行政院國家科學委員會專題研究計畫成果報告

吸引性哈巴特模型基態性質之自洽場與精確解研究

The Self-Consistent Field and Exact Solution Study of the Ground-State Properties of the Attractive Hubbard Model

計畫編號：NSC 88-2112-M-032-011
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一、摘要

本計劃中預定之各項研究已全部完成。

我們用自洽場及精確解兩種方法研究了一維吸引性哈巴特模型之基態性質及其超導-超流過渡現象。計算了基態能量、雙佔有結點濃度 D、化學勢及動能等物理量。自洽場及精確解的計算結果在電子濃度 n 及相互作用強度 $-U/t$ 的廣泛範圍內符合得很好。自洽場理論顯示, 在 n 與 $-U/t$ 變化時 BCS 超導性會平穩地過渡到局部對偶的超流性。我們發現, 在 D, n 及 BCS 有序化參數之間有簡單關係存在。

本計劃研究成果發表於國際學術期刊 [1, 2]，並在國內及國際學術會議上宣讀 [3 - 6]。

關鍵詞：電子關聯，電子相變，一維吸引性哈巴特模型，高溫超導性。

Abstract

The crossover and the ground-state properties in the one-dimensional attractive Hubbard model are studied using the exact Bethe-ansatz equations and the self-consistent field (SCF) approach. The exact and the SCF results for the ground-state energy, the concentration of double occupied sites D, the chemical potential and the kinetic energy are in good agreement for all electron concentrations n and a wide range of the coupling strength $-U/t$. The SCF theory in one dimension suggests a smooth crossover from the BCS superconductivity to the superfluidity of local pairs under variation of $-U/t$ and n. We found a simple relationship between D, n and the BCS order parameter.

Keywords: electron correlation, electron phase transition, one-dimensional attractive Hubbard model, high T_c superconductivity

二、主要成果

The crossover from weak to strong coupling superconductivity in the one-dimensional attractive Hubbard model for different concentrations of electrons is studied within the self-consistent field (SCF) theory with a renormalized chemical potential μ and compared with our results obtained by means of the exact Bethe-ansatz equations in one dimension. There are extensive evidences for the local quasi one-dimensional character of electronic structure in high temperature superconductors. Unlike the conventional superconductors in which the phase coherence and pairing occur simultaneously and at same temperature, in the underdoped cuprates there exists a separation between the pair binding regime and superconductivity regime as the doping is decreased below an optimal value. It is also well established that the pseudogap in the normal state has

essentially the same magnitude and momentum dependence as in the superconducting state. The evolution of the energy gap with the band filling n and the coupling strength $-U/t$ and the formation of the energy gap in the SCF approach are examined. The interplay between Bose condensation and the localization of electrons with purely attractive interaction is discussed in the context of existence of a pseudogap in the insulating state of the underdoped cuprates at vanishing carriers concentration. In general separation between the binding and phase coherence can be accomplished either by increasing $|U/t|$ or by decreasing n. We study the pair formation associated with the distinct change in the band structure driven by both U/t and n.

The crossover from Cooper pairing phase to Bose condensation phase as a function of $-U/t$ and n within the SCF approach is smooth. The minimum gap at zero momentum serves as a measure to distinguish the different regimes on the phase diagram, where either BCS-like (the minimum gap $E_{gap} = \Delta$ occurs at momentum $k \neq 0$) or Bose condensation behavior (the minimum gap occurs at $k = 0$) take place. We obtained a ground-state phase diagram in the n-U plane using our SCF results and found that the critical concentration n_c, above which the system undergoes the crossover from the Bose condensation regime into the BCS state, increases monotonously with increasing $-U/t$.

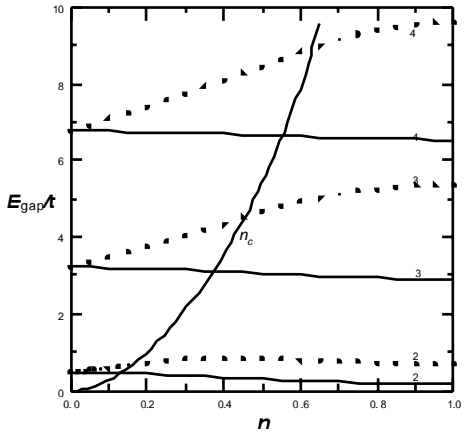

Fig. 1

In Fig. 1 we show the energy gap E_{gap} as a function of the electron concentration n in the exact theory (solid curves) and in the SCF approach (dots). The curve indexes 2 – 4 correspond to the values of the interaction strength $-U/t$ = 2.0, 6.0, 10.0.

Near zero filling the exact gap increases slowly with decreasing n, whereas the SCF gap slowly decreases (Fig. 1). The bold curve indicates a smooth evolution of the SCF gap from the BCS regime into the Bose condensation regime by increasing of U/t and decreasing of n respectively. The SCF order parameter Δ is significantly suppressed, while E_{gap} is relatively large. The SCF approach provides a common analytical relationship for the concentration of double occupied sites

$$D = n^2/4 + \Delta^2/4U^2,$$

valid for any $-U/t$ and n. Thus the order parameter Δ has physical meaning closely associated with D, rather than E_{gap}. The suppression of the superconductivity and preservation of the gap at vanishing concentration of carriers (or band filling) are consistent qualitatively with the structure of the gap (or pseudogap at finite temperatures) in the overdoped regime, which has been observed recently in low temperature tunneling experiments in YBCO and BSCCO.

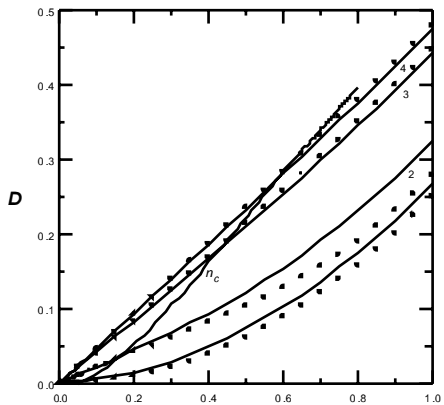

Fig. 2

The SCF data for D values follow the exact result much more closely at large values of $|U/t|$. The maximum deviation occurs at small values of $|U/t|$ near half-filled band (Fig. 2; notation is the same as in Fig. 1, the index 1 corresponds to $-U/t = 0.5$). The SCF result for D barely changes at weak coupling $|U/t| \ll 1$, while the exact result gives a linear dependence. The derivative of D with respect to $-U$ (positive slope) measures the degree to which pairing correlations are included in the SCF approach at weak coupling limit. The correlation effect in the SCF approach becomes ineffective for $|U/t| \ll 1$. In contrast, at large $|U/t|$ values the SCF approach suppresses the fluctuations and therefore slightly overestimates the exact D values.

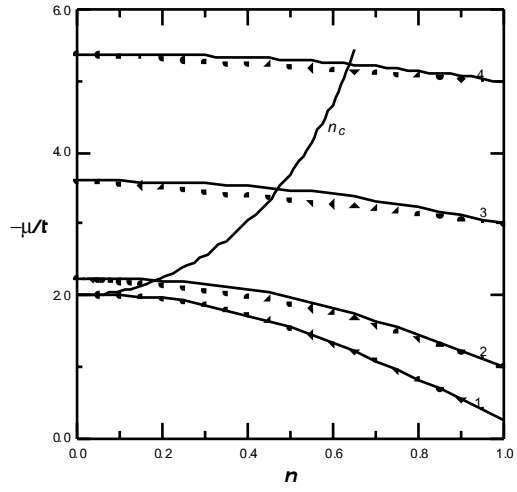

Fig. 3

The smooth character of transition is confirmed also by inspection in behavior of the ground state energy E_{GS} and the chemical potential μ.

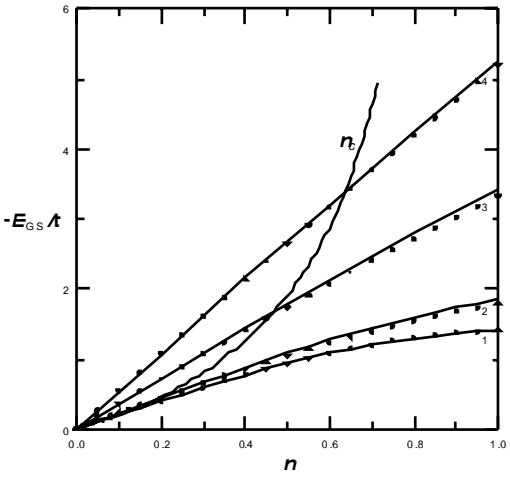

Fig 4

In Fig. 3 – Fig. 5 (Notation is the same as in Fig. 1 and 2) we show the ground-state chemical potential μ, energy E_{GS}, and kinetic energy E_{kin} as functions of n for various $-U/t$. Note that the SCF results nicely follow the exact one for all $-U/t$ values. The exact and SCF results show significant decreasing of the kinetic energy (narrowing of the effective bandwidth) by increasing $|U|/t$. The SCF approach overestimates the effect of pairing correlation in the kinetic energy at weak coupling and underestimates it at strong coupling.

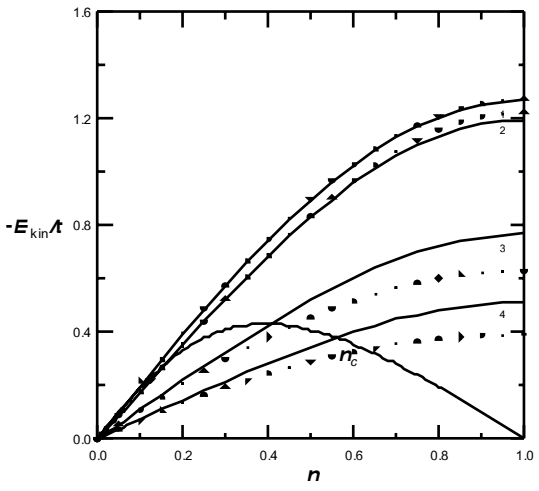

Fig. 5

The good numerical agreement of the SCF ground state results with the exact Bethe-ansatz studies suggests that the SCF theory provides the correct picture of crossover in one dimension.

Our results are published in Refs. [1, 2] and reported on national and international conferences [3 - 6].

三、參考文獻

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