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A pseudogap model beyond BCS for the cuprates: the effect of order parameter symmetry, cutoff frequency and band structure

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Abstract

We present an extension of the phenomenological pseudogap model proposed by Rodríguez-Núñez *et al* (2005 *J. Phys.: Condens. Matter* **17** 323) which relies on the assumption that the self-energy is given by $\Sigma_{\rm PG}(\mathrm{i}\omega_n) = -E_{\rm G}^2(k)\, G_0(k, -\mathrm{i}\omega_n)$, where $G_0(k, \mathrm{i}\omega_n)$ is the one-particle free Green function. Going beyond this mean-field model for the pseudogap we now take into account fluctuations of the pseudogap as $\Sigma_{\rm PG}(\mathrm{i}\omega_n) = -E_{\rm G}^2(k)\, G_{\rm PG}(k, -\mathrm{i}\omega_n)$, where $G_{\rm PG}(k, \mathrm{i}\omega_n)$ is the pseudogap one-particle Green function and $E_{\rm G}(\vec{k})$ is the value of the pseudogap parameter. We study the combined effect of α', the second-nearest neighbour in the band structure ($\epsilon(\vec{k}) = -2t[\cos(k_x) + \cos(k_y)] + 4t\alpha' \cos(k_x)\cos(k_y)$) and the cutoff frequency, $\omega_{\rm D}$, on the superconducting critical temperature, $T_{\rm c}$, as a function of the number of carriers per site, n. The effect of V/t and $\omega_{\rm D}/t$ is to increase the value of $T_{\rm c}/t$, while α' displaces $T_{\rm c,max}/t$ away from half-filling.

1. Introduction

Originally discovered by Bednordz and Müller [1] in 1986, the high-temperature superconductors (HTSCs) are still attracting a lot of interest due to their unusual physical properties, both in the normal and superconducting phases. For example, the HTSCs exhibit a pseudogap in the energy spectrum for temperatures in the interval $0 \leqslant T \leqslant T^*$. T^* is defined by Maier *et al* [2] as the crossover temperature with maximum spin susceptibility. Experimental evidence suggests that the pseudogap exists below $T_{\rm c}$, independently of the superconducting gap [3]. This agrees with energy gap evolution experiments in the tunnelling spectra of $Bi_2Sr_2CaCu_2O_{8+\delta}$ performed by Dipasupil *et al* [4]. They find that a pseudogap smoothly develops into the superconducting state gap without any tendency to close at $T_{\rm c}$. However,

intrinsic tunnelling spectroscopy shows evidence that the pseudogap and the superconducting order parameters are independent of each other [5–7].

There have been various theoretical approaches which try to explain the pseudogap opening mechanism [8]. However, having assumed the presence of the pseudogap, an understanding of its effects on the main superconducting state properties and macroscopic quantities such as the critical temperature T_c/t and the order parameter is yet to be achieved. Recently Kosuge *et al* [8] proposed a phenomenological model where the pseudogap is assumed to appear due to a BCS-type mechanism. Our purpose in this paper is to extend these ideas to include pseudogap fluctuations.

We take the pseudogap self-energy as [8]

$$\Sigma_{\mathrm{PG}}(\vec{k}, \mathrm{i}\omega_n) = -E_{\mathrm{G}}^2(\vec{k})\, G_{\mathrm{PG}}(\vec{k}, -\mathrm{i}\omega_n), \tag{1}$$

where $E_{\mathrm{G}}(\vec{k}) \equiv E_{\mathrm{G}}\,\phi(\vec{k})$ and $\phi(\vec{k}) \equiv 1, \cos(k_x) - \cos(k_y)$ for s-, d-wave order parameter symmetry, respectively. E_{G} is the value of the pseudogap parameter. $G(\vec{k}, \mathrm{i}\omega_n)$ is the pseudogap one-particle Green function, $\omega_n = T\pi(2n+1)$ is the odd Matsubara frequency and T is the absolute temperature.

According to [8], E_{G} can be calculated from superconducting fluctuations beyond a mean-field approximation. In the T-matrix formalism [9–12], the self-energy is a *bubble-diagram* involving G and the correlator, i.e., the T-matrix itself. If one assumes that the pairing fluctuations represented by the latter are strongly concentrated around zero frequency and zero wavevector (which should be valid close to T_c) one obtains equation (1) for the self-energy. In consequence, in [8–12] equation (1) is fully justified. In the T-matrix formalism, the pseudogap model goes beyond the mean-field approximation because it includes the renormalized Green function, $G(\vec{k}, \mathrm{i}\omega_n)$. Additionally, in the T-matrix formalism developed numerically in [9–12], it is shown that T_c and E_{G} (the pairing energy scale in [9]) are different for high values of pairing interaction.

This paper is organized as follows. Section 1 is devoted to an introduction and justification of the pseudogap energy scale. In section 2 we justify our proposed self-energy (equation (1)) following [8–12]. Using the pseudogap self-energy (equation (1)), which is valid close to T_c in the T-matrix formalism, we derive the diagonal one-particle Green function, $\mathcal{G}(\mathrm{i}\omega_n, \vec{k})$. In section 3 we present our numerical results and we conclude in section 4. In section 5 we give an outlook of our future work.

2. The pseudogap model beyond mean field

According to the perturbation theory of two-dimensional (2D) superconducting fluctuations developed by Kosuge *et al* [8], higher-order corrections are included by expanded terms of $\chi^{\mathrm{RPA}}(\vec{q}, \mathrm{i}\omega_m)$. Therefore the one-particle Green function $G(\vec{k}, \mathrm{i}\omega_n)$ is given by (following their notation)

$$G^{(1)}(\vec{p}, \mathrm{i}\omega_n) = \frac{1}{\mathrm{i}\omega_n + \mu - \epsilon(\vec{p}) - \sum^{(1)}(\vec{p}, \mathrm{i}\omega_n)}$$

$$\Sigma^{(1)}(\vec{p}, \mathrm{i}\omega_n) = -\Delta_f^2 \times G^{(1)}(-\vec{p}, -\mathrm{i}\omega_n)$$

$$\Delta_f^2 \equiv \frac{T}{N} \sum_{\vec{q}} K_1^{(1)}(\vec{q}, 0)$$

$$K_1^{(1)}(\vec{q}, \mathrm{i}\omega_n) = \frac{g^2\, \chi(\vec{q}, \mathrm{i}\omega_n)}{1 + g\, \chi(\vec{q}, \mathrm{i}\omega_n)}$$

$$\chi(\vec{q}, \mathrm{i}\omega_n) \equiv \frac{T}{N} \sum_{\vec{p},m} G^{(1)}(\vec{p}, \mathrm{i}\Omega_m) G^{(1)}(\vec{p}, \mathrm{i}\omega_n - \Omega_m).$$

In consequence, in the formalism of Kosuge *et al* [8], one can, in principle, calculate Δ_f self-consistently. $E_{\mathrm{G}} \equiv \Delta_f$ is the pseudogap energy scale and $G^{(1)}(\vec{k}, \mathrm{i}\omega_n) = G_{\mathrm{PG}}(\vec{k}, \mathrm{i}\omega_n)$. We take equation (1) as our starting point with $E_{\mathrm{G}}(\vec{k})$ a fixed parameter. Although Kosuge *et al*'s equations are not used in the remainder of this paper, we have included them to show that the PG order parameter is justified in their formalism.

Now our starting Hamiltonian is given by [13][5]

$$\hat{H} = \sum_{i,j;\sigma} t_{i,j} c^{+}_{i,\sigma} c_{j,\sigma} - U \sum_{i} c^{+}_{i,\uparrow} c^{+}_{i,\downarrow} c_{i,\downarrow} c_{i,\uparrow} - V \sum_{\langle i,j \rangle} c^{+}_{i,\uparrow} c^{+}_{j,\downarrow} c_{i,\downarrow} c_{j,\uparrow} \tag{2}$$

where U, V are the on-site and on-nearest-neighbours attraction, respectively. U and V allow for the presence of s- and d-wave order parameter symmetries, respectively. In equation (2), $t_{i,j}$ represents the hopping matrix elements on a 2D plane and $\langle i, j \rangle$ means next-nearest neighbours.

The T-matrix for the Hubbard model consists of the sum of the particle–particle ladder diagrams in the perturbation expansion in terms of U (local attraction). It is known that the T-matrix is the ladder approximation to the Bethe–Salpeter equation [14]

$$T(\vec{q}, \mathrm{i}\epsilon_m) = \frac{-U}{1 - U\chi(\vec{q}, \mathrm{i}\epsilon_m)}, \tag{3}$$

where $\chi(\vec{q}, \mathrm{i}\epsilon_m)$ is the independent pairing susceptibility given by

$$\chi(\vec{q}, \mathrm{i}\epsilon_m) = \frac{1}{N\beta} \sum_{\vec{k}, \mathrm{i}\omega_n} G(\vec{k}, \mathrm{i}\omega_n) G(\vec{q} - \vec{k}, \mathrm{i}\epsilon_m - \omega_n), \tag{4}$$

where $\omega_n = \pi(2n + 1)/\beta$ and $\epsilon_m = 2\pi m/\beta$, $(n = m = 0, \pm 1, \pm 2, \ldots)$ are the fermionic (odd) and bosonic (even) Matsubara frequencies, respectively, and $\beta = (k_{\mathrm{B}}T)^{-1}$ is the inverse of the absolute temperature. This approximation is supposed to be valid in the low-density limit. The corresponding one-particle Green function satisfies the Dyson equation. In the T-matrix approach the self-energy $\Sigma(\vec{k}, \mathrm{i}\omega_n)$ is given by

$$\Sigma(\vec{k}, \mathrm{i}\omega_n) = \frac{1}{N\beta} \sum_{\vec{q}, \mathrm{i}\epsilon_m} T(\vec{q}, \mathrm{i}\epsilon_m) G(\vec{q} - \vec{k}, \mathrm{i}\epsilon_m - \omega_n), \tag{5}$$

which closes the system of self-consistent equations. The results for real frequencies are obtained upon the analytic continuation, namely, $\mathrm{i}\omega_n \to \omega + \mathrm{i}0^{+}$.

Within the T-matrix formalism of [9–12] (especially equation (5) of [9] and equation (5)) we can obtain the pseudogap self-energy (equation (1)), with $E_{\mathrm{G}} \equiv 1/(N\beta) \sum_{\vec{q},m} T(\vec{q}, \mathrm{i}\varepsilon_m)$, by considering that the small values of $\vec{q}$ and ε_m give the main contribution to the summation, where ε_m are even Matsubara frequencies. Thus, we are able to justify our proposal given by equation (1), within the T-matrix formalism, for the case of s-wave symmetry (only the presence of U). The case of V follows a similar treatment.

By including the *pseudogap* self-energy (equation (1)) into the pseudogap Green function

$$G_{\mathrm{PG}}(\vec{k}, \mathrm{i}\omega_n) = [\mathrm{i}\omega_n + \mu - \epsilon(\vec{k}) - \Sigma_{\mathrm{PG}}(\vec{k}, \mathrm{i}\omega_n)]^{-1} \tag{6}$$

one obtains

$$G_{\mathrm{PG}}(\vec{k}, \omega) = \left[\frac{\omega + \epsilon(\vec{k}) - \mu}{2E^2_{\mathrm{G}}(\vec{k})} \right] \left[1 - \sqrt{1 - \frac{4E^2_{\mathrm{G}}(\vec{k})}{\omega^2 - [\epsilon(\vec{k}) - \mu]^2}} \right]. \tag{7}$$

[5] These authors were the first to propose this Hamiltonian and to study it extensively, even today, in mean-field theory.

We point out that the solution of the one-particle renormalized Green function, $G_{\rm PG}(\vec{k},\omega)$, in the presence of the pseudogap, is obtained by solving a quadratic equation for $G_{\rm PG}(\vec{k},\omega)$. Out of the two solutions of this equation we have chosen the one that allows us to obtain the one-particle free Green function in the limit $E_{\rm G}\to 0$, namely, $\lim_{E_{\rm G}\to 0} G_{\rm PG}(\vec{k},\omega) = G_0(\vec{k},\omega)$.

According to experimental data in the HTSCs, the pseudogap phase enters into the superconducting phase and becomes zero at a critical doping of $x_{\rm c} = 0.19$ (with $x = 1.0$–n), where n is the number of carriers per site. As shown by Wuyts *et al* [15], the succession of Knight shift curves ${}^{89}K_s(T)$ obtained by Alloul [16] for different doping states across the underdoped regime may be scaled to a single function of $T/E_{\rm G}$. See also [17]. These fall linearly to zero at the critical doping of $x_{\rm c} = 0.19$ and rise to the magnitude of the exchange energy, J, as $x\to 0$. We point out that the optimal doping is $x_{\rm opt} = 0.15$. This leads us to consider the effect of the PG energy scale on the superconducting properties, namely, $T_{\rm c}$ (studied in this paper) and the superconducting order parameter, $\Delta(T)$.

In the presence of a pseudogap ($E_{\rm G}\neq 0$) within the superconducting phase, we need to solve the Gorkov's equations:

$$G^{-1}_{\rm PG}(\vec{k},{\rm i}\omega_n)\mathcal{G}(\vec{k},{\rm i}\omega_n) + \Delta(\vec{k})\mathcal{F}(\vec{k},{\rm i}\omega_n) = 1 \tag{8}$$

$$G^{-1}_{\rm PG}(\vec{k},-{\rm i}\omega_n)\mathcal{F}(\vec{k},{\rm i}\omega_n) + \Delta(\vec{k})\mathcal{G}(\vec{k},{\rm i}\omega_n) = 0, \tag{9}$$

where $G^{-1}_{\rm PG}(\vec{k},{\rm i}\omega_n) \equiv 1/G_{\rm PG}(\vec{k},{\rm i}\omega_n)$ and $G_{\rm PG}(\vec{k},{\rm i}\omega_n)$ is the pseudogap one-particle Green function, equation (7). $\mathcal{G}(\vec{k},{\rm i}\omega_n)$ and $\mathcal{F}(\vec{k},{\rm i}\omega_n)$ are the diagonal and off-diagonal one-particle Green function in the superconducting phase, namely, for $0\leqslant T\leqslant T_{\rm c}$, in the Nambu formalism.

Now, taking into account the scenario where the pseudogap survives in the superconducting state, we obtain the superconducting critical temperature, $T_{\rm c}$, and the chemical potential, μ, from the two mean-field self-consistent equations

$$\pi^2 = V\,T_{\rm c}\int {\rm d}^2k\,\phi^2(\vec{k})\,\psi(\vec{k})\sum_n G_{\rm PG}(\vec{k},{\rm i}\omega_n)\,G_{\rm PG}(\vec{k},-{\rm i}\omega_n) \tag{10}$$

$$n\,\pi^2 = T_{\rm c}\int {\rm d}^2k\sum_n G_{\rm PG}(\vec{k},{\rm i}\omega_n), \tag{11}$$

where n is the number of carriers per site, $\phi(\vec{k}) = \cos(k_x) - \cos(k_y)$ and $\psi(\vec{k}) = 1$ if $|\epsilon(\vec{k}) - \mu| \leqslant \omega_{\rm D}$ (0 otherwise), where $\omega_{\rm D}$ is the cutoff frequency. We adopt the following 2D tight binding structure $\epsilon(\vec{k}) = -2\,t\,[\cos(k_x)+\cos(k_y)] + 4\,t\,\alpha'\cos(k_x)\cos(k_y)$, where t is the next-nearest hopping and $t' = \alpha'\times t$ is the second-nearest hopping matrix element.

We have performed the Matsubara summation numerically, due to the fact that the pseudogap Green function, $G_{\rm PG}(\vec{k},{\rm i}\omega_n)$, does not have a simple pole structure dependence on ω_n. However, we have expressed our $\vec{k}$-summation in a 2D integration in the usual way. In section 3, we present our results by solving the two coupled equations given previously, i.e., equations (10) and (11).

3. Numerical results

Due to the fact that our *normal* Green function has been approximated with a self-energy (equation (1)), which is beyond mean-field theory, we expect that the normal density of states (NDOS) even in the presence of the pseudogap ($E_{\rm G}\neq 0$) is going to produce a zero density of states only at $\omega = 0$. This result is independent whether we choose a s- or d-wave symmetry for the pseudogap order parameter. More specifically, the form of the density of states for both symmetries is d-type around the Fermi level.

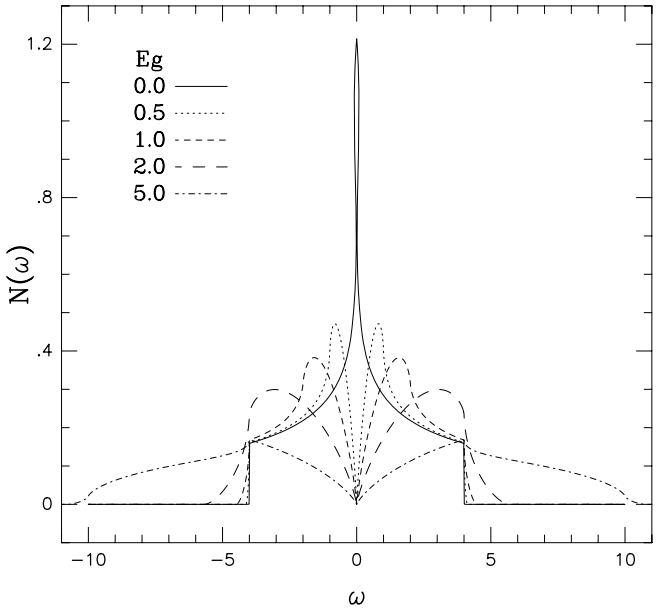

Figure 1. $N(\omega) \times \omega$ for s-wave symmetry (both for the pseudogap and the superconducting order parameters) with $\alpha' = 0.0$, and several values of E_G/t, namely, $E_G/t = 0.00, 0.50, 1.00, 2.00$ and 5.00. We see that the symmetry around $\omega = 0$ is kept due to the fact that $\alpha' = 0$ and $\mu = 0$.

Before presenting our numerical results, we define some quantities which are useful in photoemission experiments. They are the spectral function, $A(\vec{k}, \omega)$, and the density of states, $N(\omega)$. They are given by

$$\begin{aligned} A(\vec{k}, \omega) &= -\frac{1}{\pi} \lim_{\delta \to 0^+} \mathrm{Im}[\mathcal{G}(\vec{k}, \omega + \mathrm{i}\delta)] \\ N(\omega) &= \frac{1}{\pi^2} \int_0^{\pi} \mathrm{d}^2 k A(\vec{k}, \omega). \end{aligned} \tag{12}$$

In figures 1 and 2 we present the density of states, $N(\omega) \times \omega$, for s- and d-wave symmetry, respectively, for both the pseudogap and the superconducting order parameters. For these figures we have chosen $\alpha' = 0$, and several values of the pseudogap parameter ratio, namely, $E_G/t = 0.00, 0.50, 1.00, 2.00$ and 5.00. As we can see, as $\alpha' = 0$, the symmetry around half-filling, $n = 1.00$ or $\omega = 0.00$, is kept.

Comparing the two densities of states of figures 1 and 2 we observe that, except for details in the high-energy sector, for frequencies $\omega \approx 0.0$ we have a d-type pseudogap behaviour in that frequency range. For example, the density of states for d-wave symmetry is more extended than the density of states for s-wave symmetry. Approximating the full density of states for a linear behaviour around $\omega \approx 0$ is useful for performing analytical calculations, as done by Ţifrea *et al* [20]. We recall that the pseudogap behaviour has also been obtained by numerical simulations in the attractive Hubbard model [21–25].

In figure 3 we show the superconducting critical temperature, $T_c \times n$ (upper panel), and $\mu \times n$ (lower panel) for a d-wave symmetry (for both order parameters) with $\alpha' = 0$, $\omega_D/t = 0.50$ and $E_G/t = 0.50$ for several values of the pairing potential, namely, $V/t = 4.50$, 5.00, 5.50 and 6.00. From this figure it is clear that for a fixed value of V/t we should have two regions of n, to each side of half-filling, where we find superconductivity. That is the reason that we have decided to look more carefully in the parameter phase space (see figure 4).

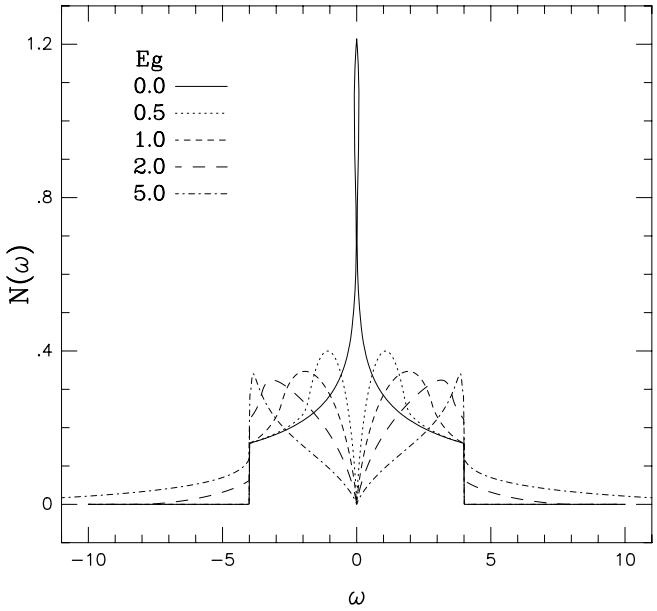

Figure 2. Same as figure 1 for d-wave symmetry.

After carefully searching the possible existence of two superconducting regions to both sides of half-filling we came to the conclusion that this is not the case. More precisely, we have found that we need reasonably large values of V/t to have superconductivity in a certain region of carrier number and after some value of V/t we have two regions with *high* values of T_c/t (two bumps, let us say) and an intermediate region with *small* values of the superconducting critical temperature. As we can see, when all this structure appears, superconductivity exists in the whole region of carrier number. In figure 4 we present the results of our search for the question posed after the results obtained in figure 3. Here, we plot $T_c \times \mu$ (upper panel) and $n \times \mu$ (lower panel) for a d-wave symmetry (for both order parameters) with $\alpha' = 0$, $\omega_D/t = 0.50$ and $E_G/t = 0.40$ for several values of the pairing potential, namely, $V/t = 6.25$, 6.30, 6.35, 6.40, 6.45 and 6.50.

To see the breaking of symmetry of $N(\omega) \times \omega$, around $\omega = 0$, we present the s-wave symmetry density of states for a set of parameters as given in figure 5. We have fixed the value of E_G/t to 2.0, while we change the values of (α', μ), as indicated in the figure.

In figure 6 we show the superconducting critical temperature, $T_c \times n$ (upper panel) and $\mu \times n$ (lower panel) for an s-wave symmetry (for both order parameters) with $\alpha' = 0$, $\omega_D/t = 0.50$ and $E_G/t = 0.50$ for several values of the pairing potential, namely, $V/t = 6.00$, 6.50, 7.00, 7.50. We see that the symmetry around half-filling is kept due the fact that $\alpha' = 0$. We also see that higher values of V are needed to obtain finite values of T_c.

By comparing figures 3 and 6, for d- and s-wave symmetries, respectively, we observe that they look completely different. For example, for the d-wave symmetry we have two maxima instead of one as is the case for the s-wave symmetry. This is likely due to the different structure of the density of states (figures 1, 2). For the case of d-wave symmetry the density of states is discontinuous at $\omega = \pm 4t$ and this gives rise to the additional maxima in the plot of $T_c \times n$ for low concentrations of n and large values of V/t. In consequence, the underlying symmetry has an important role in the resulting phase diagram.

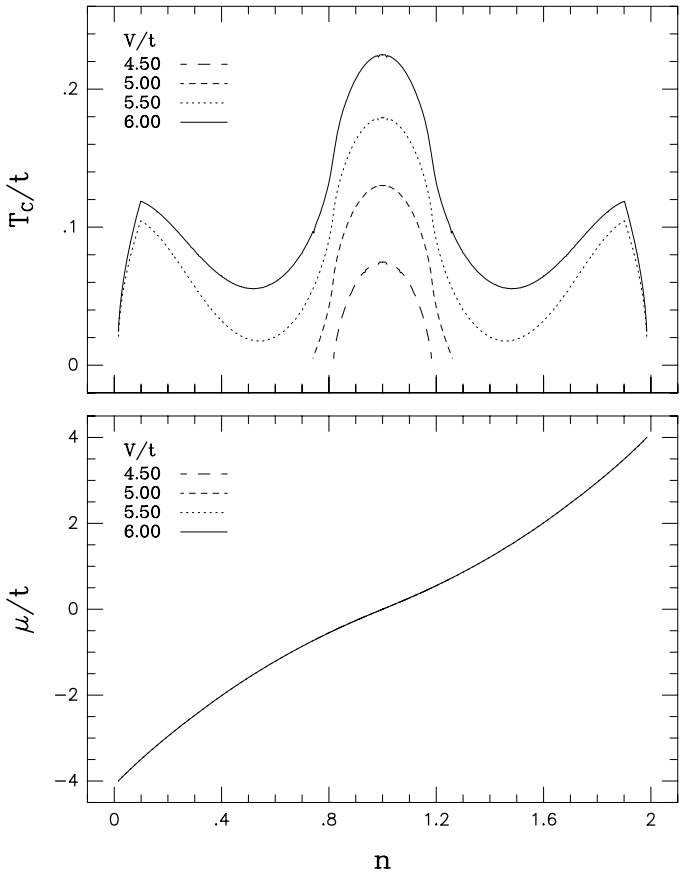

Figure 3. The superconducting critical temperature, $T_c \times n$ (upper panel) and $\mu \times n$ (lower panel) for a d-wave symmetry (for both order parameters) with $\alpha' = 0$, $\omega_D/t = 0.50$ and $E_G/t = 0.50$ and for several values of the pairing potential, namely, $V/t = 4.50$, 5.00, 5.50 and 6.00. From this figure it appears that for a fixed value of V/t we should have two regions of n, to each side of half-filling, where we find superconductivity.

Now we study the effect of second-nearest hopping, i.e., $\alpha' \neq 0$. In figure 7 we show $T_c \times n$ for a d-wave symmetry, with $\alpha' = +0.20$, $\omega_D/t = 0.5$ and several values of the pairing potential, namely, $V/t = 3.00$, 3.30, 4.00, and 4.50. We see that the effect of a positive α' is to displace the curve of T_c to the left, with respect to the one at half-filling.

4. Conclusions

Our conclusions have to be drawn from figures 1–7. The first thing to realize is that by adopting equation (1), our normal state Green function *always* produces d-wave superconductivity (see figures 1 and 2) around $\omega = 0$. Then it is sound to say that our pseudogap model is a d-wave model for the density of states around the Fermi level, at $T = T_c$. Below T_c we have to be careful about the symmetry of the density of states.

In figure 3 we present $T_c \times n$ and $\mu \times n$ for a d-wave symmetry, with $\alpha' = 0.0$, $\omega_D/t = 0.50$ and $E_G/t = 0.50$ for several values of $V/t = 4.50$, 5.00, 5.50 and 6.00. (t has been taken

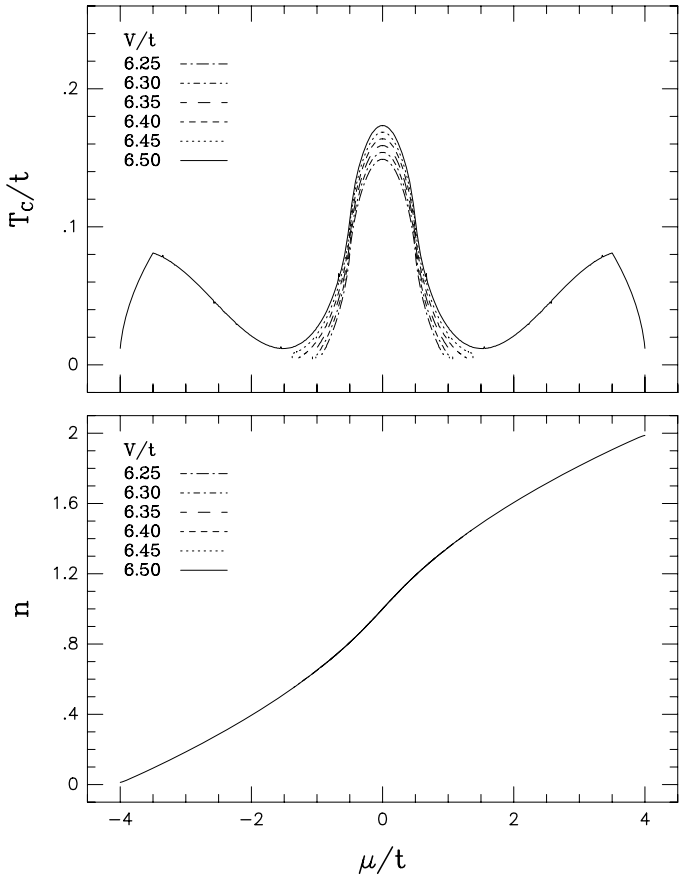

Figure 4. The superconducting critical temperature, $T_c \times \mu$ (upper panel) and $n \times \mu$ (lower panel) for a d-wave symmetry (for both order parameters) with $\alpha' = 0$, $\omega_D/t = 0.50$, $E_G/t = 0.40$ and $V/t = 6.25$, 6.30, 6.35, 6.40, 6.45 and 6.50.

the energy unit.) From this figure we observe that the symmetry around $n = 1$ is kept, since $\alpha' = 0$. We also observe that for some small values of V/t, there is no superconductivity, namely, $T_c/t = 0$, in a range of carrier concentration. From the lower panel of figures 3–7, we see that μ does not change appreciably with the considered values of V/t. In these figures 3–7, we see that the parameter controlling the symmetry around half-filling is α'. Thus, $\alpha' = +0.20$ displaces the centre of $T_c \times n$ to the left of $n = 1.0$.

We have solved numerically our two coupled self-consistent equations (10) and (11) for T_c and μ versus n for several values of (1) the pseudogap parameter, E_G/t; (2) the second-nearest hopping ratio, α'; (3) the Debye frequency, ω_D/t; and (4) the pairing interaction, V/t. The results we find are the following.

(1) Increasing the value of V/t increases the value of T_c/t, since it produces superconductivity in any channel.
(2) Increasing the value of E_G/t decreases the value of T_c/t. This has as consequence, in the case of a pseudogap dependent on carrier number, that T_c/t decreases in a very defined region of the phase space. One needs some critical value of V/t to have finite values of

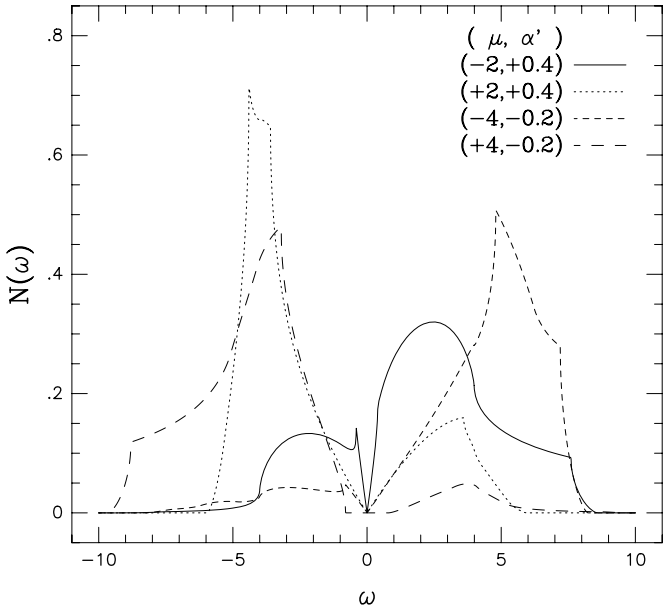

Figure 5. $N(\omega) \times \omega$ for an s-wave symmetry (both for the pseudogap and the superconducting order parameters) with $E_G/t = 2.0$, and several pair values of (α', μ).

T_c/t. This is the reason we have taken high values of V/t to find superconductivity. See figures 3–6.

(3) Decreasing the value of ω_D/t decreases the value of T_c/t. This is reasonable since we have fewer available states around the Fermi sea which contribute to the integral in equation (10).
(4) The inclusion of α', which we call the effect of the band structure, is important because it moves the *centre* of the $T_c/t \times n$ curve. The *centre* of this curve, with respect to half-filling ($n = 1$), is displaced to the left (right) if $\alpha' > 0.0$ (<0).
(5) The chemical potential is defined in the region where $T_c/t \neq 0$. However, in this region, it is almost identical for different values of V/t. This is due to the fact that μ is a global property and it depends on the number of carriers.
(6) Our model *always* produces d-wave superconductivity around the Fermi level, at T_c.

In short, we have checked that the band structure parameters α' and ω_D influence the value of T_c. In particular, $\alpha' \neq 0$ breaks the symmetry around half-filling and ω_D decreases the value of T_c. In our model of a pseudogap, beyond mean-field theory, $E_G \neq 0$ also decreases the value of T_c. Also, for $E_G \neq 0$ we have $T_c(n) \neq 0$ in an interval of n. These global results are in qualitative agreement with those in [19]. However, the dynamical properties such as the spectral function and the density of states (among others) are very different from those in [19], namely,

$$\Sigma_{PG}(\vec{k}, i\omega_n) = -E_G^2(\vec{k})\, G_0(\vec{k}, -i\omega_n), \tag{13}$$

with $G_0(\vec{k}, i\omega_n)$ been the one-particle free Green function. We should mention that the approximation given by equation (13) gives a semiconductor-type of gap for $E_G(\vec{k})/t = E_G/t =$ constant. However, for $E_G(\vec{k})/t = (E_G/t)[\cos(k_x) - \cos(k_y)]$ the pseudogap produces a d-symmetry in the density of states. This was used in [20].

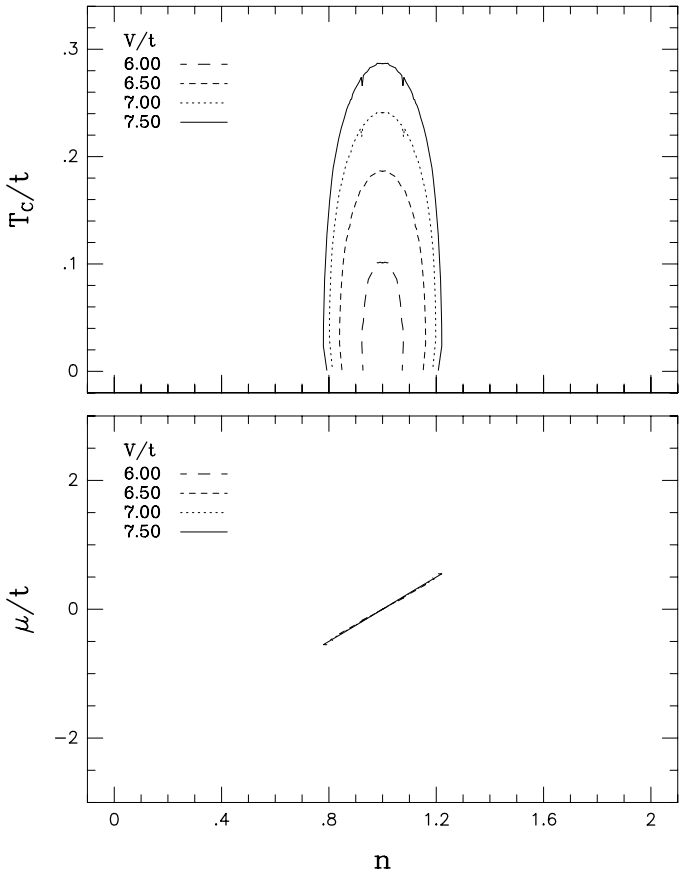

Figure 6. $T_c \times n$ (upper panel) and $\mu \times n$ (lower panel) for an s-wave symmetry (both for the pseudogap and the superconducting order parameters) with $\alpha' = 0.0$, $\omega_D/t = 0.50$ and $E_G/t = 0.50$ for several values of V/t, namely, $V/t = 6.00$, 6.50, 7.00 and 7.50. The symmetry around half-filling ($n = 1$) is kept due to the fact that $\alpha' \equiv 0$.

In this work we have considered the pseudogap order parameter coexisting and competing with the superconducting order parameter, both of the same symmetry, justifying equation (1) in the T-matrix formalism, which is valid for low values of $n \approx 0$ and for large values of $n \approx 2$, respectively. To mimic the phase diagram of the HTSCs we should include $\alpha' \neq 0$, which displays the phase diagram to the right or the left, depending on the sign of α'.

We should say a few words about the approximation used. We have considered a mean-field approximation (MFA) for the superconductivity, not for E_G. In consequence, T_c does not need to go to zero. In this MFA we may consider that our T_c refers to a quasi-2D lattice or a truly 3D lattice.

We should end by saying that in this paper we have taken $T^* \equiv E_G$. However, we have neglected any doping dependence of E_G. This is left for future work [26][6].

[6] We only say that in this case the curve $T_c \times n$ shows a deviation from parabolicity in the region where the pseudogap energy scale changes with doping.

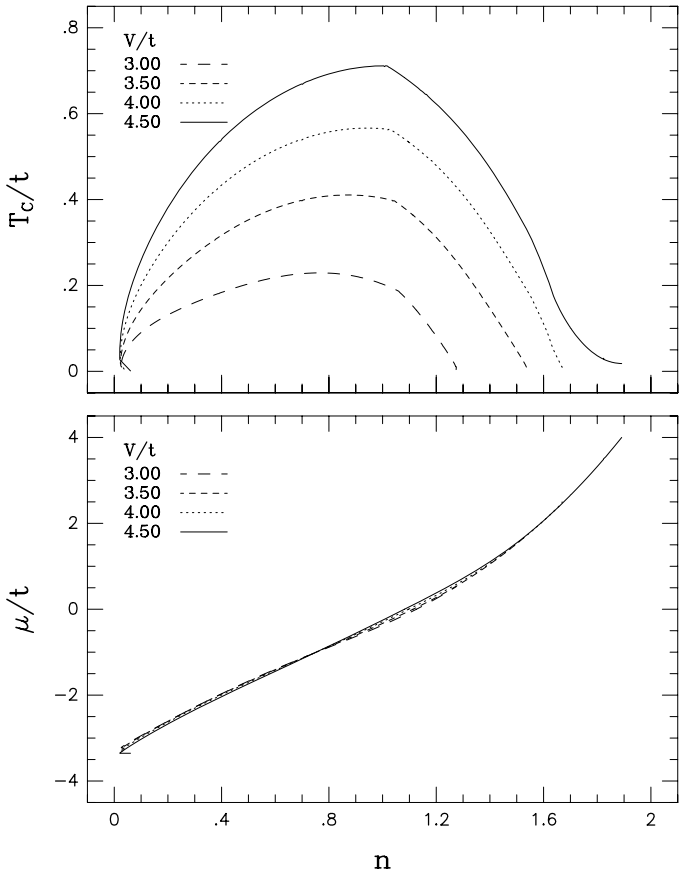

Figure 7. Same as figure 6 for a d-wave symmetry for $\alpha' = +0.20$ and $V/t = 3.00$, 3.50, 4.00 and 4.50. The symmetry around half-filling ($n = 1$) is broken due to the presence of the second-nearest hopping term, namely, $\alpha' \neq 0$.

5. Outlook

Now, with respect to the outlook, we would like to do the following.

(1) Calculate the isotope exponent, α, as a function of n. α is given from the following expression: $T_c \approx M^{-\alpha}$, where M is the isotope mass of the ions. Naturally, all the kinks which appear in the $T_c \times n$ curve are going to produce rapid changes in the isotope exponent [18].

(2) Calculate $\Delta(T) \times T$, for fixed values of n, V/t, E_G/t and α'.

(3) Calculate the BCS–BEC (Bose–Einstein condensation) crossover line, as was done in [18]. In particular, we would like to find the so-called *metallic state phase*, which is characterized by $\Delta_0 = 0$ [18].

(4) Calculate the superconducting properties, namely, the order parameter as function of temperature, below T_c, under the presence of the competing pseudogap order parameter.

(5) Reproduce the phase diagram, namely, T_c/t versus n, for the HTSCs. We believe that, for accomplishing this, we have to include second- and third-nearest neighbours.

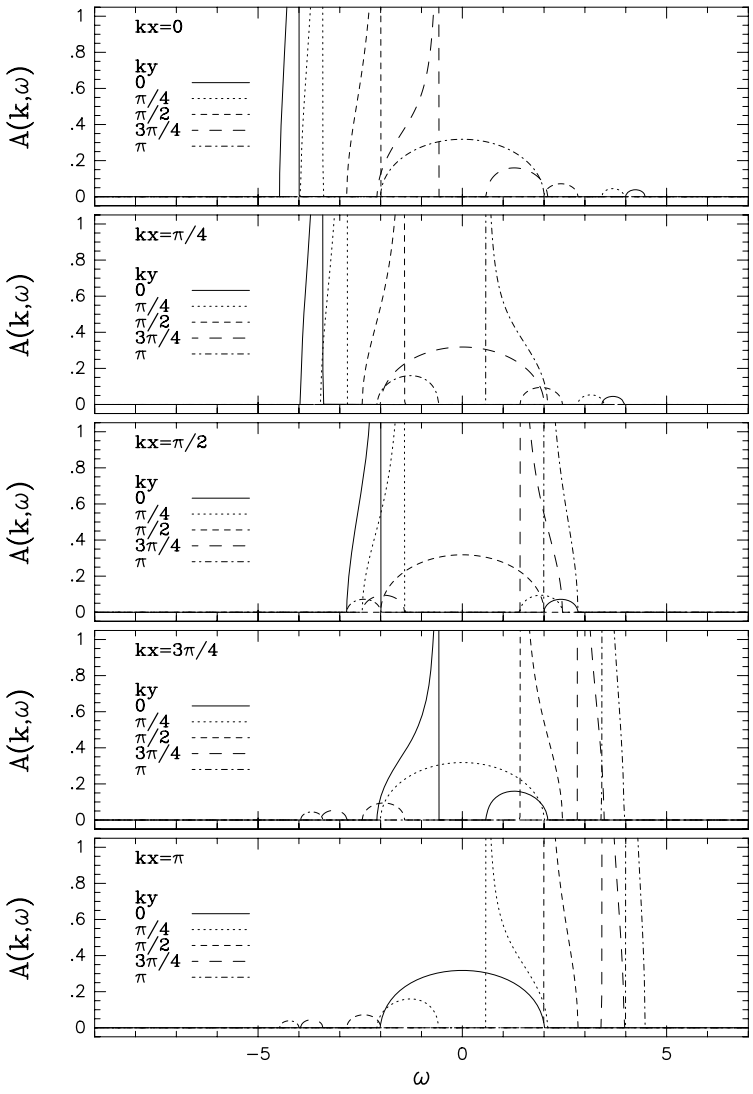

Figure 8. The s-wave symmetry spectral density $A(\vec{k},\omega)\times\omega$ for several values of k_x and k_y: $\alpha'=0$, $\mu=0.0$, $E_G/t=1.00$ and $\delta=10^{-5}$.

In order to go from the discrete version for ω_n, the Matsubara frequency representation, we need to perform the spectral theorem for the Green function as follows:

$$G(\vec{k},\mathrm{i}\omega_n)=\int_{-\infty}^{+\infty}\frac{A(\vec{k},z)\,\mathrm{d}z}{z-\mathrm{i}\omega_n}. \tag{14}$$

By performing the Matsubara frequency summation, equation (10) becomes

$$\pi^2=V\int \mathrm{d}^2k\,\phi^2(\vec{k})\,\psi(\vec{k})\int_{-\infty}^{+\infty}\mathrm{d}\omega\sum_{-\infty}^{+\infty}\mathrm{d}\omega'\frac{A_{\mathrm{PG}}(\vec{k},\omega)\,A_{\mathrm{PG}}(\vec{k},\omega')(f(\omega)-f(\omega'))}{\omega-\omega'} \tag{15}$$

$$n\,\pi^2=\int \mathrm{d}^2k\int_{-\infty}^{+\infty}\mathrm{d}\omega\,A_{\mathrm{PG}}(\vec{k},\omega). \tag{16}$$

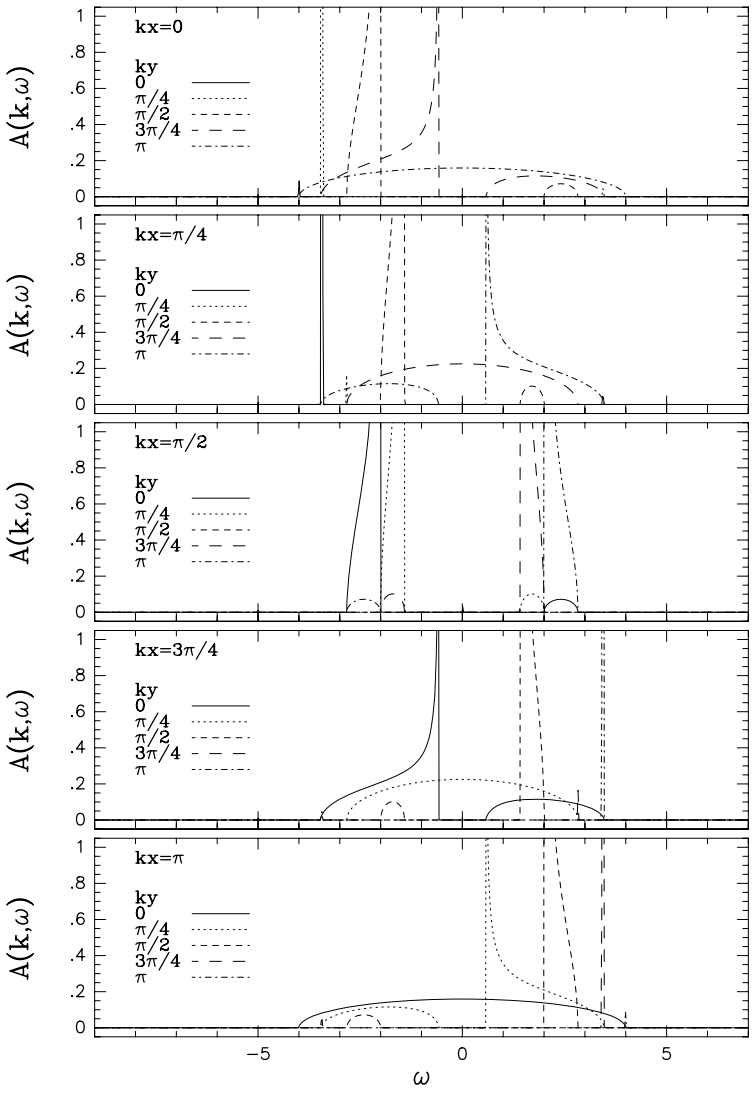

Figure 9. Same as figure 8 for d-wave symmetry.

While the spectral function, $A(\vec{k}, \omega)$, has very delicate structure (see figures 8 and 9), we prefer this form (equation (16)) to the one given by equation (11), due to the fact that it is expressed by integrals and numerical quadrature routines solve these equations quickly and with the desired accuracy. Also, we prefer integration over direct summation because the results will not depend on the number of Matsubara frequencies. In figures 8 and 9, we show the spectral function along k_x and k_y axes, for several parameters of the theory. As we can see, the spectral function has properties of quasi-particle behaviour (peak behaviour) and non-coherent behaviour (round behaviour). These features are valid for both s- and d-wave symmetries.

In figure 10 we present $A(\vec{k}, \omega) \times \omega$ and k_x for several values of k_y. In this figure, we have the following parameters: $\alpha' = 0$, $\mu = 0.00$, $E_G/t = 0.01$ and $\delta = 10^{-8}$. For this value of $E_G/t = 0.01$, the spectral function is almost a set of delta functions. This is so because the pseudogap parameter is really small.

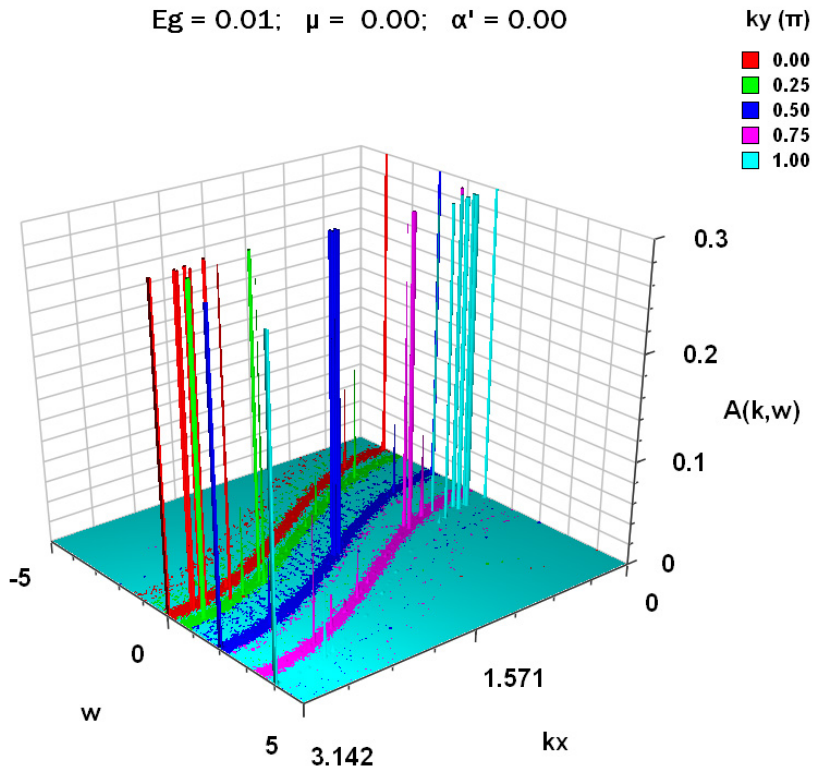

Figure 10. The s-wave symmetry spectral density $A(\vec{k}, \omega) \times \omega$ and k_x for several values of k_y: $\alpha' = 0$, $\mu = 0.00$, $E_G/t = 0.01$ and $\delta = 10^{-8}$. As we see, for this value of $E_G/t = 0.01$, the spectral function is almost a set of delta functions. Therefore, we have the almost free case due to the small value of the pseudogap value.

(This figure is in colour only in the electronic version)

Acknowledgments

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