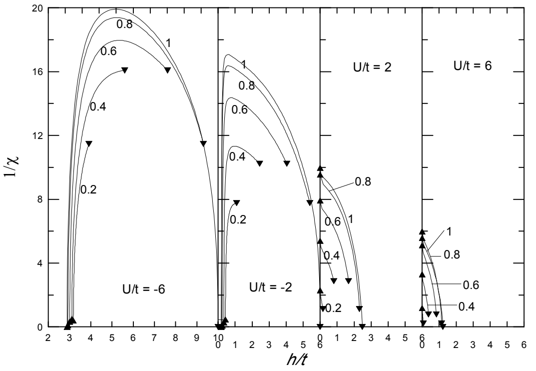

Fig. 9 The spin (magnetic) susceptibility χ in dependence on s at U/t = -6, -2, 2, 6 for various n (figures at the curves). The upward and downward triangles denote the spin onset and spin saturation correspondingly.

Because of the presence of spin energy gap at $U<0$ and h close to the spin onset critical field (upward triangles in Fig. 9) χ^{-1} increases rapidly with h for all n, while at $U>0$ there is no spin energy gap so χ^{-1} decrease monotonously with h.

Exactly at $n = 1$ the average spin s *versus h* at the critical fields of spin onset h_{c1} and spin saturation h_{c2} has infinite slop, while κ_{ch} near h_{c1} and h_{c2} is finite. Different spin and charge responses on the applied magnetic field in the vicinity of critical fields demonstrates the spin and charge separation within the one-dimensional Hubbard model.

三、計劃成果自評

We have investigated low-dimensional 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. In the one-dimensional model for the first time we have calculated and analyzed thoroughly the ground state properties and phase diagrams at zero temperature 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 magnetic crossover in the attractive model and the charge crossover in the repulsive model.

These obtained detailed and thorough results are important because they provide a reliable and firm base for the further investigation of Hubbard model in two-dimensional case and at finite temperatures. We have already done some preliminary calculations and analysis in these directions and plan to continue these studies in the nearest future.

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