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From semiconductors to superconductors: a simple model for pseudogaps

P. Nozières and F. Pistolesi[a]

Institut Laue-Langevin, BP 156, 38042 Grenoble Cedex 9, France

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Abstract. We consider a two-dimensional semiconductor with a local attraction among the carriers. We study the ground state of this system as a function of the semiconductor gap. We find a direct transition from a superconducting to an insulating phase for no doping at a critical value, the single particle excitations being always gapped. For finite doping we find a smooth crossover. We calculate the critical temperature due to both the particle excitations and the Berezinkii-Kosterlitz-Thouless transition.

PACS. 74.20.-z Theories and models of superconducting state – 74.20.Fg BCS theory and its development – 74.20.Mn Nonconventional mechanisms (spin fluctuations, polarons and bipolarons, resonating valence bond model, anyon mechanism, marginal Fermi liquid, Luttinger liquid, etc.)

1 Introduction

In the standard BCS theory of superconductors the gap Δ in the spectrum of quasiparticles is due to the breakdown of gauge symmetry at the phase transition, in much the same way as the gap in a spin density wave state is due to Bragg scattering off the doubled periodicity. The gap disappears with order and consequently $\Delta = 1.76\,T_c$ is comparable to the transition temperature T_c. Largely motivated by high temperature superconductivity, interest has grown recently in a "pseudogap" situation, in which a somewhat blurred gap Δ persists in the normal state, such that $\Delta \gg T_c$ [1]. There are many models for such a pseudogap, the simplest one being a transition from the BCS limit towards a "Bose Einstein condensation of preformed pairs": if the attraction between electrons is strong enough, bound pairs (let us say singlet) form first, with a binding energy ε_B, then below a critical temperature T_c they Bose condense. It was shown long ago that the evolution between the two limits is smooth, with however a very different physics in the strong binding limit [2]. Then the gap Δ is just the binding energy, a "molecular" quantity which has nothing to do with symmetry breaking; in contrast T_c is controlled by center of mass motion of bound pairs, which are not broken: as a result $\Delta \gg T_c$, a simple minded interpretation of the pseudogap. A similar evolution occurs for the transition from a paramagnetic metal to an antiferromagnetic insulator in half filled band: for a strong repulsion the Mott gap Δ exists irrespective of the magnetic order. The latter is only a secondary feature, while it was a key actor in the formation of Δ at weak coupling [3].

In order to build an accurate description of realistic systems one needs an interpolation between these two limits. That means including quantum fluctuations of the order parameter Δ, (mostly of its phase) which are systematically ignored in a mean field BCS calculation. That is a difficult task and the literature on the subject is large [4]. We will not attempt to review it: as usual in perturbation theories it relies on approximations that are not really controlled. We will just make a few simple qualitative comments. Grossly speaking one expects the crossover between the two limits to occur when the (zero temperature) gap Δ is comparable to the Fermi energy ε_F: they are the only energies in the problem. That can be checked explicitly for a two-dimensional system, in which phase fluctuations are enhanced, leading to the well known Kosterlitz Thouless transition [5]. The resulting transition temperature T_c^{KT} is controlled by the phase stiffness of the ground state: it can be compared to the mean field T_c^{BCS} which accounts only for pair breaking. Such an elementary calculation is sketched in Section 4: it shows that the crossover $T_c^{KT} \approx T_c^{BCS}$ occurs when $\Delta \approx \varepsilon_F/5$. There a bound pair would sit in the middle of a continuum, which makes no sense. Sure in the very strong coupling limit one returns to preformed bound pairs, but there exists a broad intermediate region near the crossover where phase fluctuations are already dominant without any bound state.

In the above model the same interaction is responsible for the gap Δ and for Bose condensation. That may well be the case and the future will tell whether high temperature superconductors pertain to such a mechanism or not. However that is not a necessity: one may also imagine that a primary gap Δ_o is due to some other mechanism that has nothing to do with superconductivity. That may be for instance a lattice distortion of some sort or a magnetic

[a] e-mail: pistoles@ill.fr

instability, as suggested by various authors [6]: the starting point is then a semiconductor rather than a metal. If a BCS attraction between electrons is added to such a system, it may lead to superconductivity, even if there were no free carriers to start from: free pairs appear spontaneously if the gain in binding energy is larger than the cost to produce free electrons and holes across the gap. Such a mechanism is actually familiar: it was introduced long ago by Kohn in his theory of excitonic insulators [7]. There the Coulomb interaction is repulsive and the bound pair (the exciton) involves an electron and a hole: excitons appear spontaneously if their binding energy is larger than the gap. What we present here is just the reverse situation in which electrons attract: bound pairs involve two electrons or two holes; at $T = 0$ they Bose condense (bound carriers are then time reversed of each other), hence superconductivity. It is clear that superconductivity will modify the real gap $\Delta_{\rm g}$ – hence the name "primary gap" for $\Delta_{\rm o}$.

The possibility of superconductivity in a semiconductor is not new: it appeared since the beginning of the BCS "era", as emphasized by the review article of Cohen [8] (for subsequent development, see [9]). However only *intraband* interactions in a doped material were included, the only new feature being the scarcity of carriers. Here we are concerned with the effect of *interband* interactions, in which carriers in both bands conspire in establishing superconducting order. That was also considered before [10], but in a somewhat different context of interband pairing, while we consider only the usual intraband pairing of time-reversed states. We show in Appendix B that the latter is energetically preferred. (An obvious question is of course whether they can occur together.)

Many features of such a "superconductivity in a semiconductor" are general, in the sense that they do not depend on the physical mechanism responsible for gap opening. We fell that such an interplay of $\Delta_{\rm o}$ and superconducting order deserves study, the more as it leads to somewhat unexpected simple conclusions. The present paper offers a very naive discussion of that problem. At this stage we have no pretense whatsoever to explain any realistic material: our only purpose is to identify and to explain qualitative features of the various limits at hand. In order to be enlightening and hopefully convincing, such an analysis must be *simple*: we therefore choose deliberately the most oversimplified model and formulation, in such a way as to have transparent results. We are perfectly aware of the many loopholes and traps of the model, and we will try to point those which we feel are important. Starting a discussion of these many complications would however be meaningless at a stage where even the feasibility of such a mechanism is an open issue [11].

In Section 2 we introduce our model, and we discuss the simplest situation in which the semiconductor is undoped: were it not for superconductivity it would be an insulator at $T = 0$. Within a mean field BCS approximation the algebra is elementary and it leads to a direct transition from insulator to superconductor at zero temperature (when the primary gap $\Delta_{\rm o}$ reaches a critical $\Delta_{\rm o}^*$). At finite T one easily calculates the order parameter Δ, the actual gap $\Delta_{\rm g}$ and the critical temperature $T_{\rm c}$: as could be surmised a pseudogap situation prevails near $\Delta_{\rm o}^*$. Section 3 is concerned with slightly doped systems: then the ground state is always conducting. With an attraction between carriers it is always superconducting. Still within a BCS mean field approximation, we explore the various limits. The interesting case is $\Delta_{\rm o} > \Delta_{\rm o}^*$, where everything is due to doping; the behaviour of gaps and critical temperature in that limit is somewhat unexpected. Up to that level the dimension of space and the nature of the gap in the Brillouin zone do not matter much: they become crucial in Section 4 which is concerned with a much more delicate issue, namely phase stiffness and Kosterlitz Thouless fluctuations. The analysis is here more speculative: as far as we can see the transition is always monitored by phase fluctuations in realistic models for the gap, in contrast to ordinary BCS metals. The reason is a very small phase stiffness, which would vanish for a filled band. In a brief conclusion we emphasize the many questions that remain open.

2 The BCS model for an undoped semiconductor

We start from a normal Fermi liquid that has a gap $2\Delta_{\rm o}$, and we choose the origin of energy at midgap. The gap may be direct or indirect in momentum space: at that stage it does not matter. Let $\rho(\xi)$ be the density of states (per spin): in a first approximation we take $\rho(\xi)$ constant: everything is symmetric around $\xi = 0$. Since the total number of states must remain the same, opening the gap $\Delta_{\rm o}$ means that the conduction band shifts from $[0, \omega_{\rm m}]$ to $[\Delta_{\rm o}, \Delta_{\rm o} + \omega_{\rm m}]$ while the valence band goes to $[-\Delta_{\rm o} - \omega_{\rm m}, -\Delta_{\rm o}]$. The conduction and valence bands are just shifted away from each other. $\omega_{\rm m}$ is a bandwidth which we assume $\gg \Delta_{\rm o}$ (the gap is small). The choice of a constant ρ is in accordance with our choice of simplicity, but it is not realistic for two reasons (i) at band edges ρ goes as $\xi^{1/2}$ in three dimensions, (ii) in usual situations states that are repelled off the gap remain in its vicinity, in an energy range which has the same order of magnitude $\Delta_{\rm o}$ (see Fig. 1); here these states are repelled at infinity. We will show in Appendix A that more realistic choices for $\rho(\xi)$ do not change the results qualitatively: they are not worth the price of complications.

We then add a local attraction U between fermions and we look for a BCS superconducting state in which electrons (or holes) are paired in singlet states with zero total momentum, $(\mathbf{k}\uparrow)$ with $(-\mathbf{k}\downarrow)$ (one the time reversed of the other). If the bottom of the band is made up of several valleys at band edge, that means pairing of electrons between symmetric valleys. We treat the problem within a mean field approximation: the Hamiltonian contains anomalous terms

$$\Delta c_{\mathbf{k}\uparrow} c_{-\mathbf{k}\downarrow}$$

where Δ is the usual order parameter, not to be confused with gaps, which must be determined self-consistently. Because of electron-hole symmetry the chemical potential μ

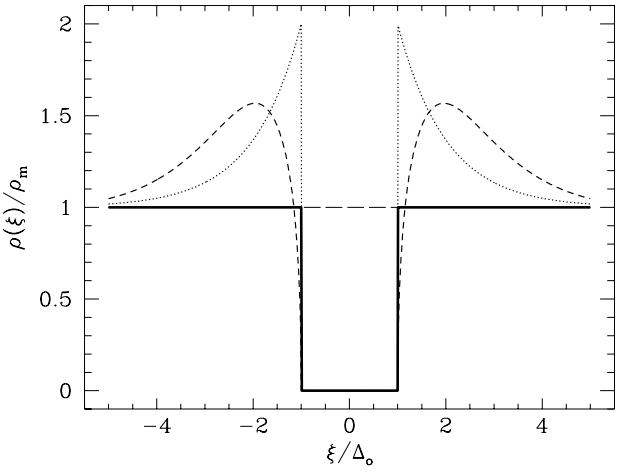

Fig. 1. Possible modification of the density of states near the band edge. The thick line correspond to the approximation used in the text. The dotted line is instead an example of a more realistic 2d case where the removed stated remain near the edge. The dashed line is a typical 3d case where the density of states vanishes at the edge with a square root dependence on the energy.

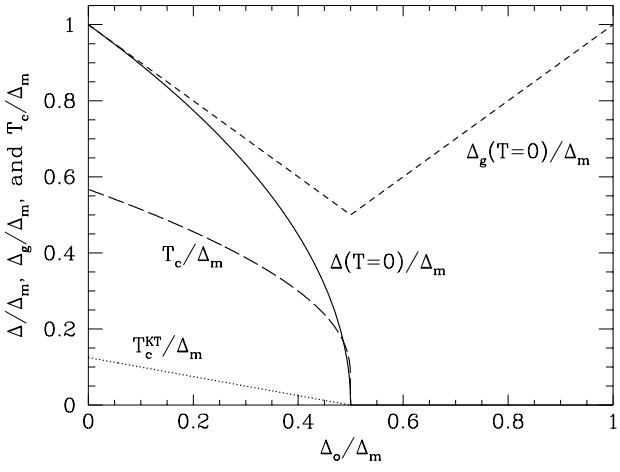

Fig. 2. Undoped case, we report as a function of Δ_o/Δ_m the following quantities: the order parameter Δ/Δ_m (continuous line), the excitation gap Δ_g/Δ_m (dashed line), the critical temperature T_c/Δ_m due to pair breaking (long dashed line), and the Kosterlitz-Thouless critical temperature T_c^{KT}/Δ_m (see Sect. 4) (dotted line).

of our undoped system remains at midgap and the reduced kinetic energy $\xi_k = (\varepsilon_k - \mu)$ starts at $\pm\Delta_o$ instead of 0. The algebra is identical to that of BCS except for that shift in the energy integration. In the absence of a gap, $\Delta_o = 0$, the order parameter Δ would take the regular metallic value Δ_m given by the familiar BCS self consistency condition

$$1 = \frac{\rho U}{2} \int_{-\omega_m}^{+\omega_m} \frac{d\xi}{\sqrt{\xi^2 + \Delta_m^2}} = \rho U \ \log \frac{2\omega_m}{\Delta_m} \cdot \qquad (1)$$

It is convenient to characterize the attraction by Δ_m instead of U. Note that for a regular metal the superconducting gap is just $\Delta_g = \Delta$. In the presence of a semiconductor gap Δ_o the self consistency equation for the *new* order parameter Δ becomes

$$1 = \rho U \ \log \left[\frac{2\omega_m}{\Delta_o + \sqrt{\Delta_o^2 + \Delta^2}} \right]. \qquad (2)$$

In order for the two equations to have a solution with the same U, we must have $\Delta_m = \Delta_o + \sqrt{\Delta_o^2 + \Delta^2}$, *i.e.*

$$\Delta = \sqrt{\Delta_m \, (\Delta_m - 2\Delta_o)}. \qquad (3)$$

Superconductivity persists with a reduced order parameter until the gap $2\Delta_o$ reaches the metallic BCS gap Δ_m: then the gain in interaction energy due to superconductivity can no longer overcome the cost of kinetic energy in producing free carriers across the gap. Note the complete analogy with excitonic insulators in which condensation produces electron-hole pairs in the presence of a repulsive U [7]. Such a model provides an elementary example of a direct *superconductor-insulator transition*, which here is sharp at $T = 0$. The quasiparticle gap Δ_g is just Δ_o in the insulating state ($\Delta = 0$). In the superconducting state it is $\sqrt{\Delta_o^2 + \Delta^2}$, *i.e.* $\Delta_g = \Delta_m - \Delta_o$. The situation is illustrated in Figure 2: note that the gap is finite when superconductivity disappears.

The calculation is easily extended at finite temperatures. The order parameter Δ becomes a function of T. We need only introduce the fermionic occupation factors in the gap equation:

$$\int_P d\xi \frac{\tanh \beta\sqrt{\xi^2 + \Delta^2}/2}{\sqrt{\xi^2 + \Delta^2}} = \int_{-\omega_m}^{\omega_m} \frac{d\xi}{\sqrt{\xi^2 + \Delta_m^2}} \cdot \qquad (4)$$

(We retain the zero temperature Δ_m as a measure of the attraction U). The integration path P takes into account the absence of states in the middle of the band: $P = [-(\Delta_o + \omega_m), -\Delta_o]$ and $[+\Delta_o, +(\omega_m + \Delta_o)]$. For $\Delta_o = 0$, equation (4) is the standard BCS gap equation, yielding the usual $\Delta(T)$ and T_c. At the other end the critical temperature goes to zero at the superconductor-insulator transition $\Delta_o^* = \Delta_m/2$ (there $\Delta = 0$ at zero temperature: there is no need of a T_c to make it vanish). The behaviour of $T_c(\Delta_o)$ is shown in Figure 2.

The approach to the transition is interesting: we subtract the $\Delta_o < \Delta_o^*$ equation (4) from the same equation at the transition, $\Delta_o = \Delta_o^*$:

$$\int_{\Delta_o^*}^{+\infty} \frac{1 - \tanh \beta_c \xi/2}{\xi} d\xi - \int_{\Delta_o}^{\Delta_o^*} \frac{\tanh \beta_c \xi/2}{\xi} d\xi = 0. \qquad (5)$$

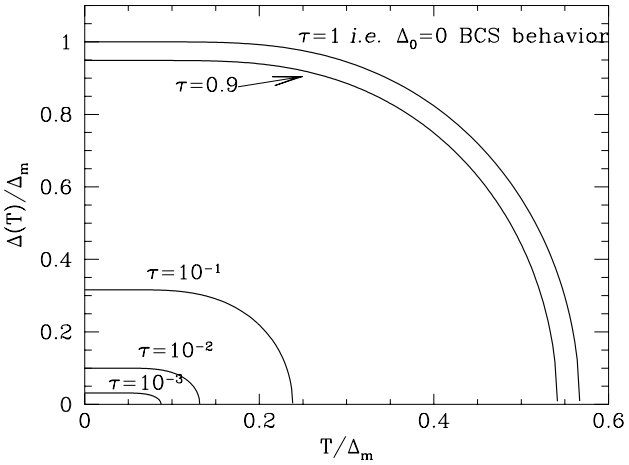

Fig. 3. $\Delta(T)$ for $\tau = 1$, 0.9, 10^{-1}, 10^{-2} and 10^{-3}. The evolution from the familiar BCS shape for large τ to a new one for τ small is evident.

When $\Delta_o \to \Delta_o^*$, T_c vanishes and we can approximate $\tanh x$ with $1 - 2e^{-2x}$. The first integral reduces then to the Exponential integral function and for large values of $\beta_c \Delta_o^*$ we obtain:

$$2\frac{T_c}{\Delta_o^*} e^{\Delta_o^*/T_c} = \frac{\Delta_o^* - \Delta_o}{\Delta_o^*} \equiv \tau. \tag{6}$$

Defining the function $w(x)$ as the solution of the transcendental equation $x = w\, e^w$, we can write T_c in terms of $w(x)$

$$T_c = \frac{\Delta_o^*}{w(2/\tau)} \cdot \tag{7}$$

The function $w(x)$ is a generalization of the logarithm and for $x \gg 1$ has the following expansion:

$$w(x) = \ln x - \ln[\ln x - \ln[\ln x - \ln \ldots]]. \tag{8}$$

The convergence of that expansion is very slow (shown in (8)), but the first term is enough to provide a rough result: the critical temperature vanishes logarithmically in $\tau[T_c \sim \Delta_o^*/\ln(2/\tau)]$.

Altogether the presence of a semiconductor gap Δ_o acts to decrease T_c, a result which is reasonable. But such a decrease should be compared to that of the zero temperature order parameter Δ, which behaves as $\sqrt{\tau}$: we see that the ratio $\Delta(T=0)/T_c$ becomes extremely small when $\Delta_o \to \Delta_o^*$, in contrast to the usual BCS result. The physical origin of that behaviour is clear: due to the finite gap Δ_g the quasi particle excitations are much less efficient in destroying the superconducting order than they would be in the BCS case, and consequently T_c increases. Such a behaviour is exemplified in Figure 3 in which we plot the order parameter $\Delta(T)$ (obtained from solving (4)) for various values of Δ_o/Δ_m: the elongated low plateau near the transition is striking.

All that discussion is based on a BCS like mean field approximation, in which condensed pair breaking is the only allowed thermal excitation, ultimately responsible for the destruction of superconductivity at T_c. Such an approximation is by no means obvious and it should be kept in mind. In practice there exist other excitations that might be more efficient in destroying superconductivity. In particular, phase fluctuations are gapless excitations and at least for Δ_o near Δ_o^* they are expected to reduce drastically the critical temperature. We will discuss this point more extensively in Section 4 for the two-dimensional system. There we find that phase fluctuations seem to be always responsible for the transition to the normal phase, even for $\Delta_o = 0$, a somewhat unexpected conclusion.

3 Doped system

We now extend our problem, allowing for a finite doping. We do it because it leads to new interesting physics: the sharp transition at Δ_o^* becomes a smooth crossover, and superconductivity persists at zero temperature for any value of Δ_o. Beyond that crossover, the superconducting behaviour is very unconventional over a broad range of parameters, in contrast to the undoped case in which queer behaviour occurred only at a specific transition point. In that respect the doped system is much more generic.

Starting from the non interacting, metallic system at $T = 0$ we suppose that the upper band is populated up to an energy $\mu_m = \varepsilon$, referred to midgap. When the gap Δ_o is restored, the "semiconductor" is doped by an amount $\delta N = 2\rho\varepsilon$ (referred to the filled valence band). In the metallic state $\Delta_o = 0$, chemical potential and superconductivity are unaffected by each other (the BCS picture is symmetric with respect to Fermi level): μ_m remains equal to ε. In the opposite limit of an insulator with no superconductivity, $\mu = \Delta_o + \varepsilon$ is pushed into the conduction band, a familiar feature of degenerate semiconductors. In between we expect no sharp superconductor-insulator transition: a weak superconducting order due to the few free carriers in the conduction band should persist at any Δ_o. Keeping Δ_m and ε fixed, we thus expect the zero temperature chemical potential μ and order parameter Δ to depend on Δ_o as showed respectively in Figures 4a and b. The transition around $\Delta_o = \Delta_m/2$ is a crossover, but with a large change of μ.

Let us assume an arbitrary temperature T. In order to fix the two parameters $\mu(T)$ and $\Delta(T)$ we need two conditions. One is the self consistency equation for the order parameter, which is the same as (4) but for the introduction of the chemical potential in the expression for the quasiparticle energy:

$$\int_P \frac{\tanh \beta E(\xi)/2}{E(\xi)} d\xi = \int_{-\omega_m}^{+\omega_m} \frac{d\xi}{\sqrt{\xi^2 + \Delta_m^2}}, \tag{9}$$

where $E(\xi) = \sqrt{(\xi - \mu)^2 + \Delta^2}$. The other one is the conservation of particle number, stating that δN is

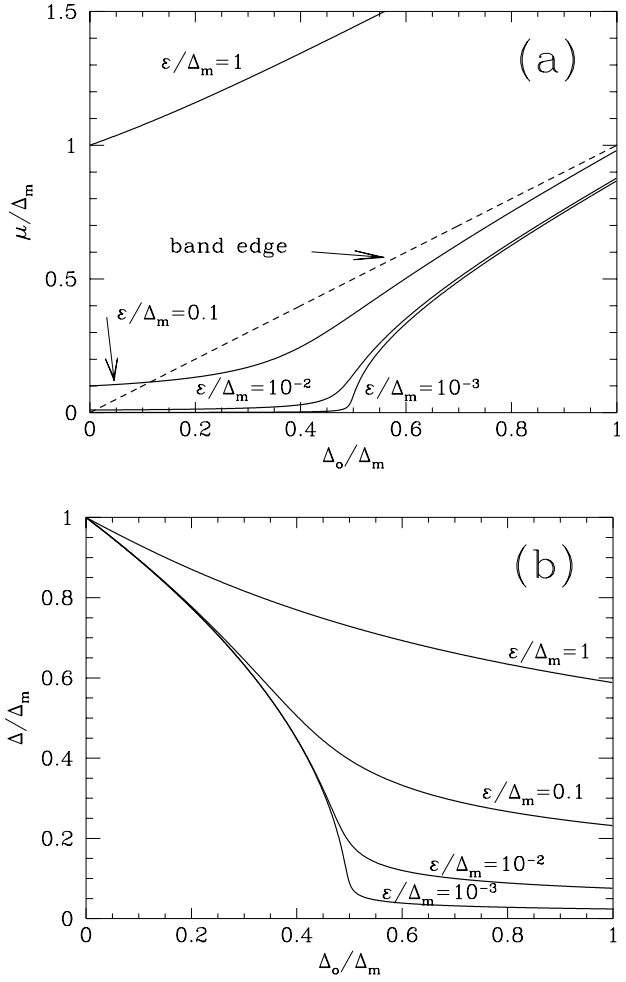

Fig. 4. (a) Chemical potential (μ) for different value of $\varepsilon/\Delta_{\rm m}$ as a function of $\Delta_{\rm o}/\Delta_{\rm m}$. The dashed line is the bottom of the upper band ($\Delta_{\rm o}/\Delta_{\rm m}$). (b) The same for the order parameter $\Delta/\Delta_{\rm m}$.

unchanged:

$$2\rho\int_P {\rm d}\xi\left[v^2(\xi)+f_{\rm F}[E(\xi)]\frac{\xi-\mu}{E(\xi)}\right]-2\rho\int_{-\omega_{\rm m}}^{0}{\rm d}\xi=\delta N, \tag{10}$$

where $f_{\rm F}(E)=1/({\rm e}^{\beta E}+1)$ is the Fermi factor for inverse temperature β and

$$v^2(\xi)=1-u^2(\xi)=\frac{1}{2}\left[1-\frac{\xi-\mu}{E(\xi)}\right] \tag{11}$$

is the familiar BCS occupation factor. The cut-off $\omega_{\rm m}$ can be sent to infinity in equations (9, 10): we are left with a system of two coupled equations.

3.1 Ground state properties

We begin by considering the zero temperature limit. In this case integrations are elementary and we obtain:

$$\begin{cases}\Delta_{\rm m}^2=\left[\Delta_{\rm o}-\mu+\sqrt{(\Delta_{\rm o}-\mu)^2+\Delta^2}\right]\left[\Delta_{\rm o}+\mu\right.\\ \qquad\left.+\sqrt{(\Delta_{\rm o}+\mu)^2+\Delta^2}\right]\\ 2\varepsilon=2\mu-\sqrt{(\Delta_{\rm o}+\mu)^2+\Delta^2}+\sqrt{(\Delta_{\rm o}-\mu)^2+\Delta^2}\end{cases}. \tag{12}$$

System (12) fixes μ and Δ as a function of the gap $\Delta_{\rm o}$ and doping $\delta N=2\rho\varepsilon$. Once they are known, the overall gap for elementary excitations is either Δ (if $\mu>\Delta_{\rm o}$) or $\sqrt{(\Delta_{\rm o}-\mu)^2+\Delta^2}$ (if $\mu<\Delta_{\rm o}$). Numerical solution of these equations is easy and it is shown in Figure 4. Simple limits can be assessed analytically as long as $\varepsilon\ll\Delta_{\rm m}$, shedding some light on the physical meaning of these results.

Consider first the "conducting" side. Here free carriers extend deep into the valence and conduction bands: the chemical potential for small doping will remain close to midgap. We can therefore expand the second equation of (12) into

$$\varepsilon=\mu\left[1-\frac{\Delta_{\rm o}}{\sqrt{\Delta_{\rm o}^2+\Delta^2}}\right]. \tag{13}$$

Doping is a small perturbation and we can use the undoped result for Δ: we thus find

$$\mu=\frac{\Delta_{\rm m}-\Delta_{\rm o}}{\Delta_{\rm m}-2\Delta_{\rm o}}\,\varepsilon+O(\varepsilon^2). \tag{14}$$

The approximation breaks down when $\varepsilon/\Delta_{\rm o}^*\sim\tau$. The crossover is very close to the superconductor-insulator sharp transition found when $\delta N=0$. Substituting that first order result for μ into the first of (12) we find the correction to Δ:

$$\Delta=2\Delta_{\rm o}^*\sqrt{\tau}+\left(\frac{\varepsilon}{\Delta_{\rm o}^*}\right)^2\frac{1+\tau}{8\,\tau^{5/2}}\Delta_{\rm o}^*+O(\varepsilon^4). \tag{15}$$

As long as $\Delta_{\rm o}<\Delta_{\rm o}^*$ doping is a minor perturbation.

In the opposite limit, we first note that an insulating state at $T=0$ is impossible. It would mean a $\Delta=0$ solution to the gap equation, *i.e.* $\Delta_{\rm m}^2=4(\Delta_{\rm o}^2-\mu^2)$, which in turn implies $\mu<\Delta_{\rm o}$. But with no Δ that means $\delta N=0$. Thus superconductivity must either extend all the way, or display a first order transition: a sharp second order transition to the insulating state is precluded. We now show that the present model has a smooth crossover.

Deep in the insulating limit, $\Delta_{\rm o}>\Delta_{\rm o}^*$, the role of equations is interchanged. The order parameter Δ will turn out to be small: consequently the gap equation which used to fix Δ now fixes μ

$$\Delta_{\rm m}^2=4(\Delta_{\rm o}^2-\mu^2)\quad\Rightarrow\quad\mu=\sqrt{\Delta_o^2-\Delta_{\rm o}^{*2}}. \tag{16}$$

Such an expansion is valid as long as $(\Delta_o - \mu) \gg \Delta$, which implies

$$\frac{\Delta_o^{*2}}{2\Delta_o} \gg \Delta \tag{17}$$

μ is still inside the band gap Δ_o. Granted μ, the other equation for δN fixes the order parameter Δ

$$\varepsilon = \frac{\delta N}{2\rho} = \frac{2\Delta^2}{{\Delta_m}^2}\sqrt{\Delta_o^2 - \Delta_o^{*2}} \quad \Rightarrow \quad \Delta = \frac{\Delta_m\sqrt{\varepsilon/2}}{\left[\Delta_o^2 - \Delta_o^{*2}\right]^{1/4}}\cdot \tag{18}$$

As surmised Δ is small for small doping ε, which justifies our calculation *a posteriori*. The condition (17) now reads

$$\varepsilon \ll \frac{\Delta_o^{*2}}{8\Delta_o}\cdot \tag{19}$$

Doping should remain small (or the gap Δ_o not exceedingly large).

When the gap exceeds that range the expansion in powers of Δ is no longer warranted. But as long as doping ε is small compared to Δ_o^* we expect the chemical potential to remain close to Δ_o, either below (inside the gap) or above (inside the continuum). We may then assume safely that $(\Delta_o + \mu) \approx 2\Delta_o \gg \Delta$. The two basic equations (12) simplify into

$$\begin{cases} \Delta_o^{*2} = \left[\Delta_o - \mu + \sqrt{(\Delta_o - \mu)^2 + \Delta^2}\right]\Delta_o \\ 2\varepsilon = \mu - \Delta_o + \sqrt{(\Delta_o - \mu)^2 + \Delta^2} \end{cases}. \tag{20}$$

Multiplying one by the other we obtain the very simple result

$$\Delta^2 = \frac{2\varepsilon\Delta_o^{*2}}{\Delta_o}$$

which joins smoothly with our former expansion (18), and which remains valid throughout the crossover $|\Delta_o - \mu| \sim \Delta$. Similarly we may eliminate the square roots from these two equations, which yields the chemical potential μ

$$\mu = \Delta_o + \varepsilon - \frac{\Delta_o^{*2}}{2\Delta_o}\cdot \tag{21}$$

For very large gaps $\Delta_o \gg \Delta_o^{*2}/\varepsilon$, the last term is negligible and we recover the usual result for a doped normal semiconductor, $\mu = \Delta_o + \varepsilon$.

Let us explore these two regimes in some more detail. When the chemical potential lies inside the gap Δ_o the real gap Δ_g is just $(\Delta_o - \mu) \gg \Delta$, of order $\Delta_o^{*2}/2\Delta_o$ as μ approaches the band edge. The relevant ratio is

$$\frac{\Delta}{\Delta_g} = \sqrt{\frac{8\varepsilon\Delta_o}{\Delta_o^{*2}}} \ll 1. \tag{22}$$

Note the strong similarity between such a regime and the Bose condensation of preformed pairs [2]. In the latter case the chemical potential μ is close to the energy of bound pairs, $\varepsilon_b/2$ per fermion and therefore it lies inside the gap. Here the reduced kinetic energy $(\xi - \mu)$ likewise never vanishes: $(\Delta_o - \mu)$ plays the role of $\varepsilon_b/2$. The resulting behaviour is similar in both cases, with a completely different physics. Here the hierarchy of energy scales is

$$\varepsilon \ll \Delta \ll \Delta_g$$

(indeed one has $\Delta^2 = 4\varepsilon\Delta_g$). In the opposite limit the chemical potential enters the conduction band: then the real gap Δ_g is just the order parameter Δ. The relevant ratio is that of Δ to the Fermi energy ε measured from the bottom of the band

$$\frac{\Delta}{\varepsilon} = \sqrt{\frac{2\Delta_o^{*2}}{\varepsilon\Delta_o}}\cdot$$

Except for a numerical factor 4 we see that $\Delta \ll \varepsilon$: we recover an ordinary BCS regime in which superconducting pairing is a small perturbation.

What is unusual is the behaviour of the order parameter $\Delta \approx \sqrt{\varepsilon}$ in that "insulating regime", for small doping ε and moderate semiconductor gap Δ_o. Such an unusual dependence $\Delta \approx \sqrt{\varepsilon}$ is due to the interplay of doping and superconductivity: (i) extrinsic carriers are needed in order to start superconductivity, but (ii) the latter does add further carriers, thereby modifying Δ. That result for the dependence on doping away from Δ_o^* should be compared with the result $\Delta = 2\Delta_o^*\sqrt{\tau}$ for the undoped system close to Δ_o^*. The two variables τ and ε act in the same way in driving the system away from the $T = 0$ critical point (we will find this behaviour again for the critical temperature).

Analytic calculations are possible only in limiting cases. In the crossover region one must resort to numerical solutions, which are quite straightforward. The result is shown in Figure 4 where system (12) is solved numerically for the values of ε indicated. Both Δ and μ clearly display the transition from a "metallic" to a "semi insulating" regime. In the latter, μ crosses the band edge when $\varepsilon \sim \Delta_o^{*2}/2\Delta_o$, separating Bose Einstein like and BCS like behaviours. Note that the chemical potential crosses the band edge Δ_o twice when ε is smaller than a critical value (see also the discussion after Fig. 7).

3.2 Finite temperature behaviour

Having a complete view of the zero temperature doped system, we consider now the effect of a finite temperature. In particular we want to investigate the critical temperature of the system. Setting $\Delta = 0$ into equations (9, 10) we obtain:

$$\int_{\Delta_o}^{\infty} d\xi \left[\frac{\tanh\beta_c(\xi - \mu_c)/2}{\xi - \mu_c} + \frac{\tanh\beta_c(\xi + \mu_c)/2}{\xi + \mu_c} - \frac{2}{\sqrt{\xi^2 + \Delta_m^2}}\right] = 2\int_0^{\Delta_o} \frac{d\xi}{\sqrt{\xi^2 + \Delta_m^2}} \tag{23}$$

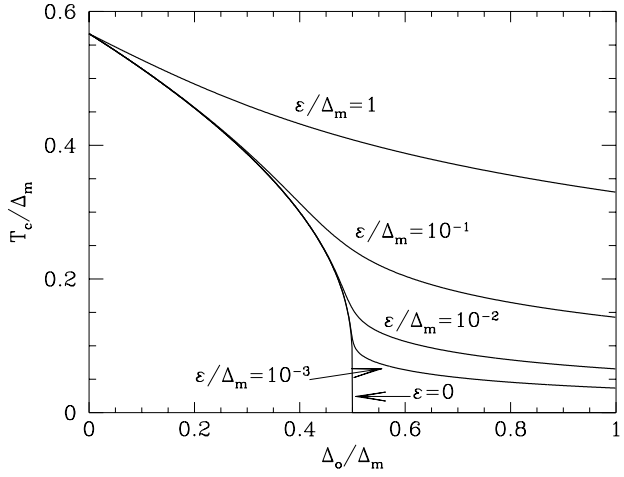

Fig. 5. Critical temperature T_c as a function of Δ_o/Δ_m for $\varepsilon/\Delta_m = 0$, 10^{-3}, 10^{-2}, 10^{-1}, and 1.

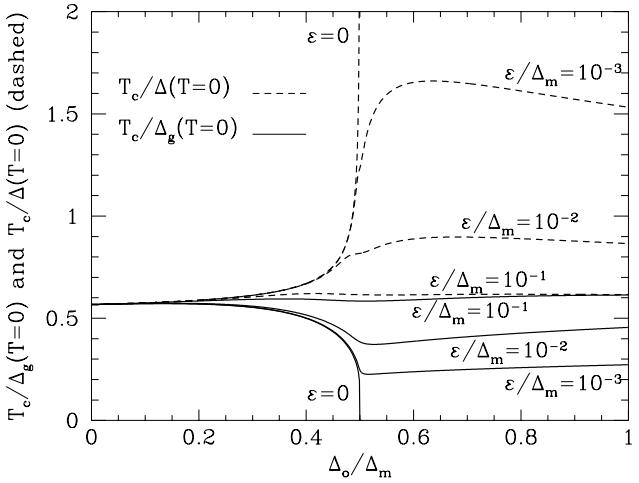

Fig. 6. $T_c/\Delta_g(T=0)$ (continuous line) and $T_c/\Delta(T=0)$ (dashed line) for different values of ε/Δ_m (indicated on the plot). The lines corresponding to $\varepsilon/\Delta_m = 10^{-1}$ are nearly constant at the BCS value of ≈ 0.57.

and

$$\varepsilon = 2\mu_c + \frac{1}{\beta_c}\log\left[\frac{1+e^{\beta_c(\Delta_o-\mu_c)}}{1+e^{\beta_c(\Delta_o+\mu_c)}}\right]. \qquad (24)$$

These equations can be easily solved numerically and the results are shown in Figure 5 for different values of ε including the undoped case. As expected from the zero temperature analysis, the critical temperature also exhibits a smooth crossover from a large to a small value, and it never vanishes for finite doping. The region $\Delta_o < \Delta_o^*$ is not much different from a standard BCS superconductor: a comparison of Figure 5 with Figure 4a clearly shows that T_c is proportional to $\Delta(T=0)$ (with the same BCS factor for $\Delta \to 0$).

A new and interesting behaviour is instead found when $\Delta_o > \Delta_o^*$. In this region the critical temperature appears to be much larger than the order parameter $\Delta(T=0)$ when $\varepsilon/\Delta_m \ll 1$. This point can easily be verified analytically. In this limit we can substitute the ground state chemical potential μ_o in equation (24). Since the critical temperature vanishes for $\varepsilon = 0$ while $\Delta_o - \mu_o > 0$ the exponentials in equation (24) are large and we can expand the expressions. At leading order in $\exp\{(\mu_o - \Delta_o)/2T_c\}$ we obtain the following equation for T_c:

$$T_c = \varepsilon\, e^{\frac{\mu_o-\Delta_o}{T_c}}. \qquad (25)$$

Again the solution can be written in terms of $w(x)$:

$$T_c = \frac{\Delta_o-\mu}{w\left[\frac{\Delta_o-\mu_o}{\varepsilon}\right]} \sim \frac{\Delta_o-\mu_o}{\ln\left[\frac{\Delta_o-\mu_o}{\varepsilon}\right]}. \qquad (26)$$

It is then clear that the ratio $T_c/\Delta(T=0)$ diverges for ε going to zero. One should note that the behaviour found for both $\Delta(T=0)$ and T_c as a function of τ is exactly the same of that found for these two quantities as a function of ε. The origin is the same since the gap at T_c in this case becomes $\Delta_o - \mu$.

We report in Figure 6 the ratio between the critical temperature T_c and the other two relevant energy scales, the zero temperature order parameter $\Delta(T=0)$ and excitation gap $\Delta_g(T=0)$ for different values of ε/Δ_m going from 0 to 10^{-1}. For small Δ_o/Δ_m the familiar BCS results of $e^\gamma/\pi \approx 0.57$ is recovered, while for $\Delta_o > \Delta_m/2$ a totally different behaviour is found. The critical temperature appears to be in between the other two quantities (for $\varepsilon \ll \Delta_m$)

$$\Delta(T=0) < T_c < \Delta_g(T=0). \qquad (27)$$

This can be easily checked analytically, since for ε going to zero Δ_g stays finite [$\Delta_g \to \Delta_0 - \sqrt{\Delta_o^2 - \Delta_m^2/4}$], while T_c vanishes logarithmically and $\Delta(T=0)$ vanishes like $\sqrt{\varepsilon}$. Thus at mean field level we have found a rather peculiar form of superconductivity, whose behaviour is totally different from the BCS one. We note that the BCS behavior is recovered also for large values of Δ_o when the chemical potential lies in the conduction band. In Figure 6 all the lines will join the BCS value 0.57 for *fixed* ε and large enough Δ_o. If ε/Δ_m is small enough, the parameter Δ_o drives the system through four different regimes. For very small Δ_o the system is in a two-band BCS regime. Increasing Δ_o the chemical potential enters the gap and the smoothed transition from a normal superconductor to a "semi-conductor" superconductor takes place. When $\Delta_o \gg \Delta_o^*$ and the chemical potential is still in the gap, the carriers in the upper band act as a strong coupling superconductor, while the lower band is nearly decoupled. For even larger $\Delta_o (> \Delta_o^{*2}/2\varepsilon)$ the chemical potential lies again in the valence band and a BCS behaviour is recovered for the upper band. The schematic phase diagram is plotted in Figure 7 where the region of positive and negative $\mu - \Delta_o$ are identified on the plane $\Delta_o - \varepsilon$. The path described above correspond to the dashed line.

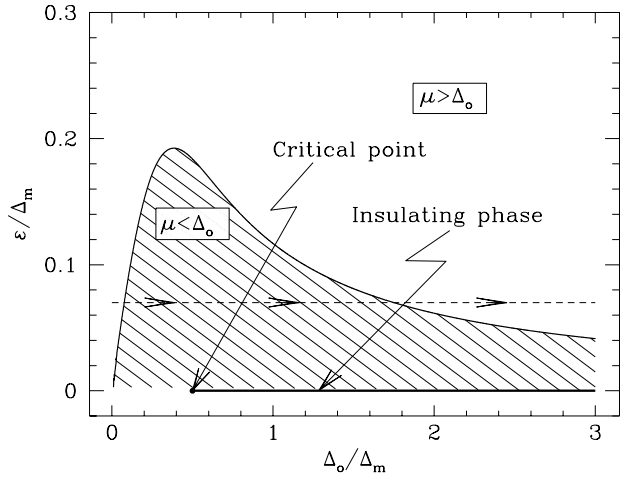

Fig. 7. Phase diagram for the chemical potential. The shaded part is the region with $\mu < \Delta_{\rm o}$. The thick line represents the insulating region of the phase diagram, for any other value of ε and $\Delta_{\rm o}$ the system is superconducting. The dashed line represents the path in the phase diagram described in the text.

All that discussion is based on a mean field, BCS like formulation. We should now ask whether such an approximation is warranted. In the next section we inquire about the effect of phase fluctuations in two dimensions, which are known to provide an alternate mechanism for the critical temperature $T_{\rm c}$, based on the creation of vortices instead of pair breaking.

4 Phase stiffness and Kosterlitz-Thouless fluctuations

We limit our discussion to a two-dimensional system for which they are known to be crucial, leading to the so called Kosterlitz-Thouless transition [5]. Although there is no strict long range order in 2d, the low temperature decay of the order parameter is algebraic up to a sharp critical temperature $T_{\rm c}^{\rm KT}$ at which the decay becomes exponential: such a transition from a "quasi superfluid" phase to a normal phase is due to the unbinding of vortex pairs. In the most naive approximation one may assume that the modulus of the order parameter is constant, the only relevant variable being its phase $\phi(\mathbf{x})$. The corresponding fluctuations are controlled by the phase stiffness J defined by the following term in the Hamiltonian

$$\Delta H = \frac{J}{2} \int {\rm d}^2 x |\nabla \phi(\mathbf{x})|^2 \tag{28}$$

J measures the resistance of the system to phase gradients. From J one infers in 2d the well-known exact critical temperature [12]

$$T_{\rm c}^{\rm KT} = \frac{\pi}{2} J \cdot \tag{29}$$

The stiffness that enters (29) is actually temperature dependent, $J(T)$. That dependence occurs both at the mean field level, through pair breaking thermal fluctuations, and via thermal fluctuations of the phase itself, which can be described within a renormalization scheme. We disregard the latter and we discuss briefly the mean field $J^{\rm MF}(T)$ which provides a neat picture of the competition between BCS and phase fluctuations [13]. $J^{\rm MF}$ vanishes at the mean field transition temperature $T_{\rm c}^{\rm MF}$, hence two possibilities: (i) $J^{\rm MF}(0) \gg T_{\rm c}$: phase fluctuations are essentially negligible except very close to $T_{\rm c}$: then $T_{\rm c}^{\rm KT}(T)$ becomes comparable to T and BCS turns into a Kosterlitz-Thouless regime; the ultimate transition is definitely in the Kosterlitz-Thouless universality class, but the relevant range is narrow and the real $T_{\rm c}$ is very close to $T_{\rm c}^{\rm MF}$. Basically BCS is correct. (ii) $J^{\rm MF}(0) \ll T_{\rm c}$: then the Kosterlitz-Thouless transition occurs well before pair breaking fluctuations become relevant: but for renormalization corrections $T_{\rm c}$ is $T_{\rm c}^{\rm KT}(0)$.

What we need is an estimate of the stiffness $J(0)$. That is easily achieved considering a superfluid flow in which pairs are condensed with center of mass momentum $\mathbf{Q}/2$ instead of $\mathbf{0}$. The corresponding phase of the order parameter is $\phi = \mathbf{Q} \cdot \mathbf{r}$ and its gradient is $\mathbf{Q}$. In order to calculate the energy of that flow we need a specific model of the band structure in momentum space: the knowledge of the density of states is not enough. Let us first consider the standard model of a 2d free electron gas, with no gap at all. The Fermi surface is a sphere with radius $k_{\rm F}$, the density of electrons with either spin is $N = k_{\rm F}^2/2\pi$. For a parabolic dispersion law, with mass m, the center of mass and relative motion of a pair are completely decoupled: the cost in kinetic energy of the superfluid flow is $N\hbar^2 Q^2/8m$. The phase stiffness is consequently

$$J = \frac{N\hbar^2}{4m} = \frac{\varepsilon_{\rm F}}{4\pi} \cdot$$

The corresponding transition temperature is $T_{\rm c}^{\rm KT} = \varepsilon_{\rm F}/8$, comparable to the Fermi energy, but noticeably smaller due to the accumulation of numerical factors. That must be compared to the BCS $T_{\rm c} \approx 0.57\Delta$; as mentioned in the introduction the crossover occurs when Δ is about a fifth of $\varepsilon_{\rm F}$, making the idea of a preformed bound state meaningless. Usual low temperature superconductors are way below that crossover and phase fluctuations are accordingly negligible.

We now turn to our gapped semiconductor: we need to specify the detailed form of the two bands. The simplest guess assumes valence and conduction bands that have a well defined extremum in the Brillouin zone, whether at the same place (direct gap), or at different places (indirect gap). Near the band edge the dispersion is parabolic, characterized by two (different) masses (the values of these masses will not enter in the final expression of the critical temperature). In a 2d system the density of states at band edge is finite, and the assumption of a constant ρ is not crucial: up to that point, our model raises no difficulty. It does however when we try to calculate the phase stiffness J. Before attempting explicit calculations, let us explain the point qualitatively. In order to set up a superfluid flow in a free electron gas, we shifted

the Fermi surface in momentum space, thereby obtaining a superfluid density $n_s = N$ and a phase stiffness $\sim \varepsilon_F$. If we do the same in a filled band we get nothing! A filled band is a single state with no degree of freedom, and shifting the distribution $n_k = 1$ produces the same state. Hence the obvious conclusion: *a filled band has no stiffness.* J can only result either from doping or from the order parameter Δ that creates free carriers even if there were none to start from. As a result the phase fluctuation T_c^{KT} is severely reduced: it becomes of order Δ, comparable to the BCS pair breaking T_c in every case. The difference with free carriers is dramatic, due to the narrow range of free carriers in momentum space.

One more general comment is in order: is it possible to go smoothly from the semiconductor to the metal? Put another way, does a reduction of the gap Δ_o to 0 drive us back to a regular Fermi liquid metal? As long as we were dealing with the density of states ρ only, the answer was "yes" in 2d: where free carriers sat in the Brillouin zone was of no concern. When calculating the phase stiffness J the answer is "no". The standard situation is an indirect gap which closes when the minimum of the conduction band is lower than the top of the valence band. Thereafter free carriers exist even in the normal state, but they remain localized near the corresponding band extrema. The insulator with no Fermi surface will not turn suddenly into a metal with a large Fermi surface (a sphere for free carriers). Instead a small Fermi surface will appear near the band extrema, responsible for the very small superfluid density (and phase stiffness). Such a behaviour should be contrasted with the 1d case, in which a smooth transition is possible. The standard example is the appearance of a commensurate spin density wave at zone edge: the resulting antiferromagnetic order produces Bragg scattering and opens a gap Δ_o. Near the gap the band dispersion is hyperbolic, returning to the normal metal behaviour when the distance $(\varepsilon - \varepsilon_0)$ to the band bottom ε_o exceeds Δ_o: in such a case the transition metal $\rightarrow$ semiconductor is smooth. But then the physics is completely different, as usual in 1d geometries. We see no realistic 2d system that could provide a smooth transition and a large superfluid density (that would mean a gap spread over the whole Fermi surface and translating together with it).

We now turn to the calculation of J, putting all the pairs in a state of total momentum $\mathbf{Q}$ and looking at the variation of the total energy. The BCS calculation for the energy is unmodified but for the following transformation

$$\xi_k \rightarrow \Xi_k(Q) = (\xi_{\mathbf{k}+\mathbf{Q}/2} + \xi_{-\mathbf{k}+\mathbf{Q}/2})/2\,. \tag{30}$$

where $\xi_{\mathbf{k}}$ is the dispersion relation of the band. This transformation changes only the kinetic energy: in our case we have for the two bands:

$$K(Q) = 2\sum_{\mathbf{k}\in \mathrm{v}} v_k^2[\Xi^{\mathrm{v}}_{\mathbf{k}}(\mathbf{Q}) - \mu] + 2\sum_{\mathbf{k}\in \mathrm{c}} v_k^2[\Xi^{\mathrm{c}}_{\mathbf{k}}(\mathbf{Q}) - \mu]. \tag{31}$$

Since the shift of $\mathbf{Q}$ of a filled band does not change the kinetic energy of the band we can write:

$$K(Q) = 2\sum_{\mathbf{k}\in \mathrm{v}} (\xi^{\mathrm{v}}_k - \mu) - 2\sum_{\mathbf{k}\in \mathrm{v}} u_k^2[\Xi^{\mathrm{v}}_{\mathbf{k}}(\mathbf{Q}) - \mu] + 2\sum_{\mathbf{k}\in \mathrm{c}} v_k^2[\Xi^{\mathrm{c}}_{\mathbf{k}}(\mathbf{Q}) - \mu]. \tag{32}$$

We use at this point the hypothesis that in the region where u_k and v_k are significantly different from zero the two bands are parabolic. We can thus expand Ξ for small Q:

$$\Xi^{\mathrm{v}}_{\mathbf{k}}(\mathbf{Q}) \simeq \xi^{\mathrm{v}}_k - \frac{Q^2}{8m_{\mathrm{v}}} \quad \text{and} \quad \Xi^{\mathrm{c}}_{\mathbf{k}}(\mathbf{Q}) \simeq \xi^{\mathrm{c}}_k + \frac{Q^2}{8m_{\mathrm{c}}} \tag{33}$$

where $m_{\mathrm{c/v}}$ are the effective masses of the two bands. The expression for K becomes:

$$K(Q) = K(0) + \frac{Q^2}{4m_{\mathrm{v}}}\sum_{\mathbf{k}\in \mathrm{v}} u_k^2 + \frac{Q^2}{4m_{\mathrm{c}}}\sum_{\mathbf{k}\in \mathrm{c}} v_k^2. \tag{34}$$

By introducing the 2-dimensional density of states per spin: $\rho = m/2\pi$ we obtain:

$$K(Q) - K(0) = \frac{Q^2}{8\pi}\left[\int_{-\infty}^{-\Delta_o} u(\xi)^2 \mathrm{d}\xi + \int_{\Delta_o}^{+\infty} v(\xi)^2 \mathrm{d}\xi\right], \tag{35}$$

and the masses simplify from the expression. We thus obtain for J:

$$J = \int_{\Delta_o}^{+\infty} \frac{\mathrm{d}\xi}{8\pi}\left[2 - \frac{\xi+\mu}{\sqrt{(\xi+\mu)^2+\Delta^2}} - \frac{\xi-\mu}{\sqrt{(\xi-\mu)^2+\Delta^2}}\right], \tag{36}$$

and since the integration is elementary we can write a closed expression for T_c^{KT}

$$T_c^{KT} = \frac{\sqrt{(\Delta_o-\mu)^2+\Delta^2} + \sqrt{(\Delta_o+\mu)^2+\Delta^2} - 2\Delta_o}{16}\,. \tag{37}$$

We comment this result in the two cases of $\varepsilon = 0$ and of finite doping.

In the undoped case the expression simplifies even more. In the superconducting region, $\Delta_o < \Delta_o^*$, we find

$$T_c^{KT} = (\Delta_m - 2\Delta_o)/8 \tag{38}$$

T_c^{KT} is thus comparable to the order parameter Δ, in contrast to a BCS superconductor, a spectacular consequence of the severe reduction in phase stiffness. The behavior near the transition point is easily understood. There the gap is large as compared to Δ and the density of free carriers v_k^2 lies in the tail of the BCS distribution: it is of the order $\rho\Delta^2/\Delta_m$. The stiffness is accordingly of the same order, leading to (38). Our conclusion is that the transition to the normal state is always due to unbinding of vortices, in sharp contrast to the weak coupling BCS limit.

We consider now the case of large Δ_o. We can use the approximation used in (20) and keeping the lowest order in Δ/Δ_o in equation (37) we find:

$$T_c^{KT} = \frac{\varepsilon}{8}\left[1 + \frac{\Delta_o^{*2}}{2\Delta_o^2}\right]. \quad (39)$$

As expected T_c^{KT} is proportional to the stiffness of a single band with Fermi energy $= \varepsilon$, this result is true for any sign of $\mu - \Delta_o$ provided $\mu \sim \Delta_o \gg \Delta$. The factor of proportionality is greater than one indicating that the lower band is contributing to the stiffness. This result implies that even in the doped system (for $\varepsilon \to 0$) the lowest critical temperature is T_c^{KT} due to binding-unbinding transitions of the vortices. The anomalous large value of the critical temperature found at mean field is thus never reached in reality. This result is not changed by a more realistic model for the dispersion relation as shown in Appendix A.

Conclusions

Superconductivity is usually concerned with a regular metal, in which free carriers exist at the Fermi level. We show here that superconductivity can also occur in semiconductors as soon as carriers in either band feel an attraction. The semiconductor is characterized by a gap $2\Delta_o$, the origin of which is not specified. The attraction is characterized by the superconducting gap Δ_m that would exist in a regular metal. The relevant parameters are the ratio Δ_o/Δ_m and the doping of the semiconductor.

Superconductivity may happen even in an undoped semiconductor in which no free carriers exist in the normal state at $T = 0$, as soon as the gain in superconducting energy $\sim \Delta_m$ exceeds the cost in producing carriers $\sim \Delta_o$. Such a situation is completely equivalent to excitonic insulators, in which electrons repel instead of attracting: then electrons and holes attract and they form bound excitons. If the binding energy is larger than the gap these excitons appear spontaneously. In our model we find a sharp transition at a specific value $\Delta_o^* \sim \Delta_m$ (the precise value depends on details of the density of states). The ground state is superconducting if $\Delta_o < \Delta_o^*$, insulating if $\Delta_o > \Delta_o^*$. Near the transition it departs from the familiar BCS regime: the order parameter Δ, the real quasiparticle gap Δ_g and the critical temperature T_c are such that

$$\Delta \ll T_c \ll \Delta_g.$$

That may be viewed as a "pseudogap" behaviour, monitored by the competition between semiconducting and superconducting features.

In the undoped case only the vicinity of the transition point Δ_o^* is unusual. This is no longer true when the semiconductor is doped: then the sharp transition becomes a crossover and superconductivity extends all the way. Nothing very spectacular happens when $\Delta_o < \Delta_o^*$: the effect of a small doping is minor. In contrast the "semiinsulating region" $\Delta_o > \Delta_o^*$ is extremely unusual: that is the main result of our paper. Past the crossover the chemical potential first remains inside the band gap. We then find a superconducting state very reminiscent of the Bose Einstein condensation of preformed pairs. The order parameter Δ is proportional to the square root of doping, and the characteristic energies display the same pseudogap ordering as in [2]. That behaviour prevails until the gap reaches $\Delta_o^{*2}/\varepsilon$, where ε is a typical Fermi energy in the conduction band. Then the chemical potential enters the conduction band and, after a transient region, the system returns to a single band BCS superconductor that involves only extrinsic carriers. The range of anomalous behaviour is very broad, and thus generic.

The main body of the paper is concerned with the simplest conceivable model, with a constant density of states ρ (a sensible choice for a 2d system), and a mean field treatment "à la BCS", both at zero and at finite temperatures. The only new feature is the presence of the semiconductor gap Δ_o. The problem is then studied both analytically and numerically. Both simplifications can be questioned: we now address the issues in succession.

A constant density of states is not realistic for two reasons: (i) it ships the gap states to infinity, while standard mechanisms for a small gap leave the states close to where they originated from, in an energy range $\sim \Delta_o$ (ii) in 3d the density of states $\rho(\xi)$ starts as $\sqrt{\xi}$ near band edge. Improvements are explored in Appendix A, where other densities of states are tried, still within a mean field picture. Numerical results show that the qualitative evolution remains the same. In the undoped case the sharp superconductor-insulator transition is just shifted, the square root behaviour of Δ being unaffected. In the doped case the calculation can be carried out explicitly in the anomalous region, if

$$\Delta \ll \Delta_o - \mu \ll \Delta_o.$$

Free carriers at $T = 0$ are then mostly in the conduction band and their density v_k^2 is small, of order Δ^2. Our main result, Δ proportional to the square root of doping, is maintained (with modified coefficients). We conclude that the physics described in this paper is not too sensitive to details of $\rho(\xi)$. We did not consider the case of a Fermi surface close to a Van Hove singularity, as found in a nested 2d system. That could definitely be done.

Departures from mean field behaviour is a more delicate problem. Thermal fluctuations of the phase of Δ are controlled by the phase stiffness J. In ordinary metals J is comparable to the Fermi energy: phase fluctuations are small and a mean field picture is correct except very close to T_c^{MF} (where fluctuations turn to a Kosterlitz-Thouless transition in 2d). In our semiconductor we show that J is only due to free carriers (it would be $\equiv 0$ for a filled band). J is comparable to the Fermi energy and thus small: it follows that the phase fluctuation mechanism for T_c always prevails (at least in 2d and for $\Delta_o < \Delta_m^2/\varepsilon$): that is the second unexpected result of our analysis. Simple considerations are enough in order to provide orders of magnitude, but a real quantitative theory is still lacking.

Granted these difficulties, we only tackled the problem, our goal being to emphasize simple physical ideas.

Many important questions remain open. For instance one should worry about the origin of the semiconducting gap Δ_o. If it arises from another instability (lattice distortion, magnetism, etc...), does superconductivity react on that primary instability? If it does we face a coupled problem, in which Δ depends on Δ_o and in reverse Δ_o depends on Δ. A self consistent calculation is required, and it may lead to unexpected fixed points [14]. Another issue is the relevance of interband pairing, as envisaged in [10]. Even if it is not the primary effect, it may affect the quantitative results. (It seems that such am interplay of intra and interband pairing is crucial in understanding the smooth transition of the stiffness when the gap Δ_o closes to zero in a 1D band.) These remarks open exciting possibilities, which we did not approach. As it stands our paper is only an exploration.

This work evolved from long discussions with Guy Deutscher: we are grateful to him for his helpful advice. We are also grateful to Prof. J. Friedel for pointing out reference [10] of which we were not aware.

Appendix A: Non constant density of states

In this appendix we consider a more realistic form for the density of states, in which the states removed from the energy region $[-\Delta_o, \Delta_o]$ remain in the vicinity of the edge. We explore two simple cases: a discontinuous density of states (typical of 2d system) and a density of states that vanishes at Δ_o with a square root of $\xi - \Delta_o$ (typical of a 3d case). These two possibilities are shown in Figure 1. We solve the equations numerically showing that the qualitative behaviour found for constant density of states is not changed.

Equations (9, 10) can be easily generalized when the density of states is not constant:

$$\begin{cases} \displaystyle\int_{P'} \rho(\xi) \left[v^2(\xi) + f_{\rm F}[E(\xi)] \frac{\xi - \mu}{E(\xi)} \right] \mathrm{d}\xi = \int_{-\omega_{\rm m}}^{\varepsilon} \rho_{\rm m}(\xi)\, \mathrm{d}\xi \\ \displaystyle\int_{P'} \rho(\xi) \frac{\tanh \beta E(\xi)/2}{E(\xi)}\, \mathrm{d}\xi = \int_{-\omega_{\rm m}}^{+\omega_{\rm m}} \frac{\rho_{\rm m}(\xi)}{\sqrt{\Delta_{\rm m}^2 + \xi^2}}\, \mathrm{d}\xi \end{cases} . \tag{A.1}$$

In this equations $\rho_{\rm m}(\xi)$ and $\rho(\xi)$ are the densities of states of the metallic and insulating phase respectively. The integration path is now $P' = [-\omega_{\rm m}, -\Delta_o]$ and $[\Delta_o, +\omega_{\rm m}]$, since we conserve the number of states by deforming ρ and not by shifting the whole band. The function $\rho(\xi)(\geq 0)$ is thus constrained by the conservation of the number of states when passing from the metallic to the insulating phase:

$$\int_{P'} \rho(\xi)\, \mathrm{d}\xi = \int_{-\omega_{\rm m}}^{\omega_{\rm m}} \rho_{\rm m}(\xi)\, \mathrm{d}\xi. \tag{A.2}$$

It is clear that in order to fulfill equation (A.2) $\rho(\xi)$ must depend on Δ_o too.

Equations (A.1) are quite general. We will consider two specific simple cases. We assume that $\rho_{\rm m}$ is constant, and that $\rho(\xi)$ is defined in the two cases by the following expressions:

$$\begin{cases} \rho_1(\xi)/\rho_{\rm m} = 1 + \mathrm{e}^{-x} \\ \rho_2(\xi)/\rho_{\rm m} = \dfrac{2+\pi}{\sqrt{\pi}} \sqrt{x}\, \mathrm{e}^{-x} + \dfrac{x^2}{1+x^2} \end{cases} \tag{A.3}$$

where $x = (|\xi| - \Delta_o)/\Delta_o$ and $\rho = 0$ for $|\xi| < \Delta_o$ (*cf.* Fig. 1, the dotted line correspond to ρ_1 and the dashed line to ρ_2). The numerical results for Δ and μ in the zero temperature case are reported in Figure 8 for the discontinuous density of states (ρ_1), and in Figure 9 for the second one. There is no qualitative difference with Figure 4. Different shapes of the density of states correspond to different values of the ratio $\Delta^*/\Delta_{\rm m}$, always keeping it of order 1[1].

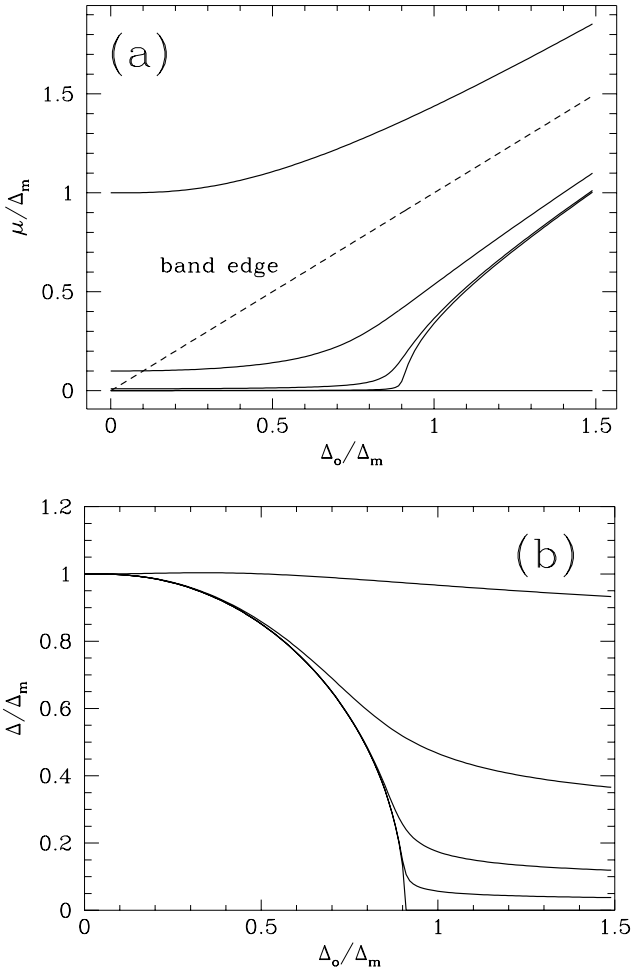

Fig. 8. Zero temperature numerical results for the density of states $\rho = \rho_1$ (discontinuous one): (a) Chemical potential, and bottom of the upper band (dashed). (b) Order parameter Δ. $\varepsilon/\Delta_{\rm m}$ take the following values: 0, 10^{-3}, 10^{-2}, 10^{-1}, 1.

[1] Although the energy range over which $\rho(\xi)$ varies is of order Δ_o, we have tried a more general form in which that energy scale is different from Δ_o. The maximal variation of Δ_o^* obtained is an increase of a factor $e \approx 2.71$ when all the removed states are accumulated at the edge.

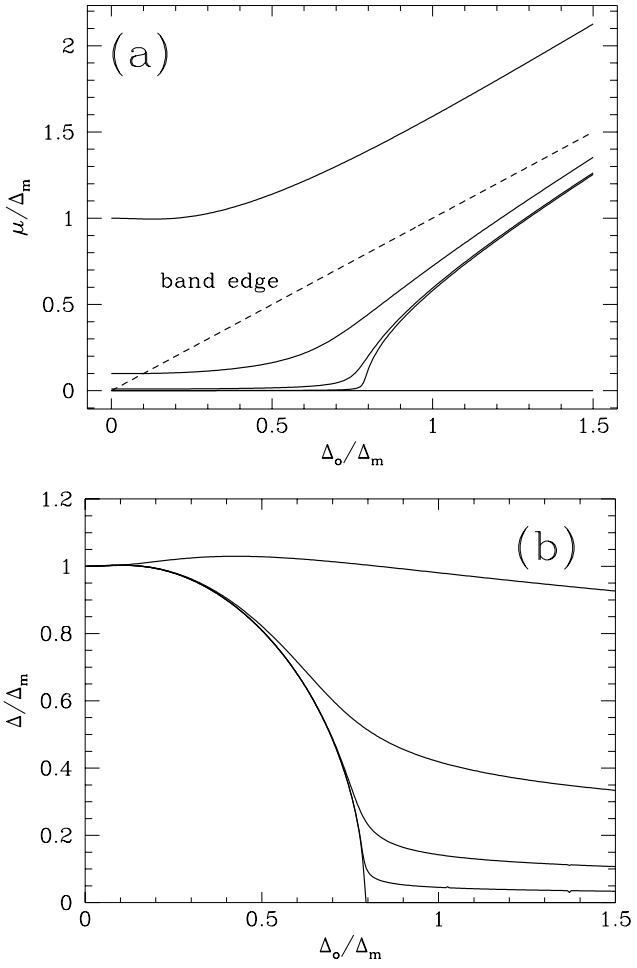

Fig. 9. Numerical results for the density of states $\rho = \rho_2$ (square root). Conventions are the same of Figure 8.

Most of the results can be understood analytically. Let us first consider how the order parameter vanishes at the transition for no doping. In this case Δ is small and we can expand E in the second of (A.1). After the equation for the critical Δ_o is subtracted we obtain:

$$0 = \int_{\Delta_o^*}^{+\infty} \frac{\rho_{\Delta_o^*}(\xi) - \rho_{\Delta_o}(\xi)}{\xi} \mathrm{d}\xi - \frac{1}{\Delta_o} \int_{\Delta_o}^{\Delta_o^*} \rho(\xi)\mathrm{d}\xi + \Delta^2 \int_{\Delta_o^*}^{+\infty} \frac{\rho_{\Delta_o}}{2\xi^3}. \quad \text{(A.4)}$$

The last term for $\tau \to 0$ ($\Delta_o \to \Delta_o^*$) yields simply $\Delta^2(\tau)$ multiplied by a constant. The second term vanishes like $\tau^{1+\alpha}$ if $\rho(\xi) \sim (\xi - \Delta_o)^\alpha$. This term is always subleading compared to the first term that vanishes linearly in τ. We thus conclude that the dependence $\Delta \sim \tau^{1/2}$ is quite general. This is not surprising for a mean field theory.

For finite doping and $T = 0$ it is interesting to study the dependence of Δ on ε. In particular we can readily obtain this dependence analytically when $\Delta_o \gg \Delta_m$. We distinguish the two cases $\mu < \Delta_o$ and $\mu > \Delta_o$. When $\Delta_o \gg \Delta_o - \mu \gg \Delta$ the lower band is nearly decoupled and the conservation of particles gives:

$$\delta N = 2\varepsilon\rho_m \approx \int_{\Delta_o}^{\infty} \rho(\xi) \frac{\Delta^2}{2(\xi-\mu)^2} \approx \frac{\Delta^2}{2} \frac{\rho(\Delta_o - \mu)}{\Delta_o - \mu}. \quad \text{(A.5)}$$

We thus recover $\Delta \sim \varepsilon^{1/2}$ for a general density of states, again a mean field exponent. Note that the coefficient involves the density of states on an energy scale $\sim (\Delta_o - \mu)$ (measured from the bottom of the conduction band). This fact does not invalidate the conclusion since the chemical potential is practically independent on ε, determined as usual by the gap equation.

For Δ_o large enough μ sits again in the valence band, and the limit $\Delta_o \gg \mu - \Delta \gg \Delta$ is reached. In this case the BCS theory applies in the upper band and one recovers the familiar exponential behavior of Δ on the inverse of the density of states at the Fermi energy.

Concerning the critical temperature we have verified that using the density of states ρ_1 one recovers the same behaviour found for a constant density of states: near the transition point and for small doping it vanishes like $1/w(1/\tau)$ or $1/w(1/\varepsilon)$. In the BCS region ($\Delta_o \gg \Delta_m^2/\varepsilon$) the usual BCS T_c is recovered.

We can readily calculate the phase stiffness if we assume that the dispersion relation depends only on $\mathbf{k}^2$. In this case we can generalize the results for the variation of the kinetic energy:

$$\Xi_{\mathbf{k}}(\mathbf{Q}) = \xi_k + \xi_k' \frac{Q^2}{4} + \xi_k'' \frac{(\mathbf{kQ})^2}{2} + O(Q^4), \quad \text{(A.6)}$$

where $\xi' \equiv \mathrm{d}\xi(k^2)/\mathrm{d}(k^2)$. Using this expression for the kinetic energy and the invariance under rotation we obtain for each band:

$$\frac{\mathrm{d}E(Q)}{\mathrm{d}Q^2} = 2 \sum_{\mathbf{k}\in\text{band}} v_k^2 \left[\frac{\xi_k'}{4} + \frac{\xi_k''}{2} \frac{k^2}{2} \right]. \quad \text{(A.7)}$$

The derivatives of the dispersion relation can be related to the density of states: $\xi_k' = 1/4\pi\rho$ and $\xi_k'' = -\rho'/16\pi^2\rho^3$. Putting everything together we obtain for our problem the same phase stiffness J as in (36), but with an additional factor $A(\xi)$ in the integrand of (36) [provided $\rho(\xi) = \rho(-\xi)$]:

$$A(\xi) = 1 - \frac{\rho'(\xi)}{\rho(\xi)^2} \int_{\Delta_o}^{\xi} \rho(x)\mathrm{d}x. \quad \text{(A.8)}$$

When the density of states is constant $A(\xi)$ is 1. One can show that the integral of $[A(\xi) - 1]$ is equal to Δ_o: it thus gives the contribution of the additional states to the phase stiffness. The various contributions to the phase stiffness are just rearranged and we find that the shape of $\rho(\xi)$ does not affect qualitatively the dependence of the phase stiffness on the important parameters Δ_o and ε. Moreover the quantitative change is not enough to let T_c^{KT} become larger than the T_c given by particle excitations. Thus the phase fluctuations should always be responsible for the transition to the normal phase. (Except for very large Δ_o at fixed ε where the BCS limit is recovered.)

Appendix B: Interband pairing

In this paper we have considered pairing of time reversed state within the same band. If we indicate with $a_{k\sigma}$ and $b_{k\sigma}$ the destruction operators for the lower and upper band respectively, the possible pairings considered in the main body of the paper are: $\langle a_{k\uparrow} a_{-k\downarrow}\rangle$ and $\langle b_{k\uparrow} b_{-k\downarrow}\rangle$. The two bands are then coupled by the interband interaction, which is assumed identical to the intraband interaction.

Another model of pairing in a two band semiconductor was proposed some years ago by Kohmoto and Takada [10] (see also [15]). The main difference with our proposal is that in that case the paired states are not time-reversed one of the other, specifically electrons of different bands are paired: $\langle a_{k\uparrow} b_{-k\downarrow}\rangle$. (The spin was not included in the original formulation and it is introduced here for comparison with our work). The mean field calculations predicts at $T = 0$ a first order transitions from an insulator to a superconductor. We discuss briefly in this Appendix this model [10] and we compare it to ours in one simple case.

The main difference arise from the fact that the kinetic energies of the paired states are different: one expects that the energy cost should accordingly be larger. Although it is possible to have interactions that favor only one of the two possible states, when the strength of the interaction is the same in the two channels the intraband pairing should be favoured due to the lower (kinetic) energy cost. We demonstrate this fact in a simple case.

We consider a local interaction of the form

$$-U \int \mathrm{d}x\, \rho(x)\rho(x),$$

where $\rho(x) = \sum_\sigma \psi^\dagger(x)_\sigma \psi\ (x)_\sigma$ and $\psi_\sigma(x) = a_\sigma(x) + b_\sigma(x)$. The antiparallel spin component of this interaction can be reduced to two terms:

$$V_1 = -2U \int \mathrm{d}x\, \left(a^\dagger_\uparrow a^\dagger_\downarrow + b^\dagger_\uparrow b^\dagger_\downarrow\right)\left(a_\downarrow a_\uparrow + b_\downarrow b_\uparrow\right), \quad \text{(B.1)}$$

$$V_2 = -2U \int \mathrm{d}x\, \left(a^\dagger_\uparrow b^\dagger_\downarrow - a^\dagger_\downarrow b^\dagger_\uparrow\right)\left(b_\downarrow a_\uparrow - b_\uparrow a_\downarrow\right). \quad \text{(B.2)}$$

V_1 would induce the pairing suggested in this paper, while V_2 is needed in order to obtain the state proposed by Kohmoto and Takada. We consider the simplest case of constant density of states ρ, symmetric bands, and no doping ($\mu = 0$). We also keep the energy cut-off $\Delta_\mathrm{o} + \omega_\mathrm{c} = \omega_\mathrm{m}$ finite. We can then evaluate the Hamiltonian on the respective trial wave functions. For the intraband pairing proposed in this paper the ground state wavefunction is:

$$|\psi_1\rangle = \prod_{\mathbf{k}} \left(u_k + v_k\, b^\dagger_{k\uparrow} b^\dagger_{-k\downarrow}\right)\left(v_k + u_k\, a^\dagger_{k\uparrow} a^\dagger_{-k\downarrow}\right)|\mathrm{vac}\rangle \quad \text{(B.3)}$$

while for the state proposed in reference [10] the wavefunction takes the form:

$$|\psi_2\rangle = \prod_{\mathbf{k}} \left(\frac{1 + a^\dagger_{k\uparrow} b^\dagger_{-k\downarrow}}{\sqrt{2}}\right)\left(\frac{1 - a^\dagger_{k\downarrow} b^\dagger_{-k\uparrow}}{\sqrt{2}}\right)|\mathrm{vac}\rangle. \quad \text{(B.4)}$$

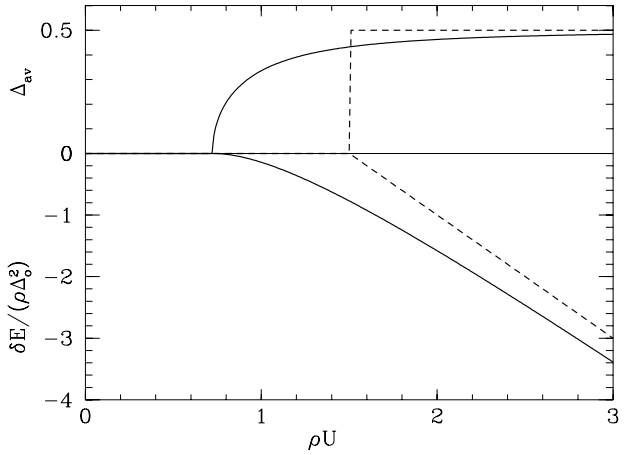

Fig. 10. Comparison of the ground state energies of the state presented in this paper (full lines) and of the one proposed in reference [10] (dashed line). The upper part of the plot shows the order parameter for the two models.

Here the singlet state has been chosen to take maximal advantage of the interaction. The energy difference with respect to the normal state (δE) is in the two cases:

$$\delta E_1 = \rho\left[2\Delta_\mathrm{o}\omega_\mathrm{c} + \omega_\mathrm{c}^2 - (\Delta_\mathrm{o} + \omega_\mathrm{c})\sqrt{(\Delta_\mathrm{o} + \omega_\mathrm{c})^2 + \Delta^2} + \Delta_\mathrm{o}\sqrt{\Delta_\mathrm{o}^2 + \Delta^2}\right], \quad \text{(B.5)}$$

$$\delta E_2 = \rho\omega_\mathrm{c}\left[2\Delta_\mathrm{o} + \omega_\mathrm{c} - 2U\omega_\mathrm{c}\rho\right], \quad \text{(B.6)}$$

where the value of Δ in (B.5) is given by the usual gap equation: $1 = 2\rho U \int_{\Delta_\mathrm{o}}^{\Delta_\mathrm{o}+\omega_\mathrm{c}} \mathrm{d}\xi/\sqrt{\xi^2 + \Delta^2}$. The minimum value of the interaction ($U^{\min}$) for which δE changes sign determines the transition from the insulating to the superconducting phase. For the two states we have respectively $\rho U_1^{\min} = 1/2\ln(1 + \omega_\mathrm{c}/\Delta_\mathrm{o})$ and $\rho U_2^{\min} = 1/2 + \Delta_\mathrm{o}/\omega_\mathrm{c})$. Thus $U_1^{\min} < U_2^{\min}$ always. Moreover explicit evaluation of the energy shows that the energy gain of the intraband pairing state is always larger than the interband one. In Figure 10 we plotted δE in the two cases when $\delta\omega_\mathrm{c}/\Delta_\mathrm{o} = 1$. The transition is second order in case (1), first order in case (2). We report also the average of the order parameter over the states that participate to the pairing:

$$\Delta_\mathrm{av} = \frac{\sum_k u_k v_k}{\sum_k 1}, \quad \text{(B.7)}$$

which clearly displays the nature of the transition.

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