Specific heat of a non-local attractive Hubbard model

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Abstract

The specific heat of an attractive (interaction $G < 0$) non-local Hubbard model is investigated. We use a two-pole approximation which leads to a set of correlation functions. In particular, the correlation function $\langle S_i \cdot S_j \rangle$ plays an important role as a source of anomalies in the normal state of the model. Our results show that for a given range of $G$ and $\delta$ where $\delta = 1 - n_T (n_T = n_+ + n_-)$, the specific heat as a function of the temperature presents a two peak structure. Nevertheless, the presence of a pseudogap on the anti-nodal points $(0, \pm \pi)$ and $(\pm \pi, 0)$ eliminates the two peak structure, the low temperature peak remaining. The effects of the second nearest neighbor hopping on the specific heat are also investigated.

Keywords: D. Hubbard model, D. pseudogap, D. specific heat

1. Introduction

The phenomenology of high-$T_c$ Superconductors (HTSC) has brought several fundamental issues \cite{1}. One of these issues is certainly the nature of the pseudogap found in some of those materials. In the possible competing scenarios on the nature of the pseudogap, one should mention two of them. Assuming that the pseudogap occurs below a temperature $T^*$: (i) the pseudogap would be due to the formation of incoherent pairs until that a superconducting phase develops below the critical temperature $T_c$ \cite{2,3}; (ii) the pseudogap would be due to short-range fluctuations of magnetic nature which below a certain temperature $T_{\text{mag}}$ would give rise an ordered state ending at a Quantum Critical Point (QCP) which can coexist with the SC phase \cite{4}. Nevertheless, despite of the intense debate, the complete explanation for the nature of the pseudogap is clearly an unsolved question.

Quite recently, an attractive Hubbard model with non-local interaction \cite{5,6} has been considered using a two pole approximation \cite{7,8}. Although our model is not fully realistic for HTSC, it allows superconductivity with $d_{\text{xy}}$-wave symmetry \cite{9} and also can be quite useful to bring information on the possible sources of the pseudogap. In Refs. \cite{5,6}, it has been obtained the evolution of the Fermi surface from a closed shape to a hole pocket shape as well as the behavior of the $\chi$ with a maximum at $\delta'$ where $\delta = 1 - n_T (n_T = n_+ + n_-)$, and then, decreasing when $\delta < \delta'$. Remarkably, both results can be traced from one single mechanism, i. e. from short range antiferromagnetic (AF) correlations. To be precise, for a proper range of temperature and doping these correlations distort the renormalized quasi-particles bands shifting by $\Delta_c$ the flat region on the anti-nodal points $((0, \pm \pi))$ and $(\pm \pi, 0))$ to energies below the chemical potential $\epsilon_c$ \cite{5}. As a consequence, a pseudogap $\Delta_{PG} \approx \Delta_c$ emerges in the DOS close to the chemical potential.

The mechanism discussed in the previous paragraph also favors the existence of $d$-wave superconductivity in the attractive non-local Hubbard model \cite{5}. This occurs because the magnetic correlations enhance the density of states at the van Hove singularity (VHS) providing more electrons able to form superconducting pairs. It should be noticed, that is exactly the non-locality of the attractive interacting term which triggers the short range AF correlations within the two pole approximation for the attractive Hubbard model.

The electronic specific heat $C(T)$ is an important quantity giving relevant information about the pseudogap and the mechanisms behind it. Mostly important, the close relation between the specific heat and the density of states allows a theoretical investigation about effects of correlations, in particular, the magnetic ones.

Therefore, we present here a systematic study of the specific heat using the attractive non-local Hubbard model within the two pole approximation. This approximation allows to deal properly with the regime of strong correlations. In particular, we assume that there is also next-neighbor hopping. As will be shown below, this hopping furnishes an additional mechanism to amplify magnetic correlations and, therefore modifies the DOS, thus affecting the specific heat.

2. The model

The model investigated is a two-dimensional one-band Hubbard model \cite{5,10} which is given by:

$$H = \sum_{(ij)\sigma} t_{ij} d_{i\sigma}^d d_{j\sigma} + \frac{G}{2} \sum_{(ij)\sigma} n_{i\sigma} n_{j-\sigma} - \mu \sum_{i\sigma} n_{i\sigma} \quad (1)$$
where \( d_{i\sigma}^\dagger(d_{i\sigma}) \) is the fermionic creation (annihilation) operator at site \( i \) with spin \( \sigma = \{\uparrow, \downarrow\} \) and \( n_{i\sigma} = d_{i\sigma}^\dagger d_{i\sigma} \) is the number operator. The quantity \( t_j \) represents the hopping between sites \( i \) and \( j \) and \( \langle \ldots \rangle \) indicates the sum over the first and the second-nearest-neighbors of \( i \) and \( \mu \) is the chemical potential. The second term in \( H \) takes into account the interaction between the electrons in which \( G \) is a non-local attractive potential. The bare dispersion relation is given by

\[
\varepsilon_k^\mu = 2t[\cos(k,a) + \cos(k,a)] + 4t_z \cos(k,a) \cos(k,a)\quad \text{where} \quad i \text{is the first-neighbor and} \quad t_2 \text{is the second-neighbor hopping amplitudes and} \quad a \text{is the lattice parameter.}
\]

In the two-poles approximation proposed by Roth \([7, 8]\), the Green’s function matrix is defined as

\[
G(\omega) = N(\omega N - E)^{-1} N
\]

in which \( N \) and \( E \) are the normalization and the energy matrices, respectively \([8]\).

The specific heat is given by \( C(T) = \frac{\partial}{\partial T} \ln Z \) where \( Z \) is the partition function, \( T \) the temperature. In the grand canonical ensemble, the specific heat is the energy of a chemical potential \( E \equiv E(\mu(T)) \), where \( \mu \) changes with the temperature. Therefore, the calculation of \( C(T) \) must be performed keeping \( \langle n \rangle \) constant in the \( T - \mu \) plane \([11]\). The energy per atom is \( E = \frac{\langle H \rangle}{N} \) (\( N \) being the number of sites of the system) and can be written \([12]\):

\[
E = \frac{i}{2N} \lim_{T \to 0} \sum \epsilon_k \int_{-\infty}^{\infty} f(\omega) \langle \omega + \mu + \epsilon_k \rangle [G_{\epsilon,\epsilon}(\omega + i\delta) - G_{\epsilon,\epsilon}(\omega - i\delta)]\, d\omega
\]

where \( f(\omega) \) is the Fermi function and \( G_{\epsilon,\epsilon}(\omega) \) is a Green’s function of the type

\[
G_{\epsilon,\epsilon}(\omega) = \frac{Z_{\epsilon,\epsilon}(\tilde{k})}{\omega - \omega_{\epsilon,\epsilon}(\tilde{k})} + \frac{Z_{\epsilon,\epsilon}(\tilde{k})}{\omega - \omega_{\epsilon,\epsilon}(\tilde{k})}
\]

with the spectral weights \( Z_{\epsilon,\epsilon}(\tilde{k}) \) and the renormalized bands \( \omega_{\epsilon,\epsilon}(\tilde{k}) \) defined in App \( \text{(Appendix A)} \).

Combining \( C(T) = \frac{\partial}{\partial T} \ln Z \) with equations \( 2 \) and \( 3 \) we obtain

\[
C(T) = \int_{-\infty}^{\infty} F(\omega)\, d\omega
\]

with \( F(\omega) = f'(\omega) g(\omega) + f(\omega) g'(\omega) \) and \( f'(\omega) = \frac{1}{\pi} \frac{\partial f(\omega)}{\partial \omega} \). The function \( g(\omega) \) is defined as

\[
g(\omega) = \frac{1}{2N} \sum_{i=1}^{2} \sum_{\epsilon,\epsilon} \tilde{Z}_{\epsilon,\epsilon}(\tilde{k}) \delta(\omega - \omega_{\epsilon,\epsilon}(\tilde{k}))
\]

where \( \tilde{Z}_{\epsilon,\epsilon}(\tilde{k}) = (\omega_{\epsilon,\epsilon}(\tilde{k}) + \mu + \epsilon_k) \omega_{\epsilon,\epsilon}(\tilde{k}) Z_{\epsilon,\epsilon}(\tilde{k}) \).

The spin-spin correlation function discussed in the numerical results section is given by

\[
\langle S_i^\tau S_j^\sigma \rangle = \langle S_i^\tau S_j^\sigma \rangle - h_{ij} \langle S_i^\tau S_j^\sigma \rangle
\]

and \( h_{ij} \) defined in App \( \text{(Appendix A)} \).

3. **Numerical results**

(i) **Specific heat for \( t_2 = 0 \)**

The specific heat for the Hubbard model with only nearest neighbor hopping, is shown in the left panel in figure \( 1 \) for \( n_T = 0.90 \) and different values for the interaction \( G \). For \( G = 0.0 \), the specific heat presents a Schottky anomaly \([13]\) with a maximum at \( k_B T = 0.90|t| \). If \( |G| \) is increased, the peak in \( k_B T = 0.90|t| \) is preserved and a second peak emerges at \( k_B T = 0.20|t| \), as can be observed for \( G = 1.5t \). For high values of \( |G| \), for instance \( G = 3.0t \), the peak at low temperature dominates and the specific heat shows only a single peak. The right panel in figure \( 1 \) shows the spin-spin correlation function \( \langle S_i^\tau S_j^\sigma \rangle \).

Another feature observed in \( C(T) \) is the presence of a crossing point at \( k_B T \approx 0.8|t| \). Such crossing point is a characteristic of the specific heat of many correlated systems \([14]\). In order to understanding the temperature dependence of \( C(T) \), let us analyze \( F(\omega) \) and \( g(\omega) \) defined above. Figure \( 2 \) shows \( g(\omega) \) for \( n_T = 0.90 \) and different values of \( G \). The figure \( 2 \) presents \( f'(\omega) \) for \( G = 1.5t \) and different values of \( k_B T \). The \( F(\omega) \) is shown in figure \( 4 \). The \( g(\omega) \) shown in figure \( 2 \) presents an important feature, namely, both the positive area associated to the lower Hubbard band and the negative area related to the upper Hubbard band enhance as \( |G| \) increases. As a consequence, the low temperature peak on \( C(T) \) is favored by \( G \) while the high temperature peak is suppressed by \( G \), as can be observed in figure \( 1 \). For intermediate values of \( G \), there is a temperature in which the negative area in \( g(\omega) \) associated to the upper Hubbard band gives the maximum contribution to \( F(\omega) \) leading to a local minimum in \( C(T) \) at this temperature. This is the reason why at moderated values of \( G \), both the low and high temperature peaks coexist on \( C(T) \) as can be observed in figure \( 1 \) for \( G = 1.5t \).

The right panel in figure \( 1 \) shows that \( \langle S_i^\tau S_j^\sigma \rangle \) is large at low temperatures and increases with \( |G| \). As discussed in references \([14, 15] \), the \( \langle S_i^\tau S_j^\sigma \rangle \) modify the renormalized band structure by enlarging the flat region near the anti-nodal points.
\( \langle S_i \cdot S_j \rangle \) decreases and its effect becomes negligible. The density of states for different temperatures and \( G \) are shown in figure (3). In (3a), \( G = 1.0t \) and the chemical potential \( \mu \) intercepts the density of states \( \rho(\omega) \) below the peak associated to a VHS, for all values of temperatures shown in the figure. In (3b), in which \( G = 1.5t \), \( \rho(\omega = \mu) \) is maximum for \( k_B T = 0.2|t| \), while for \( k_B T = 0.4|t| \), \( \mu \) intercepts \( \rho(\omega) \) after the VHS where \( \rho(\omega = \mu) \geq 0 \) (see the inset). It is interesting to note that the specific heat presents a peak just at \( k_B T = 0.2|t| \) and a local minimum at \( k_B T = 0.4|t| \) (see figure 1). This occurs because at low temperatures the function \( f'(\omega) = \frac{\partial f(\omega)}{\partial \omega} \) (7) (\( f(\omega) \) is the Fermi function) is very close to the chemical potential. In this case the position of chemical potential on \( \rho(\omega) \) plays an important role. For \( G = 3.0t \), figure (3c) shows that the chemical potential intercepts \( \rho(\omega) \) on the VHS when \( k_B T = 0.2|t| \). However, for \( k_B T = 0.4|t| \) and \( k_B T = 0.9|t| \), \( \mu \) is found within the gap, where \( \rho(\omega = \mu) = 0 \). Figure (a) shows the specific heat for different values of \( n_T \). Notice that when \( n_T \) decreases the peak at low temperature disappears. This occurs because the \( \langle S_i \cdot S_j \rangle \) becomes small decreasing the density of states at the VHS. Moreover, the low occupation moves the chemical potential \( \mu \) away from the VHS. On the other hand, if \( n_T \) increases, \( \langle S_i \cdot S_j \rangle \) is enhanced, \( \mu \) moves closer to the VHS and as consequence the low temperature peak in \( C(T) \) enlarges. Figure (4b) shows the spin-spin correlation function \( \langle \hat{S}_i \cdot \hat{S}_j \rangle \) for the same parameters as in the upper panel. Figure (4c) shows that at low temperatures, the specific heat exhibits a maximum for a given \( n_T \). At high temperatures the maximum disappears. Figure (4d) displays the spin-spin correlation function \( \langle \hat{S}_i \cdot \hat{S}_j \rangle \) for the same parameters as in the upper panel.
density of states. The main figure shows a pseudogap starts to decrease and closes for different values of $t_2/|t|$. The inset shows $k_BT'/|t|$ as a function of the modulus of the interaction $G$.

(ii) Specific heat for $t_2 \neq 0$

The figure 5(a) presents the specific heat as a function of temperature for different values of the second nearest-neighbors amplitude $t_2$. The low temperature peak in the specific heat is strongly enhanced by $t_2/|t|$. This occurs because $t_2$ enhances $\langle S_i \cdot S_j \rangle$ and enlarges the flat regions on the renormalized bands resulting in a high density of states on the VHS. As a consequence, the low temperature peak on $C(T)$ increases while the high temperature peak is not affected because temperature suppresses $\langle S_i \cdot S_j \rangle$. The lower panel in figure 5(b) shows the behavior of $\langle S_i \cdot S_j \rangle$ for the same parameters as in 5(a). Figure 5(c) shows that the effects of $t_2/|t|$ on $C(T)$ are more intensive at low temperatures where $\langle S_i \cdot S_j \rangle$ is stronger. Furthermore, there is a maximum on $C(T)$ in $t_2/|t| \approx 0.5$ but, this maximum does not show at high temperatures. Figure 5(d) shows $\langle S_i \cdot S_j \rangle$ for the same parameters as in 5(c). In figure 6 we present the renormalized band structures and the effective spectral weights for $k_BT'/|t| = 0.2$ and several values of $t_2/|t|$. We observe that a pseudogap $\Delta_{PG}$ emerges from $t_2/|t| = 0.2$ and persists until $t_2/|t| = 0.6$. Moreover, the pseudogap is maximum for $t_2/|t| \approx 0.5$ which is just the value of $t_2/|t|$ for which $C(T)$ is maximum (see figure 5). The inset in the upper panel of figure 6 shows in detail the pseudogap $\Delta_{PG}$ for $t_2/|t| = 0.5$. Indeed, for $t_2/|t| = 0.5$, the presence of the pseudogap gives rise to a wide flattening in $\omega_{S_{i\sigma}}(k)$ along the direction $(0, \pi)-(0, 0)$, which increases the density of states at the VHS and also produces a peak on $g(\omega)$. When $t_2/|t|$ increases, the pseudogap opens and the region of $Z_{S_{i\sigma}}(k)$ near $(0, \pi)$ becomes positive resulting in an enhancement of the specific heat. Nevertheless, for $t_2/|t| > 0.5$, the pseudogap starts to decrease and closes for $t_2/|t| \sim 0.6$. The lower panel in figure 6 shows that the negative region on $Z_{S_{i\sigma}}(k)$ increases with $t_2/|t|$. However, at low temperatures such regions do not contribute to $C(T)$ because they are associated to the upper Hubbard band. On the other hand, when the temperature increases, the negative regions of $Z_{S_{i\sigma}}(k)$ become relevant and affect the specific heat (see $C(T)$ for $k_BT'/|t| = 0.9$ in the upper panel in figure 5(c)).

Figure 7 displays the temperature $T'$ below which a pseudogap appears on the renormalized band as shown in figure 6 (left panel). The pseudogap lines are displayed for different intensities $t_2/|t|$ and a common feature is that $k_BT'/|t|$ increases with the total occupation $n_T$. Nevertheless, we observed that from $t_2/|t| = 0.05$ to $t_2/|t| = 0.30$ the pseudogap lines start in $(k_BT'/|t| > 0)$. This occurs because above $n_T \approx 0.80$ and below a critical value of $k_BT'/|t|$, the spin-spin correlations become so strong that distort the renormalized band sufficiently to close the pseudogap. Therefore, in the present scenario, the pseudogap is observed in a range of $G$, $t_2$, $n_T$ and $T$ in which the spin-spin correlations are typical for a $(G/t \geq 1)$ regime. The inset in figure 7 shows the pseudogap line as a function of $|G|$. The $k_BT'/|t|$ increases with $|G|$ because $G$ favors the correlations $(\langle S_i \cdot S_j \rangle)$ (see the right panel of figure 1) which, in the present scenario, are responsible for the pseudogap. For $|G| \lesssim 0.5|t|$, the systems becomes weakly correlated and the pseudogap closes because the chemical potential reaches the upper Hubbard band.

4. Conclusions

The specific heat $C(T)$ of an attractive extended Hubbard model has been studied within a two-pole approximation 2,8. It has been verified that $C(T)$ as a function of temperature shows a two peak structure. A systematic analysis of $C(T)$ in terms of the renormalized band structure allowed us to identify the mechanisms behind the two peak structure. Indeed, the low temperature peak is associated to the lower Hubbard band while the high temperature peak is related to the upper Hubbard band. If $\mu$ is near a van Hove singularity (VHS) the low temperature peak is enhanced due to the close relation between specific heat and density of states. On the other hand, the upper Hubbard band contributes with a positive and also a negative portion for $C(T)$. For small $G$, the contribution is positive but when $|G|$ increases the negative portion dominates and the high temperature peak on $C(T)$ is suppressed. It should be stressed that the AF magnetic correlations associated to the spin-spin correlation function $\langle S_i \cdot S_j \rangle$ affects the behavior of the peaks on the specific heat. This occurs because $\langle S_i \cdot S_j \rangle$ changes the renormalized band structure resulting in an enhancement or a decrease of the density of states, mainly, on the VHS. The lower temperature peak is more affected by this effect because the VHS contributes significantly to that peak which is the only one preserved when $|G|$ increases. The low temperature peak is also deeply dependent on the occupation $n_T$. At low $n_T$ the chemical potential $\mu$ is far from the VHS. Therefore, the low density of states on $\mu$ is not sufficient to induces the low temperature peak on $C(T)$.

It has been verified that if the second nearest-neighbor hopping $t_2/|t|$ is present, these same $\langle S_i \cdot S_j \rangle$ correlations induce a pseudogap on the renormalized band structure. The pseudogap opens at the anti-nodal points $(0, \pm \pi)$ and $(\pm \pi, 0)$ suggesting a $d$-wave symmetry for it. Nevertheless, the pseudogap and the two peak structure on $C(T)$ do not coexist. Indeed, the second nearest-neighbor hopping $t_2/|t|$ enhances the spin-spin correlations which increases the low temperature peak on $C(T)$ and suppresses the high temperature peak.
In summary, the present results for an attractive non-local Hubbard model suggest that in presence of a pseudogap the specific heat has a single peak structure which is closely related to short-range AF magnetic correlations.

Appendix A.

Within the two-pole approximation proposed in reference [7], the spectral weights and renormalized bands have the general form:

\[
Z_{\alpha\sigma}(k) = \frac{1}{2} - (-1)^{l} \left[ \frac{\alpha - \epsilon_{k} + W_{k\sigma}}{2X_{k\sigma}} \right] (A.1)
\]

\[
\omega_{\alpha\sigma}(k) = \frac{\beta + \epsilon_{k} + W_{k\sigma} - 2\mu}{2} + (-1)^{l} \left[ \frac{X_{k\sigma}}{2} \right]. (A.2)
\]

Also, \(\alpha = \frac{G_{1} + \epsilon_{n\sigma}(G_{1} - 2G_{2})}{n_{\sigma}(1-n_{\sigma})} - 2G_{1}\), \(\beta = \frac{G_{1} + \epsilon_{n\sigma}(G_{1} - 2G_{2})}{n_{\sigma}(1-n_{\sigma})} + X_{k\sigma}\) and \(X_{k\sigma} = \sqrt{(G - \epsilon_{k} + W_{k\sigma})^{2} + 4G_{1}(\epsilon_{k} - W_{k\sigma}) + \tilde{G}}\) with \(\tilde{G} = \frac{G_{1} + \epsilon_{n\sigma}(G_{1} - 2G_{2})}{n_{\sigma}(1-n_{\sigma})}\) and \(G = \frac{G_{1} + \epsilon_{n\sigma}(G_{1} - 2G_{2})}{n_{\sigma}(1-n_{\sigma})}\). The effective interactions \(G_{1}\) and \(G_{2}\) are defined as \(G_{1} = G \sum_{n\sigma} \langle n_{\sigma}\rangle\) and \(G_{2} = G \sum_{n\sigma} \langle n_{\sigma}\rangle\) where \(\langle n_{\sigma}\rangle = n_{\sigma}^{2} - \frac{n_{\sigma}m_{\sigma}n_{\sigma}m_{\sigma}}{1 - b_{\alpha\sigma} b_{\alpha\sigma}}\). The band shift \(W_{k\sigma}\) is given by \(W_{k\sigma} = \frac{1}{n_{\sigma}(1-n_{\sigma})} \sum_{\vec{k}} \epsilon(\vec{k} - \vec{q}) F_{\sigma}(\vec{q})\), where \(\epsilon(\vec{k} - \vec{q})\) is given in terms of \((\vec{S}_{\vec{k}} \cdot \vec{S}_{\vec{q}})\) and the Fourier transform of \(n_{\sigma\sigma}\) and \(m_{\sigma\sigma}\) defined as \(n_{0\sigma} = \langle d_{\sigma}^{\dagger} d_{\sigma} \rangle = \frac{1}{N} \sum_{\vec{k}} \sum_{l} G_{\sigma\sigma}^{(1)}(\vec{k}) \epsilon_{l}^{\dagger} \vec{k}^{l}\), and \(m_{j\sigma} = \langle d_{\sigma}^{\dagger} d_{j-\sigma} \rangle = \frac{1}{N} \sum_{\vec{k}} \sum_{l} F_{\sigma l} G_{\sigma\sigma}^{(2)}(\vec{k}) \epsilon_{l}^{\dagger} \vec{k}^{l}\), where \(F_{\sigma l} \Gamma(\omega) \equiv \int \frac{d\omega}{\omega} \frac{\delta(\omega) \Gamma(\omega)}{\omega}\) is a general Green’s function. The Green’s functions \(G_{\sigma\sigma}^{(1)}\) and \(G_{\sigma\sigma}^{(2)}\) are obtained as in reference [3]. Finally, the correlation functions \((\vec{S}_{\vec{k}} \cdot \vec{S}_{\vec{q}})\) and \(h_{j\sigma\sigma}\) introduced in section 6 are \((\vec{S}_{\vec{k}} \cdot \vec{S}_{\vec{q}}) = \frac{1}{(1-n_{\sigma})} \left( n_{\sigma}^{2} - h_{1\sigma}^{(1)} \right)\) and \(h_{j\sigma\sigma} = \frac{n_{\sigma} n_{\sigma}^{2} - h_{1\sigma}^{(1)}}{1 + h_{1\sigma}^{(1)} + h_{1\sigma}^{(1)} + h_{1\sigma}^{(1)}}\).

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