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DENSITY OF STATES AND SUPERCONDUCTING CRITICAL TEMPERATURE *V s* THE NUMBER OF CARRIERS IN A TRIANGULAR LATTICE UNDER THE APPLIED PRESSURE

Densidad de Estado y Superconductividad Crítica en la Relación de Temparatura *Vs*. El Número de Carrier en una Red Triangular Dependiete de la Presión Aplicada

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Abstract

We propose a band structure for a triangular lattice with nearest neighbor hopping, in terms of parameters which depend on applied pressure to the sample. Such a lattice is a representation of the compound, $Na_xCoO_2 \cdot y\ H_2O$, (Sodium Cobalt Oxyhydrate), which is superconducting at a critical temperature of $T_C \approx 5\ K$. We calculate the density of states, $N(\omega)$ *vs* ω, for several values of the parameters which depend on pressure, distorting in this way the geometry of the lattice. We observe the frequency dependence of the density of states for the different parameters. For zero pressure, we have obtained a density of states which is not symmetric around $\omega = 0$. which is a different result with respect to a square lattice in 2–D. We also study the superconducting critical temperature, T_C, as function of the chemical potential, μ. T_C and μ are calculated from two self–consistent *BCS* equations. As a natural result, we have studied the effect of pressure on T_C, relating the different van Hove singularities, which appear in the density of states, with the different T_C;$_{\max}$'s. We then prove that $_{ns} = {}_{\mathrm{mv}}$, where $_{ns}$ is the number of logarithmic singularities and $_{\mathrm{mv}}$ is the number of T_C;$_{\max}$'s. We compare our results with relevant results in the literature.

Key words: superconducting, density of states, band structures

Resumen

Proponemos una estructura de bandas para una red triangular con saltos a los primeros vecinos, en término de parámetros que dependen de la presión aplicada a la muestra. Tal red es representativa del compuesto, $Na_xCoO_2 \cdot yH_2O$, el cual superconduce a una temperatura crítica de $T_C \approx 5\ K$. Calculamos la densidad de estados, $N(\omega)$ *vs* ω, para varios valores de los parámetros vs. presión, distorcionando de esta forma la geometría de la red. Observamos que la densidad de estados vs. frecuencia depende de los parámetros seleccionados. Para presión nula, hemos obtenido una densidad de estados que nos simétrica alrededor de $\omega = 0$, un resultado diferente para la red cuadrada en 2 – D. También hemos estudiado T_C *vs* el potencial químico, los cuales son calculados auto–consistentemente. Como un resultado esperado, hemos estudiado el efecto de la presión sobre T_C, relacionando las diferentes singularidades de van Hove, las cuales aparecen en la densidad de estados, con los máximos de T_C. Entonces probamos que el número de máximos en T_C son iguales al número de singularidades de van Hove que aparecen en $V(\omega)$. Hemos comparado nuestros resultados con los resultados relevantes en la literatura científica.

Palabras clave: superconductividad, densidad de estado, estructura de banda

1 Introduction

Just recently the compound Sodium Cobalt Oxyhydrate ($Na_xCoO_2 \cdot yH_2O$) was discovered, which presents superconducting properties at $T_c \approx 5\ K$ (Takada *et al.*, 2003). $Na_xCoO_2 \cdot yH_2O$ must be hydrated to superconduct (Takada *et al.*, 2003), and its triangular CoO_2 layers provide an intriguing contrast with the square CuO_2 layers of the high–temperature superconductors. Such compound, in its solid state, corresponds to a triangular lattice with equal lattice sides (Pereg-Barnea & Hsiu-Hau, 2005) as it is shown in Fig. 1. Superconductivity is induced on the CoO_2 layer, which a triangular lattice by the presence of *Co*. This superconductivity is considered non–conventional (Ishida *et al*., 2003; Fujimoto *et al*., 2004) from a point of view of its symmetry, in that the Cooper pairs are not in a spin singlet state with s–wave symmetry, as with conventional superconductors (Mazini & Hohannes, 2005).

Additionally to this exotic (non–conventional) superconductivity, magnetism has been discovered in this compound. This magnetic phase is located near the superconducting phase (Ishara *et al.*, 2005; Sahurai *et al.*, 2005). This may led to the interpretation that the superconducting phase has a magnetic origen. According to (Laverock *et al.*, 2007) the explanation for superconductivity in sodium cobalt oxides when hydrated with water is due to the properties of some small elliptically shaped pockets predicted to be electronically dominant Fermi surface sheet, which they have detected experimentally by using *x*–ray Compton scattering.

For example, the discover of superconductivity, with $T_c \leq 5\ K$ in the compound $Na_{0.35}CoO_2 \cdot 1{:}3H_2O$ has renewed the interest in the physical properties of the undoped compound Na_xCoO_2 (Bernhard *et al*., 2007). Its rich phase diagram includes several phases with extraordinary properties of electromagnetic and thermoelectric types. Among its key features we can mention:

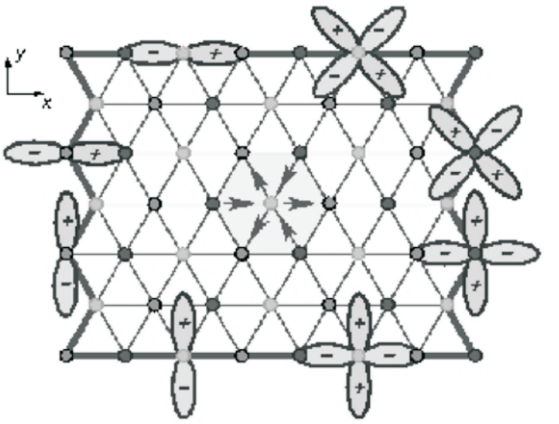

Fig. 1. Scheme for the triangular lattice in 2–*D*'s. In the proposed band structure we have taken into account the nearest neighbor hopping matrix element. The parameters α and β allow us to distort the lattice. $\gamma = 0.001$, $N_x = N_y = 1000$.

1. Its triangular coordination of *Co* which favours non–conventional base states.

2. Anomalous electromagnetic properties which are not confined to the regime of Mott insulator for $x \to 0$, but for $x \to 1$, where we expect a band insulator.

Due to the fact that we have strong differences in the experimental results (Mazin & Hohannes, 2005), especially on the symmetry of the *SC* order parameter, we have started the study of these materials by the evaluation of the density of states, under the application of static pressure. These contradictory reports have led to an unprecedented number of proposals (Kobayashi *et al*., 2003; Higemoto *et al*., 2004; Kuroki *et al*., 2004; Motrunik & Lee, 2004; Sa *et al*., 2004; Watanabe *et al.*, 2004; Yokoi *et al.*, 2004; Johannes *et al.*, 2005; Kato *et al.*, 2005; Yanase *et al.*, 2005) for the pairing symmetry, each in agreement with some particular subset of available data.

According to Mazin and Johannes (2005), the remaining symmetries left are of *f*–type.

However, as they themselves say, the synthesis of single–crystal Na_xCoO_2 . yH_2O is difficult, and polycrystalline samples often show inhomeneities in the distribution of *Na* and in the H_2O accumulation (Chen *et al.*, 2004; Ueland *et al.*, 2004). After being synthesized, the compound is chemically unstable at ambient pressure and humidity (Foo *et al.*, 2005), which makes its handling and characterization very problematic. In order to arrive to their conclusions, they use three conditions:

1. Two dimensionality. Electronic band structure calculations for this compound show an anisotropy in the Fermi velocity, which is supported by experimental measured resistency anisotropy of $10^3 - 10^4$ (Jin *et al.*, 2005). This implies that the transport along the *c*–axis is probably incoherent.

2. Absence of a finite superconducting gap. In all the experimental works on the density of states at the Fermi level (Fujimoto *et al.*, 2004; Yokoi *et al.*, 2004; Yan *et al.*, 2005) the authors conclude that there is not an exponential behavior of the superconducting gap for $T \to 0$. However, (Kobayashi *et al.*, 2003; Yokoi *et al.*, 2004; Kobayashi *et al.*, 2005; Kobayashi *et al.*, 2006) have carried out various kinds of experimental studies and revealed by measuring, specifically, the ^{59}Co–*N M R* Knight shifts that the spin–inglet pairing is realized in this compound. They have also found that the rate of the Tc suppression by non–magnetic impurities is small (Yokoi *et al.*, 2004). These results are explained by considering the *s*–wave order parameter symmetry.

3. Absence of superconductivity–induced spontaneous magnetic moments below the superconducting critical temperature (Uemura *et al.*, 2004), Tc.

Then, again, because of all these problems, we have decided to concentrate on *s*–wave superconductivity only to obtain some consequences of the triangular lattice under pressure. The consideration of other symmetries is not a problem from the computational point of view. Consideration of other symmetries changes the numerical values of Tc, which is a global quantity.

From the analysis of the density of states (Kittel, 1976), we can observe the behavior of this quantity, with pressure, in the non–superconducting phase. This free density of states depends on the lattice tight binding band (see Eq. 1).

$$\epsilon(\vec{k})/2t = -\cos(k_x) + \alpha\cos(\frac{k_x}{2} + \frac{\sqrt{3}k_y}{2}) + \beta\cos(\frac{k_x}{2} - \frac{\sqrt{3}k_y}{2}) \quad (1)$$

In Eq. (1) t has dimensions of energy and it represents the hopping integral of wave functions in the lattice neighbor sites in 2–*D*. In Eq. (1) α and β are parameters which satisfy the following conditions $\alpha \leq 1$ and $\beta \leq 1$. When $\alpha = \beta = 1$ our sample is free of pressure, namely, we have the perfect lattice, and Eq. (1) becomes

$$\epsilon(\vec{k})/2t = -\cos(k_x) + 2\cos(\frac{k_x}{2}) \times \cos(\frac{\sqrt{3}k_y}{2}) \quad (2)$$

The structure of this paper is as follows. In Section 2 we present the self–consistent equations, valid in mean–field approximation, or *BCS* approximations. These equations will be solved in Section 3, where we present the numerical solutions. Finally, we conclude in Section 4.

2. The Self–Consistent Problem: Description of the Method

The numerical algorithm of the density of states, $N(\omega)$, for a triangular lattice, was calculated using the usual definition:

$$N(\omega) = \frac{1}{N}\sum_{\vec{k}} \delta\left(\omega - \epsilon(\vec{k})\right) \quad , \tag{3}$$

where $N = N_x \times N_y$ is the number of points in the 2–*D* reciprocal space. In Eq. (3) we have assumed that the dominant symmetry of the superconducting order parameter is of *s*–wave, namely, $\vec{k}$–independent. This condition is not fully satisfied in the compound $Na_xCoO_2 \,.\, yH_2O$, since this material is a non–conventional superconductor. However, for another types of symmetries the main features found in this paper remain. $\delta(x)$ is the Dirac delta function which has dimensions of inverse energy.

For solving our self–consistent equations we will approximate the Dirac delta function by the following expression:

$$\delta(x) \approx \lim_{\gamma \to 0^+} \frac{1}{\pi}\frac{\gamma}{x^2 + \gamma^2} \quad . \tag{4}$$

In what follows we will use $\gamma = 0.01 - 0.001$. See the following figures. The calculation of T_c *vs* μ and *n vs* μ (or T_c *vs n*) is based in the following two self–consistent coupled equations:

$$\begin{aligned} \frac{1}{V} &= \frac{1}{N}\sum_{\vec{k}} \frac{\tanh(\frac{\epsilon(\vec{k})-\mu}{2\,k_B T_c})}{2(\epsilon(\vec{k}) - \mu)}\varphi^2(\vec{k}) \\ \rho &= \frac{1}{2} - \frac{1}{2\,N}\sum_{\vec{k}} \tanh(\frac{\epsilon(\vec{k}) - \mu}{2\,k_B T_c}) \quad , \end{aligned} \tag{5}$$

where k_B is the Boltzmann constant. T_c has dimensions of $\hbar_B T_c/t$ (See Section 3). V , in Eq. (5), is the absolute value of the pairing interaction which gives rise to the Cooper pairing. As we have said earlier we have solved our two coupled equations (5) numerically. To solve Eqs. (5) we have used $V/t = 1.0$. In Eq. (5) $\varphi(\vec{k})$ is a factor which takes care of the symmetry of the order parameter. For *s*–wave symmetry, $\varphi(\vec{k}) \equiv 1 \;\; \forall \vec{k}$, while for *d*–wave symmetry we should take $\varphi(\vec{k}) = \cos(k_x) - \cos(k_y)$, etc.

It is important to point out that the number of points is crucial in the determination of T_c, since the curve becomes smooth when the number of the lattice points is increased. In our case, we have obtained smooth results for $N_x = N_y = 1000$ or $N =$ 1,000,000. The smoothness of the T_c curve is important for the calculation of the isotope exponent, α', which depends on partial derivatives of T_c with respect to μ and ω_D (Rodríguez & Schmidt, 2003; Rodríguez & Schmidt, 2006; Rodríguez & Schmidt, 2008).

3. Results and Discussion

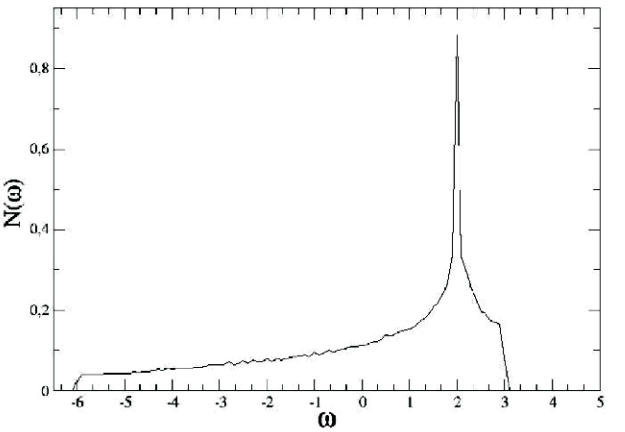

Fig. 2. Density of States for a perfect triangular lattice with $N = N_x \times N_y = 1000 \times 1000$ points. $\gamma =$ 0.001.

The density of states for an undistorted triangular lattice is shown in Fig. 2. This density of states is not symmetric with respect to any frequency, ω, as it is the case for a perfect square lattice. The frequency interval is $\omega/t \in (-6, 2)$. The van Hove singularity of the density of states is located at $\omega/t = 2$. We will see later than the positions of the logarithmic singularities of $N(\omega)$ are related to the maxima of the superconducting critical temperatures, namely, to $T_{c,max}$. This is a consequence of the greater amount of reciprocal space states available which contribute to

superconductivity, around the chemical potential.

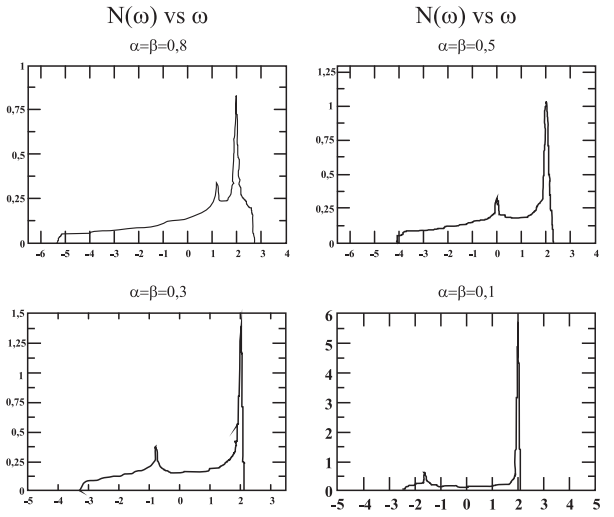

Fig. 3. $N(\omega)$ *vs* ω/t for different values of $\alpha = \beta$, especifically, for 0.8, 0.5, 0.3 and 0.1, respectively. Horizontal scale is ω/t. Here $N_x = N_y = 1000$ and $\gamma = 0.01$.

By deforming the perfect triangular lattice we obtain different van Hove singularities for different values of α and β (Eq. 1). These results are shown in Figs. 2–6. In the case of $\alpha = \beta = 0$, we reproduce a 1–D lattice, since we totally compress the lattice along the y–axis (there is not dependence on k_y, in the reciprocal space). For this case ($\alpha = \beta = 0$) the density of states is symmetric around $\omega/t = 0$, with twomaxima at $\omega/t = \pm 2.0$ (Fig. 6).

Let us compare Fig. 6 and the last Fig. 3 of, this with $\alpha = \beta = 0.1$. We see that these figures will coincide if $\alpha = \beta = 0$ (as a tendency), which is the one–dimensional case. However, for $\alpha = \beta = 0.1$ we observe a logarithmic singularity around $\omega/t = 2.0$ and another one starting to appear at $\omega/t = -2.0$. This shows us that our density of states are consistent between them.

The modification of $N(\omega)$, by applying pressure to the lattice, is obvious, since the density of states depends on the band structure.

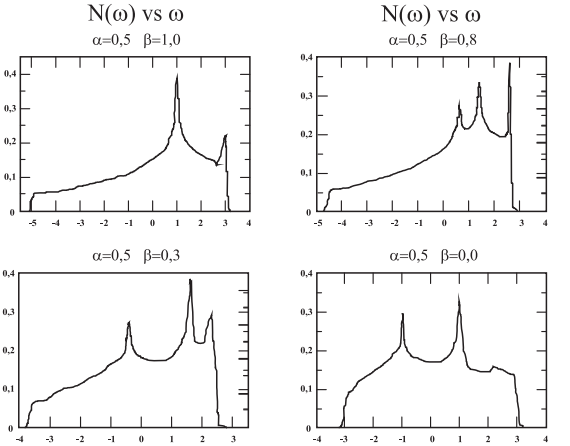

Fig. 4. $N(\omega)$ *vs* ω/t for different values of $\alpha = \beta$, namely, for $\alpha = 0.5$ and $\beta = 1.0, 0.8, 0.3, 0.0$. Horizontal scale is ω/t. We see that when we reduce β, with a smaller α, more logarithmic singularities appear in the density of states. We have taken $N_x = N_y = 1000$ and $\gamma = 0.01$.

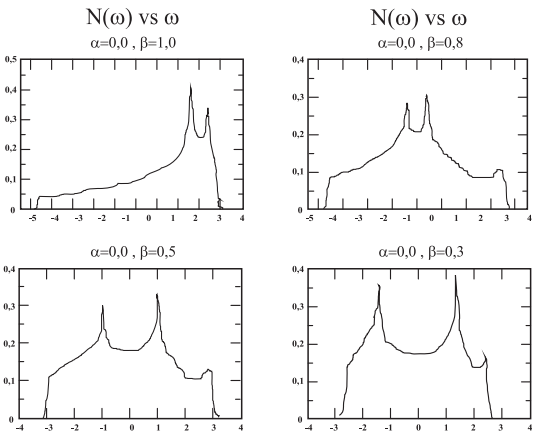

Fig. 5. $N(\omega)$ *vs* ω/t for different values of $\alpha = \beta$, namely, for $\alpha = 0.5$ and $\beta = 1.0, 0.8, 0.3, 0.0$. Horizontal scale is ω/t. We have taken $N_x = N_y = 1000$ and $\gamma = 0.01$.

As we have previously said we find that $n_s = m_v$. This has to be like this because *BCS* theory is valid close to the chemical potential and if the density of states around the chemical potential has a van Hove singularity, then we have a great number of states available to produce superconductivity or the Cooper pairs. So, the singularities and the peaks of T_c are related and, in

consequence, $n_s = m_v$.

The study of the effect of the band structure on the superconducting properties, namely, for $T \leq T_c$, is left for the future. With Eqs. (3) we can calculate the isotope exponent, namely, α', which is defined by the following relation:

$$T_c \propto M^{-\alpha} , \qquad (6)$$

where M is the isotope mass of the substituted ion. Such isotope exponent or isotope effect is determined experimentally if we substitute one of the elements of the triangular lattice (Co) by an isotope ion, with different isotopic mass, M.

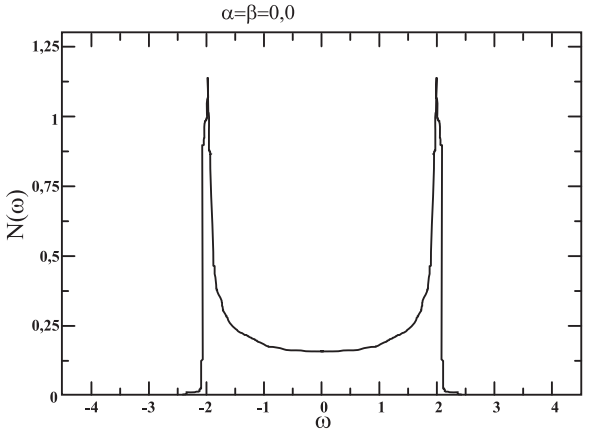

Fig. 6. $N(\omega)$ *vs* ω/t for $\alpha = \beta = 0.0$. This density of states corresponds to a 1–D lattice, which is obtained if we apply static pressure. We have taken $N_x = N_y = 1000$ and $\gamma = 0.01$.

4. Conclutions

We have calculated the density of states for a triangular lattice which has undergo applied pressure. When we change the parameters of the band structure, namely, α and β, we obtain variations on the location and the number of van Hove singularities.

For the case of a perfect triangular lattice we obtain only one logarithmic singularity for the density of states, namely, at $\omega/t = 2.0$. On the other hand, we got $T_{c,max} = 0.05$, for $\mu/t = 2.0$, or $\rho = 0.75$.

The relations T_c *vs* ρ and $N(\omega)$ *vs* μ in the perfect triangular lattice do not present symmetry around particular values. In particular, we have proved that $n_s = m_v$, where n_s is the number of van Hove singularities and mv is the number of maxima of T_c.

We leave for future work the evaluation of the superconducting properties, namely, $\Delta(T)/t$ *vs* T/t, where $\Delta(T)$ is a absolute temperature dependence of the order parameter, for $T \leq T_c$, for different values of pressure parameters α and β.

We would like to ending by pointing out a delicate aspect of our numerical calculations. The number of points both in real and reciprocal space, $N = N_x \times N_y$, is a very crucial parameter in results presented here. For example, $N_x = N_y = 500$ is a reasonable value for the calculation of the density of states and the super-conducting critical temperature, T_c. However, if we wish to perform the calculation of the isotope exponent, α' (Eq. (6)), then we have to go over to the continuous description by means of the following transformation:

$$\frac{1}{N}\sum_{\vec{k}} g(\vec{k}) \rightarrow \frac{1}{(2\pi)^2}\int_{-\pi}^{+\pi} g(\vec{k}) d^2k \quad . \quad (7)$$

The reason to do that is due to the fact that the isotope exponent depends on the lattice points, or N, and, it is a quantity which presents rapid changes as function of ρ or μ. In consequence, with the use of continuous approximation, we can use some of the numerical routines which have been developed for these cases. To predict that the behavior of α' *vs* ρ should be complex, as it was found in (Rodríguez & Schmidt, 2003; Rodríguez & Schmidt, 2006; Rodríguez & Schmidt, 2008).

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