Van Hove Singularity and Superconductivity in Disordered 

\textbf{Sr}_2\textbf{RuO}_4

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Abstract

On the basis of a simple model we analyse the influence of disorder on critical temperature $T_C$ in p–wave superconductors. The disorder is treated by means of the Coherent Potential Approximation (CPA) and we focus our attention on the effect of a van Hove singularity near Fermi energy $E_F$. For the appropriate values of its parameters our model reproduces the experimentally found behaviour of \textbf{Sr}_2\textbf{RuO}_4.

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I. INTRODUCTION

The perovskite structure of Strontium Ruthenate, Sr$_2$RuO$_4$ is very similar to that of HTS copper oxides. However, its superconducting transition temperature $T_C$ is relatively low ($T_C \approx 1$ K) [1]. Nevertheless, recent reports indicate that its Cooper pairs are not of the usual s–wave symmetry. In fact they suggest that this material features triplet pairing and is a superconducting analogue of the $^3$He superfluid system [1-4]. Clearly, the possibility of exotic pairing engenders interest in the effects of disorder on the superconducting properties. Moreover, studies of the electronic structure [2,3] have identified an extended van Hove singularity close to the Fermi energy $E_F$, and therefore one may wonder whether the van Hove scenario could lead to a rise in $T_C$ with doping. Evidently, since doping the system always increases the disorder one should investigate both aspects simultaneously.

II. THE MODEL

We base our discussion on the extended negative U Hubbard Hamiltonian:

$$H = \sum_{i\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + \frac{1}{2} \sum_{ij} U_{ij} \hat{n}_i \hat{n}_j - \sum_i (\mu - \varepsilon_i) \hat{n}_i,$$

where $\hat{n}_i = \hat{n}_{i\uparrow} + \hat{n}_{i\downarrow}$ and $\hat{n}_{i\sigma}$ is the usual, site occupational number operator $c^\dagger_{i\sigma} c_{i\sigma}$. Evidently the above $\hat{n}_i$ is the charge operator on site labelled $i$, $\mu$ is the chemical potential, which at $T = 0$ is equal to Fermi energy $E_F$. Disorder is introduced into the problem by allowing the local site energy $\varepsilon_i$ to vary randomly from site to site. Finally, $c^\dagger_{i\sigma}$ and $c_{i\sigma}$ 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 $U_{ij}$ is the attractive interaction ($i \neq j$) which causes superconductivity.

In the Hartree-Fock-Gorkov approximation the equation for the Green’s function $G(l, j; \omega_n)$, corresponding to the Hamiltonian in Eq. 1, is given by:

$$\sum_l \begin{bmatrix} (\omega_n + \mu - \varepsilon_i) \delta_{il} + t_{il} & \Delta_{il} \\ \Delta^*_{il} & (\omega_n - \mu + \varepsilon) \delta_{il} - t_{il} \end{bmatrix} G(l, j; i\omega_n) = \delta_{ij},$$

(2)
where $\omega_n$ is Matsubara frequency. Let us define the random potential $V^{\varepsilon_i}$ by:

$$V^{\varepsilon_i} = \begin{bmatrix} \varepsilon_i & 0 \\ 0 & -\varepsilon_i \end{bmatrix},$$

(3)

where $\varepsilon_i$ is uniformly distributed on the energy interval $[-\delta^2, \delta^2]$. The Green’s function for an impurity, described by $V^{\varepsilon_i}$ in Eq. 3, embedded in the medium, described by $\Sigma(\omega_n)$ is given by:

$$G^{\varepsilon_i}(i, i, \omega_n) = \{1 - G^C(i, i, \omega_n)[V^{\varepsilon_i} - \Sigma(\omega_n)]\}^{-1} G^C(i, i, \omega_n),$$

(4)

Following the usual CPA procedure we demand that the coherent potential Greens function $G^C(i, i; \omega_n) = (\omega_n - \epsilon_k - \Sigma(\omega_n))^{-1}$ satisfy the relation:

$$G^C(i, i, \omega_n) = \langle G^{\varepsilon_i}(i, i, \omega_n) \rangle = \frac{1}{\delta} \int_{-\delta/2}^{\delta/2} \exp(i \varepsilon_i) G^{\varepsilon_i}(i, i, \omega_n).$$

(5)

Evidently, Eq. 5 completely determines, that is to say can be solved for, $\Sigma(\omega_n)$.

Let us now proceed further with the CPA strategy [5] and determine the averaged Greens function matrix $\langle G(i, j; \omega_n) \rangle$ subject to the self consistency conditions:

$$\overline{\Sigma}_{ij} = |U_{ij}| \frac{1}{\beta} \sum_n e^{i\omega_n \eta} \langle G_{12}(i, j; \omega_n) \rangle, \quad \overline{\pi} = \frac{2}{\beta} \sum_n e^{i\omega_n \eta} \langle G_{11}(i, i; \omega_n) \rangle.$$  

(6)

In this paper we assumed nearest neighbour electron hopping and pairing on a two dimensional lattice. In Figure 1a and b we have presented Fermi surfaces for $n = 0.55$ and $n = 1$ respectively. The latter case correspond to the situation, where the Fermi Energy, $E_F$, is located exactly at the van Hove singularity.

### III. CRITICAL TEMPERATURE AND RESIDUAL RESISTIVITY

The linearised gap equation for the critical temperature $T_C$ of p-wave superconducting phase transition reads as follows [6]:

$$1 = |U| T_C \sum_n e^{i\omega_n \eta} \frac{1}{N} \sum_{\vec{k}} \frac{2(sin k_x)^2}{(\omega_n - \epsilon_{\vec{k}} - \Sigma_{11}(\omega_n))(\omega_n + \epsilon_{\vec{k}} - \Sigma_{22}(\omega_n))}.$$  

(7)
A useful measure of disorder is the resistivity $\rho$. Thus we shall study the relationship between $\rho$ and $T_C$. The Residual resistivity $\rho$ for low temperature can be obtained from the Kubo–Greenwood formula. For the disordered two dimensional systems at hand [7]:

$$\rho = \left\{ \frac{2e^2}{\pi \hbar c N} \sum_k 4(\sin k_x)^2 t^2 \left[ \text{Im} G_{11}^{C}(\mathbf{k}, 0) \right]^2 \right\}^{-1}, \quad (8)$$

where $e$ is the electron charge, $\hbar$ is Plank constant and $c$ is the distance between RuO$_2$ planes.

In short, we have solved the CPA equations (Eqs. 4,5) for various system parameters (Eq. 1) and calculated both $T_C$ and residual resistivity $\rho$.

To illustrate how effective a van Hove singularity can be in raising $T_C$, in Fig. 2a we present $T_C$, calculated for clean systems and normalised to its maximal value $T_C^{\text{max}}$, versus band filling $n$ for various values of $U/t$. Clearly, $T_C$ is peaked at $n = 1$, where the Fermi energy $E_F$ is exactly at the van Hove singularity. For small enough interaction $U$ it is enlarged by a factor of 7. Going further we turn to our results for the disordered case. Thus, in Fig. 2b, we plotted $T_C$ versus residual resistivity $\rho$ as calculated by the CPA procedure described above. The parameters $U/t = -0.702$ as well as band filling $n = 0.55$ were chosen so that the $T_C$ vs. $\rho$ curve reproduce the experiments [1]. Unlike the Born approximation limit, the CPA residual resistivity is dependent on the strength of disordered potential, $\delta$, nonlinearly. This is illustrated in Fig. 3a, where the different curves correspond to different band fillings $n$. The pronounced nonlinearity for $n=1$ is due to a van Hove singularity being near $E_F$. As shown in Fig. 3b this give rise to an interesting upturn as $\rho \to 0$ in the $T_C$ vs. $\rho$ plot.

IV. REMARKS AND CONCLUSIONS

Our results confirm that, similarly to d–wave superconductors [5], in the case of p–wave pairing the critical temperature $T_C$ is very sensitive function of nonmagnetic diagonal disorder. Nevertheless, they suggest that in Sr$_2$RuO$_4$ doping could lead to higher value of
critical temperature $T_C$. Here we used uniform distribution of site energy levels $\varepsilon_i$ as the simplest model of disorder. Clearly further study of the problem would include a more sophisticated impurity model, and more realistic band structure.

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FIGURES

FIG. 1. Fermi surfaces for the one band electron structure with nearest neighbour hoping:
\[ \epsilon_k = -2t(\cos k_x + \cos k_y), \]
and two different band fillings: \( n = 0.55 \) (a), \( n = 1.00 \) (b).

FIG. 2. (a) \( T_C \) for the clean system versus band filling \( n \) for various interactions \( U \). (b) \( T_C \) versus residual resistivity fitted for Sr\(_2\)RuO\(_4\). The diamonds are the data of Ref. [1].

FIG. 3. (a) Residual resistivity versus strength of disordered potential \( \delta (\epsilon_i \in [-\frac{\delta}{2}, \frac{\delta}{2}]) \) for various band fillings \( n \). (b) \( T_C \) versus residual resistivity for various band fillings \( n \).
[Fig. 1] Fermi surfaces for the one band electron structure with nearest neighbour hoping: $\varepsilon_k = -2t(\cos k_x + \cos k_y)$, and two different band fillings: $n = 0.55$ (a), $n = 1.00$ (b).
[Fig. 2] (a) $T_C$ for the clean system versus band filling $n$ for various interactions $U$. (b) $T_C$ versus residual resistivity fitted for $Sr_2RuO_4$. The diamonds are the data of Ref. [1].
[Fig. 3] (a) Residual resistivity versus strength of disordered potential $\delta$ ($\epsilon_i \in (-\delta, \delta)$) for various band fillings $n$.  (b) $T_C$ versus residual resistivity for various band fillings $n$. 