Proceedings of the European Conference "Physics of Magnetism '99", Poznań 1999

VAN HOVE SINGULARITY AND SUPERCONDUCTIVITY IN DISORDERED Sr_2RuO_4

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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 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 Sr_2RuO_4.

PACS numbers: 74.62.Dh, 74.25.Dw, 74.25.Fy

1. Introduction

The perovskite structure of strontium ruthenate, Sr_2RuO_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.

2. The model

We base our discussion on the extended negative U Hubbard Hamiltonian

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

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 a site labelled i, μ 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 ε_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 σ, 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 function $\boldsymbol{G}(i,j;\mathrm{i}\omega_n)$, corresponding to the Hamiltonian in Eq. (1), is given by

$$\sum_l \begin{bmatrix} (\mathrm{i}\omega_n + \mu - \varepsilon_i)\delta_{il} + t_{il} & \Delta_{il} \\ \Delta^*_{il} & (\mathrm{i}\omega_n - \mu + \varepsilon_i)\delta_{il} - t_{il} \end{bmatrix} \boldsymbol{G}(l,j;\mathrm{i}\omega_n) = \mathbf{1}\delta_{ij}, \quad (2)$$

where ω_n is Matsubara frequency. Let us define the random potential $\boldsymbol{V}^{\varepsilon_i}$ by

$$\boldsymbol{V}^{\varepsilon_i} = \begin{bmatrix} \varepsilon_i & 0 \\ 0 & -\varepsilon_i \end{bmatrix}, \quad (3)$$

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

$$\boldsymbol{G}^{\varepsilon_i}(i,i,\mathrm{i}\omega_n) = \{\mathbf{1} - \boldsymbol{G}^{\mathrm{c}}(i,i,\mathrm{i}\omega_n)[\boldsymbol{V}^{\varepsilon_i} - \boldsymbol{\Sigma}(\mathrm{i}\omega_n)]\}^{-1}\boldsymbol{G}^{\mathrm{c}}(i,i,\mathrm{i}\omega_n). \quad (4)$$

Following the usual coherent potential approximation (CPA) procedure we demand that the coherent potential Green function $\boldsymbol{G}^{\mathrm{c}}(i,i;\mathrm{i}\omega_n) = \boldsymbol{G}^0(i,i;\mathrm{i}\omega_n\mathbf{1} - \boldsymbol{\Sigma}(\mathrm{i}\omega_n))$, where $\boldsymbol{G}^0(i,i,\mathrm{i}\omega_n)$ is the Green function for the clean system with $\varepsilon_i = 0$ for every site i, satisfies the following relation:

$$\boldsymbol{G}^{\mathrm{c}}(i,i,\mathrm{i}\omega_n) = \langle \boldsymbol{G}^{\varepsilon_i}(i,i,\mathrm{i}\omega_n)\rangle = \frac{1}{\delta}\int_{-\delta/2}^{\delta/2} \mathrm{d}\varepsilon_i \, \boldsymbol{G}^{\varepsilon_i}(i,i,\mathrm{i}\omega_n). \quad (5)$$

Evidently, Eq. (5) completely determines that it can be solved for $\boldsymbol{\Sigma}(\mathrm{i}\omega_n)$.

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

$$\overline{\Delta}_{ij} = |U_{ij}|\frac{1}{\beta}\sum_n \exp(\mathrm{i}\omega_n\eta)\langle G_{12}(i,j;\mathrm{i}\omega_n)\rangle, \quad \overline{n} = \frac{2}{\beta}\sum_n \exp(\mathrm{i}\omega_n\eta)\langle G_{11}(i,i;\mathrm{i}\omega_n)\rangle. \quad (6)$$

In this paper we assumed nearest neighbour electron hopping and pairing on a two-dimensional lattice. In Fig. 1a and b we have presented Fermi surfaces

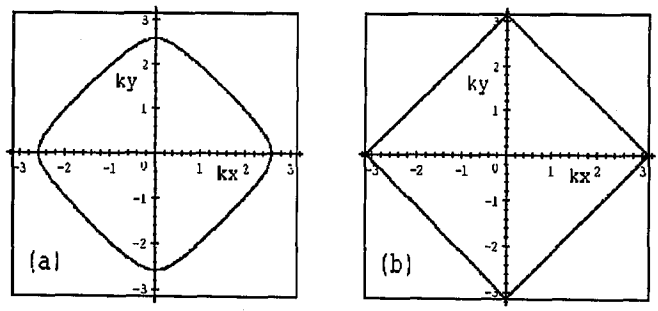

Fig. 1. Fermi surfaces for the one-band electron structure with nearest neighbour hopping: $\epsilon_k = -2t(\cos k_x + \cos k_y)$, and two different band fillings: $n = 0.55$ (a), $n = 1.00$ (b).

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.

3. 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]:

$$1 = \frac{|U|T_c}{N} \sum_{n,k} \exp(i\omega_n \eta) \frac{2(\sin k_x)^2}{[i\omega_n - \epsilon_k + \mu - \Sigma_{11}(i\omega_n)][i\omega_n + \epsilon_k - \mu - \Sigma_{22}(i\omega_n)]}. \quad (7)$$

A useful measure of disorder is the resistivity ρ. Thus we shall study the relationship between ρ and T_c. The residual resistivity ρ for low temperature can be obtained from the Kubo–Greenwood formula. For the disordered two-dimensional systems at hand [7]

$$\rho = \left\{ 2\frac{e^2}{\pi\hbar c} \frac{1}{N} \sum_{k} 4(\sin k_x)^2 t^2 [\mathrm{Im} G^c_{11}(k, 0)]^2 \right\}^{-1}, \quad (8)$$

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 ρ.

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^{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 a 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 ρ 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. ρ curve reproduces the experiments [1]. Unlike the Born approximation limit, the CPA residual resistivity is dependent on the strength of disordered potential, δ, nonlinearly. This is illustrated in Fig. 3a, where the different curves correspond

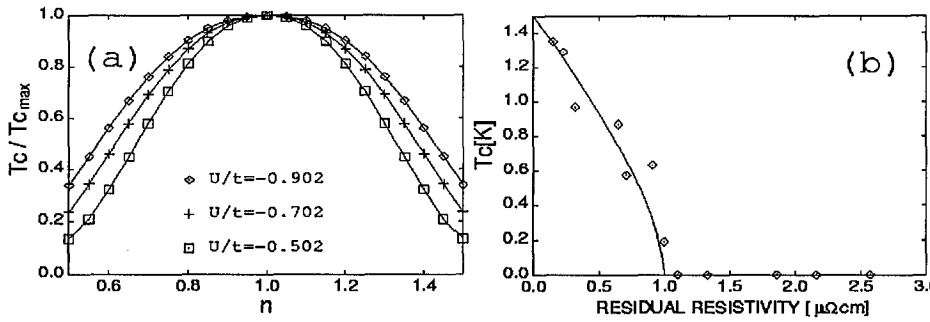

Fig. 2. (a) T_c for the clean system vs. band filling n for various interactions U. (b) T_c vs. residual resistivity fitted for Sr_2RuO_4. The diamonds are the data of Ref. [1].

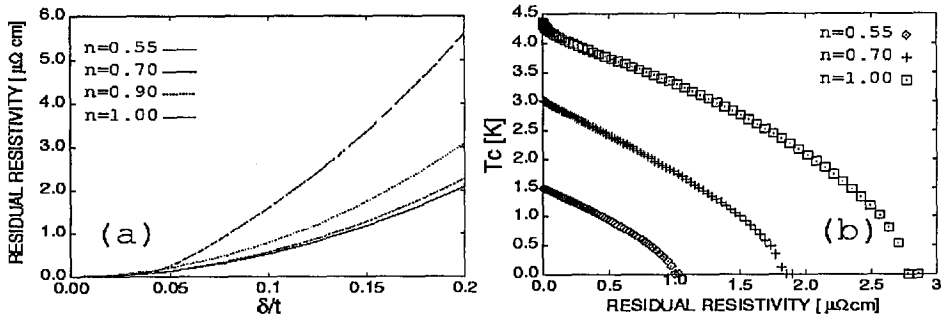

Fig. 3. (*a*) Residual resistivity vs. strength of disordered potential $\delta(\epsilon_i \in [-\delta/2, \delta/2])$ for various band fillings n. (b) T_c vs. residual resistivity for various band fillings n.

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 gives rise to an interesting upturn as $\rho \to 0$ in the T_c vs. ρ plot.

4. Remarks and conclusions

Our results confirm that, similarly to *d*-wave superconductors [5], in the case of *p*-wave paring the critical temperature T_c is a very sensitive function of nonmagnetic diagonal disorder. Nevertheless, they suggest that in Sr_2RuO_4 doping could lead to a higher value of critical temperature T_c. Here we used uniform distribution of site energy levels ε_i as the simplest model of disorder. Clearly a further study of the problem would include a more sophisticated impurity model, and a more realistic band structure.

Acknowledgments

The authors would like to thank Dr A.M. Martin, Prof. K.I. Wysokiński for helpful discussions and Prof. A.P. Mackenzie for the experimental data. This work has been partially supported by the Committee for Scientific Research grant No. 2P03B05015 and EPSRC grant No. GR/L22454.

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