

Dimensional crossover of the superfluid state in the attractive Hubbard model

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Abstract. The superfluid state in the attractive Hubbard is studied for the stacked square lattices to simulate the two- to three-dimensional crossover effects. We use the variation cluster approximation to calculate the order parameter and pair coherence length from the weak-coupling BCS state to the strong-coupling BEC state at $T = 0$ K. We show that in the weak-coupling BCS region the density of states at Fermi level plays an important role in the dimensional crossover of the superfluid state but in the strong-coupling BEC region the quantum fluctuations depending on the dimensionality of the system play an essential role.

1. Introduction

The physics of the crossover between the weak-coupling Bardeen-Cooper-Schrieffer (BCS) regime and the strong-coupling Bose-Einstein condensed (BEC) limit has long been one of the major issues in condensed matter physics [1, 2]. In systems of ultracold fermionic atoms [3], a tunable pairing interaction associated with the Feshbach resonance enables one to observe the crossover between the BCS- and BEC-type superfluid states experimentally [4]. Recently, the two-dimensional (2D) phenomena have been discussed in the ultracold fermionic gases prepared by modifying the 1D optical lattices. Also, by tuning the strength of a periodic potential of the optical lattice, the 2D to three-dimensional (3D) crossover behaviors have been investigated in a very controlled manner [5, 6, 7, 8, 9].

In this paper, motivated by the above development in the field, we study the dimensional crossover effects in the ultracold fermionic systems, focusing in particular on their superfluid states. Here, we adopt the attractive Hubbard model for spin-1/2 fermionic atoms and simulate the dimensional crossover using the 2D square lattices stacked with the controllable interplaner hopping parameter. We employ the variational cluster approximation (VCA), one of the quantum cluster methods, where unlike in the dynamical-mean-field-theory (DMFT) calculations the effects of spatial correlations of atoms can be taken into account. We thereby calculate the order parameter and pair coherence length from the weak-coupling BCS to strong-coupling BEC states as a function of the interplaner hopping parameter at $T = 0$ K. We will show that in the weak-coupling BCS region the density of states (DOS) at the Fermi level plays an important role in the dimensional crossover but the quantum fluctuation due to dimensionality of the system plays an important role in the strong-coupling BEC region.



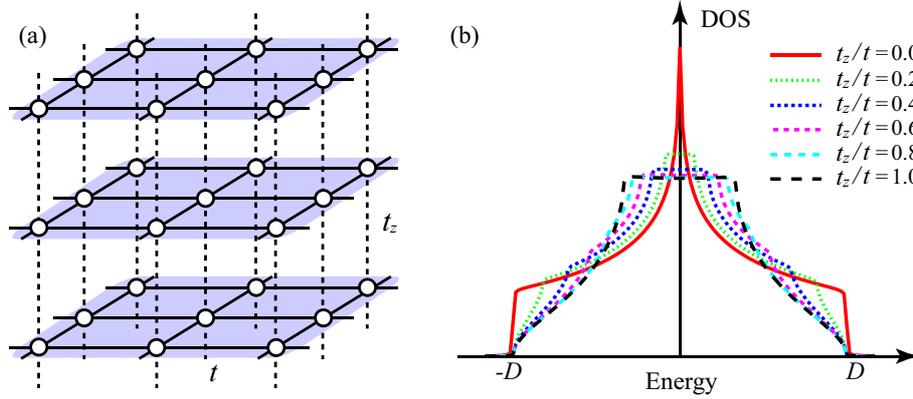


Figure 1. (a) The stacked 2D square lattices and (b) DOS of the noninteracting band structure of our model.

2. Model and method

2.1. Attractive Hubbard model with the interplaner hopping parameter

To discuss the dimensional crossover in the superfluidity, we consider the attractive Hubbard model defined on the stacked square lattices shown in Fig. 1(a). The Hamiltonian reads

$$\mathcal{H} = - \sum_{\langle i,j \rangle, \sigma} t_{ij} \left(c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.} \right) - U \sum_i n_{i\uparrow} n_{i\downarrow} - \mu \sum_{i,\sigma} n_{i\sigma}, \quad (1)$$

where $c_{i\sigma}$ ($c_{i\sigma}^\dagger$) is the annihilation (creation) operator of a fermion with spin σ ($=\uparrow, \downarrow$) at site i and $n_{i\sigma}$ is the number operator of a fermion with spin σ at i site. t_{ij} is the hopping parameter between the nearest-neighbor sites $\langle ij \rangle$, U (> 0) is the attractive on-site Hubbard interaction and μ is the chemical potential. In this paper, we assume the system of stacked 2D square lattices coupled with the interplaner hopping parameter [see Fig. 1(a)]: we assume the hopping parameters in the xy -plane as $t_{ij} = t$ and those of the z -direction as $t_{ij} = t_z$. The dimensional crossover is thus controlled by t_z with $0 \leq t_z \leq t$, where $t_z = 0$ for the 2D square lattice and $t_z = t$ for the 3D cubic lattice. The bandwidth of the noninteracting band structure $D = 4t + 2t_z$ is used as the unit of energy when we consider the calculated physical quantities at different t_z values. It is well known that the s -wave superfluid state is realized in this model in the two and higher dimensions at $T = 0$ K for all values of U (> 0) and in the entire particle density [10, 11, 12]. In particular, the BCS-BEC crossover in the attractive Hubbard model has been studied in detail by DMFT [13, 14, 15, 16, 17, 18] and also recently by VCA [19]. However, not much is known of its dimensional crossover.

2.2. Variational cluster approximation

We employ the method of VCA [20, 21], which is based on the self-energy functional theory (SFT) [22]. The trial self-energy for the variational method is generated from the exact self-energies of the disconnected finite-size clusters, which act as a reference system. The variational Hamiltonian is defined as $\mathcal{H}' = \mathcal{H} + \mathcal{H}_{\text{pair}} + \mathcal{H}_{\text{local}}$ with

$$\mathcal{H}_{\text{pair}} = \Delta' \sum_i \left(c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger + \text{H.c.} \right) \quad (2)$$

$$\mathcal{H}_{\text{local}} = \varepsilon' \sum_{i,\sigma} n_{i\sigma}, \quad (3)$$

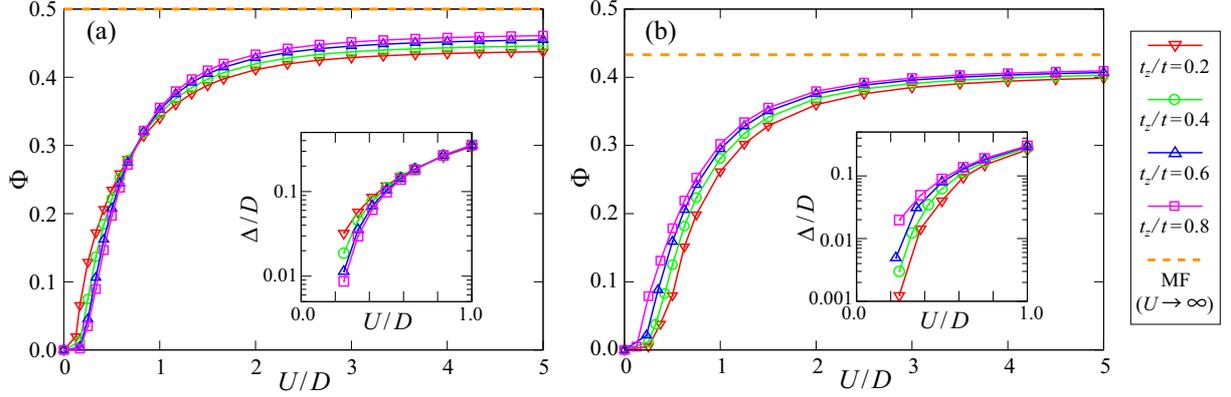


Figure 2. Calculated t_z dependence of the anomalous expectation value $\Phi = \langle c_{i\uparrow}c_{i\downarrow} \rangle$ and order parameter $\Delta = U\Phi$ as a function of U/D at (a) half and (b) quarter filling. The insets enlarge the weak-coupling region.

where the Weiss field for the s -wave pairing Δ' and the on-site potential ε' are the variational parameters. We use the Nambu formalism $\Psi_i^\dagger = (c_{i\uparrow}^\dagger, c_{i\downarrow})$ to solve the eigenvalue problem by the Lanczos exact-diagonalization method. We hereafter denote all the $2L_c \times 2L_c$ Nambu matrices by a 'hat' on top. We use a $L_c = 2 \times 2 \times 2 = 8$ site cluster as a reference system, whereby the effects of spatial correlations within this cluster are taken into account exactly. Within the SFT, the grand potential at $T = 0$ K is given by

$$\Omega = \Omega' - \frac{1}{N} \oint_C \frac{dz}{2\pi i} \sum_{\mathbf{K}} \ln \det [\hat{\mathbf{I}} - \hat{\mathbf{V}}(\mathbf{K})\hat{\mathbf{G}}'(z)], \quad (4)$$

where Ω' is the grand potential of the reference system, $\hat{\mathbf{I}}$ is the unit matrix, $\hat{\mathbf{V}}$ is the hopping parameter between the adjacent clusters and $\hat{\mathbf{G}}'$ is the exact Green's function of the reference system. \mathbf{K} -summation is made in the reduced Brillouin zone of the superlattice and the contour C of the frequency integral encloses the negative real axis. The variational parameters Δ' and ε' are optimized based on the variational principle, i.e., $(\partial\Omega/\partial\Delta', \partial\Omega/\partial\varepsilon') = (0, 0)$. The solution with $\Delta' \neq 0$ corresponds to the superfluid state. The average particle density $n (= \langle n_{i\sigma} \rangle)$ is expressed as

$$n = \frac{1}{NL_c} \oint_C \frac{dz}{2\pi i} \sum_{\mathbf{K}} \sum_{i=1}^{L_c} \mathcal{G}_{ii}(\mathbf{K}, z), \quad (5)$$

where \mathcal{G} is the diagonal term of the $L_c \times L_c$ matrix $\hat{\mathcal{G}}(\mathbf{K}, \omega) = [\hat{\mathbf{G}}'^{-1}(\omega) - \hat{\mathbf{V}}(\mathbf{K})]^{-1}$. The chemical potential μ is determined to keep the particle density at a given value of n .

3. Results of calculations

3.1. Order parameter

Let us first discuss the anomalous expectation value $\Phi = \langle c_{i\uparrow}c_{i\downarrow} \rangle$; the order parameter is given by $\Delta = U\Phi$. Within the framework of VCA, this is defined as

$$\Phi = \frac{1}{NL_c} \oint_C \frac{dz}{2\pi i} \sum_{\mathbf{K}} \sum_{i=1}^{L_c} \mathcal{F}_{ii}(\mathbf{K}, z), \quad (6)$$

where \mathcal{F} is the anomalous (or off-diagonal) term of the Green's function $\hat{\mathcal{G}}(\mathbf{K}, \omega)$.

In Fig. 2, we show the calculated results for Φ as a function of U/D at half and quarter fillings. In the weak-coupling region, where $U/D \ll 1$, we find that Φ increases exponentially with U and moreover, with increasing t_z , Φ decreases at half filling and increases at quarter filling. These behaviors may be understood within the BCS mean-field theory, where the order parameter is given as $\Delta \propto \exp[-1/U\rho(\varepsilon_F)]$ with the DOS at the Fermi level $\rho(\varepsilon_F)$. Thus, Φ increases exponentially with U . Also, the dimensional crossover from 2D to 3D may be understood via the behavior of $\rho(\varepsilon_F)$ [see Fig. 1(b)]; the DOS of the 2D square lattice has a van Hove singularity at the Fermi level at half filling, which decreases with increasing t_z , but $\rho(\varepsilon_F)$ at quarter filling increases with increasing t_z . The dimensional crossover (or the t_z dependence) of Φ in the weak-coupling region may thus be understood.

In the strong-coupling region, where $U/D \gg 1$, we find that Φ increases with increasing t_z , irrespective of the band filling (see Fig. 2). At $U/D \rightarrow \infty$, Φ is given by $\sqrt{n(1-n)}$ in the mean-field theory, irrespective of the spatial dimension of the system, and thus $\Phi = 1/2$ at half filling ($n = 1/2$ per spin) and $\Phi = \sqrt{3}/4$ at quarter filling ($n = 1/4$ per spin). Now, in the strong-coupling region with finite U/D values, we can understand the behavior of Φ in terms of the effective spin-1/2 Heisenberg model in a magnetic field, which is obtained by the strong-coupling expansion of the attractive Hubbard model. The Hamiltonian reads $\mathcal{H}_{\text{eff}} = \sum_{\langle i,j \rangle} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j - h \sum_i S_i^z$, where we use the particle-hole transformation $a_{i\uparrow} = c_{i\uparrow}$ and $a_{i\downarrow} = (-1)^i c_{i\downarrow}^\dagger$ [23], and define the spin operator $\mathbf{S}_i = \sum_{\alpha,\beta} a_{i\alpha}^\dagger \sigma_{\alpha\beta} a_{i\beta} / 2$. The exchange interaction is given by $J_{ij} = 4t_{ij}^2/|U|$ with $J_{ij} = J = 4t^2/|U|$ in the xy -plane and $J_{ij} = J_z = 4t_z^2/|U|$ in the z -direction, and the magnetic field is given by $h = 2\mu + |U|$. The superfluid state in the original model thus corresponds to the magnetically ordered state in the xy -plane in the effective model; e.g., the superfluid states at half ($n = 0.5$) and quarter ($n = 0.25$) fillings correspond, respectively, to the magnetically ordered states in the xy -plane with total magnetizations of $m = \sum_i \langle S_i^z \rangle / N = 0$ (with nonvanishing local moments) and $m = 0.25$. From this mapping, we may argue that in 2D, where the system has strong quantum spin fluctuations due to its low dimensionality, the superfluidity (and order parameter) is suppressed stronger than in 3D, as is consistent with our calculated results shown in Fig. 2. This argument also explains why the values of Φ obtained in VCA are smaller than the mean-field values neglecting quantum fluctuations.

3.2. Pair coherence length

Let us then discuss the spatial extension of the Cooper pair. Here, we calculate the pair coherence length ξ from the condensation amplitude $F(\mathbf{k})$ calculated by the cluster perturbation theory (CPT) [24]. The anomalous Green's functions are calculated by CPT with the optimized variational parameters, which are defined as

$$\mathcal{F}_{\text{cpt}}(\mathbf{k}, \omega) = \frac{1}{L_c} \sum_{i,j=1}^{L_c} \mathcal{F}_{ij}(\mathbf{k}, \omega) e^{-i\mathbf{k} \cdot (\mathbf{r}_i - \mathbf{r}_j)}, \quad (7)$$

and the condensation amplitude is given by

$$F(\mathbf{k}) = \oint_C \frac{dz}{2\pi i} \mathcal{F}_{\text{cpt}}(\mathbf{k}, z), \quad (8)$$

from which the pair coherence length ξ is given by [19, 25]

$$\xi^2 = \frac{\sum_{\mathbf{k}} |\nabla_{\mathbf{k}} F(\mathbf{k})|^2}{\sum_{\mathbf{k}} |F(\mathbf{k})|^2}. \quad (9)$$

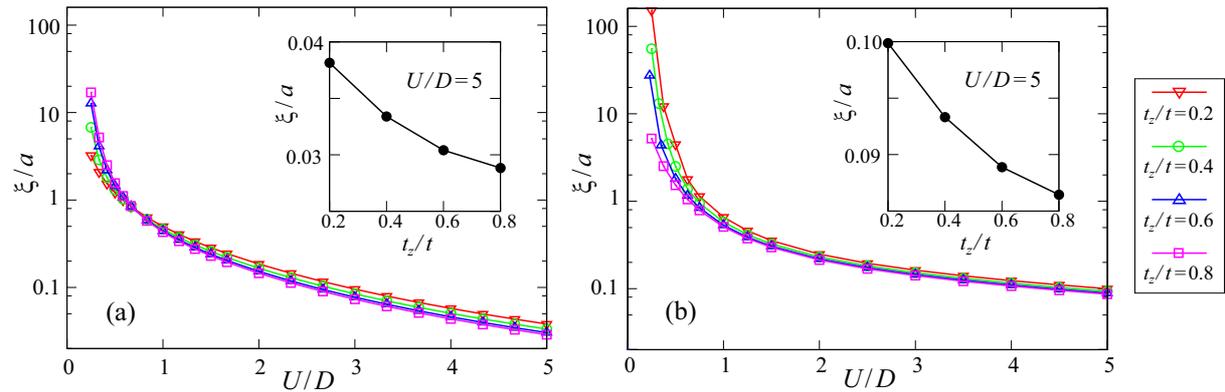


Figure 3. Calculated pair coherence length ξ as a function of U/D at (a) half and (b) quarter fillings. The insets show the t_z dependence of ξ at $U/D = 5$.

In Fig. 3, we show the calculated result for ξ as a function of U/D at half and quarter fillings. In the weak-coupling region, ξ is much larger than the lattice constant a . With increasing U , ξ decreases smoothly to smaller values, and in the strong-coupling region, it becomes much smaller than the lattice constant. Thus, a smooth crossover occurs from the weakly paired BCS-like state ($\xi \gg a$) to the tightly paired BEC state ($\xi \ll a$). In the weak-coupling BCS region, ξ is enhanced with increasing t_z at half filling but is suppressed with increasing t_z at quarter filling. This behavior may be understood just as in the behavior of Φ , where the value of $\rho(\varepsilon_F)$ plays an important role in the BCS region: i.e., ξ is suppressed (enhanced) with increasing (decreasing) $\rho(\varepsilon_F)$. In the BEC region, on the other hand, the pairs are tightly bounded with increasing t_z both at half filling and at quarter filling. In the strong-coupling region, the quantum fluctuations play an important role, which are suppressed in higher dimensions, just as in the behavior of Φ . ξ is thus suppressed and the pairs are more tightly bound with increasing t_z (or decreasing the quantum fluctuations) as shown in the insets of Fig. 3.

4. Summary

Motivated by the experimental realization of the dimensional crossover of the superfluidity in the ultracold fermionic systems, we have studied the superfluidity of the attractive Hubbard model defined on the 2D square lattices stacked with the interplaner hopping parameter. Using the method of VCA, we have calculated the order parameter and pair coherence length in the parameter regions from the weak-coupling BCS to strong-coupling BEC states. We have shown that in the weak-coupling BCS region the DOS at the Fermi level plays an important role in the dimensional crossover of the superfluid state but in the strong-coupling BEC region the quantum fluctuations depending on the dimensionality of the system play an essential role in its dimensional crossover.

Acknowledgments

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