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Effect of local potential variations in the model of hole superconductivity

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In the model of hole superconductivity the strength of the pairing interaction depends on the local carrier density. This gives rise to a dependence of the gap function Δ_k on the band energy ϵ_k. Fluctuations in the local potential energy will result in different values of Δ_k at the Fermi energy and hence in different values of the local energy gap. In particular, the energy gap can be sharply reduced. We study this behavior by numerical solution of the Bogoliubov–de Gennes equations for the model. The behavior is contrasted with what occurs in the attractive Hubbard model, where local potential fluctuations have negligible effect. The physical origin of this behavior and the possible relevance to high-T_c oxides is discussed.

1. Introduction

Experimental estimates of the superconducting energy gap in high-T_c oxides have yielded a wide spread in gap values [1]. Results vary between different techniques, such as infrared and tunneling, and within the same technique depending on experimental conditions. Furthermore, the broadening of the resistive transition in a field observed in high-T_c oxides [2] suggests the existence of a distribution of gap values and the fact that critical currents are low [3] suggests that there are regions in the superconductor with reduced order parameter.

In this paper we examine the effect of local potential variations on the energy gap in the model of hole superconductivity [4,5]. In this model the energy gap function Δ_k depends on the band energy ϵ_k. It was suggested in ref. [4] that this would give rise to high sensitivity to non-magnetic disorder. Recently, Marsiglio [6] has studied the effect of non-magnetic disorder on T_c in this model, and found that T_c can be strongly depressed. Here, we study the effect of local potential fluctuations on the local energy gap (as measured in a tunneling experiment), by numerical solution of the Bogoliubov–de Gennes equations [7] for the model. We find that such fluctuations can cause large variations in the local energy gap, suggesting a possible explanation for the above-mentioned observations.

2. Formalism

The Hamiltonian is given by [5]

$$H = -\sum_{i,j,\sigma} t_{ij}^{\sigma} (c_{i\sigma}^{+} c_{j\sigma} + \text{h.c.}) + \sum_i U_i n_{i\uparrow} n_{i\downarrow} + \sum_{ij} V_{ij} n_i n_j + \sum_i \epsilon_i n_i , \tag{1a}$$

$$t_{ij}^{\sigma} = t_{ij} + (\Delta t)_{ij} (n_{i,-\sigma} + n_{j,-\sigma}) . \tag{1b}$$

Here, the operators describe holes in a d-dimensional hypercubic lattice. For generality, we allow the interactions U_i, V_{ij} as well as the site energy ϵ_i to depend on position, although in the numerical calculations we will only consider variations in ϵ_i. The hopping t_{ij} as well as the hopping interaction $(\Delta t)_{ij}$ are assumed to be constants t, Δt between nearest-neighbor sites, and zero otherwise.

We introduce the local expectation values

$$a_i = \langle c_{i\downarrow} c_{i\uparrow} \rangle , \tag{2a}$$

$$b_{ij} = \langle c_{i\downarrow} c_{j\uparrow} \rangle , \tag{2b}$$

and the local order parameters

$$\Delta_{ii} = -U_i a_i + \sum_j (\Delta t)_{ij}(b_{ij} + b_{ji}) \tag{3a}$$

$$\Delta_{ij} = (\Delta t)_{ij}(a_i + a_j) - V_{ij}\frac{b_{ij} + b_{ji}}{2}, \tag{3b}$$

with i, j nearest neighbor sites. The Bogoliubov–de Gennes (BdG) equations for this model are obtained in the usual way [7], by performing a mean-field decoupling of the interactions in eq. (1) and a Bogoliubov transformation to quasi-particle operators. This results in the matrix equations

$$E_n u_n = \epsilon u_n - \Delta v_n, \tag{4a}$$

$$E_n v_n = -\epsilon v_n - \Delta^+ u_n, \tag{4b}$$

for the quasi-particle energies E_n and eigenvector amplitudes u_n, v_n. Here,

$$(\epsilon)_{ij} = (\epsilon_i - \mu)\,\delta_{ij} - t_{ij}, \tag{5a}$$

$$(\Delta)_{ij} = \Delta_{ij}. \tag{5b}$$

μ is the chemical potential and the index n labels the particular eigenvalue and eigenvector. We also implicitly include the renormalization of the single-particle hopping t_{ij} due to the hopping interaction [5]. The only difference with the usual case [7] is that the order parameter Δ has here off-diagonal matrix elements in addition to diagonal ones. The self-consistency conditions are

$$\Delta_{ii} = -U_i \sum_n u_{ni} v_{ni}^* (1-2f_n) + \sum_j (\Delta t)_{ij} \sum_n (u_{ni} v_{nj}^* + u_{nj} v_{ni}^*)(1-2f_n), \tag{6a}$$

$$\Delta_{ij} = (\Delta t)_{ij} \sum_n (u_{ni} v_{ni}^* + u_{nj} v_{nj}^*)(1-2f_n) - \frac{V_{ij}}{2} \sum_n (u_{ni} v_{nj}^* + u_{nj} v_{ni}^*)(1-2f_n). \tag{6b}$$

with f_n the Fermi function for energy E_n.

In the absence of disorder ($\epsilon_i = 0$ for all i, U_i, V_{ij} constants) the eigenvector index n becomes the wavevector k and the solution of these equations takes the form

$$u_n = e^{ikR_i} u_k, \tag{7a}$$

$$v_n = e^{ikR_i} v_k. \tag{7b}$$

Defining

$$\Delta_k = \sum_j e^{ik(R_j - R_i)} \Delta_{ij} \tag{8a}$$

and

$$\epsilon_k = -\sum_j e^{ik(R_j - R_i)} t_{ij}, \tag{8b}$$

eq. (4) yields

$$u_k v_k^* = \frac{\Delta_k}{2E_k}, \tag{9a}$$

$$E_k = \sqrt{(\epsilon_k - \mu)^2 + \Delta_k^2}; \tag{9b}$$

and eq. (6) gives rise to the usual BCS equation [4]. The gap function is parametrized as

$$\Delta_k = \Delta_m \left(\frac{1}{z} \sum_\delta e^{ik\delta} + c \right), \tag{10a}$$

where δ runs over nearest neighbor sites, or equivalently

$$\Delta_k = \Delta_m \left(-\frac{\epsilon_k}{D/2} + c \right), \tag{10b}$$

with $D = 2zt$ the bandwidth, with z the number of nearest neighbors. For the local order parameters we have

$$\Delta_{ii} = \Delta_m c, \tag{11a}$$

$$\Delta_{ij} = \frac{\Delta_m}{z}. \tag{11b}$$

The minimum quasi-particle energy, the "energy gap", is [4]

$$E_k^{\min} \equiv \Delta_o = \frac{\Delta(\mu)}{a}, \tag{12a}$$

$$a = \left(1 + \left(\frac{\Delta_m}{D/2} \right)^2 \right)^{1/2}, \tag{12b}$$

and it occurs at the values of k where the band energy is

$$\epsilon_k = \mu + \frac{1}{a}\frac{\Delta_m}{D/2}\Delta_o \tag{13}$$

as can be seen from minimization of eq. (9b). Figure 1 shows a typical example of the gap function and quasi-particle energy plotted versus band energy.

That disorder in the site energies ϵ_i will have a large effect on the energy gap in this model can be seen as

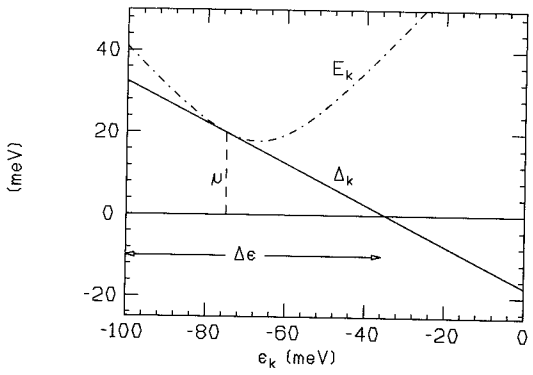

Fig. 1. Gap function Δ_k and quasi-particle energy E_k vs. band energy ϵ_k for a representative case. $D=0.2$ eV. Only the lower half of the (hole) band is shown. The range of values of site energies ($\Delta\epsilon$) that would cause the energy gap to vary between 0 and its maximum value is indicated.

follows. Consider first a situation where ϵ_i varies slowly over distances of the order of the coherence length. In that case we would simply solve the usual BCS equations with a constant $\epsilon_i \equiv \epsilon_o(r)$ in each region r, to obtain the parameters Δ_m and c in eq. (10a). The resulting critical temperature T_c and energy gap Δ_o are a function of the (local) carrier density $n(r)$ [4], which in turn depends on the site energy $\epsilon_o(r)$; for a constant density of states,

$$n(r)=1+\frac{\mu+\epsilon_o(r)}{D/2}. \tag{14}$$

From eq. (14) we deduce that if T_c is non-zero in a range of hole densities from 0 to n_{max}, the gap will vary between zero and its maximum value in a range of site energies

$$\Delta\epsilon=n_{max}\frac{D}{2} \tag{15}$$

Instead, if ϵ_i varies over distances of the order of the coherence length or shorter it becomes necessary to solve the full BdG equations. However, to a first approximation we may argue that the parameters Δ_m and c will be unaffected by very short-distance fluctuations. The "local band energy" will be given by

$$\epsilon_k(r)=\epsilon_k+\epsilon_o(r) \tag{16}$$

and minimization of the quasi-particle energy

$$E_k(r)=\sqrt{(\epsilon_k(r)-\mu)^2+\Delta_k^2} \tag{17}$$

leads to a local quasi-particle gap

$$\Delta_o(r)=\frac{\Delta(\mu-\epsilon_o(r))}{a}. \tag{18}$$

Thus, the local gap can be read off from fig. 1 by simply shifting μ along the horizontal axis a distance $\epsilon_o(r)$. The range in site energies where the gap varies between 0 and its maximum value is simply the region of the horizontal axis to the left of where the gap function crosses zero in fig. 1, i.e.

$$\Delta\epsilon=\frac{D}{2}(1+c). \tag{19}$$

Now the parameter c is found to have a weak dependence on carrier density [4], and at the point where T_c goes to zero it can be found exactly as [8]

$$c=-(1-n_{max}). \tag{20}$$

Replacement of eq. (20) in eq. (19) yields a result identical to eq. (15). Thus, a similar sensitivity of the local energy gap to disorder is expected in both regimes of slowly varying and rapidly varying fluctuations with respect to the coherence length.

3. Numerical results

To study the effect of disorder on scales of the order of or less than the coherence length we solve the BdG equations numerically by an iterative Newton–Raphson method. For computational reasons we restrict ourselves to a one-dimensional lattice of $N=20$ sites. We choose parameters so that the range of densities where T_c is non-zero is rather large, so that several densities can be studied on the finite size lattice. The parameters used were $U=5$ eV, $\Delta t=0.25$ eV, $V=0$, $t=0.03$ eV. They give rise to a maximum T_c of 160 K and a range of hole densities where T_c is non-zero from $n=0$ to $n=1.1$, as shown in fig. 2. Although this is not realistic for the high-T_c oxides, the qualitative effects discussed here depend only on the existence of a finite gap slope in the gap function. Fig. 3 shows the energy gap function eq. (10) obtained from solving the BCS equation, for four values of the chemical potential. These values were chosen as the lowest ones that lie half-way between the allowed kinetic energy values on the finite lattice ($\epsilon_k=-2t\cos k$, with k an integer multiple of $2\pi/N$)

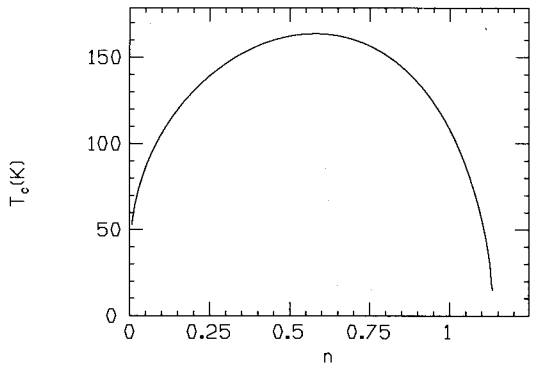

Fig. 2. Critical temperature vs. hole concentration for the one-dimensional model discussed in the text. $U=5$ eV, $\Delta t=0.25$ eV, $V=0$, $t=0.03$ eV.

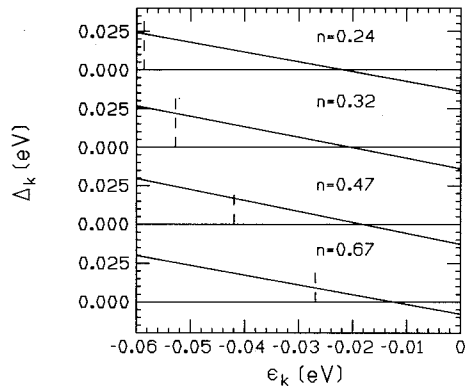

Fig. 3. Gap function vs. band energy for 20 site chain discussed in the text. The values of the chemical potential, indicated by the dashed lines, are $\mu=-t[\cos(\pi r/10)+\cos(\pi(r+1)/10], 0\leqslant r\leqslant 3$. The corresponding densities are given in the figure.

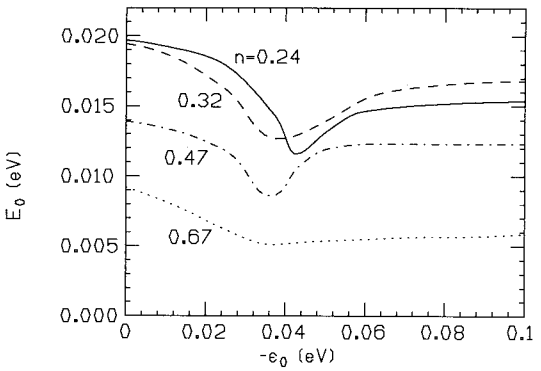

Fig. 4. Effect of disorder on a single site on the minimum quasi-particle energy E_o, for the one-dimensional chain discussed in the text. The abscissa gives the site energy of site zero, all other sites have site energies $\epsilon_i=0$. Parameters are given in the text. The different curves correspond to different carrier densities (numbers next to the curves).

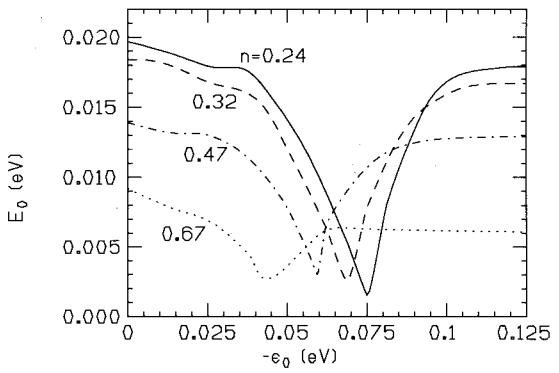

Fig. 5. Same as fig. 4 for disorder on two neighboring sites. Values of $\epsilon_o=\epsilon_1$ are given in the abscissa. Parameters are the same as in fig. 4.

to minimize finite lattice effects. The values of the hole density at the critical temperature are given in the figure, below T_c these values change by less than 5% down to $T=0$. (In the absence of superconductivity the hole densities would approach the values $n=0.1$, 0.3, 0.5 and 0.7 for these values of the chemical potential.)

Figures 4 and 5 show the minimum quasi-particle energy obtained from numerical solution of eqs. (4) – (6) for various hole densities. In fig. 4 we vary the site energy ϵ_i on a single site, and in fig. 5 on two adjacent sites. It can be seen that the energy gap is depressed by site energy disorder, particularly when two adjacent site energies are varied. The coherence length for these cases, obtained from the average size of the pair wavefunction [4], ranges from 1.3 to 1.6 lattice spacings in the range of densities shown. It can be seen that a somewhat smaller disorder is needed to depress the energy gap as the density increases, as one would expect from the previous considerations and the form of the gap function, fig. 3. The relative depression of the energy gap decreases as the density increases, presumably due to the increase in coherence length with density.

In contrast, fig. 6 shows the effect of site disorder for an attractive Hubbard model. As expected, site disorder has essentially no effect in this model. Re-

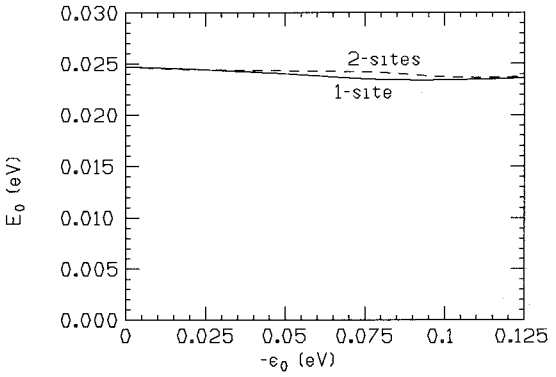

Fig. 6. Effect of on-site energy disorder in the attractive Hubbard model. $t=0.03$ eV, $U=-0.09$ eV, $n=0.35$. $T_c=150$ K. The coherence length is $\xi=0.44$ lattice spacings. The full and dashed lines show the effect of changing one and two neighboring site energies, as in figs. 4 and 5 respectively.

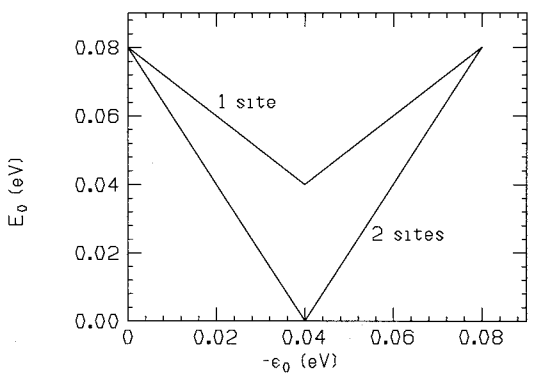

Fig. 7. Minimum quasi-particle excitation energy in the strong coupling limit for different site energies on one and two sites, as given by eqs. (21)–(23), for $\epsilon_b=0.08$ eV.

sults obtained for other densities show similar behavior.

The behavior found in figs. 4 and 5 can also be qualitatively understood from a strong coupling point of view. In the strong coupling limit of this model the single hole hopping amplitude is zero [9]. The pair binding energy $\epsilon_b=-2\mu$, with μ the chemical potential, arises from delocalization of the pair. Consider first the case of a potential well at a single site (zero), with energy $\epsilon_o<0$. The excitation energy corresponding to breaking up a pair and localizing one of the holes at sites 0 is

$$E_{ex}=\epsilon_o-2\mu=\epsilon_o+\epsilon_b, \tag{21}$$

and it decreases linearly with increasingly negative ϵ_o. For $|\epsilon_o|>\epsilon_b/2$, however, the ground state acquires one extra hole localized at site zero, and the lowest excitation energy is given by the cost in promoting this hole to another site:

$$E_{ex}=-\epsilon_o. \tag{22}$$

Similarly, if there are two sites with negative site energy ϵ_o, the difference in energy between having two holes localized at these sites and having them paired and delocalized is easily seen to be

$$E_{ex}=|2\epsilon_o+\epsilon_b|. \tag{23}$$

Figure 7 shows the behavior predicted by eqs. (21)–(23). It can be seen that it qualitatively resembles the results found in figs. 4 and 5.

4. Tunneling density of states

In a point contact tunneling experiment one measures the local density of states. With a scanning tunneling microscope and a tip of atomic dimensions it is in principle possible to obtain atomic resolution. Thus one can sample the site density of states

$$\rho_i(\omega)=\sum_n [\,|u_{ni}|^2\,\delta(\omega-E_n) + |v_{ni}|^2\,\delta(\omega+E_n)\,]. \tag{24}$$

We obtain an estimate of this quantity on our finite lattice by broadening the δ-functions to Lorentzians:

$$\rho_i(\omega)\approx\frac{\Gamma}{\pi}\sum_n \times\left[\frac{|u_{ni}|^2}{(\omega-E_n)^2+\Gamma^2}+\frac{|v_{ni}|^2}{(\omega+E_n)^2+\Gamma^2}\right]. \tag{25}$$

Figure 8 shows the behavior of this quantity for one case, at the impurity site and at a distant site. The eigenvector corresponding to the lowest eigenvalue in the BdG equations is localized around the site where the potential is lower, and this gives rise to a reduced gap in the local density of states in this region. Far away from the impurity site the density of states coincides with the results obtained for a uniform chain, as shown in fig. 8 (although differences

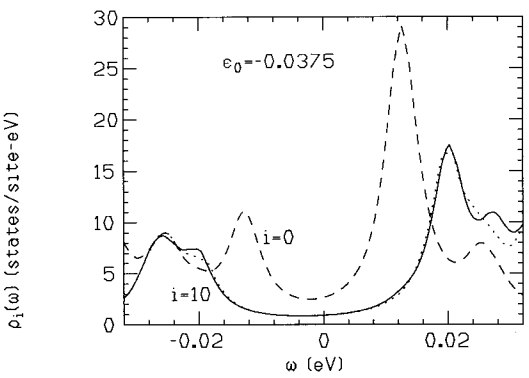

Fig. 8. Site density of states, eq. (24), in the one-dimensional chain. $n=0.32$, $\epsilon_o=-0.0375$, for sites $i=0$ (dashed line) and $i=10$ (full line). The dotted line gives the results for a uniform chain. $\Gamma=0.0032$ eV.

appear for energies higher than shown in the figure). The asymmetric shape of the tunneling characteristics has been discussed elsewhere [4].

Figure 9 shows the local density of states at the impurity site for various values of the local potential, both negative ((a)) and positive ((b)). In the case of negative potential the tunneling gap becomes progressively smaller, as expected; in the positive case instead the gap remains of constant size but the low energy spectral weight at the impurity site diminishes (and is transferred to high energy structure, not shown in fig. 9).

Calculations for other cases show similar behavior. If the tip in the tunneling probe does not have atomic dimensions one would measure an average of eq. (24) over a finite number of sites. Still, our results illustrate that tunneling measurements at different points in a sample can exhibit large variations due to variations in the local potential energy.

We have also evaluated the tunneling density of states for the attractive Hubbard model. Consistent with the results for the lowest eigenvalue found in fig. 6, the tunneling gap remains essentially unchanged at the impurity site (there is, however, some redistribution of the amplitude of the spectral weight even in this case).

5. Discussion

We have considered here the effect of non-magnetic disorder on the quasi-particle energy gap in the

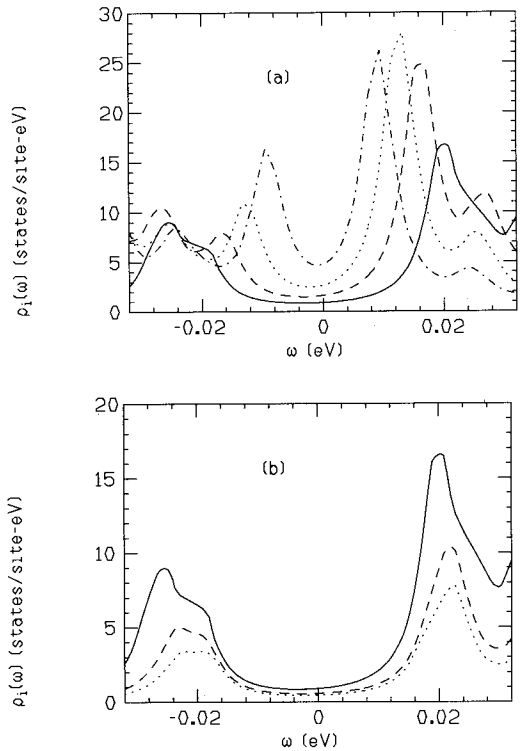

Fig. 9. Site density of states in the one-dimensional chain at the impurity site for (a) negative and (b) positive potential values. $n=0.32$, $\Gamma=0.0032$ eV. In (a), the solid, dashed, dotted and dash-dotted lines correspond to $\epsilon_o=0$, $\epsilon_o=-0.025$, $\epsilon_o=-0.0375$ and $\epsilon_o=-0.045$ respectively. In (b), the solid, dashed and dotted lines correspond to $\epsilon_o=0$, $\epsilon_o=0.025$ and $\epsilon_o=0.0375$ respectively.

model of hole superconductivity. For cases where potential fluctuations occur over distances larger than the coherence length the effect can be simply inferred from the dependence of the critical temperature on carrier concentration in this model [4]. More generally one may argue that the experimental observation that T_c varies strongly with carrier concentration [10] implies a sensitivity to potential fluctuations that change the local carrier density. For disorder on length scales of the order of or shorter than the coherence length, variations in the energy gap will occur due to the finite slope of the gap function. We studied this effect by numerical solution of the BdG equations for a case with finite gap slope and a case with zero gap slope (attractive Hubbard model). In the latter no change in the energy gap occurred on varying the on-site energy, while in the former the energy gap could be sharply depressed by on-site disorder. We also calculated the local density of

states and found that it exhibits a reduced gap in the region of depressed local potential. THe scale of disorder that gives rise to variations in the energy gap is of order $\Delta\epsilon = n_{max}D/2$ (eq. (15)). With $n_{max} \sim 0.2$ in high-T_c oxides and bandwidth D of order 0.5 eV or smaller, fluctuations of such magnitude are easily generated by impurities, defects or vacancies. Additionally, on approaching the surface of a sample one may expect changes in the local potential energy and hence different energy gaps from experimental techniques that are sensitive to bulk or surface regions.

The different sensitivity of the model of hole superconductivity and the attractive Hubbard model to site disorder can be understood as follows: in the former the strength of the attractive interaction (generated by Δt) depends on the character of the wavefunctions at the Fermi energy (whether bonding or antibonding) [5], while in the latter it does not. A change in on-site energies changes the strength of the interaction in the model of hole superconductivity due to the fact that for higher (lower) on-site energies the wavefunction at the Fermi energy becomes more bonding (antibonding) like. For the attractive Hubbard model a similar effect of disorder would be obtained by varying the local strength of the on-site attraction U_i. We have verified by numerical solution of the BdG equations that indeed such disorder in the attractive Hubbard model depresses the energy gap. In real materials the largest effect of non-magnetic disorder is likely to be to change the local potential energy rather than the strength of any electron–electron interation; thus we would expect real materials described by the model of hole superconductivity to be more sensitive to non-magnetic disorder than those described by attractive Hubbard or similar models, particularly if the slope of the gap function is large. Anderson's "theorem" [11] is not expected to hold in these non-weak-coupling situations.

There is another physical argument that can be invoked to understand the sensitivity of the mechanism of hole superconductivity to non-magnetic disorder: because in this model pairing originates in the *kinetic energy* gained by the paired holes,local potential fluctuations that tend to localize the hole around that region are naturally pair-breaking, as they reduce the kinetic energy. In contrast, in models where the pairing interaction originates in potential rather than kinetic energy such as the attractive Hubbard model, paired carriers can spend increasing time in the region of depressed local potential without suffering a reduction in their pairing energy, and thus such fluctuations are not strongly pair-breaking. This argument is only in appearance different from the one discussed above: the facts that in the model of hole superconductivity pairing originates in kinetic energy gain and that the gap function has a finite slope are intimately connected.

To conclude, one may argue that the considerations in this paper lend support to the applicability of the model of hole superconductivity to high-T_c oxides. Observation of energy gap variations and sensitivity to disorder [1–3] suggest that the gap function cannot be constant, and the possibility of higher angular momentum pairing immediately comes to mind; however, on the other hand various observations suggest that the superconducting state is isotropic *s*-wave rather than higher angular momentum [12]. These combined observations thus suggest that the gap function varies in directions perpendicular to constant energy surfaces and is constant on constant energy surfaces, as described by the model of hole superconductivity (eq. (10b)). Of course there could be other models that exhibit similar properties.

Acknowledgement

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