The Effect of Non-Magnetic Disorder on a D-Wave Superconductor in the Presence of a Van Hove Singularity

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We apply the Coherent Potential Approximation (CPA) to an extended Hubbard model to describe disordered superconductors with d-wave pairing. We discuss the pair-breaking effect caused by non-magnetic disorder in the presence of a Van Hove singularity. It is shown that singularities soften the suppression of a superconducting critical temperature.

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I. INTRODUCTION

According to the Anderson theorem, magnetic impurities which break the time reversal symmetry influence substantially the properties of a superconductor while non-magnetic ones have a negligible effect. However the original treatment of the influence of magnetic and non-magnetic impurities on superconductors had been applied to classic BCS superconductors \cite{1–3} with a uniform pairing potential; the problem has recently been reexamined for exotic superconductors with a short coherence length $\xi$ and with an anisotropic order parameter.

Gyoergy et al. and Moradian et al. \cite{4, 5} have shown that, even for s-wave superconductors, the theorem was only asymptotically true in the limit of large $\xi$, where the spatial fluctuations of the order parameter were small enough. On the other hand, for high temperature superconductors with d-wave symmetry of the order parameter modulated in $k$ space, the assumption of uniform order parameter has already been broken for a clean system. As a consequence of that, the non-magnetic impurities mixing wave vectors $k$ of the pairing potential $\Delta_k$ act on the superconductivity in a similar way as the magnetic ones, leading to a pair breaking effect \cite{6–15}.

Another important feature of high temperature superconductors is connected with singularities in the density of states. Here, the distance between the chemical potential and Van Hove singularity has been found to be relatively small \cite{16–19}. This has led to the formulation of the Van Hove scenario for high temperature superconductors, which says that an optimal critical temperature is reached when the chemical potential $\mu$ passes through the Van Hove singularity $E_v$ in the normal density of states \cite{19, 20}. However, doping with charge carriers not only changes the density in the system but also smears the den-
sity of states, eliminating its singularities and, especially for anisotropic superconductors, simultaneously introducing the electron pair–breaking phenomenon [6, 12, 13].

II. THE MODEL AND APPROXIMATIONS

We start from the single band Hubbard model with an attractive extended interaction, which is described by the following Hamiltonian [21]:

\[
H = \sum_{ij, \sigma} t_{ij} c_{i, \sigma}^\dagger c_{j, \sigma}^\phantom{\dagger} + \frac{1}{2} \sum_{ij} U_{ij} n_i n_j - \sum_i (\mu - \varepsilon_i)n_i .
\]

(1)

In the above \( n_i = n_{i\uparrow} + n_{i\downarrow} \) is the charge on the site labeled \( i \), \( \mu \) is the chemical potential. Disorder is introduced into the problem by allowing the local site energy \( \varepsilon_i \) to vary randomly from site to site, \( c_{i, \sigma}^\dagger \) and \( c_{i, \sigma}^\phantom{\dagger} \) are the Fermion creation and annihilation operators for an electron on site \( i \) with spin \( \sigma \), \( t_{ij} \) is the amplitude for hopping from site \( j \) to site \( i \), and, finally, \( U_{ij} \) is the attractive interaction (\( U_{ij} < 0 \)), between electrons on neighbour sites \( (i \neq j) \).

Here we will assume, for simplicity, that the random site energy \( \varepsilon_i \) has a uniform distribution \( \varepsilon_i \in [-\delta/2, \delta/2] \). Following the usual way, we shall apply the Coherent Potential Approximation (CPA), meaning that the coherent potential \( \Sigma(E) = \Sigma(i, i; E) \) [11, 12, 15], in a site approximation, is defined by the zero value of an averaged t-matrix \( T(i, i; E) \):

\[
< T_\alpha(i, i; E) > = \sum_\alpha P_\alpha T_\alpha(i, i; E)
\]

\[
= \langle (V_\alpha - \Sigma^\sigma(E))(1 - [V_\alpha - \Sigma(E)]G(i, i; E))^{-1}\rangle = 0 ,
\]

where \( \alpha \in [1, 2, ..., N] \) specifies the site energy occupation, \( \varepsilon_i \), of the lattice site \( i \) with equal probability \( P_\alpha = 1/N \).

Apart from the examined disorder Eq. (1) has on site character, the disordered potential \( V_\alpha \), and consequently the coherent potential \( \Sigma(E) \), have their diagonal representation:

\[
V_\alpha = \begin{bmatrix} \varepsilon_i & 0 \\ 0 & -\varepsilon_i \end{bmatrix} , \quad \Sigma(E) = \begin{bmatrix} \Sigma_{11}(E) & 0 \\ 0 & \Sigma_{22}(E) \end{bmatrix} .
\]

(3)

In the limit of a long coherence length \( \xi \), both types of fluctuations, in phase [22, 23] as well as in amplitude [24], are negligible. Thus staying in this limit one can use the constant bond approximation [12, 15]:

\[
|\Delta_{ij}| \rightarrow |\Delta_{ij}| = \Delta_0 \quad \text{for all nearest neighbour sites } i, j.
\]

(4)

Thus the Fourier transform in 2D k-space of the d-wave pairing potential \( \Delta_{ij} \) and the hopping integral \( t_{ij} \) can be written as:

\[
\Delta_k = \Delta_0 \eta_k/2 , \quad \eta_k = 2(\cos k_x - \cos k_y) ,
\]

(5)
\[ \epsilon_k = t \gamma_k, \quad \gamma_k = 2(\cos k_x + \cos k_y). \]  

Then the averaged Green function \( \overline{G}(i, i; E) \) can be expressed as follows:

\[
\overline{G}(i, i; E) = \frac{1}{N} \sum_k \overline{G}(k; E) = \frac{1}{N} \sum_k \left[ \frac{E + \epsilon_k + \mu - \Sigma_{11}(E)}{\overline{\Sigma}_k}, \quad \frac{E + \epsilon_k - \mu - \Sigma_{22}(E)}{\overline{\Sigma}_k} \right].
\]

The set of equations (2), (3), and (7) ought to be solved together with the corresponding formulae for the chemical potential \( \mu \), which satisfies the following:

\[
n = -\frac{2}{\pi} \int_{-\infty}^{\infty} dE \text{Im} \overline{G}_{11}(i, i; E) \frac{1}{1 + \exp \beta E},
\]

where \( n \) is the number of electrons per lattice site, and the gap equation for \( \overline{\Delta}_{ij} \) is

\[
\overline{\Delta}_{ij} = \frac{U_{ij}}{\pi} \int_{-\infty}^{\infty} dE \text{Im} \overline{G}_{12}(i, j; E) \frac{1}{1 + \exp \beta E},
\]

where \( \beta \) is the inverse of temperature \( \beta = 1/k_B T \), \( k_B \) denotes the Boltzmann constant.

III. CRITICAL TEMPERATURE IN THE PRESENCE OF DISORDER AND A VAN HOVE SINGULARITY

In this section we will apply the derived formulae Eqs. (7–9) to find the simultaneous effects of disorder and a Van Hove singularity. It should be noted that the final effect is not clear, because the disorder usual reduces the critical temperature while the singularity enhances it. The interplay of these two effects for a weak disorder should be taken into account with equal footing and treated self-consistently, because disorder influences the density of states smearing any singularities.

The linearized gap equation (7) in the Hartree-Fock-Gorkov approximation [11, 21] is

\[
1 = \frac{|U_{ij}|}{\pi} \int_{-\infty}^{\infty} dE \tanh \left( \frac{E}{2k_B T_c} \right) \text{Im} \frac{\overline{G}_{11}(E)}{2E - \text{Tr} \Sigma(E)},
\]

where \( T_c \) is the critical temperature. \( \overline{G}_{11}(E) \) is an averaged electron Green function which defines the weighted density of states of the d-wave electron states \( \overline{N}_d(E) \) [12]:

\[
\overline{N}_d(E) = -\frac{1}{\pi} \text{Im} \overline{G}_{11}(E) = -\frac{1}{\pi N} \sum_k \text{Im} \frac{\eta_k^2}{4 E - \Sigma_{11}(E)} \frac{1}{E - \Sigma_{11}(E) - \epsilon_k + \mu}.
\]

Note that \( N_d(E) \) differs from a simple electron density of states (DOS) \( N(E) \):

\[
\overline{N}(E) = -\frac{1}{\pi} \text{Im} \overline{G}_{11}(E) = -\frac{1}{\pi N} \sum_k \text{Im} \frac{1}{E - \Sigma_{11}(E) - \epsilon_k + \mu}.
\]
by an additional weight $\eta_k$ in the above integral.

In Fig. 1 we show the weighted d-wave density of states $N_d(E)$ in the presence of disorder for various $\delta (\varepsilon_i \in [-\delta/2, \delta/2])$ and the electron density of states $N(E)$ for the clean system. It is clear that the weighted density of states $N_d(E) \sim -\ln(E)$ for the clean system have a logarithmic behaviour similar to $N(E)$ around the Van Hove singularity at $E_v = 0$, satisfying the criterion of the Van Hove scenario [25]. On the other hand, for disordered systems $N_d(E)$ becomes a smooth function (Fig. 1) with a maximum at $E = 0$. Gonczarek and Mulak [26] investigated various types of such maxima, showing that they also enhance the critical temperature $T_c$ effectively.

Note also, that the Van Hove scenario works better for superconductors with a relatively small transition temperature $T_c$ (which corresponds to a small interaction parameter $U_{ij}$). This can be easily seen in the following function:

$$F(T_c, E) = \frac{2T_c}{(E)} \tanh \left( \frac{E}{2T_c} \right),$$  \hspace{1cm} (13)

which is present in the gap equation (10) for a clean system, $\Sigma_{11}(E)=0$. This can be interpreted as an effect leading to a natural cut-off $E_c$ around the chemical potential $\mu = E_v = 0$ (Fig. 1(a)). If the temperature $T_c$ is small, then the function $F(T_c, E)$ is non-zero in the narrow range of energies around $\mu$ only. In fact in the limit $T_c \to 0$ it tends to the Dirac delta function ($F(T_c, E) \to \delta(E)$), and the cut-off is limited to the neighbourhood of the $E = \mu = 0$ point (Fig. 2).

Note that for finite $T_c$, $E_c \approx 2T_c$. Consequently, the logarithmic Van Hove singularity
in the density of states near $\mu$ has the form
\begin{equation}
N(E) \approx -N_0 \ln \left| \frac{E - \mu}{D} \right| ,
\end{equation}
and we get the Labbe-Bok formula for $T_c$ [20]:
\begin{equation}
T_c \sim \exp \left\{ -\frac{1}{\sqrt{|N_0 U|}} \right\} .
\end{equation}

In our case this effect is associated with a relative increase of \text{Im}$\Sigma_{11}$($E$) (Fig. 3), which can be referred to stronger non-elastic electron scattering. This is a pair breaking factor known from the Abrikosov-Gorkov pair breaking formula, formulated originally for magnetic and adapted for non-magnetic disorder [2, 12]:
\begin{equation}
\ln \left( \frac{T_c}{T_{c0}} \right) = \psi \left( \frac{1}{2} \right) - \psi \left( \frac{1}{2} + \rho_c \right),
\end{equation}
where $\rho_c = |\Sigma_{11}(0)|/(2\pi T_c)$ is a pair-breaking parameter and $T_{c0}$ is the critical temperature of a clean superconductor.

It is interesting that the most efficient pair breaking phenomenon should be present for the maximum value of \text{Im}$\Sigma_{11}(E)$ at $E = 0$ and coincides with the maximum of $N_d(E)$. For a disordered case, Eq. (10) can be rewritten in terms of Matsubara frequencies $\omega_n = \frac{\pi}{\beta}(2n + 1)$ as
\begin{equation}
1 = \frac{|U|}{2k_B T_c} \sum_n \frac{\overline{G^{t}_{11}(i\omega_n)}}{2i\omega_n - \text{Tr} \Sigma(i\omega_n)} .
\end{equation}
FIG. 3: Imaginary part of the self energy $-\text{Im}\Sigma(E)$ for various strengths of the disorder $\delta$.

FIG. 4: (a) $N_d(i\omega)$ versus $\omega$ : full line ‘1’, the fitting curve $c/(\omega + b)$ for $c = 0.95$ and $b = 0.35$ : dashed line ‘2’. (b) $T_c$ versus $|\Sigma|$ : ‘1’ the standard Abrikosov-Gorkov formula (Eq. (16)) , ‘2’ results obtained from Eq. (19), ‘3’ results from numerical solving of the gap equation (Eq. (10)) for $U = -2t$.

In Fig. 4(a) we show the density $N_d(i\omega) = -\text{Im}G(i\omega_n)/\pi$ versus the imaginary frequency $\omega$, where $E = i\omega$ for the chemical potential at the Van Hove singularity $\mu = E_v = 0$ (for $n=1$, Fig. 1).

In the standard treatments [2, 6, 12], $N(i\omega)$ or $N_d(i\omega)$ was assumed to be constant. However in the present case, due to the Van Hove singularity, it depends strongly on $\omega$. The corresponding weighted density $N_d(i\omega)$ can be roughly approximated by a simple formula

$$N_d(i\omega) = \frac{c}{\omega + b},$$

(18)
where $c$ and $b$ are constants (Fig. 4(a)). Approximating also $\Sigma(i\omega) = -i|\Sigma_0|\text{sgn}(\omega)$, we get from Eq. (17) the analytic pair-breaking formula [15]:

$$\psi\left(\frac{1}{2}\right) - \psi\left(\frac{1}{2} + \frac{b}{2\pi T_c}\right) = \psi\left(\frac{1}{2} + \rho_c\right) - \psi\left(\frac{1}{2} + \rho_c + \frac{b}{2\pi T_c}\right),$$

(19)

where $\rho_c = |\Sigma_0|/(2\pi T_c)$ is again a pair-breaking parameter.

Note that for large $b$ ($b \to \infty$) Eq. (19) transforms into the standard Abrikosov-Gorkov equation (Eq. (16)). Fig. 4(b) presents the comparison between these analytic formulae as well as the numerical results obtained from the gap equation (Eq. (10)). Both analytic and numerical results (Fig. 4(b)) show that the Van Hove singularity makes the superconducting state more robust in the presence of disorder.

IV. CONCLUSIONS

Analyzing the effect of disorder on a disordered d-wave superconductor, we have found the additional influence of the Van Hove singularity. In the presence of a weak disorder $\delta < t$ we observe only a small change of the weighted density of states $N_d$ (Fig. 1). At the same time we observe the rapid degradation of $T_c$, which is connected with the pair-breaking effect (Eqs. (17,19)). Interestingly, the Van Hove singularity modifies the standard Abrikosov-Gorkov formula, originally obtained for a constant density of states, increasing the critical value of $|\Sigma_0|$, which destroys the superconducting phase (Fig. 4(b)). The analytic formula (Eq. (19)) obtained for this simple assumption was the principal result of the present paper. The final result of weaker pair-breaking is in qualitative agreement with the experimental results on Zn substitutions [27–29] and other numerical investigations [7, 12, 15], which treated disorder and the Van Hove singularity using a self-consistent procedure.

It should be noted, however, that our treatment neglected order parameter fluctuations which can occur in the strong coupling limit [22, 23]. Such fluctuations have also been found to make the mechanism of $T_c$ suppression by disorder [8, 9] less efficient. Similar results of a weaker effect of disorder on superconductivity has been also obtained, without involving the Van Hove singularity, by the assumption of an anisotropic character of impurity scatterers [13].

References