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Specific heat of a Hubbard model on the pseudogap and superconducting regions

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OBJECTIVE:

The main objective of the present work is to investigate the specific heat of the repulsive Hubbard model including the pseudogap and also the superconducting region. Superconductivity with $d_{x^2-y^2}$ -wave pairing is considered and the effects of such superconductivity on the specific heat, are also analyzed.

INTRODUCTION:

The Hubbard model is considered one of the simplest model which describes the behavior of correlated electron system. Considerable attention is devoted to this model mainly after the discovery of the high temperature superconductors (HTSC). Although the Hubbard model has been largely investigated the existence of pseudogap and superconductivity are still open questions. The analysis of the specific heat structure can give us some informations about this regions.

METODOLOGY:

The Hubbard model which has been largely used to describes strongly correlated electron systems is investigated here by the Green's functions technique. The equations of motion of the Green's functions are treated by using a two poles approximation [1,2].

The Hubbard model considers the hopping to first (t) and second (t_2) nearest neighbors and also a Coulomb interaction between electrons with opposite spins and localized in the same site i. The model is given by:

$$H = \sum_{<<ij>>\sigma} t_{ij} c_{i\sigma}^{+} c_{j\sigma} + U \sum_{i} n_{i\sigma} n_{i-\sigma} - \mu \sum_{i\sigma} n_{i\sigma}$$

in which $c_{i\sigma}^{+} c_{j\sigma}$ is the fermionic creation (annihilation) operator and $\sigma = \{\uparrow\downarrow\}$ represent the spin. $n_{i\sigma} = c_{i\sigma}^{+} c_{i\sigma}$ is the density operator, t_{ij} is the hopping integral between sites i and j which are nearest-neighbors. The symbol <<…>> indicates the sum over the first and second-nearest-neighbors.

The equation of motion of the Green's functions is:

$$\omega\langle\langle A;B\rangle\rangle = \frac{1}{2\pi i}\langle[A,B]_+\rangle + \langle\langle [A,H];B\rangle\rangle$$

In order to treat the equation of motion above, Roth [2,3] proposed to rewrite the commutator as:

$$[A_n, H] = \sum_m K_{nm} A_m$$

where

$$\mathbf{K} = \mathbf{E}\mathbf{N}^{-1}$$

with

$$\mathbf{E}_{nm} = \left\langle \left[\left[A_n, H \right], A^+{}_m \right]_+ \right\rangle$$

and

$$\mathbf{N}_{nm} = \left\langle \left[A_n , \overset{+}{A}_m \right]_+ \right\rangle .$$

E and **N** are respectively, the energy and the normal matrices.

The $\{A_m\}$ is a set of operators that must to represent the most important excitations of the system. In the present case the set of operators is $\{c_{i\sigma}, c_{i\sigma}n_{i-\sigma}, c^{+}_{i-\sigma}, n_{i\sigma}c^{+}_{i-\sigma}\}$ and the Green's functions of our interest are:

$$G_{11\mathbf{k}}(\omega) = \frac{\eta - \gamma_{\mathbf{k}}^{2}[\omega + E_{11}]^2}{n^2(1-n)^2(\omega^2 - E_{1\mathbf{k}}^2)(\omega^2 - E_{2\mathbf{k}}^2)}$$

and

$$G_{13\mathbf{k}}(\omega) = \frac{-\gamma_{\mathbf{k}}[n(1-n)U]^2}{n^2(1-n)^2(\omega^2 - E_{1\mathbf{k}}^2)(\omega^2 - E_{2\mathbf{k}}^2)}$$

with $\eta = n^2(1-n)^2(\omega^3 + \omega^2\alpha_2 + \omega\alpha_1 + \alpha_0)$, $\alpha_0 = -\xi_1\xi_2(W_{\mathbf{k}} + U(1-n)) - \dfrac{E_{11}\gamma_{\mathbf{k}}^2}{n^2(1-n)^2}$,

$\alpha_2 = E_{11}$, $\alpha_1 = -\xi_1\xi_2 - (\xi_1 + \xi_2)(W_{\mathbf{k}} + U(1-n)) - \dfrac{\gamma_{\mathbf{k}}^2}{n^2(1-n)^2}$, and $E_{11} = \xi_1 + \xi_2 - (W_{\mathbf{k}} + U(1-n))$.

$E_{1\mathbf{k}}^2 = \xi_{1\mathbf{k}}^2 + \frac{\gamma_{\mathbf{k}}}{n^2(1-n)^2} \frac{E_{11}^2 - \xi_{1\mathbf{k}}^2}{\xi_{2\mathbf{k}}^2 - \xi_{1\mathbf{k}}^2}$ and $E_{2\mathbf{k}}^2 = \xi_{2\mathbf{k}}^2 + \frac{\gamma_{\mathbf{k}}}{n^2(1-n)^2} \frac{\xi_{2\mathbf{k}}^2 - E_{11}^2}{\xi_{2\mathbf{k}}^2 - \xi_{1\mathbf{k}}^2}$ are the renormalized bands in the superconducting state.

Also, $\xi_{1\mathbf{k}} = \frac{U + \varepsilon_{\mathbf{k}} + W_{\mathbf{k}} - 2\mu}{2} - \frac{X_{\mathbf{k}}}{2}$ and $\xi_{2\mathbf{k}} = \xi_{1\mathbf{k}} + X_{\mathbf{k}}$ are the renormalized bands in the normal state.

The non interacting energy band is:

$$\varepsilon_{\mathbf{k}} = 2t(\cos k_x a + \cos k_y a) + 4t_2 \cos k_x a \cos k_y a \ .$$

The quantity $X_{\mathbf{k}}$ is given by $X_{\mathbf{k}} = \sqrt{(U - \varepsilon_{\mathbf{k}} + W_{\mathbf{k}})^2 + 4nU(\varepsilon_{\mathbf{k}} - W_{\mathbf{k}})}$ and the band shift

$$W_{\mathbf{k}\sigma} = \frac{w_0 + \varepsilon(\mathbf{k}) w_1}{n_\sigma(1-n_\sigma)} ,$$

with $w_1 = \frac{1}{4}(< N_j N_i > - < N_j >< N_i >) + < \mathbf{S}_j \mathbf{S}_i > - < c_{j\sigma}^+ c_{j-\sigma}^+ c_{i-\sigma} c_{i\sigma} >$ e

$w_0 = -\sum_{<j>i} i < c_{i\sigma}^+ c_{j\sigma} (1 - n_{i-\sigma} - n_{j-\sigma})$.

A analytical expression for the specific heat

The analytical expression for the specific heat has been obtained following the formalism presented in reference [3].

The equation of motion for operator $c_{i\sigma}(t)$ is

$$i\frac{d}{dt}c_{i\sigma}(t)=\sum_j(t_{ij}-\mu\delta_{ij})c_{j\sigma}+Uc_{i\sigma}n_{i-\sigma},$$

multiplying by $c_{i\sigma}^{+}$ both sides of the equation above, making the sum in *i* and σ and taking the average of the ensemble we obtain

$$\sum_{i\sigma}\frac{d}{dt}<c_{i\sigma}^{+}c_{i\sigma}(t)>=\sum_{ij\sigma}(t_{ij}-\mu\delta_{ij})<c_{i\sigma}^{+}c_{j\sigma}>+U\sum_{i\sigma}<n_{i\sigma}n_{i-\sigma}>.$$

Considering the it ***H*** average

$$<H>=\sum_{ij\sigma}t_{ij}<c_{i\sigma}^{+}c_{j\sigma}>+\frac{U}{2}\sum_{i\sigma}<n_{i\sigma}n_{i-\sigma}>-\mu\sum_{i\sigma}<n_{i\sigma}>$$

and combing it with $\sum_{i\sigma}\frac{d}{dt}<c_{i\sigma}^{+}c_{i\sigma}(t)>$, we get:

$$\sum_{i\sigma}\frac{d}{dt}<c_{i\sigma}^{+}c_{i\sigma}(t)>=\sum_{ij\sigma}(t_{ij}-\mu\delta_{ij})<c_{i\sigma}^{+}c_{j\sigma}>2<H>-2\sum_{ij\sigma}t_{ij}<c_{i\sigma}^{+}c_{j\sigma}>+2\mu\sum_{i\sigma}<n_{i\sigma}>$$

by using the correlation function definition

$$\left\langle B(t'),A(t)\right\rangle = i\lim_{\varepsilon\to 0}\int_{-\infty}^{\infty}\frac{\left[G^{AB}(\omega+i\varepsilon)-G^{AB}(\omega-i\varepsilon)\right]}{e^{\beta\omega}+1}e^{-i\omega(t-t')}d\omega$$

it is possible to obtain <H> explicitly. Then, through the relation $E=\frac{<H>}{N}$ we get the energy per atom of the system. The specific heat *c(T)* is defined $c(T)=\frac{\partial E}{\partial T}$. Therefore,

$$c(T)=\frac{i}{2N}\lim_{\varepsilon\to 0^{+}}\int_{-\infty}^{\infty}\frac{\partial}{\partial T}\sum_{k\sigma}(\varepsilon_k+\mu+\omega)\Gamma_k(\omega\pm i\varepsilon)f(\omega)d\omega$$

where $f(\omega)=\frac{1}{e^{\frac{\omega}{k_B T}}+1}$ is Fermi function and $\Gamma_k(\omega\pm i\varepsilon)=\left[G^{AB}(\omega+i\varepsilon)-G^{AB}(\omega-i\varepsilon)\right]$

with $A(t)=c_{i\sigma}(t)$ and $.B(t'=0)=c_{i\sigma}^{+}$.

NUMERICAL RESULTS:

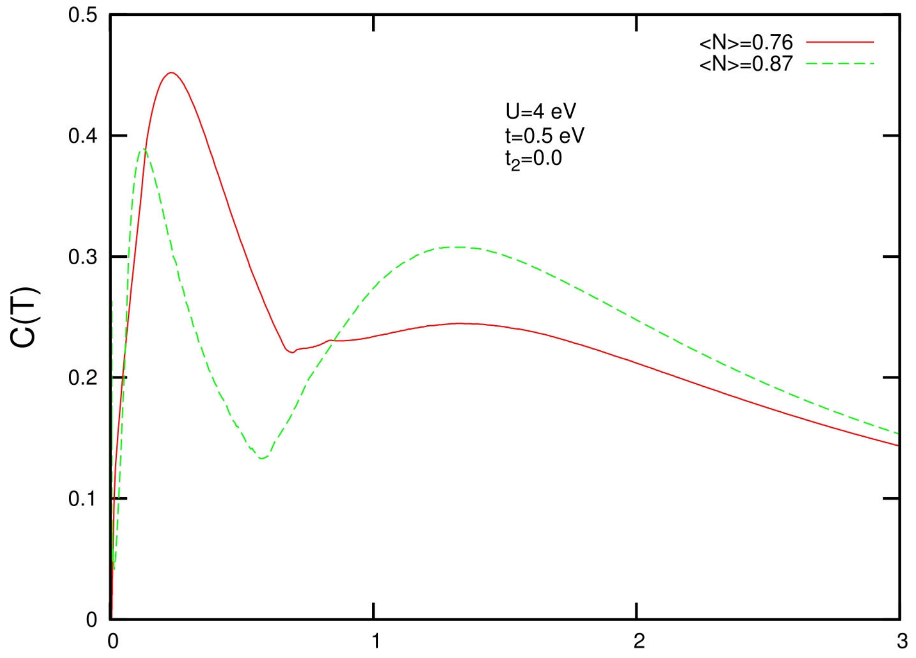

FIG. 1: Specific heat as a function of the temperature for different values of <N>.

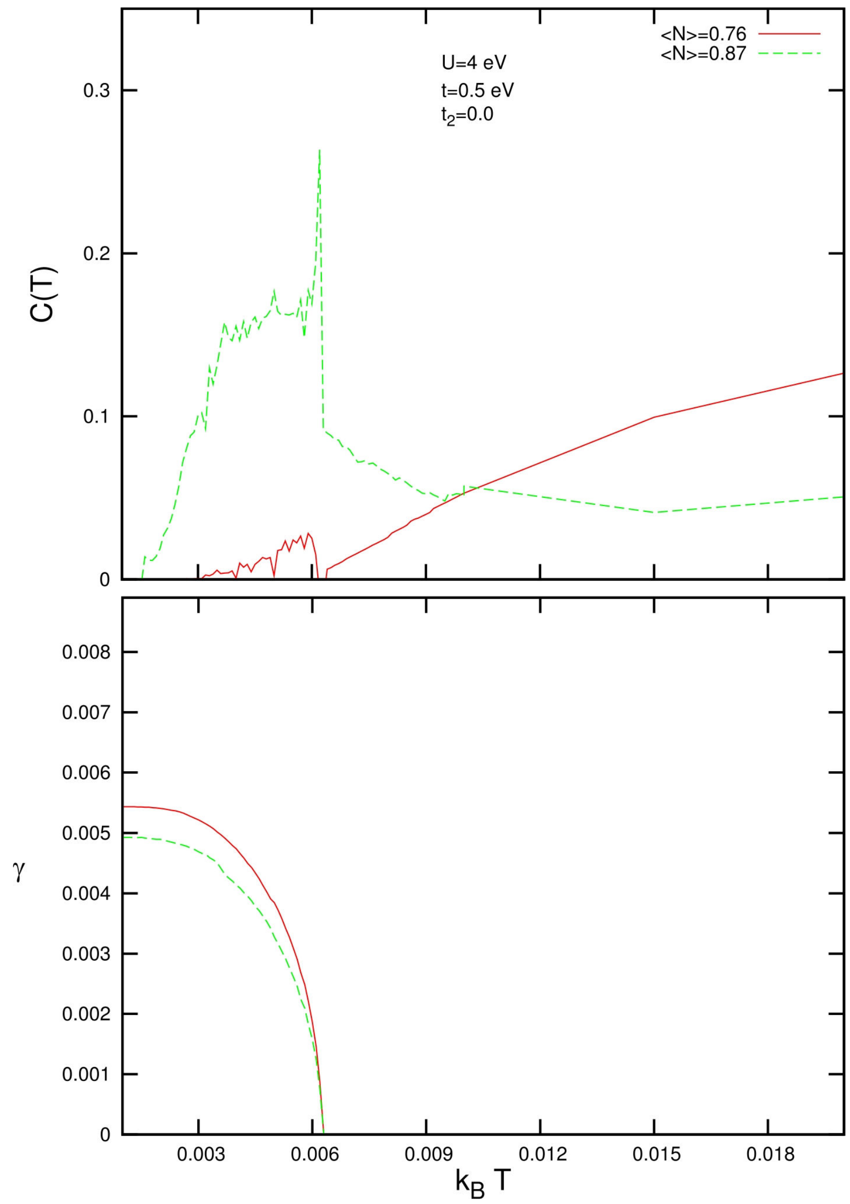

FIG. 2: In the upper panel, the specific heat as a function of the temperature for different values of <N>. The lower panel shows the superconducting order parameter.

CONCLUSIONS:

The numerical results show that the specific heat presents the peak at the superconducting critical temperature Tc. Furthermore, above Tc, C(T) is characterized by a two peaks structure which is a characteristic of the Hubbard model. The next step in the present work is to include pseudogap effects associated to antiferromagnetic correlations.

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