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The effect of a pseudogap on the superconducting critical temperature and on the superconducting order parameter of the same symmetry

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Abstract

We study numerically the superconductivity in a system whose normal state is characterized by the presence of a phenomenological pseudogap, E_g/t, in the energy spectrum, for $0 \leqslant T \leqslant T^*$. T^* is called the crossover temperature and it is defined in the high-temperature superconductors (HTSC) where the static spin susceptibility, $\chi(T)$, is a maximum. At T^* one also observes the formation of a pseudogap in the density of states around the chemical potential (Maier *et al* 2002 *Preprint* cond-mat/0208419). In order to fix ideas, we have chosen the pseudogap and the superconducting gap to have the same symmetry. We have adopted the scenario where the pseudogap and the superconducting gap are independent of each other (Tallon and Loram 2001 *Physica* C **349** 53), for which the pseudogap enters in the superconducting phase going down to zero at zero temperature. We have found that $\forall E_g/t \neq 0$ we require a critical value of the superconducting interaction, V/t, to produce a finite superconducting critical temperature, T_c/t, and the superconductor order parameter at $T/t = 0$, Δ_0/t. These results have been obtained for both $\mu/t = 0$ and $\mu/t \neq 0$. We have obtained a phase diagram, namely, V/t versus E_g/t, at half-filling. We have compared our results with the analytical calculations of Ţifrea *et al* (2002 *Physica* C **371** 104), the recent work of Ţifrea and Moca (2003 *Preprint* cond-mat/0307362 (2004 *Europhys. J.* B, at press)) and other relevant theoretical results.

1. Introduction

Originally discovered by Bednorz and Müller [1] in 1986, the high-temperature superconductors (HTSC) are still attracting a lot of interest due to their unusual physical properties, both in the normal and in the superconducting phases. For example, in the normal state, the HTSC exhibit a pseudogap in the energy spectrum in the temperature range $0 \leqslant T \leqslant T^*$. T^* is defined by Maier *et al* [2] as the crossover temperature where the spin susceptibility is a maximum. There is experimental evidence obtained by the group of Tallon and Loram [3–7] that the pseudogap persists below T_c/t, independently of the superconducting gap. This interpretation is in agreement with the experiment on energy gap evolution in the tunnelling spectra of Bi2Sr2CaCu2$_{8+\delta}$ performed by Dipasupil *et al* [8]. They find that the pseudogap smoothly develops into the superconducting state gap with no tendency to close at T_c/t.

Further proof that the pseudogap and the superconducting gap are independent of each other is given in the experiments of Krasnov *et al* [9] where, by applying a magnetic field to their samples, they managed to destroy the superconducting gap while the pseudogap remained. They conclude that the pseudogap and the superconducting gap coexist in Bi-2212, using intrinsic tunnelling spectroscopy.

Krusin-Elbaum *et al* [10] have applied pulsed magnetic fields of higher intensity and they have studied the H versus T diagram of Bi-2212. They have not been able to close their pseudogap with pulsed magnetic fields up to 60 T.

The pseudogap (PG) phenomenon has several origins. For example, Fujimoto [11] has considered the PG in a BCS pairing model with a long but finite interaction range. Vertex corrections for the self-energy are important in this study. Other authors consider that the PG is due to phase fluctuations [12–16]. They have succeeded in explaining the pseudogap observed in ARPES, NMR, and tunnelling spectroscopy experiments. In these studies the single-particle self-energy is calculated using the t-matrix approximation.

Domańsky and Ranninger [17] consider that the PG has its origin in the boson–fermion model. Very recently, Kaminski *et al* [18] have found, using angle-resolved photoemission experiments with circularly polarized light, that in the pseudogap state, left-circularly polarized photons give a different photocurrent to right-circularly polarized photons, and therefore the state below T^* is rather unusual, in that it breaks time reversal symmetry [19].

Yanase and co-workers [20] consider that the pseudogap phenomenon is due to superconducting fluctuations in the Hubbard model. They have implemented the FLEX approximation and the self-consistent t-matrix approximation.

Since the work of Iguchi *et al* [21], there has appeared the percolation theory for high-T_c superconductivity. de Mello and co-workers [22] have put forward this approach in which they assume that the charge density varies in the sample. Because of that, there is a distribution of $T_c(r)$. T^* is the maximum of all $T_c(r)$.

Posazhennikova and Coleman [23] have studied the quenched disordered formulation of the pseudogap problem. Their theory of the pseudogap is induced by the fluctuations of the order parameter. They average the free energy of the pseudogap system over the quenched disordered distribution of the order parameter.

Prelovšek and Ramšak [24] have obtained the pseudogap both analytically and numerically using the equation of motion approach for the t–J model of strongly correlated electron systems. At the level of the self-energy they have decoupled the spin and single-particle fluctuations. According to their interpretation, the value of the pseudogap temperature is $T^* \approx 2J/3$, where the spin susceptibility, $\chi(T)$ has a maximum. They also discuss the presence of a second crossover temperature, T_{sg}, which has been identified in connection with the decrease of the NMR relaxation rate $1/T_1$ for $T < T_{sg}$.

Vilk and Tremblay [25] have also obtained a single-particle pseudogap in the Hubbard model using a non-perturbative approach.

Chakravarty, Laughlin, and co-workers [26–28] have proposed a candidate for the pseudogap order parameter due to orbital antiferromagnetism or d density wave (DDW) order, which is characterized by a local order parameter that distills the universal physics underlying the staggered flux state.

In this paper we do not adopt a physical mechanism for the opening of the pseudogap in the normal state density of states. We rather exploit its consequences for two macroscopic quantities in the superconducting state, namely, the superconducting critical temperature, T_c/t, and the superconducting order parameter at $T = 0$, Δ_0/t. The reader is referred to [29] where a general study of critical points in the cuprate phase diagram is considered.

This paper is organized as follows. In section 2, we present the pseudogap model, following the steps of Ţifrea *et al* [30]. In section 3 we present our numerical results. In section 4 we present a discussion and conclusions.

2. The pseudogap model

We assume, as was done in [30], that the PG and the normal one-particle self-energy are related by the following relation:

$$\Sigma(\vec{k}, \mathrm{i}\omega_n) \equiv -E_g^2\, G_0(\vec{k}, -\mathrm{i}\omega_n), \tag{1}$$

where $G_0(\vec{k}, \mathrm{i}\omega_n)$ is the free one-particle Green function and E_g is the width of the PG. $\vec{k}$ is the wavevector and $\omega_n = 2\pi T(n + 1/2)$ is the odd Matsubara frequency, with n an integer. With this choice of self-energy is easy to show that the 'PG' Green function is given by

$$G(\vec{k}, \mathrm{i}\omega_n) = \frac{u_{\vec{k}}^2}{\mathrm{i}\omega_n - E_{\vec{k}}} + \frac{v_{\vec{k}}^2}{\mathrm{i}\omega_n + E_{\vec{k}}}, \tag{2}$$

where the notation is the same as that in [30]. In equation (1) we have chosen the pseudogap of pure s symmetry, since we wish to look for details overlooked in [30]. Later on, we also consider d wave symmetry as well.

We stress the fact that the authors of [30] did not find critical pairing interactions to have $T_c/t \neq 0$ and $\Delta_0/t \neq 0$. These considerations have been properly taken into account by Pistolesi and Nozières [31] in a model similar to the present one.

We could include damping effects in equation (2), by making the following substitution: $\mathrm{i}\omega_n \to \mathrm{i}\omega_n + \mathrm{i}\Gamma$, where Γ is a pure complex quantity, as has been done by Andrenacci and Beck [32].

Equation (2) is similar to a BCS solution for the pseudogap Green function because we have adopted a self-energy which is similar to a BCS-like self-energy. In consequence, we are treating the pseudogap in a BCS approximation.

The superconducting state in the HTSC is assumed to be of the BCS type, due to the presence of well-defined quasi-particles. The characteristic equation is obtained from the usual Gorkov equations, with the specification that in our case the normal state one-particle Green function is given by equation (2). In this way, the two BCS equations will include the PG effect as follows:

$$\begin{aligned} &G^{-1}(\vec{k}, \mathrm{i}\omega_n)\, \mathcal{G}(\vec{k}, \mathrm{i}\omega_n) + \Delta \mathcal{F}^{\dagger}(\vec{k}, \mathrm{i}\omega_n) = 1 \\ &\Delta^* \mathcal{G}(\vec{k}, \mathrm{i}\omega_n) - G^{-1}(\vec{k}, -\mathrm{i}\omega_n) \mathcal{F}^{\dagger}(\vec{k}, \mathrm{i}\omega_n) = 0, \end{aligned} \tag{3}$$

where $\mathcal{G}(\vec{k}, \mathrm{i}\omega_n)$ and $\mathcal{F}^{\dagger}(\vec{k}, \mathrm{i}\omega_n)$ are the diagonal and off-diagonal BCS Green functions, respectively. $G^{-1}(\vec{k}, \mathrm{i}\omega_n)$ is the pseudogap one-particle Green function given by equation (2).

This interpretation of the pseudogap phenomenon is equivalent to making the following choice in the T-matrix approximation [33–35] for the superconducting self-energy:

$$\sum(\vec{k}, \mathrm{i}\omega_n) = \begin{bmatrix} \Sigma(\vec{k}, \mathrm{i}\omega_n) & \Delta \\ \Delta^* & \Sigma(\vec{k}, \mathrm{i}\omega_n) \end{bmatrix} \tag{4}$$

where $\Sigma(\vec{k}, \mathrm{i}\omega_n)$ is given by our assumption (equation (1)). As we can see, this assumption, by construction, produces two gaps, one coming for the normal state self-energy and the other one coming from Δ in equation (4). Our approach is completely different from that of the Chicago group [36–39] where they have an effective gap, given by $\Delta_{\mathrm{eff}} = \sqrt{\Delta^2 + E_{\mathrm{g}}^2}$, where $\Delta \equiv \Delta(T)$. Their approach is equivalent to taking $\Delta/t = 0$ in our equation (4) and replacing $\Sigma(\vec{k}, \mathrm{i}\omega_n)$ by the diagonal self-energy (equation (1)), with $E_{\mathrm{g}} \to \sqrt{E_{\mathrm{g}}^2 + \Delta^2}$.

Solving our BCS equation in the presence of the pseudogap (equation (3)), we obtain for the superconducting one-particle Green functions, $\mathcal{G}(\vec{k}, \mathrm{i}\omega_n)$ and $\mathcal{F}^{\dagger}(\vec{k}, \mathrm{i}\omega_n)$, the following expressions:

$$\begin{aligned} \mathcal{G}(\vec{k}, \mathrm{i}\omega_n) &= \frac{G^{-1}(-\vec{k}, -\mathrm{i}\omega_n)}{G^{-1}(\vec{k}, \mathrm{i}\omega_n)\, G^{-1}(-\vec{k}, -\mathrm{i}\omega_n) + |\Delta|^2} \\ \mathcal{F}(\vec{k}, \mathrm{i}\omega_n) &= \frac{\Delta}{G^{-1}(\vec{k}, \mathrm{i}\omega_n)\, G^{-1}(-\vec{k}, -\mathrm{i}\omega_n) + |\Delta|^2}. \end{aligned} \tag{5}$$

Performing the fraction decomposition, we see that $\mathcal{G}(\vec{k}, \mathrm{i}\omega_n)$ and $\mathcal{F}(\vec{k}, \mathrm{i}\omega_n)$ can be expressed as

$$\mathcal{G}(\vec{k}, \mathrm{i}\omega_n) = \sum_{i=1}^{4} \frac{\alpha_i(\vec{k})}{\mathrm{i}\omega_n - \omega_i(\vec{k})} \tag{6}$$

$$\mathcal{F}(\vec{k}, \mathrm{i}\omega_n) = \Delta \sum_{i=1}^{4} \frac{\beta_i(\vec{k})}{\mathrm{i}\omega_n - \omega_i(\vec{k})} \tag{7}$$

where

$$\omega_{\pm}^2 = E_{\vec{k}}^2 + \frac{|\Delta|^2}{2} \pm |\Delta| \sqrt{E_{\mathrm{g}}^2 + \frac{|\Delta|^2}{4}} \tag{8}$$

$$E_{\vec{k}}^2 \equiv \epsilon(\vec{k} - \mu)^2 + E_{\mathrm{g}}^2 \tag{9}$$

$$\omega_1(\vec{k}) = +|\,\omega_+| \qquad \omega_2(\vec{k}) = -|\,\omega_+| \tag{10}$$

$$\omega_3(\vec{k}) = +|\,\omega_-| \qquad \omega_4(\vec{k}) = -|\,\omega_-| \tag{11}$$

and $\epsilon(\vec{k}) = -2\,t\,[\cos(k_x) + \cos(k_y)]$ is the free tight binding band in two dimensions and μ the chemical potential. For all the calculations presented in section 3 we choose $t = 1$ as our unit of energy. In equations (6) and (7), the spectral weights, $\alpha_i(\vec{k})$ and $\beta_i(\vec{k})$, for $i = 1, 2, 3, 4$, are given by

$$\alpha_1(\vec{k}) = \frac{\gamma_1^{+}(\vec{k})[[\omega_1]^2 - [\epsilon(\vec{k})]^2]}{4\Delta\, \omega_1(\vec{k}) \sqrt{E_{\mathrm{g}}^2 + |\Delta|^2/4}}$$

$$\alpha_2(\vec{k}) = \frac{\gamma_1^{-}(\vec{k})[[\omega_1]^2 - [\epsilon(\vec{k})]^2]}{4\Delta\, \omega_1(\vec{k}) \sqrt{E_{\mathrm{g}}^2 + |\Delta|^2/4}}$$

$$\alpha_3(\vec{k}) = \frac{-\gamma_3^+(\vec{k})[[\omega_3]^2 - [\epsilon(\vec{k})]^2]}{4\Delta\ \omega_3(\vec{k})\sqrt{E_g^2 + |\Delta|^2/4}}$$

$$\alpha_4(\vec{k}) = \frac{-\gamma_3^-(\vec{k})[[\omega_3]^2 - [\epsilon(\vec{k})]^2]}{4\Delta\ \omega_3(\vec{k})\sqrt{E_g^2 + |\Delta|^2/4}}$$

$$\gamma_i^+(\vec{k}) = \left[\frac{u_{\vec{k}}^2}{\omega_i(\vec{k}) + E_{\vec{k}}} + \frac{v_{\vec{k}}^2}{\omega_i(\vec{k}) - E_{\vec{k}}}\right]^{-1}$$

$$\gamma_i^-(\vec{k}) = \left[\frac{u_{\vec{k}}^2}{\omega_i(\vec{k}) - E_{\vec{k}}} + \frac{v_{\vec{k}}^2}{\omega_i(\vec{k}) + E_{\vec{k}}}\right]^{-1}$$

$$\beta_1(\vec{k}) = -\beta_2(\vec{k}) = \frac{[\omega_1]^2 - [\epsilon(\vec{k})]^2}{4\Delta\ \omega_1(\vec{k})\ \sqrt{E_g^2 + |\Delta|^2/4}}$$

$$\beta_3(\vec{k}) = -\beta_4(\vec{k}) = \frac{[\omega_3]^2 - [\epsilon(\vec{k})]^2}{4\Delta\ \omega_3(\vec{k})\ \sqrt{E_g^2 + |\Delta|^2/4}}.$$

From our approach we see that the effective superconducting order parameter in the quasi-particle spectrum is not given by the Chicago group simple expression. Our effective superconducting order parameter is given by $\Delta_{\rm eff} = \sqrt{2\Delta\sqrt{E_g^2 + \Delta^2/4}}$, which reduces to the BCS result when $E_g/t = 0$, namely, $\Delta_{\rm eff} = \Delta$, as it should.

We have to solve the $T/t = T_c/t$ equation, with $\Delta/t = 0$, and the gap equation for $\Delta = \Delta_0$, at $T \equiv 0$. For the first problem the following equations have to be solved:

$$\frac{1}{V} = \frac{1}{2\,N_x N_y}\sum_{n_x,n_y}\frac{\phi^2(\vec{k})}{\sqrt{[\epsilon(\vec{k}) - \mu]^2 + \phi^2(\vec{k})E_g^2}}\tanh\left(\frac{\sqrt{[\epsilon(\vec{k}) - \mu]^2 + E_g^2}}{2k_B T_c}\right) \tag{12}$$

$$\rho = \frac{1}{2\,N_x N_y}\sum_{n_x,n_y}\left\{1 - \frac{\epsilon(\vec{k}) - \mu}{\sqrt{[\epsilon(\vec{k}) - \mu]^2 + \phi^2(\vec{k})E_g^2}}\right\}\tanh\left(\frac{\sqrt{[\epsilon(\vec{k}) - \mu]^2 + E_g^2}}{2k_B T_c}\right), \tag{13}$$

here V/t is the absolute value of the pairing interaction, ρ the carrier density per site and per spin and μ the chemical potential. The weight function ϕ is equal to 1 for s wave symmetry, whereas $\phi(\vec{k}) = \cos(k_x) - \cos(k_y)$ for d wave symmetry. Naturally, other kinds of combined symmetries could be considered.

In order to obtain the superconducting gap at $T = 0$ K we have to solve the following set of equations:

$$\frac{1}{V_d} = \frac{1}{2\,N_x N_y}\sum_{n_x,n_y}\frac{1}{\Delta_0\sqrt{\Delta_0^2 + 4E_g^2}}\left[\frac{A_0^2}{\sqrt{[\epsilon(\vec{k}) - \mu]^2 + A_0^2}} - \frac{B_0^2}{\sqrt{[\epsilon(\vec{k}) - \mu]^2 + B_0^2}}\right] \tag{14}$$

$$\rho = \frac{1}{2\,N_x N_y}\sum_{n_x,n_y}\left[\alpha_2(\vec{k}) + \alpha_4(\vec{k})\right] \tag{15}$$

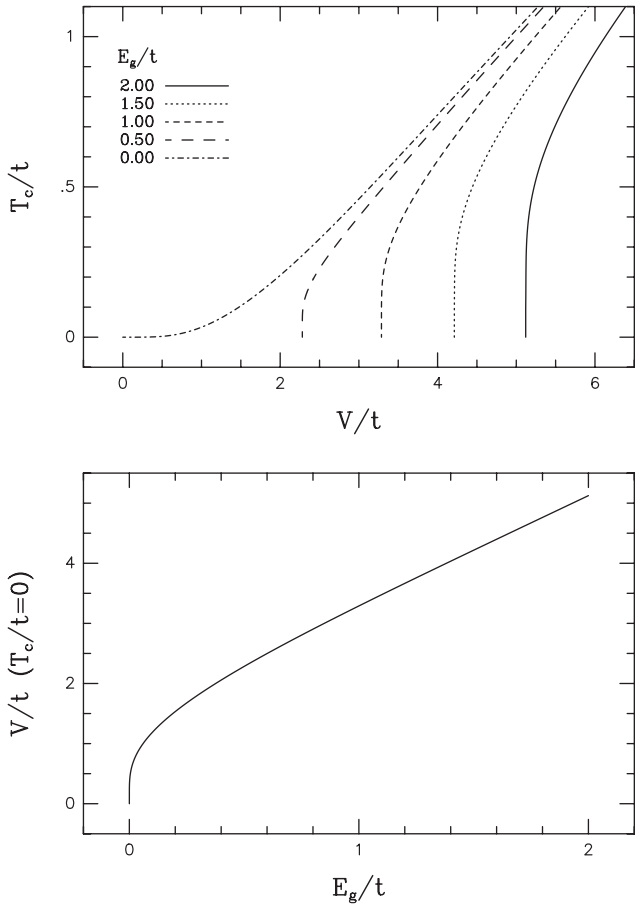

Figure 1. T_c/t versus V/t for several values of the pseudogap parameter, E_g/t, for the case of pure s wave symmetry. For $E_g/t \neq 0$ there is a critical interaction potential, $V/t = V_c^{T_c}/t$, below which $T_c/t = 0$. For example, for $E_g/t = 0.50$ we find $V_c^{T_c}/t \approx 2.25$ in units of t. In the lower panel of this figure we present the critical interaction as a function of the pseudogap parameter, when $T_c/t \to 0$.

where

$$A_0^2(B_0^2) \equiv E_g^2 + \tfrac{1}{2}\left[\Delta_0^2 \pm \Delta_0\sqrt{\Delta_0^2 + 4E_g^2}\right] \tag{16}$$

and $\alpha_2(\vec{k})$ and $\alpha_4(\vec{k})$ are defined as previously.

In the above k-sums we use $k_x = 2n_x\pi/N_x$ and $k_y = 2n_y\pi/N_y$, with $n_x = 0, 1, \ldots, N_x - 1$, and $n_y = 0, 1, \ldots, N_y - 1$. However numerical solutions for our discrete system in two dimensions were obtained in an integral form. We have used a relative tolerance of 10^{-5} to solve equations (12)–(15) iteratively. From these equations we conclude that $A_0^2 = \Delta_0^2$ and $B_0^2 = 0$ when $E_g/t = 0$. In equations (16), $\Delta_0 \equiv \Delta(T = 0)$, i.e., the order parameter at absolute temperature.

3. Numerical results

3.1. Results for zero chemical potential, i.e. a half-filled band

In figure 1 we present T_c/t versus V/t for several values of the pseudogap parameter, E_g/t, for the case of pure s wave symmetry. We observe that there is a critical value of the interaction potential, $V_c^{T_c}/t$, for having T_c/t. As we will see in the results for Δ_0/t versus V/t, there is also a critical value of the pairing potential below which $\Delta_0/t = 0$. In the case of V_c coming

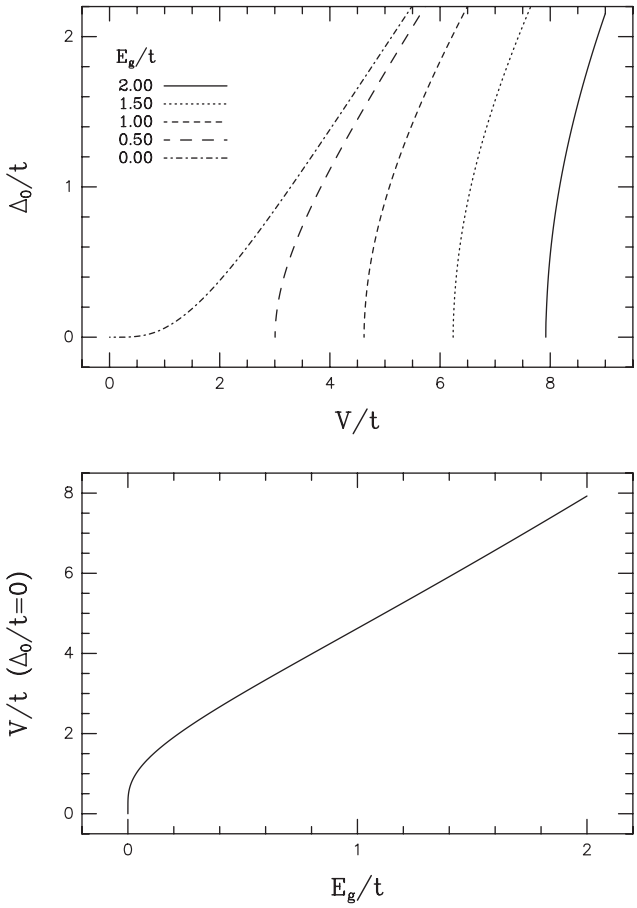

Figure 2. Δ_0/t versus V/t for several values of the pseudogap parameter, E_g/t (s wave symmetry). For $E_g/t \neq 0$ there is a critical interaction potential, $V/t = V_c^{\Delta_0}/t$, below which $\Delta_0/t = 0$. For example, for $E_g/t = 0.50$ we find $V_c^{\Delta_0}/t \approx 3.00$. In the lower panel of this figure we have presented the critical interaction as a function of the pseudogap.

from $\Delta_0/t \to 0$, these two critical pairing interactions are different. These critical pairing interactions were not discussed in [30]. However, they were considered in a similar model by Pistolesi and Nozières [31].

In figure 2 we present Δ_0/t versus V/t for several values of E_g/t, when the pseudogap and the superconducting order parameter, at $T = 0$, have the same symmetry, namely, pure s wave pairing symmetry. We see that we need a critical interaction potential, $V_c^{\Delta_0}/t \neq 0$, when $E_g/t \neq 0$, in order to have $\Delta_0/t \neq 0$. The comments made in relation to figure 1 also apply here. From figure 2, for $E_g/t = 0.50$, $V_c^{\Delta_0}/t \approx 3.00$. Comparing figures 1 and 2, we see that for a fixed value of E_g/t, $V_c^{T_c}/t \leqslant V_c^{\Delta_0}/t$. This straightforward result implies that the ratio $2\Delta_0(V, E_g)/k_B T_c(V, E_g)$ is well defined only for $V \geqslant V_c^{\Delta_0}/t$, for a fixed value of E_g/t.

We have re-done the numerical calculations of the gap equation at $T/t = 0$, namely, equation (14), with $B_0 \equiv 0$. Our results are shown in the next figure (figure 3). From this figure we observe that the critical interaction potential is $V_c^{\Delta_0}/t = 0$, for any value of the pseudogap parameter. According to the results for Δ_0/t versus V/t, we can re-obtain the

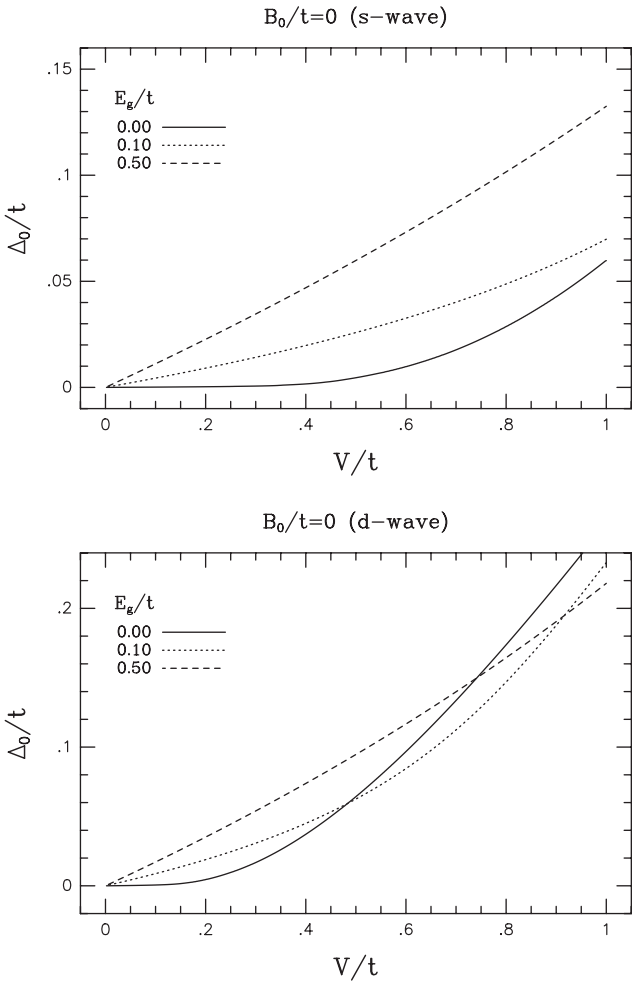

Figure 3. Δ_0/t versus V/t for several values of the pseudogap parameter, E_g/t. Following the approximation of [30], we have taken $B_0 \equiv 0$.

related results of [30] if we take $B_0 = 0$. However, the critical pairing potential resulting from the calculations of T_c/t versus V/t is always present in our calculations. This is due to the presence of the pseudogap at T_c/t (equation (12))[4].

In figure 3 we plot Δ_0/t versus V/t for several values of the pseudogap parameter, E_g/t, when we adopt the approximation of [30], namely, $B_0 \equiv 0$. This approximation does not produce a critical value of the interaction potential. In consequence, $V^{\Delta_0} = 0$, $\forall\ E_g/t$. As our equation (12) does not have the presence of the factor B_0, we cannot perform this approximation. Because of this, T_c/t always needs a critical value of the interaction, $\forall\ E_g/t \neq 0$.

In figure 4, upper part, we present the superconducting density of states, $\mathcal{N}(\omega)$ versus ω, for a fixed value of $E_g/t = 0.50$ and several values of the superconducting gap, Δ_0/t. (We have not obtained self-consistency for our equation (12).) With the purpose of speeding up this calculation, we have approximated the Dirac delta function of the one-particle spectral function, $\mathcal{A}(\vec{k}, \omega)$, as a Lorentzian. Remember that $\mathcal{A}(\vec{k}, \omega) \equiv -(1/\pi)\ \lim_{\delta \to 0^+} \mathrm{Im}\{\mathcal{G}(\vec{k}, \omega + \mathrm{i}\delta)\}$ and that

[4] We thank Professor R Micnas and Professor R Frésard for this interpretation.

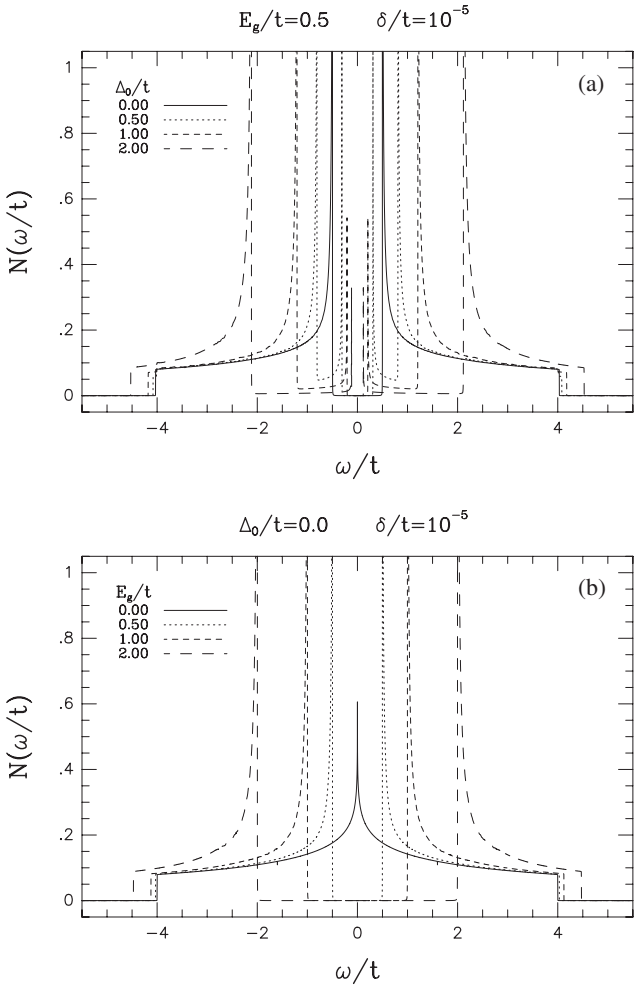

Figure 4. The density of states, $N(\omega)$ versus ω, for (a) a fixed value of $E_g/t = 0.50$ and several values of the superconducting gap, Δ_0/t (upper panel), and (b) several values of Δ_0/t at a fixed value of $E_g/t = 0.0$ (lower panel). This state is what we call the 'normal state' or 'pseudogap phase'. However, it should be called a 'semiconducting phase' according to [31]. The spectral density is obtained with the use of $\mathcal{G}(\vec{k}, i\omega_n)$ coming from equation (5). The parameter $\delta/t = 10^{-5}$ is used to approximate the Dirac delta functions of our one-particle spectral density with Lorentzians.

$$\mathcal{N}(\omega) = \frac{1}{N_x N_y} \sum_{n_x, n_y} \mathcal{A}(\vec{k}, \omega). \tag{17}$$

From figure 4 we observe that in the superconducting density of states, for $E_g/t \neq 0$, we have four symmetric peaks around the chemical potential ($\omega/t = 0$). The two internal peaks are due to the superconducting gap, Δ_0/t, and the peaks further away are due to the pseudogap. However, the SC peaks have less spectral weight than the PG peaks. These results are similar to the ones found by Capezzali *et al* [41, 42] using quantum phase fluctuations for the attractive Hubbard model. However, we know that in the superconducting state the superconducting quasi-particles are well defined. This implies that they should have larger spectral weights than the peaks coming from the pseudogap. This is a drawback of our approximation.

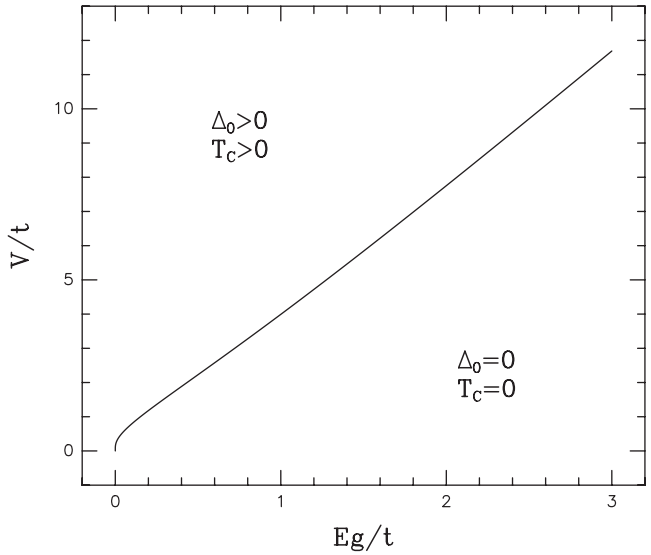

Figure 5. The phase diagram, V/t versus E_g/t, for $\alpha' = 0$ for a pseudogap and a superconducting order parameter with the same symmetry, namely, s wave symmetry. These calculations are done at half-filling. Above the line shown, we have a BCS-type superconductor. Below it, we have an insulator-type material.

We have stated that our density of states is not completely correct if we want to discuss the HTSC, because in the superconducting phase the weight of the superconducting quasi-particles must be larger than the weight of the pseudogap. To change this scenario we need to try another approximation for the pseudogap (equation (1)), probably choosing lifetime effects for it.

At this point, our model is similar to that of [31], since we pass from a semiconductor phase (full gapped density of states) to a superconducting state as shown in our figure 4. However, our model is different to that of [31] because they have imposed a cut-off energy around the Fermi surface. Our calculation is done $\forall\, \vec{k}$ on the Brillouin zone.

In figure 5 we present the main results of section 3.1. In this figure we have a phase diagram, namely, V/t versus E_g/t, for half-filling and for s wave symmetry. Above this line we have a BCS superconductor, with both $T_c/t \neq 0$ and $\Delta_0/t \neq 0$. Below this line we have $T_c/t = \Delta_0/t = 0$, which is a semiconductor-like solution for s wave symmetry.

In consequence, for a finite pseudogap E_g we need a minimum pairing interaction V in order to create a superconducting state. This is due to the fact that our electronic structure, with $E_g \neq 0$, corresponds to an insulator [46][5], so we need a finite pairing attraction in order to promote two electrons to the chemical potential, so that they can get paired. Furthermore, $\Delta_0 \equiv 0 \rightarrow T_c \equiv 0$, since Δ_0 is a factor multiplying both sides of the self-consistent equation which is used to evaluate both T_c and Δ_0. In other words, the fact that $\Delta_0 = 0$ implies that T_c is zero, by definition. This is the criterion used in figure 5.

3.2. $\Delta(T)$ versus T/t for both s and d symmetries at half-filling

The results presented here will not change the main conclusions of this paper for the case when both order parameters have d symmetry, where $\phi(\vec{k}) = \cos(k_x) - \cos(k_y)$. In figure 6 we present T_c/t versus V/t (upper panel) and Δ_0/t versus V_d/t (lower panel) at $E_g/t = 0$ for both pure s wave and $d_{x^2-y^2}$ symmetry ($\cos(k_x) - \cos(k_y)$). The only difference that we see with respect to the pure s wave symmetry case is the different values of the superconducting critical temperature, T_c/t, and the superconducting order parameter, Δ_0/t. The results for

[5] Due to the presence of a phenomenological pseudogap, we have found that we have a 'metallic' phase, which is the one present in figure 5, in the region where $\Delta_0 = 0$.

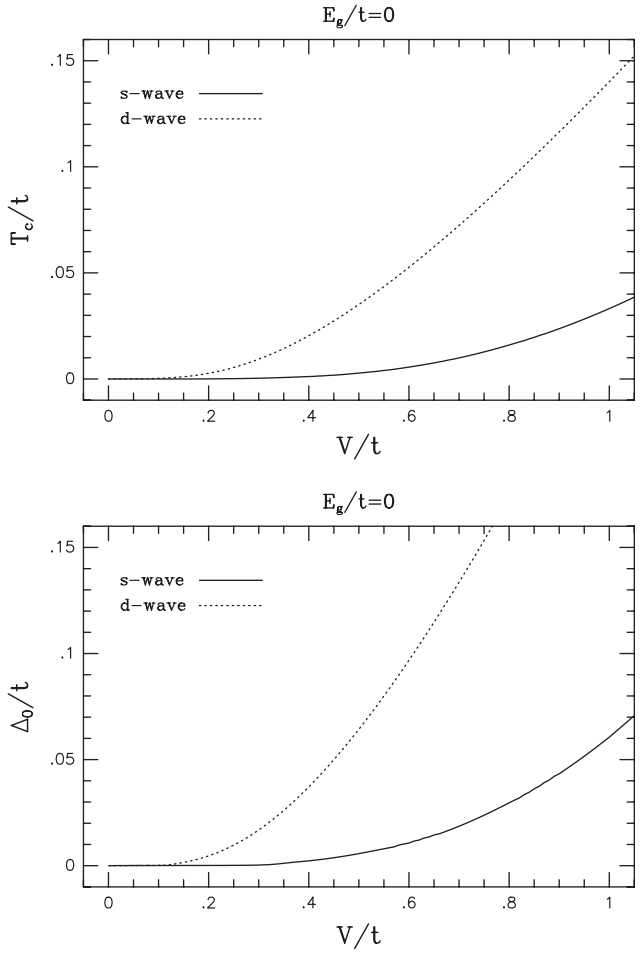

Figure 6. T_c/t versus V/t (upper panel) and Δ_0/t versus V/t (lower panel) at $E_g/t = 0$ for two different order parameter symmetries. 's wave' means the pure symmetric order parameter and 'd wave' refers to the $d_{x^2-y^2}$ symmetry order parameter. See the text for more details.

$E_g/t = 0$ for the d wave symmetry order parameter are at odds with the ones published by den Hertog [40] and Soares *et al* [43]. However, our results are in agreement with [44, 45]. In the lower part of figure 4 we present the normal state density of states, namely, when $\Delta/t = 0$. For this density of states we see only a gap, i.e., the one due to the presence of the pseudogap.

Let us try to understand why we have $\Delta(T) = 0$ for $T = 0$ in figures 7 and 8. In those figures, we see some kind of re-entrant superconductivity. In order to understand this behaviour, for the case of d wave symmetry, we present in figure 9 $A^2(\Delta_0)$ versus Δ and $B^2(\Delta_0)$ versus Δ_0. These two quantities are the two contributions (after summation is carried out) which appear in equation (14) (the gap equation). From this figure, we observe that at both limits the two factors cancel out. However, the first factor is always dominant for most values of Δ_0. In consequence, for small values of Δ_0 and increasing values of E_g/t the two contributions cancel each other and we need strong values of V/t to overcome the pseudogap. Then, the vanishing of the order parameter, for $E_g/t = 0$, at $T = 0$ is due to the presence of these subtracting factors. This is the origin of the re-entrant superconductivity, which is a major consequence of the presence of the pseudogap.

In order to justify figure 5, we now include figures 7 and 8. In figure 7 we plot $\Delta(T)/t$ versus T/t, for s wave symmetry, for $V_d/t = 2.5$ for several values of E_g/t. We observe

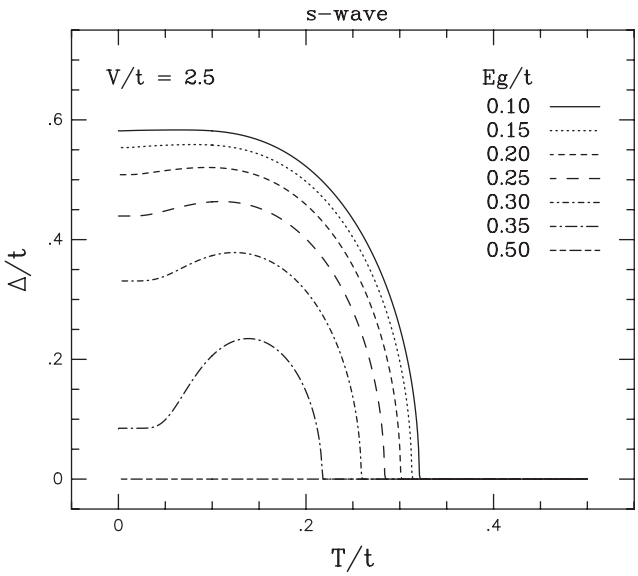

Figure 7. $\Delta(T)/t$ versus T/t, when $V/t = 2.50$, for s wave symmetry and half-filling. Here we have chosen $E_g/t = 0.10, 0.20, 0.25, 0.30, 0.35, 0.50$. From this figure we observe that the critical interaction is between 0.35 and 0.50.

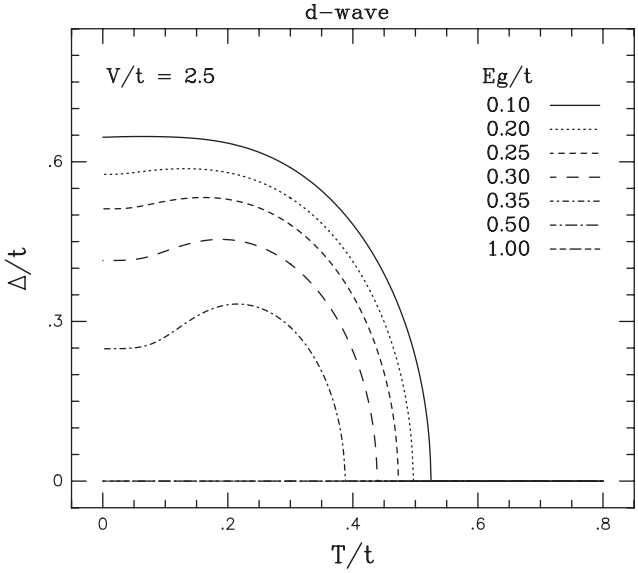

Figure 8. $\Delta(T)/t$ versus T/t, when $V/t = 2.50$, for d wave symmetry and half-filling. Here we have chosen $E_g/t = 0.10, 0.20, 0.25, 0.30, 0.35, 0.50, 1.00$. From this figure we observe that the critical interaction is between 0.50 and 1.00.

that $\Delta(T) \equiv 0$ for $E_g/t = 0.50$. In figure 8 we present $\Delta(T)/t$ versus T/t, for d wave symmetry, $V/t = 2.5$, for several values of E_g/t. In the last figure we observe that $\Delta(T) \equiv 0$ for $E_g/t = 1.00$.

Let us recall that the value of T_c/t is obtained from the gap equation, when $\Delta(T)/t \to 0^+ \neq 0$. In the case where $\Delta(T) = 0$, as in the case of s wave symmetry shown in figure 7 ($E_g/t = 0.5$) and in figure 8 ($E_g/t = 1.00$) for d wave symmetry, we are allowed to define $T_c/t \equiv 0$. In consequence, when $\Delta(T) = 0$, $T_c = 0$. In consequence, this is the argument used to construct figure 5.

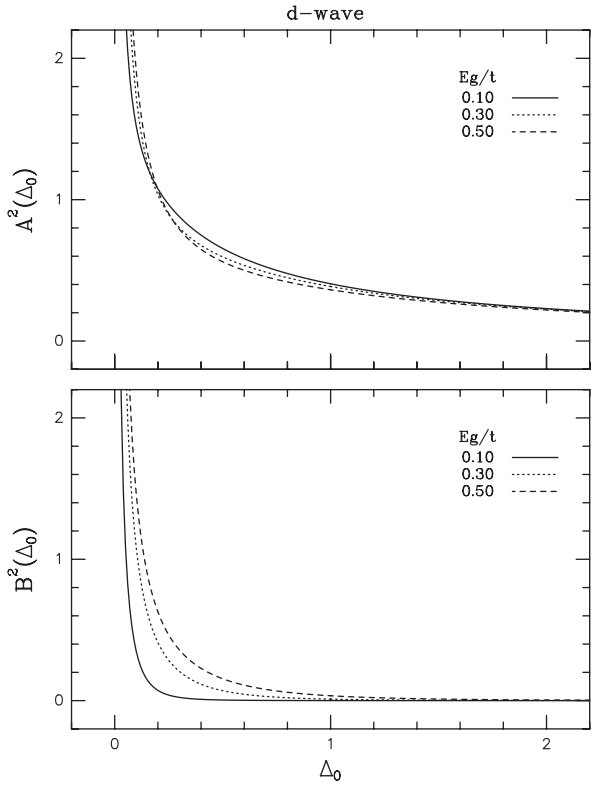

Figure 9. $A^2(\Delta_0)$ versus Δ and $B^2(\Delta_0)$ versus Δ_0, for d wave symmetry, at $\mu = 0$, for different values of E_g/t, namely $E_g/t = 0.1$, 0.3, and 0.5. We see that the first factor, i.e., $A^2(\Delta_0)$, is almost always greater than the second factor, namely, $B^2(\Delta_0)$. Only for small and large values of Δ_0 do they tend to be equal.

3.3. Results taking into account a non-zero chemical potential

In this subsection we present results obtained when we consider values of the chemical potential, μ, that are different from zero, corresponding to various band fillings.

In figure 10 we present the superconducting critical temperature, T_c/t, versus ρ and μ/t versus V/t, with the pseudogap parameter $E_g/t = 0.10$, for several values of the pairing potential, namely, $V_d/t = 1.50, 2.00, 2.50$, and 3.00, for the case of pure s wave symmetry. We observe that T_c/t is symmetric around half-filling, namely, for $\rho = 0.50$. We also observe that $T_c/t \neq 0$ in a certain window of carrier concentration.

In figure 11, we present T_c/t versus V/t, for $\rho = 0.90$ and several values of the pseudogap, namely, $E_g/t = 0.10, 0.20, 0.30, 0.40$, and 0.50. For example for $E_g/t = 0.10$, $V_c^{T_c}/t \approx 2.35$. For $E_g/t = 0.4$ and 0.5, $T_c = 0$. These results are in agreement with those of section 3.1, i.e., when we do not have self-consistency for the chemical potential.

In figure 12, we present T_c/t versus V_d for $\rho = 0.50$, for several values of the pseudogap parameter, namely, $E_g/t = 0.10, 0.20, 0.30, 0.40$, and 0.50, for the case of pure d wave symmetry. In this case $\Delta_0(\vec{k}) = \Delta_0(\cos(k_x) - \cos(k_y))$. We see that for $\rho = 0.50$, the chemical potential is pinned at $\mu/t = 0$. If we compare these results with the ones of figure 10, we observe that $T_c^d \geqslant T_c^s$, for the same values of V/t and E_g/t. Also, we observe that $V_c \approx 2.30$, for d wave symmetry with $E_g/t = 0.1$.

4. Discussion and conclusions

In this paper we have considered the pseudogap and the superconducting order parameter to have the same symmetry, namely, either s wave or d wave symmetry. This is a reasonable

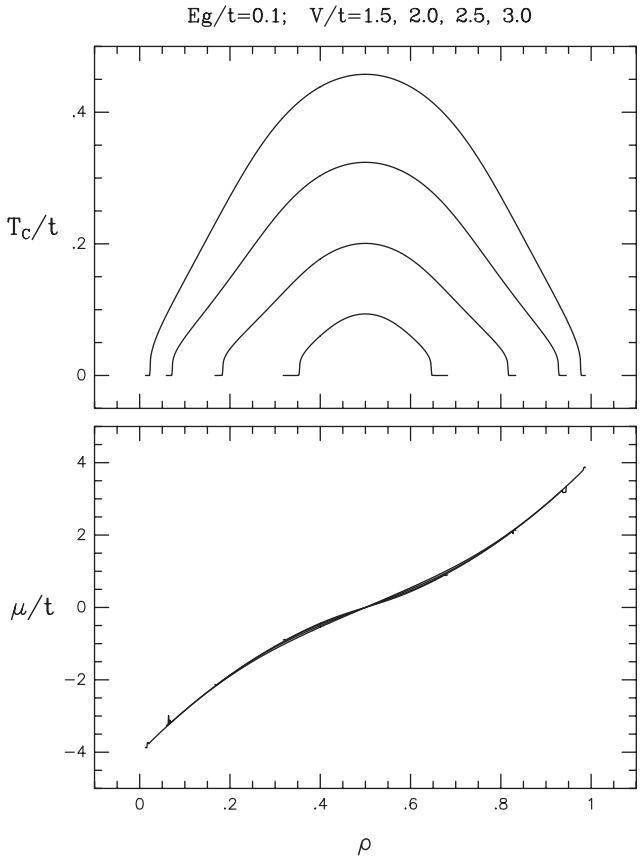

Figure 10. T_c/t versus ρ for the pseudogap parameter, $E_g/t = 0.10$, for several values of the pairing potential, namely, $V/t = 1.50$, 2.00, 2.50, and 3.00, for the case of pure s wave symmetry. T_c/t goes up for larger values of V/t.

scenario since it has been shown that the observed symmetry of the order parameter cannot be fitted with just the lowest harmonics of the d wave order parameter [47–50]. Furthermore, a recent experiment with twisted Josephson junctions in the Bi cuprates [51] favours an extended s wave order parameter, and has shown the absence of a d wave part in the order parameter. Leaving aside controversial issues, we have adopted the point of view that the pseudogap and the superconducting order parameter have the same symmetry. With this point of view in mind and following the model of Ţifrea *et al* [30], we have studied their model to treat delicate points such as the critical interaction potential.

We have chosen a free tight binding model given by nearest neighbours (nn; see the discussion after equations (8)–(11)). However, we could include next nearest neighbour (nnn) hopping, as was done by Soares *et al* [43] and Tobijaszewska and Micnas [52]. In [43], the nnn hopping parameter, t', has been used to study the crossover between the BCS regime and the BEC limit, while in [52], the next nearest neighbour hopping parameter has been used to fit Uemura-type [53–55] plots, i.e., critical temperature versus temperature phase stiffness plots. Other authors [56] have used the t' hopping term to fit T_c/t and the isotope exponent, α, in the different cuprate families. In consequence, the nnn hopping parameter should be taken into account in future calculations.

We repeat that our approach is different from that of the Chicago group. For example, Kao *et al* [39] have plotted the density of states, at $T/t = 0$, for both the *intrinsic* and *extrinsic* schools of the pseudogap (see [39] for details). Their two densities of states are completely

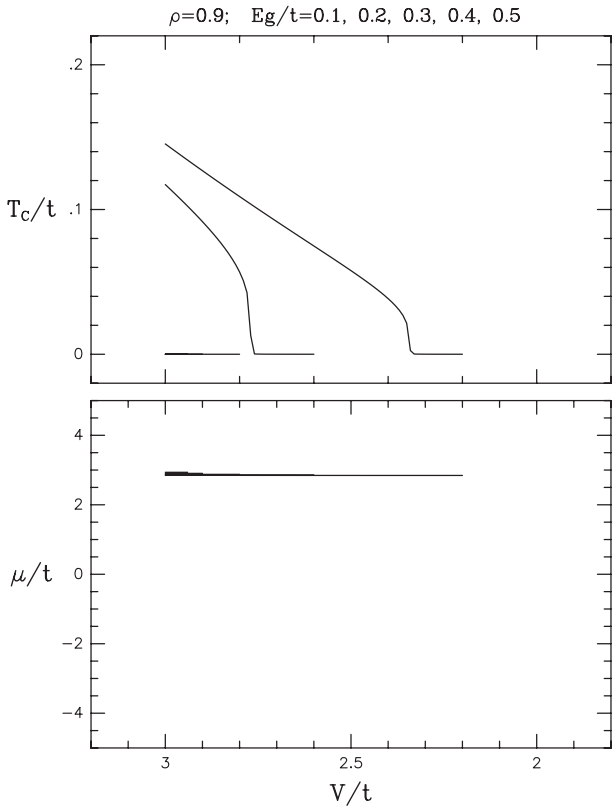

Figure 11. T_c/t versus V/t for $\rho = 0.90$, for several values of the pseudogap parameter, namely, $E_g/t = 0.10$, 0.20, 0.30, 0.40, and 0.50, for the case of pure s wave symmetry. We observe that for $E_g/t = 0.4$ and 0.5, $T_c = 0$.

different to the ones presented here in figure 2 (lower panel). This implies that their approach and that of the present work are completely different, as was pointed out in section 2 (refer to the discussion about the t-matrix formulation around equation (4)).

As we have said in section 3.1, $\Delta_0/t = 0$ due to the fact that the system behaves as an insulator. This being so, we need to have a finite pairing interaction in order to promote two electrons to the chemical potential so that they can form a pair and that $\Delta_0/t \neq 0$.

When $E_g/t = 0$, $R \approx 3.5$ in the BCS approximation, with $R \equiv 2\Delta_0(V, E_g)/k_B T_c(V, E_g)$. We end up by saying that in [30], even though this is for a superconductor order parameter with d wave symmetry, they do not find our critical interaction. We have implemented numerical calculations for d wave symmetry (see figure 12) and the results are qualitatively similar, even though there are some quantitative differences. The authors of [30] have recently applied their pseudogap model to calculate the specific heat behaviour of high-temperature superconductors in the underdoped regime [57]. Let us recall that they have done self-consistent calculations for the order parameter. However, they have not considered the effect of the chemical potential. The presence of the pseudogap down to $T = 0$ K produces metallic regions in the ground state, for s and d wave symmetries [58], which are absent in the model discussed in [44, 45]. We have also seen that the results for sections 3.1–3.3 are consistent, since they produce a critical attractive interaction.

In summary, we have numerically implemented a model which has a pseudogap (really, it is a semiconductor gap, since damping effects have been neglected in our calculations) in the one-particle energy spectrum of quasi-particles in the temperature range $0 \leqslant T \leqslant T^*$. We have investigated the effect of E_g/t on the two basic parameters of the BCS theory, T_c/t

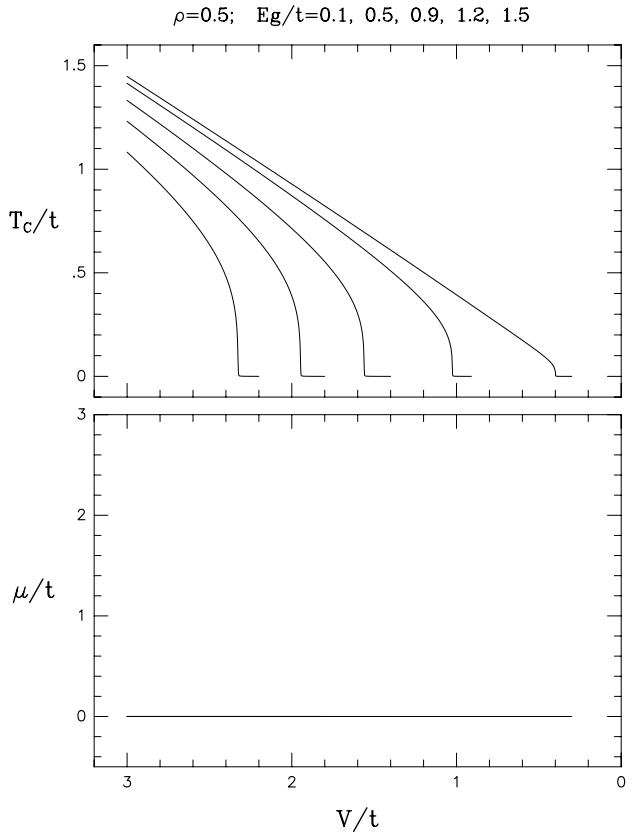

Figure 12. T_c/t versus V/t for $\rho = 0.50$, for several values of the pseudogap parameter, namely, $E_g/t = 0.10$, 0.20, 0.30, 0.40, and 0.50, for the case of pure d wave symmetry.

and Δ_0/t. We have found that for $E_g/t \neq 0$ a critical pairing potential emerges from our calculations, since $\Delta_0/t = 0$ implies that $T_c/t = 0$. In consequence, in order to define the ratio $R \equiv 2\Delta_0(V, E_g)/k_B T_c(V, E_g)$ we need to work with $\Delta_0/t \geqslant 0$. Figure 5 represents the main results of the present work. See also the discussion after figures 7–9 which explains the phase diagram presented in this paper. We have also found that the critical potential is valid for both $\mu/t = 0$ and $\mu/t \neq 0$. In this paper we have not considered the effect of impurities, i.e., dirty superconductors, as was recently done by Dahm *et al* [59], for $Bi_2Sr_2CaCu_2O_8$. However, Kaminski *et al* [60] have studied the anisotropy of the scattering rate in cuprate superconductors for the same compound, adopting the following expression for the scattering rate: Im $\Sigma = a + b\omega$. They say that the anisotropy is probably not due to impurity scattering, but rather related to the same interaction as gives rise to the pseudogap. Without touching these delicate points (probably valid around the Fermi surface or along certain directions in the Brillouin zone), we remark that the consequence of adopting a pseudogap as is done in [30] is the presence of a critical interaction for obtaining superconductivity, for both s and d wave symmetries.

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The present paper began with the initial participation of D Romero and L Sánchez, who after some time left the group. The interpretation given here is completely new (see [61]) and the numerical calculations presented here resulted from computer calculations performed at LANA, Universidade Federal de Santa Maria, Brazil. These calculations were carried out in a cluster of 16 CPUs.

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