Interplay Between Condensation Energy, Pseudogap, and the Specific Heat of a Hubbard Model in a $n$-Pole Approximation

A. C. Lausmann · E. J. Calegari · S. G. Magalhaes · C. M. Chaves · A. Troper

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Abstract The condensation energy and the specific heat jump of a two-dimensional Hubbard model, suitable to discuss high-$T_c$ superconductors, are studied. In this work, the Hubbard model is investigated by the Green’s function method within a $n$-pole approximation, which allows to consider superconductivity with $d_{x^2-y^2}$-wave pairing. In the present scenario, the pseudogap regime emerges when the antiferromagnetic correlations become sufficiently strong to move to lower energies the region around of the nodal point $(\pi, \pi)$ on the renormalized bands. It is observed that above a given total occupation $n_T$, the specific heat jump $\Delta C$ and also the condensation energy $U(0)$ decrease signaling the presence of the pseudogap.

Keywords Superconductivity · Pseudogap · Specific heat · Condensation energy · Hubbard model

1 Introduction

It is believed that the two-dimensional Hubbard model [1] is able to capture the essential physics of the high-temperature superconductivity (HTSC) in copper-oxides [2, 3]. In such systems, understanding the interplay between the superconductivity and the
pseudogap regime could be the key to clarify the mechanisms behind the unconventional superconductivity. Experimental results for some cuprates indicate a close relation among specific heat, condensation energy, and the pseudogap [4–7]. More precisely, due to the presence of a pseudogap on the normal state density of states, the jump in the specific heat and the superconducting condensation energy decrease below a given doping. Besides, according to references [3,8], the HTSC phase diagram can be separated in two regimes: a weak coupling regime and a strong coupling regime [3,8]. The weak coupling regime could be described, approximately, in terms of the conventional BCS superconductivity while the strong coupling regime would be governed by unconventional superconductivity. In this scenario, the pseudogap is a property of the strong coupling regime [3]. In this context, the investigation of the specific heat and the condensation energy of two-dimensional Hubbard model may give us important insights about the physics of the HTSC.

In the present work, the normal-state pseudogap and the superconducting regime of a two-dimensional Hubbard model is investigated within the Green’s functions technique [9,10]. The pseudogap emerges on the strongly correlated regime in which the antiferromagnetic (AF) correlations associated with the spin–spin correlation function $\langle S_i \cdot S_j \rangle$ becomes sufficiently strong to open a pseudogap in the region $(\pi, 0)$ on the Fermi surface. Such normal-state pseudogap is also observed in the $(\pi, 0)$ point of the renormalized surface.

### 2 Model and Method

The repulsive ($U > 0$) one band two-dimensional Hubbard model [1] studied here is

$$
H = \sum_{\langle\langle ij\rangle\rangle}\sigma t_{ij}c_{i\sigma}^\dagger c_{j\sigma} + \frac{U}{2} \sum_{i\sigma} n_{i,\sigma} n_{i,-\sigma} - \mu \sum_{i\sigma} n_{i\sigma},
$$

which takes into account hopping to first and second nearest neighbors. The quantity $\mu$ represents the chemical potential, $n_{i,\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$ is the number operator, and $c_{i\sigma}^\dagger$ ($c_{i\sigma}$) is the fermionic creation (annihilation) operator at site $i$ with spin $\sigma = \{\uparrow, \downarrow\}$. We use the Green’s function technique in the Zubarev’s formalism [11]. The equation of motion of the Green’s functions are treated within the $n$-pole approximation introduced by Roth [9,10]. In this procedure, a set of operators $\{\hat{A}_n\}$ is introduced in order to describe the most important excitations of the system. The $n$-pole approximation assumes that the commutator $[\hat{A}_n, \hat{H}]$, which appears in the equation of motion of the Green’s functions, can be written as $[\hat{A}_n, \hat{H}] = \sum_m K_{nm} \hat{A}_m$, where the elements $K_{nm}$ are determined by anti-commuting both sides of this relation with the operator set $\{\hat{A}_n\}$ and taking the thermal average. We get $\mathbf{K} = \mathbf{E}\mathbf{N}^{-1}$ with

$$
E_{nm} = \langle [\hat{A}_n, \hat{H}], \hat{A}_m^\dagger \rangle_+ \quad \text{and} \quad N_{nm} = \langle [\hat{A}_n, \hat{A}_m^\dagger]_+ \rangle.
$$

In terms of $\mathbf{E}$ and $\mathbf{N}$, the Green’s function matrix is $\mathbf{G}(\omega) = \mathbf{N}(\omega \mathbf{N} - \mathbf{E})^{-1}\mathbf{N}$. Both $\mathbf{E}$ and $\mathbf{N}$ can be determined through Eq. 2 if the set of operators $\{\hat{A}_n\}$ is known. As we
are interested in investigating both the normal and the superconducting regimes, we use the operator set \( \{ \hat{A}_n \} = \{ \hat{c}_{i\sigma}, \hat{c}_{i\sigma}^\dagger, \hat{n}_{i\sigma}, \hat{n}_{i\sigma}^\dagger \} \).

The energy per particle can be obtained from the Green’s function following the procedure described by Kishore and Joshi [12]. For the Hubbard model introduced in Eq. 1, the internal energy per particle in the superconducting state is

\[
E = \frac{1}{2L} \sum_{k,\sigma} \sum_{i=1}^{4} Z_{i,k\sigma} (\varepsilon_k + \mu + E_{i,k\sigma}) f(E_{i,k\sigma}) - \mu n_T \tag{3}
\]

where \( n_T = n_{-\sigma} + n_{\sigma} \) is the total occupation, \( Z_{i,k\sigma} \) are the spectral weights [10] of the Green’s function \( G_{k,\sigma}^{(1)} = \langle \langle \hat{c}_{k\sigma}^\dagger \rangle \hat{c}_{k\sigma} \rangle \), and \( f(\omega) \) is the Fermi function. In the superconducting state, the renormalized bands are

\[
E_{i,k\sigma} = (-1)^{(j+1)} \sqrt{\omega_{j,k\sigma}^2 + \frac{(-1)^{(j+1)} |\gamma_k|^2 [(\varepsilon_k + U n_{-\sigma} - \mu)^2 - \omega_{j,k\sigma}^2]}{n_{-\sigma}^2 (1 - n_{-\sigma})^2 (\omega_{2,k\sigma}^2 - \omega_{1,k\sigma}^2)}} \tag{4}
\]

with \( j = 1 \) if \( i = 1 \) or 2, and \( j = 2 \) if \( i = 3 \) or 4, \( \gamma_k = 2t\gamma (\cos(k_x a) - \cos(k_y a)) \) is the gap function and \( \gamma \) is the superconducting order parameter with \( d_{x^2-y^2} \)-wave symmetry [10]. In the normal state, the renormalized bands are

\[
\omega_{j,k\sigma} = \frac{U + \varepsilon_k + W_{k,\sigma} - 2\mu}{2} - (-1)^{(j+1)} \frac{X_{k,\sigma}}{2} \tag{5}
\]

where \( X_{k,\sigma} = \sqrt{(U - \varepsilon_k + W_{k,\sigma})^2 + 4n_{-\sigma}U(\varepsilon_k - W_{k,\sigma})} \) is the unperturbed band energy \( \varepsilon_k = 2t[\cos(k_x a) + \cos(k_y a)] + 4t_2 \cos(k_x a) \cos(k_y a) \), where \( t \) is the first-neighbor and \( t_2 \) is the second-neighbor hopping amplitudes. \( W_{k,\sigma} \) is a band shift that depends on the correlation function [10, 13] \( \langle S_i \cdot S_j \rangle \).

The specific heat jump is \( \Delta C = \left[ \frac{C_S - C_N}{C_N} \right]_{T=T_c} \) with \( C_{S,N} = \frac{\partial E_{S,N}}{\partial T} \), \( E_S \), and \( E_N \) being the energy per particle in the superconducting and in the normal state, respectively. \( E_N \) is obtained from Eq. 3 keeping the superconducting order parameter equal to zero (\( \gamma = 0 \)). Now, let us define \( U(T) = F_N - F_S \) as the difference between the normal \( (F_N) \) and the superconducting \( (F_S) \) states Helmholtz free energy. The superconducting condensation energy is defined as

\[
U(0) = E_N - E_S \tag{6}
\]

3 Results

The main focus of the present work is the strong coupling regime in which unconventional superconductivity may occur. For this purpose, we analyzed the renormalized bands, the superconducting condensation energy and the specific heat jump as a function of the total occupation \( n_T \) and of the interaction \( U \).
Figure 1 shows the renormalized band $\omega_{1,\sigma k}$. In the left panel, $\omega_{1,\sigma k}$ is shown for different values of the total occupation $n_T$. The inset displays the region near the point $(\pi, 0)$ in which a pseudogap develops when the occupation is increased. For instance, when $n_T = 0.81$, the band intersects the Fermi energy $\varepsilon_F$, but for $n_T = 0.85$, the band does not reach the Fermi energy giving rise to a pseudogap between the band and $\varepsilon_F$. The right panel shows $\omega_{1,\sigma k}$ for $n_T = 0.85$ and different interactions $U$. The inset highlights a pseudogap on $(\pi, 0)$ for $U = 8.0|t|$ and $U = 10.0|t|$ and the absence of pseudogap for $U = 6.0|t|$. In the $n$-pole approximation used in this work [9,10], the Green’s functions naturally present a pole structure which contains the spin–spin correlation function [10] $\langle S_i \cdot S_j \rangle$. In the present scenario, the pseudogap emerges when the correlation function $\langle S_i \cdot S_j \rangle$ becomes sufficiently strong to move to lower energies the region of the nodal point $(\pi, \pi)$ of the renormalized band $\omega_{1,\sigma k}$. This occurs because the renormalized band $\omega_{1,\sigma k}$ is deeply influenced by the momentum structure of the spin–spin correlation function [14] $\langle S_i \cdot S_j \rangle$. Due to the antiferromagnetic character [10] of $\langle S_i \cdot S_j \rangle$, the region of the nodal point $(\pi, \pi)$ of $\omega_{1,\sigma k}$ is strongly affected (see Fig. 1). As a consequence, a pseudogap arises at the anti-nodal point $(\pi, 0)$. Moreover, the $\langle S_i \cdot S_j \rangle$ is very sensitive to $n_T$ and $U$, and indeed, $\langle S_i \cdot S_j \rangle$ increases [15] with $n_T$ and $U$. Therefore, when $\langle S_i \cdot S_j \rangle$ reaches a critical value $|\langle S_i \cdot S_j \rangle|_{c}$, the pseudogap emerges.

The density of states (DOS) for the renormalized band $\omega_{1,\sigma k}$ is shown in Fig. 2 for different occupations $n_T$. The vertical line in $\omega = 0$ indicates the position of the Fermi energy $\varepsilon_F$ and the model parameters are shown in the figure. When $n_T$ increases, the correlations become stronger, resulting in a narrowing of the density of states. However, the most important feature observed in the DOS is the reduction of the DOS on $\varepsilon_F$ for $n_T \gtrsim 0.83$. Such reduction is an effect of the presence of a pseudogap in the strongly correlated regime of the system.

The condensation energy $U(0)$ as a function of the total occupation $n_T$ is shown in Fig. 3a. Note that $U(0)$ increases with $n_T$, reaches a maximum, and then starts to decrease. The depletion of $U(0)$ for a $n_T$ greater than a given value is related to the development of a pseudogap near the anti-nodal points on the Fermi surface. This result
Fig. 2 The density of states (DOS) for different occupations $n_T$. The vertical line in $\omega = 0$ indicates the position of the Fermi energy $\varepsilon_F$. The inset shows the region near the Fermi energy $\varepsilon_F$. For $n_T \gtrsim 0.83$ the DOS at $\varepsilon_F$ is decreased indicating the presence of a pseudogap (Color figure online).

is in qualitative agreement with experimental data obtained for some cuprate systems [5,6]. Figure 3b shows $\langle S_i \cdot S_j \rangle$ as a function of $n_T$. The horizontal dotted line indicates approximately the value of $\langle S_i \cdot S_j \rangle$, from which the system enters in the underdoped strong coupling regime. Figure 3c displays the behavior of the condensation energy $U(0)$ as a function of the interaction $U$ for several occupations. It is interesting to note that there is an optimal value of $U$ which produces a maximum $U(0)$. However, such optimum value changes with the occupation $n_T$. This feature is associated to the opening of the pseudogap which occurs in the strong coupling regime. Therefore, if $n_T$ decreases, a higher value of $U$ is necessary for the system to access the strong coupling regime.
Fig. 4 The jump in the specific heat as a function of the total occupation (see the text) (Color figure online)

regime. The correlation function $\langle S_i \cdot S_j \rangle$ shown in Fig. 3d may serve as a parameter to indicate that the system is reaching the strong coupling regime. As in Fig. 3b, the horizontal dotted line indicates approximately the value of $\langle S_i \cdot S_j \rangle$, from which the system enters in the underdoped strong coupling regime. The results for condensation energy $U(0)$ versus $n_T$, Fig. 3a, are in qualitative agreement with a method based on the resonating valence bond (RVB) spin liquid [16] and also with results from the fluctuation-exchange (FLEX) approximation [17]. In the FLEX approximation, $U(0)$ increases with $U$ but does not present a maximum like the one observed in Fig. 3c. There are no available results for $U(0)$ versus $U$ in the RVB method [16].

Figure 4 shows the specific heat jump $\Delta C$ as a function of $n_T$. Note that initially the $\Delta C$ increases slightly with $n_T$ but, above $n_T \approx 0.83$, $\Delta C$ starts to decrease. The decreasing in $\Delta C$ is an evidence of the presence of a pseudogap in the underdoped regime and is close related to the development of a pseudogap on the density of states (DOS) (see Fig. 2). The decrease of the DOS on $\varepsilon_F$ when $n_T$ increases is directly related to the pseudogap on $\varepsilon_F$ and agrees with a high-resolution photoemission study [18] of $\text{La}_2-x\text{Sr}_x\text{CuO}_4$ which suggests that a pseudogap is mainly responsible for the similar behavior between the specific heat jump and the DOS($\varepsilon_F$) observed in the underdoped regime. This result for $\Delta C$ agrees at least qualitatively, with a method based on the resonating valence bond (RVB) spin liquid [16] in which the specific heat jump and the condensation energy decrease due to the opening of a pseudogap in the underdoped regime. Also, the result for $\Delta C$ shown in Fig. 4 is in qualitative agreement with the experimental data for some cuprates [4,5].

4 Conclusions

In this work, we have investigated the superconducting condensation energy $U(0)$ and the specific heat jump $\Delta C$ of a two-dimensional Hubbard model. The results show that both $U(0)$ and $\Delta C$ decrease in the strong coupling underdoped regime. It has been verified that this behavior is related to the opening of a pseudogap at the anti-nodal point $(\pi, 0)$ on the renormalized band $\omega_{1,\sigma k}$. In the strong coupling regime, the correlation function $\langle S_i \cdot S_j \rangle$ present in the band shift becomes sufficiently strong to move to lower energies the renormalized band $\omega_{1,\sigma k}$ in the region of the nodal point $(\pi, \pi)$.
and as a consequence, a pseudogap opens in the ($\pi$, 0) point. The results obtained here corroborate the scenario that attributes the pseudogap to the strong correlations present in the underdoped regime [8].

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