Phase diagram and magnetic correlations in one-dimensional repulsive Hubbard model with magnetic field

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The generalized self-consistent field (GSCF) theory for the one-dimensional repulsive Hubbard model at half-filling is examined in the presence of magnetic field h in wide range of interaction strength U/t. The evolution of the energy gap in the presence of magnetc field describes a magnetic crossover from *itinerant* magnetism of weakly bound electron-hole pairs with $k_F = \pi/2$ to the *localized* magnetic regime, with the Bose condensation of local electron-hole pairs ($k_F = 0$).

§1. Introduction

The Bethe-ansatz formalism and solutions for some ground-state and thermodynamic properties in the presence of magnetic field for the one-dimensional (1d) Hubard model have been known for more than few decades.[1] The recent numerical calculations of ground-state in entire parameter space of electron concentration n, interaction strength U/t and magnetic field h give solid ground for testing and interpretation of approximate solutions.[2,3] In this paper we apply the GSCF approach along with the exact results and study electron-hole (exciton) BCS-like pairing, which at half-filling ($n = 1$) describes magnetic crossover driven by U/t and h from itinerant state into Bose-Einstein condensation regime and correspondingly find certain distinction between the magnetic ordering with well-developed magnetic moment (*localized*) and the band-like (*itinerant*) magnetism. This magnetic crossover closely resembles the analogies to the BCS-Bose condensation for superconducting crossover in the attractive model.[4,5]

§2. Energy gap

Below we examine within the GSCF approach the evolution of the energy gap in the momentum space for various U/t and h at half-filling ($n = 1$). From the quasi-particle energy spectrum one can find that until $2sU + h \geq 4t$ the Fermi-impulse remains equal to π. But at $2sU + h < 4t$ the location of the maximal energy of quasi-particles in the occupied band moves and thus

$$k_F = \begin{cases} \pi & \text{if} \quad 2sU + h \geq 4t \\ \arccos\left(-(2sU + h)/4t\right) & \text{if} \quad 2sU + h < 4t. \end{cases}$$
$$(2.1)$$

The energy gap is

$$E_{\text{gap}} = \begin{cases} \sqrt{(2sU + h - 4t)^2 + |\Delta_\pi^{(+)}|^2} & \text{if} \quad 2sU + h \geq 4t \\ |\Delta_\pi^{(+)}| & \text{if} \quad 2sU + h < 4t, \end{cases}$$
$$(2.2)$$

where s is the average longitudinal spin, t is the electron hopping constant between the neighboring sites and $\Delta_q^{(+)} \equiv -(2U/N_{\text{latt}}) \sum \exp(-iqr_j)\langle c_{j\uparrow}^+ c_{j\downarrow}\rangle$ is antiferromagnetic (AF) order parameter.

Earlier we studied in an entire range of coupling strength and electron concentration the crossover from the itinerant BCS state into the Bose condensation regime within the attractive Hubbard model at arbitrary filling ($0 \leq n \leq 1$) in the absence of magnetic field ($h = 0$).[3] Now we see an analogous crossover for $U > 0$ case at half-filling and $h \neq 0$. At $n = 1$ due to the electron-hole symmetry, the value q minimizing the energy is $q = \pi$. The Fermi-impulse increases from $k_F < \pi$ to $k_F = \pi$ driven by U/t and h. Such a weak singular behavior of the energy gap at $U > 0$ case gives rise to the crossover from itinerant into the localized magnetic regime.[6] In fact the Hubbard model with $n = 1$ and $U > 0$ can be reinterpreted in terms of electron-hole, using the electron-hole transformation.[8–10] The transformed Hubbard model is also equivalent to the two-orbital model of spinless fermions.[11,12] It is easy to check that under the electron-hole transformation the Hubbard model ($U > 0$) at $n = 1$ in the presence of h becomes equivalent to $U < 0$ one for electron-hole concentration $n \Rightarrow 1 - 2s$, where the renormalized chemical potential $\bar{\mu} \Rightarrow -\bar{h}/2$ and the BCS order parameter for $U < 0$ $\Delta_0^{(-)} \Rightarrow \Delta_\pi^{(+)}$ (where $\Delta_0^{(-)} \equiv -(2|U|/N_{\text{latt}}) \sum \langle c_{j\uparrow}^+ c_{j\downarrow}^+\rangle$).

Note that at the crossover $\bar{h} = h + 2sU$ approaches the limit $\bar{h} \to 4t$ with $k_F = \pi$, in contrast the chemical potential of electron-hole pairs, $\bar{\mu} = \mu + n|U|/2$ decreases and approaches to $-2t$ with the corresponding momentum $k_F = 0$. At the transition the chemical potential $\bar{\mu}$, driven by the coupling strength or magnetic field, intersects the bottom of the conduction band $-2t$ and leads to the transition of electron-hole pairs from the band-like

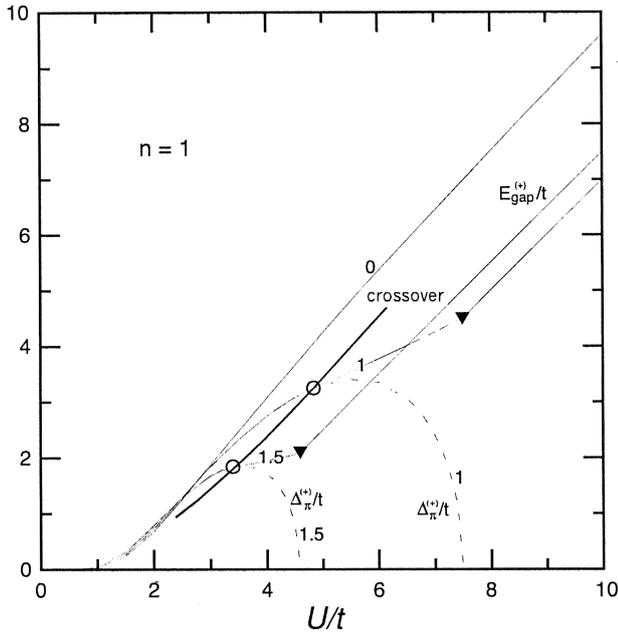* Present address: Department of Physics, Tamkang University, Tamsui, Taiwan 251, R.O.C.

Fig. 1.   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 labeling the curves). The thick solid curve and the circles correspond the spin (magnetic) crossover. The triangles mark the longitudinal spin saturation.

Fig. 2.   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* h/t for $n = 1$ and various U/t (figures labeling the curves). The thick solid curve and the circles correspond the spin (magnetic) crossover. The triangles mark the longitudinal spin saturation.

(itinerant) behavior into the localized magnetic regime.[6]

It is easy to show that $h_{cross} \leq h_{sat}$, i.e h_{cross} never exceeds the critical field for the longitudinal spin saturation h_{sat}. Thus the spin crossover always occurs in the phase of non-zero transverse spin ($S_\perp \neq 0$) with non-saturated longitudinal spin ($s < 1/2$). Analogously, at given $h \leq 4t$ we have the critical interaction strength $U_{cross} = (4t - h)/2s$. At given $U \leq 4t$ the critical magnetic field h_{cross} for spin crossover is determined from (2.1),

$$h_{cross} = 4t - 2sU. \tag{2.3}$$

§3.   Results

The formula (2.2) is illustrated in Figs. 1. At $h = 0$ the energy gap E_{gap} is identical to the order parameter $\Delta_\pi^{(+)}$ and both increase with U/t. However in applied magnetic field, the energy gap becomes distinct from the order parameter, when $E_{gap}^{(+)}(U)/t$ intersects the boundary of magnetic crossover (bold curve). Apparently $\Delta_\pi^{(+)}(U)$ (Fig. 1) is non-monotonous and vanishes at magnetic saturation U_{sat}, while the gap monotonously increases with U/t. The variation of $E_{gap}^{(+)}(U)/t$ is linear above U_{sat} and is identical to the exact gap.

For comparison in Fig. 2 we present the results of energy gap E_{gap} versus h/t for various U/t. The Energy gap decreases with h/t at large U/t and is non-monotonic function of h at intermediate at weak coupling. The GSCF approach is exact for all $h \geq h_{sat}(U)$, where $h_{sat}(U) = \sqrt{16t^2 + U^2} - U$. Above the saturation $E_{gap}^{(+)}(h)/t$ increases with h/t linearly, while $\Delta_\pi^{(+)}(h) \equiv 0$ at $h \geq h_{sat}(U)$.

We also calculate the expectation value of square local spin components, after averaging over all the lattice sites

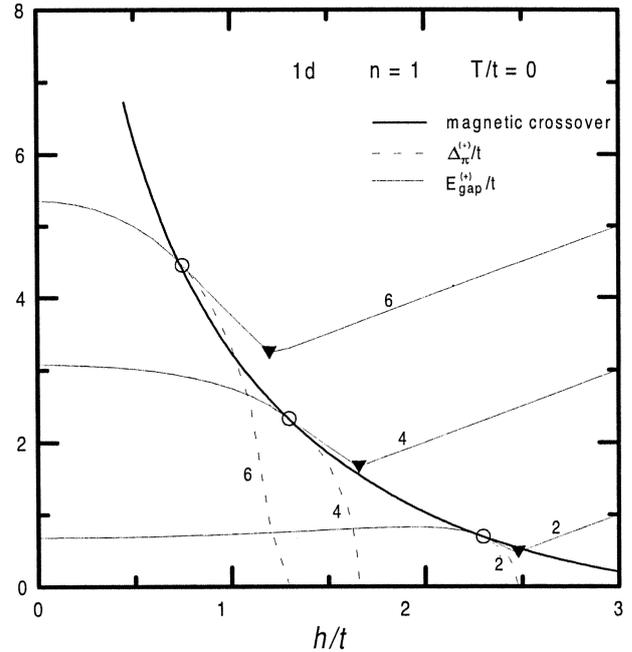and taking the square root we obtain the root-mean-square local spin[6]

$$s_{rmsl} = \frac{1}{2}\left(n - 2D^{(+)}\right)^{1/2}, \tag{3.1}$$

where $D^{(+)}$ is the expectation value for the concentration of doubly occupied sites

$$D^{(+)} \equiv \frac{1}{N_{latt}} \sum_j \left\langle c_{j\uparrow}^+ c_{j\downarrow}^+ c_{j\downarrow} c_{j\uparrow} \right\rangle. \tag{3.2}$$

Evidently for $n = 1$ the maximal value of s_{rmsl} is $1/2$ and the minimal value is $2^{-3/2} \approx 0.35355$ (at $U/t = h/t = 0$, $D^{(+)} = 1/4$). In Fig. 3 the GSCF longitudinal spin s and the r.m.s. local spin both relatively close follow the exact result. The GSCF results for s and s_{rmsl} *versus* U/t increase monotonously and intersect (at $h \neq 0$) the corresponding bold curves for the boundary of the magnetic crossover. The system is in the regime of itinerant magnetism or localized magnetism below or above these curves respectively. The upper bold curve describes the magnetic crossover for the r.m.s. local spin and in a wide range of U/t this curve is located in close vicinity to the saturation limit with $s_{rmsl} = 1/2$. The magnetic crossover reflects the changes in the local (short-range) characteristics such as the r.m.s. local spin (magnetic moment) rather than long range magnetic ordering (magnetization). At $h = 0$ the r.m.s. local spin never intersects the bold curve and therefore there is no magnetic crossover from localized to itinerant magnetism in the absence of magnetic field no matter how strong is the interaction strength U/t. Naturally, at arbitrary given $U < U_{sat}$ or $h < h_{sat}$ below spin saturation the r.m.s. local spin s_{rmsl} is always greater than the longitu-
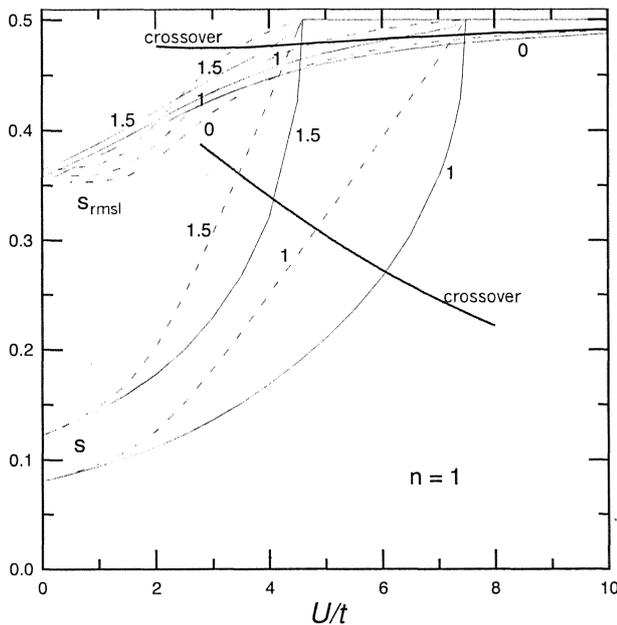
Fig. 3. The ground state root-mean-square local spin s_{rmsl} and longitudinal spin s for $n = 1$ as a function of U/t at various h/t (figures labeling the curves) in the Bethe-ansatz (the thin solid curves) and the GSCF (the dashed curves) approaches. At $h = 0$ for both exact and GSCF $s = 0$ independently of U/t. The thick solid curves mark the spin crossover.

dinal spin s (see Fig. 3). At spin saturation $(U \geq U_{sat}$ or $h \geq h_{sat})$ s_{rmsl} and s are equal.

The boundary for a crossover from itinerant to localized magnetism on a curve $1 - 2s$ versus U/t fully reproduces the GSCF boundary phase diagram n versus $|U|$, obtained for the attractive Hubbard model.[3] The phase with $n = 0$ $(U < 0)$ corresponds to saturated phase $s = 1/2$ $(U < 0)$, while $n = 1$ $(U < 0)$ is equivalent to non-magnetic phase $s = 0$ $(U > 0)$.

The GSCF theory at $n = 1$ and $h \neq 0$ displays the spin charge separation, where antiferromagnetic order parameter $\Delta_\pi^{(+)}$ is different from the electron-hole excitation gap $E_{gap}^{(+)}$.

In conclusion, the GSCF theory provides a qualitative and quantitative description of the main ground-state properties for the Hubbard model in the presence of magnetic field.[6] The GSCF theory displays an exact map-

ping and equivalency between $U > 0$ and $U < 0$ Hubbard models in entire space of n and s for bipartite lattices in 1d case.[6,10] The GSCF theory $(U > 0)$ at $n = 1$ in the presence of $h \neq 0$ displays the spin charge separation between the spin and charge excitations, where antiferromagnetic order parameter $\Delta_\pi^{(+)}$ is distinct from the electron-hole excitation gap $E_{gap}^{(+)}$. This in turn gives rise to a smooth magnetic crossover of bound electron-hole pairs (excitons) from an itinerant magnetism with relatively small band-like moment ($s_{rmsl} \approx 1/2$) to a localized magnetsm of Bose condensated electron-hole pairs with well developed local moment.

The overall picture of magnetic crossover is found independent on the details of the electronic structure and the results are similar to the simple case of constant density of states. The work currently in progress is aimed to apply the GSCF approach for studies magnetic crossover within the Hubbrd model in higher dimensions.

Acknowledgements

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