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Superconductivity, magnetism and mapping between the attractive and repulsive Hubbard models

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The exact Bethe-ansatz and generalized self-consistent field (GSCF) ground-state properties of the one-dimensional (1d) Hubbard model for $U > 0$ and $U < 0$ are compared. The GSCF approach displays full mapping between $U > 0$ and $U < 0$ models.

KEYWORDS: Hubbard model, Bethe-ansatz, off-diagonal long-range order, ferromagnetism

§1. Introduction

One of the interesting features of the Hubbard model is the existing symmetry between $U > 0$ and $U < 0$ cases. It has been known for a long time that the positive-U model at half-filling ($n = 1$) can be mapped into the negative-U model for zero magnetic field ($h = 0$) and general electron concentration n by performing electron-hole transformation on one of the spin species.[1–5] In fact we recently found the strong equivalency between the BCS-BC crossover for the electron pairs in superconductivity for $U < 0$ at general concentration n and corresponding magnetic crossover for $U > 0$, driven by magnetic field $h \neq 0$, from itinerant BCS-like magnetism of weakly bound electron-hole pairs into the localized magnetic regime (local pairs).[6–9]

One of the motivations of this article is to make use of the existing knowledge about the repulsive and attractive Hubbard model in any dimension by extending the mapping between the ground state properties and various phenomena in the superconductivity and magnetism for an entire parameter space U/t, magnetic field h and electron concentration $0 \leq n \leq 1$. A rigorous proof was given that the unique ground state of the negative-U Hubbard model on some bipartite lattices possesses off-diagonal long-range order (ODLRO) within the finite range of electron concentration, regardless of lattice dimensions (d).[10] Another important exact result is the Nagaoka's theorem about the itinerant ferromagnetism for one hole in $d > 1$ bipartite lattices at large-U limit.[11]

Using the analogy between $U > 0$ and $U < 0$ Hubbard models one can show the correspondence (mapping) between the Nagaoka xy ferromagnetism in the vicinity of half-filling and ODLRO 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 generalized mean field (GSCF) results in one dimesion.[6,7]

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§2. Mapping

The bipartite Hubbard lattice (N_{latt}-even) with $U > 0$ can be reinterpreted in terms of electron-hole pairs for two-orbital model of spinless fermions with intrasite attraction $U < 0$[4,5] through the performance of the electron-hole transformation on the electron operators for one of species (spin-up)[1–3] such as

$$b^+_{i\downarrow} = c^+_{i\downarrow}\ , \qquad b^+_{i\uparrow} = (-1)^i c_{i\uparrow}\ . \tag{2.1}$$

$$b_{i\downarrow} = c_{i\downarrow}\ , \qquad b_{i\uparrow} = (-1)^i c^+_{i\uparrow}\ , \tag{2.2}$$

where i is the lattice site number.

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 $\Delta^{(+)}_{\mathbf{q}} \Rightarrow \Delta^{(-)}_{\pi-\mathbf{q}}$. Note that for $\bar{h}/2 \equiv (h + 2Us)/2$ the corresponding parameter $-\bar{h}/2 \Rightarrow \bar{\mu} \equiv \mu + U\bar{n}/2$ in the transformed Hamiltonian with $U < 0$ plays the role of a renormalized chemical potential $\bar{\mu}$ for the electron-hole pairs concentration $n \Rightarrow 1 - 2s$.

With the use of the newly defined creation and annihilation operators we find a simple relation between the repulsive $U > 0$ and attractive $U < 0$ Hubbard models for arbitrary $h > 0$ and all n. The self-consistent equations for $U > 0$ are equivalent to those obtained within the attractive Hubbard model.[7–9] Earlier we analyzed these self-consistent and Bethe-ansatz equations for the attractive Hubbard model and repulsive Hubbard models in an entire range of $|U|/t$, n and h, and found various stable inhomogeneous magnetic and superconducting states .[7]

§3. Results

Here we present the results of calculations as a functions of general electron concentration n and average longitudinal spin (magnetization) s. In Fig. 1 the mapping between $U > 0$ and $U < 0$ models in the GSCF approach along with exact solution are shown for the kinetic energy at half-filling ($U > 0$) and in the presence of magnetic field ($U < 0$) in the entire space of $1 - 2s$ and n respec-

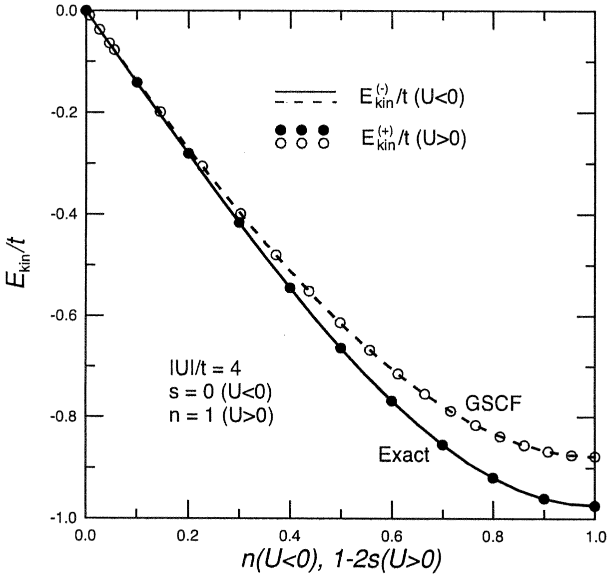

Fig. 1. The GSCF and exact ground state kinetic energies for the attractive ($E^{(-)}_{\rm kin}/t$) and repulsive ($E^{(+)}_{\rm kin}/t$) Hubbard models at $|U|/t = 4$ as a function as a function of n ($s = 0$) and as a function $1 - 2s$ ($n = 1$) respectively.

tively. The variation of the GSCF order parameter $\Delta^{(+)}_{\pi}$ *versus* $1 - 2s$ at $n = 1$ for $U > 0$ closely follows the the variation of $\Delta^{(-)}_0$ *versus* n at $s = 0$ for $U < 0$. The kinetic energy $E^{(+)}_{\rm kin}$ for $U > 0$ at $n = 1$ can be calculated by differentiating the energy with respect to t

$$E^{(+)}_{\rm kin} = \frac{1}{N_{\rm latt}} \sum_k \frac{(\epsilon_k - h/2 - sU)\,\epsilon_k}{\sqrt{(\epsilon_k - h/2 - sU)^2 + \left(\Delta^{(+)}_{\pi}\right)^2/4}}. \quad (3.1)$$

The variation of $E^{(-)}_{\rm kin}$ versus n at $U < 0$ is analogous to the variation of $E^{(+)}_{\rm kin}$ at $U > 0$. Indeed in Fig. 1 our calculations show a perfect matching between $E^{(-)}_{\rm kin}$ *versus* n for at $U < 0$, $E^{(+)}_{\rm kin}$ *versus* $1 - 2s$ for $U > 0$.

It can be seen that under the electron-hole transformation $n \Leftrightarrow 1 - 2s$ and $q \Leftrightarrow \pi - q$[9] there is a symmetry between

$$\bar{E}^{(-)} = E^{(-)} - \left(\frac{n}{2} - s\right) U \quad (3.2)$$

($U < 0$) and

$$\bar{E}^{(+)} = E^{(+)} \quad (3.3)$$

($U > 0$) at $s \Leftrightarrow (1 - n)/2$ where $E^{(-)}$ and $E^{(+)}$ are the energies of the attractive and repulsive Hubbard models respectively (see Fig. 2). Using this symmetry one can easily calculate other physical quantities.

In summary, 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.

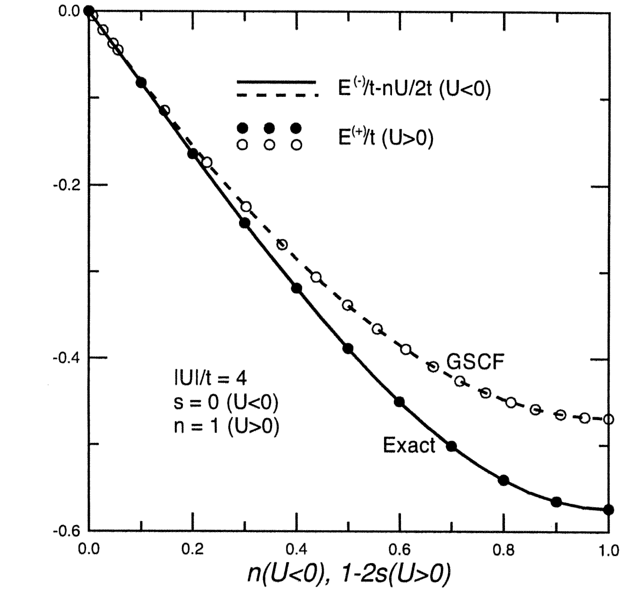

Fig. 2. The GSCF and exact results for the attractive ($\bar{E}^{(-)}/t = E^{(-)}/t - nU/2t$) and repulsive ($\bar{E}^{(+)}/t = E^{(+)}/t$) Hubbard models ($E^{(-)}$ and $E^{(+)}$ are the ground state energies) at $|U|/t = 4$ as a function of n ($s = 0$) and as a function of $1 - 2s$ ($n = 1$) respectively.

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