A microscopic theory of layered high T_c superconductors

A K RAJAGOPAL[†], S S JHA[*] and S D MAHANTI[‡]

*Tata Institute of Fundamental Research, Homi Bhabha Road, Bombay 400 005, India
†Naval Research Laboratory, Washington D C 20375, USA
‡Department of Physics and Astronomy, Michigan State University, East Lansing, Michigan 48824, USA

Abstract. A generalized Gorkov formalism of superconductivity in a layered system with non-primitive lattice structure is given. This is used to justify theoretically a model of high T_c oxide superconductors proposed recently by one of us (SSJ). A numerical estimation of the critical temperature as a function of the number of superconducting layers is mentioned.

Keywords. Gorkov formalism; microscopic theory; layered superconductors; non-primitive lattice structure.

1. Introduction

In order to develop a generalized BCS pairing theory for the new high T_c layered superconducting compounds, whose crystal structures are complicated orthorhombic and tetragonal non-primitive lattices with several atoms in the unit cell (Yvon and Francois 1989) we need to first set up a complete set of band functions. From these a layer representation is developed. These are non-orthogonal between different layers and overcomplete, but are very useful in the formal conceptualization of the layer model of superconductivity proposed recently by one of us (Jha 1987, 1988, 1989). The many-body theory using such states can then be used to develop the Gorkov formalism of superconductivity. In the interest of brevity, we shall discuss in this paper only the equation for the critical temperature in such a theory in the second section. This general scheme is then shown to reduce to the linearized gap equation developed by Jha (1987) under certain conditions, which seem to be appropriate for the new high T_c systems. Details of this formulation will be published separately (Rajagopal and Jha 1991). In the third section we use this to show how one can estimate T_c as a function of the number of inequivalent superconducting layers in the system. In the final section, a brief summary of the scope of this work is given.

2. The critical temperatures in the layered high T_c systems

In terms of the layer band functions, $\phi_{b_j k}(\mathbf{r}\,|\,j)$, which are the eigenfunctions of a reduced hamiltonian for only one layer j per unit cell so that b_j is the band index appropriate to the layer j and $\mathbf{k}$ is a 3-D wave vector arising from the full 3-D lattice periodicity of the jth layer, and the associated layer band energy, $\varepsilon_{b_j k}$, even the one particle hamiltonian is of the form

$$\hat{\mathscr{H}}_0 = \frac{1}{S}\sum_{\sigma}\sum_{jb_j j'b'_{j'}}\int_{\mathrm{IBZ}}\frac{\mathrm{d}^3 k}{(2\pi)^3}\langle jb_j\mathbf{k}|\mathscr{H}_0|j'b'_{j'}\mathbf{k}\rangle C^{\dagger}_{jb_j k\sigma}C_{j'b'_{j'}k\sigma} \tag{1}$$

Here $C^{\dagger}$, C are the usual creation, annihilation operators for the carriers, s is the total number of layers in the unit cell ($j = 1, \cdots s$). Equation (1) contains interlayer "hopping" or "tunneling" terms for the charge carriers to go from one layer to another. In fact, we have

$$\langle jb_j \mathbf{k} | \mathscr{H}_0 | j'b'_{j'} \mathbf{k} \rangle = \varepsilon_{b_j \mathbf{k}} \langle b'_j \mathbf{k} | b_j \mathbf{k} \rangle + \langle b_j \mathbf{k} | \tilde{V}_j | b_j \mathbf{k} \rangle$$

$$= \sum_b \langle b'_{j'} \mathbf{k} | b\mathbf{k} \rangle E_{b\mathbf{k}} \langle b\mathbf{k} | b_j \mathbf{k} \rangle, \tag{2}$$

where $\tilde{V}_j$ is the periodic potential arising from all other layers other than the jth layer. The second equation in (2) relates the layer band energies and matrix elements to the full 3-D band energies $E_{b\mathbf{k}}$ and the overlaps of the layer-to-layer wavefunctions as well as layer-to-crystal band functions. For brevity we introduce the notation $\alpha \equiv j, b_j$. The gap equations in the linearized form needed for discussing the critical temperature T_c is then defined by the following equations:

$$\Delta_{\mathbf{k}}(\beta\alpha) \equiv \sum_{n_1 = -\infty}^{\infty} \Omega \int_{\mathrm{IBZ}} \frac{d^3 k'}{(2\pi)^3} \sum_{\alpha',\alpha_1} \langle \beta\mathbf{k}, \alpha - \mathbf{k} | V_{\mathrm{int}} | \alpha'_1 - \mathbf{k}', \alpha_1 k' \rangle$$

$$\times F_{\mathbf{k}'}(\alpha, \alpha'_1; \omega_{n_1}), \tag{3}$$

$$\sum_{\alpha\alpha'} [(\omega_n + \mu - \varepsilon_{\alpha\mathbf{k}}) \langle \beta\mathbf{k} | \alpha\mathbf{k} \rangle - \langle \beta\mathbf{k} | \tilde{V}_\alpha | \alpha\mathbf{k} \rangle] \tilde{\mathscr{G}}_{\mathbf{k}}^{(0)}(\alpha\alpha'; \omega_n) \langle \alpha'\mathbf{k} | \beta'\mathbf{k} \rangle$$

$$\cong \langle \beta\mathbf{k} | \beta'\mathbf{k} \rangle, \tag{4}$$

$$\sum_{\alpha\alpha'} [(-\omega_n + \mu - \varepsilon_{\alpha\mathbf{k}}) \langle \alpha\mathbf{k} | \beta\mathbf{k} \rangle - \langle \alpha\mathbf{k} | V_\alpha | \beta\mathbf{k} \rangle] \tilde{F}_{\mathbf{k}}^{\dagger}(\alpha\alpha'; \omega_n)$$

$$\cong \sum_{\alpha\alpha'} \Delta_{\mathbf{k}}^*(\beta\alpha) \tilde{\mathscr{G}}_{\mathbf{k}}^{(0)}(\alpha\alpha'; \omega_n) \langle \alpha'\mathbf{k} | \beta'\mathbf{k} \rangle. \tag{5}$$

The chemical potential μ is determined by the condition of the given total number of change carriers in the system

$$N_c = -\frac{i}{\tau} \sum_{n = -\infty}^{\infty} \sum_{\alpha\alpha'} \Omega \int_{\mathrm{IBZ}} \frac{d^3 k}{(2\pi)^3} \langle \alpha'\mathbf{k} | \alpha\mathbf{k} \rangle \tilde{\mathscr{G}}_{<\mathbf{k}}(\alpha\alpha'; \omega_n)$$

$$\omega_n = (2n + 1)\pi/\tau, \quad n = 0, \pm 1, \pm 2, \ldots, \tau = -i\beta, \beta = 1/k_B T. \tag{6}$$

Here $\Omega = abc$ is the volume of the unit cell, IBZ under the k-integrations indicate the first Brillouin zone integration. We have displayed these equations in their full glory to indicate the places where the various contributions arise. A variety of models can now be obtained based on a variety of approximations tailored to suit the system. Incidentally this theory reduces to the 3-D band scheme if we drop the layer indices and keep just the band indices and note that the overlaps become Kronecker deltas and $\varepsilon_{\alpha\mathbf{k}}$ are identified as band energies, $E_{b\mathbf{k}}$.

The gap parameters are in general of the form $\Delta_{\mathbf{k}}(\beta\alpha)$ indicating that there can be interlayer pairing possible and they obey the equations after some algebra

$$\Delta_{\mathbf{k}}(\beta\alpha) = \frac{-\Omega}{2} \int_{\mathrm{IBZ}} \frac{d^3 k'}{(2\pi)^3} \sum_{\alpha_1,\alpha_1} \langle \beta\mathbf{k}, \alpha - \mathbf{k} | V_{\mathrm{int}} | \alpha'_1 - \mathbf{k}', \alpha_1 k' \rangle$$

$$\times \left[\frac{\tanh \beta_c \xi_{\alpha'_1 \mathbf{k}'}/2 + \tanh \beta_c \xi_{\alpha_1 \mathbf{k}'}/2}{\xi_{\alpha'_1 \mathbf{k}'} + \xi_{\alpha_1 \mathbf{k}'}} \right] \Delta_{\mathbf{k}'}(\alpha_1 \alpha'_1). \tag{7}$$

Here $\xi_{\alpha k} \equiv \bar{\varepsilon}_{\alpha k} - \mu$, $\bar{\varepsilon}_{\alpha k}$ now includes mean field contributions from V_{int} and

$$N_c = \sum_\alpha \Omega \int_{IBZ} \frac{d^3 k}{(2\pi)^3} \frac{1}{(\exp(\beta_c \xi_{\alpha k}) + 1)} + O(\Delta^2). \tag{8}$$

From (3) to (5) we see that there are interlayer contributions to single-particle energies as well as to the pairing of charge carriers. It could be argued that the overlaps of interplanar wavefunctions are negligible in the oxide superconductors because of the layer separations and weak interlayer interactions. This argument carried to pairing across planes makes possible to drop the interplanar superconducting parameter $\Delta_k(\beta\alpha)$ ($\beta \neq \alpha$) from further consideration. Furthermore we may for simplicity take only one band for each layer so that no complication of interband sums even within the same layer occurs. With these approximations, we may then write (7) in terms of layer index j and wave vector $\mathbf{k}$:

$$\Delta_k(j) = \frac{-\Omega}{2} \int \frac{d^3 k'}{(2\pi)^3} \sum_{j'} \langle jk\, j - \mathbf{k} | V_{int} | j' - \mathbf{k'} j' \mathbf{k'} \rangle$$

$$\left[\frac{\tan h\beta_c \xi_{j'k'}/2}{\xi_{j'k'}} \right] \Delta_{k'}(j'). \tag{9}$$

This is the equation that Jha (1987) derived in his original work. In the next section, we employ this to estimate T_c as a function of number of layers in the system.

3. T_c as a function of number of layers—an estimation

The critical temperature T_c with Cooper pairing restricted to carry within the same conduction layers is determined by the nontrivial solution of the gap equation (9). If in (9) we employ $\mathbf{k}$-independent interaction parameters by averaging $\langle jk\, j - \mathbf{k} | V_{int} | j' - \mathbf{k'} j' \mathbf{k'} \rangle$ over the angles between $\mathbf{k}$ and $\mathbf{k'}$ on the Fermi surface i.e. use $\bar{V}_{jj'}$, then we only need to examine T_c given by that solution of the determinental equation

$$\det |I_j(T_c)\delta_{j,j'} + \lambda_{j,j'}| = 0, \tag{10}$$

where we have further approximated

$$I_j(T_c) = \Omega \int_{IBZ} \frac{d^3 k'}{(2\pi)^3} \tan h(\beta_c \xi_{j'k'}/2)/2\xi_{j'k'} \simeq N_j(0) \ln\left(\frac{1 \cdot 13\hbar\Omega}{k_B T_c}\right) \tag{11}$$

and

$$\lambda_{j,j'} = [N_j(0)]\bar{V}_{jj'}[N_{j'}(0)]^{1/2}. \tag{12}$$

Here, $N_j(0)$ is the density of states of the jth layer at the Fermi energy and $\hbar\Omega$ is a common cut-off energy for $\bar{V}_{jj'}$. This determinental equation takes simple forms when applied to Tl_1- or Tl_2- or Bi_2 systems and then T_c can be estimated as a function of the number of layers. It is found (Rajagopal and Jha 1990) after further considerations that the largest T_c attainable for asymptotically large number of layers is 143 K in a model describing Tl_1- and Tl_2-systems and 136 K in the Bi_2-system.

In the next section we give a brief summary and scope of this development.

4. Conclusions and scope of the work

We have given here a generalized Gorkov formulation of superconductivity in a layered system with *non-primitive* lattice structure in view. In the past a theory for primitive lattice structure with single layer per unit cell has been examined by Klemm and Scharnberg (1981) with a view to study the anisotropy of critical magnetic fields. Ginzburg-Landau phenomenological approach for superconductivity in layered system has been considered by Bulaevskii *et al* (1989) and Birman and Lu (1989). By appropriate analysis of equations (3) to (5) we have given a microscopic derivation of the Ginzburg-Landau theory. We have also worked out a general two-layer model in detail, to examine the various aspects of interlayer coupling, k-dependence in the single particle energies, interaction energies etc so as to understand the implications of the approximations made here.

Acknowledgements

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