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An electron–phonon model for anisotropic transport in single-crystal $YBa_2Cu_3O_{7-x}$

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Abstract. In terms of the Block–Wannier basis, we present an electron–phonon model Hamiltonian with quasi-two-dimensional character of the electron dynamics for the calculation of the normal-state transport coefficients in the high-T_c oxides. The physical picture of this model is that the in-plane resistivity originates from both the intra-plane and the inter-plane electron–phonon scattering, while the out-of-plane transport comes from the hopping conduction of electrons via phonon emission and absorption. The results obtained can be used to explain the nearly linear temperature dependences of the in-plane resistivity, the out-of-plane conductivity and thermopower observed in single-crystal $YBa_2Cu_3O_{7-x}$.

1. Introduction

In the current search to discover why the superconducting transition temperature T_c in YBCO is so high, there has been interest in the normal-state transport properties exhibiting strong anisotropies and anomalous temperature dependences [1–16]. It is widely expected that a better understanding of the unusual transport behaviour in YBCO might offer valuable clues to the mechanism for high T_c superconductivity. Earlier data [1–4] on ceramic YBCO material give linear temperature dependences for both the resistivity ρ and the Hall number density $n_H = 1/eR_H$ with $R_H > 0$. Recent measurements [5–9] on single-crystal YBCO show that the in-plane transport properties resemble those found in ceramic samples, indicating that the dominant contribution to the conduction of a ceramic sample comes from crystallites with current flow in the Cu–O planes. On the other hand, Tozer *et al* [5] reported that the resistivity anisotropy ρ_c/ρ_{ab} is 30 at room temperature and increases to about 80 as the temperature is lowered. At the same time, the temperature dependences of the out-of-plane transport coefficients are quite different from those of the corresponding in-plane quantities. The thermopower S_c along the c axis exhibits metallic behaviour [6, 7], while the out-of-plane resistivity ρ_c appears to be semiconducting [5, 8] and it satisfies the empirical formula $A/T + BT$ proposed by Anderson and Zou [10]. The Hall coefficient, measured with a magnetic field applied parallel to the Cu–O planes, is negative or electron-like [5, 9], while the sign of S_c is positive [6, 7], indicating hole-like conduction according to the usual viewpoint. These anisotropic transport properties are very anomalous and difficult to be understood from a simple transport theory for common metals or semiconductors.

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In this paper we are going to clarify several points of the unusual normal-state transport properties in YBCO.

(1) The origin of such strong anisotropies in the transport properties of YBCO.

(2) A unified explanation for the nearly linear temperature dependences of ρ_{ab}, $\sigma_c(=1/\rho_c)$ and S_c observed in single-crystal YBCO.

(3) Whether the electrons or holes give the dominant contribution to the conduction along the c axis.

Both structure analysis and band-structure calculation indicate the essentially two-dimensional nature of electron dynamics in YBCO. It is the highly two-dimensional character of the electron structure in YBCO that leads to the strong anisotropies in the transport properties. Although a number of interesting mechanisms for the high T_c superconductivity have been suggested, neither one to date can be considered generally accepted. In spite of these (phonon or non-phonon) mechanisms we believe that the normal-state transport of the high T_c oxides is essentially caused by the electron–phonon interaction. As we show below, owing to the nearly two-dimensional confinement of the carriers to Cu–O planes, phonons play entirely different roles for the carrier transports parallel and perpendicular to the Cu–O planes. The in-plane resistance originates from the electron–phonon scattering, while the out-of-plane conductance comes from the electron hopping via phonon emission and absorption. We propose an electron–phonon model Hamiltonian describing the above physical picture, from which the nearly linear temperature dependences of ρ_{ab}, σ_c and S_c can be deduced. At the same time, we point out that for the phonon-assisted hopping conduction between adjacent planes, the sign of the thermopower S_c is opposite to that of carrier charge, in contrast with the usual case. Thus, from the positive thermopower found in single-crystal YBCO [6, 7], one would infer that the carriers which give the dominant contribution to the out-of-plane transport are electrons rather than holes. This conclusion is also consistent with the electron-like Hall coefficient observed in the measurement [5] on single-crystal YBCO.

2. Anisotropic electron–phonon model

The system under consideration is composed of Cu–O planes, each coupled weakly with its nearest-neighbour ones. The carriers (electrons or holes) are free to move within the two-dimensional Cu–O planes, but have strong localised behaviour along the c axis. For such a system an appropriate basis set for the starting point of the transport calculation is the electron wavefunctions in a mixed Bloch–Wannier representation

$$\psi(r, z) = S^{-1/2} \sum_{k,n} \exp(\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{r})\varphi(z - nd)c_{k,n} \tag{1}$$

which are Bloch-like with respect to translations parallel to the Cu–O planes with $\boldsymbol{k}$ and $\boldsymbol{r}$ as the two-dimensional wavevector and coordinate variables, respectively. $\varphi(z - nd)$ is the Wannier function which is well localised around the nth Cu–O plane with n the plane index and d the spacing between adjacent Cu–O planes. S is the area of the Cu–O plane. In terms of the Bloch–Wannier basis set (1) and the second-quantisation representation, the Hamiltonian for an electron–phonon system in the presence of a constant electric field $\boldsymbol{E} = (\boldsymbol{E}_\parallel, E_z)$ can be expressed as follows

$$H = H_{\mathrm{eE}} + H_{\mathrm{e}} + H_{\mathrm{ph}} + H_{\mathrm{e\text{–}ph}} \tag{2}$$

$$H_{\mathrm{eE}} = -e \sum_n N_n(\boldsymbol{E}_\parallel \cdot \boldsymbol{R}_n + E_z nd) \tag{3}$$

$$H_e = \sum_{k,n} \varepsilon_{kn} c_{kn}^+ c_{kn} \tag{4}$$

$$H_{ph} = \sum_{Q,\lambda} \Omega_{Q\lambda} b_{Q\lambda}^+ b_{Q\lambda} \tag{5}$$

$$H_{e\text{-}ph} = \sum_{k,Q,\lambda,n} M_{nn}(Q,\lambda) c_{k+q,n}^+ c_{kn} \varphi_{Q\lambda} + \sum_{k,Q,\lambda,n} \{M_{n,n+1}(Q,\lambda) c_{k+q,n}^+ c_{k,n+1} \varphi_{Q\lambda} + \text{HC}\} \tag{6}$$

with $\varphi_{Q\lambda} = b_{Q\lambda} + b_{\bar{Q}\lambda}^+$. Here H_{eE} is the interaction for the system of carriers with the external field. $(\boldsymbol{R}_n, nd)$ is the coordinate of the centre of mass of carriers for the nth Cu–O plane and N_n is the corresponding number of carriers. H_e is the Hamiltonian for the decoupled two-dimensional electron systems, in which $c_{kn}^+(c_{kn})$ denote electron creation (annihilation) operators corresponding to the basis vector $|\boldsymbol{k}, n\rangle$ in (1), $\varepsilon_{kn} = \boldsymbol{k}^2/2m^* + \varepsilon_{0n}$ with m^* the effective carrier mass and ε_{0n} the energy at the centre of the lowest miniband in the c direction. H_{ph} represents the phonon Hamiltonian in which $b_{Q\lambda}^+$ $(b_{Q\lambda})$ are creation (annihilation) operators for phonon with wave vector $\boldsymbol{Q}$ in branch λ, $\Omega_{Q\lambda}$ is the phonon energy, and $\boldsymbol{Q} = (\boldsymbol{q}, q_z)$ with $\boldsymbol{q}$ and q_z respectively as the phonon momentum parallel and perpendicular to the Cu–O planes. $H_{e\text{-}ph}$, the last term in (2), contains the intra-plane and inter-plane electron–phonon interactions with $M_{n,n}(\boldsymbol{Q}, \lambda)$ and $M_{n,n+1}(\boldsymbol{Q}, \lambda)$ as the respective interaction matrix elements in the Bloch–Wannier basis set (1). Using the standard procedure [17] to calculate the electron–phonon interaction matrix element, we relate $M_{n,m}(\boldsymbol{Q}, \lambda)$ to the usual matrix element $M(\boldsymbol{Q}, \lambda)$ in the three-dimensional Bloch representation as

$$M_{n,m}(\boldsymbol{Q}, \lambda) = M(\boldsymbol{Q}, \lambda) \int \mathrm{d}z \exp(q_z z) \varphi^*(z - nd) \varphi(z - md). \tag{7}$$

It is easily seen that $|M_{nm}(\boldsymbol{Q}, \lambda)|^2$ depends only upon the absolute value of the difference $n - m$, and the magnitude of the non-diagonal term $(n \neq m)$ is much smaller than that of the diagonal term $(n = m)$. If q_z in the integrand of (7) is taken to be zero, we shall obtain that $M_{nm}(\boldsymbol{Q}, \lambda) = M(\boldsymbol{Q}, \lambda)\delta_{nm}$, which reduces to the pure two-dimensional model. In the present model electrons from a given Cu–O plane may hop via phonon emission and absorption to its neighbours. The assumption of weak coupling between planes allows the neglect of all non-diagonal matrix elements except those coupling nearest neighbour planes. The subscript m in $M_{n,m}(\boldsymbol{Q}, \lambda)$ in equation (6) is therefore taken to be n and $n \pm 1$.

In the following, starting from the identical Hamiltonian given by (2)–(6), we shall derive the expressions for the in-plane resistivity ρ_{ab} and the out-of-plane conductivity σ_c of the system in the presence of a weak electric field. In order to apply the linear response theory to the calculations for ρ_{ab} and σ_c, we separate the Hamiltonian (2) into two parts

$$H = H_0 + H' \tag{8}$$

where $H_0 = H_e + H_{ph}$ is the unperturbed part while $H' = H_{eE} + H_{e\text{-}ph}$ is the (small) perturbation. We imagine that at time $t = -\infty$ the electric field was absent and the electron–phonon interaction was turned off. The electron systems of various Cu–O planes were decoupled from phonons and from each other. The noninteracting electron gas, together with the phonon system, is considered to be in a state of thermal equilibrium

with a temperature T. Thus, the initial condition for the density matrix can be chosen to be

$$\rho(t=-\infty)=\rho_0=Z^{-1}\exp[-(H_e+H_{ph}-\mu N)/T] \tag{9}$$

where μ is the chemical potential of the electron gas and Z is the partition function.

3. In-plane resistivity

We first calculate the in-plane resistivity ρ_{ab} of the system in the presence of a weak field E_x perpendicular to the c axis. An expression for ρ_{ab} can be obtained from the equation of motion for the centre-of-mass momentum P_x:

$$\dot{P}_x=-i[P_x,H]=NeE_x-i\sum_{K,Q,\lambda,n}M_{nn}(\boldsymbol{Q},\lambda)q_x c^+_{k+q,n}c_{kn}\varphi_{Q\lambda}$$

$$-i\sum_{K,Q,\lambda,n}\{M_{n,n+1}(\boldsymbol{Q},\lambda)q_x c^+_{k+q,n}c_{k,n+1}\varphi_{Q\lambda}+\text{HC}\}. \tag{10}$$

In the steady state, the centre of mass of carriers moves with a constant speed v_e along the x direction and the ensemble average of $\dot{P}_x$ is zero at all times:

$$\langle\dot{P}_x(t)\rangle=0, \tag{11}$$

which is called the force-balance equation.

According to the theory of linear response of statistical systems to perturbations [18], for any operator A, the ensemble average $\langle A\rangle$ in the presence of H' is given to the lowest order by

$$\langle A\rangle=\langle A\rangle_0-i\int_{-\infty}^{0}dt\,\langle[A,H'(t)]\rangle_0, \tag{12}$$

where $\langle\cdots\rangle_0=\text{Tr}(\cdots\rho_0)$ denotes averaging with the equilibrium statistical operator (9), the square bracket with a comma stands for the commutator of two operators, and

$$A(t)=e^{iHt}A\,e^{-iHt}$$

is the operator A in the Heisenberg picture; for example [19]

$$c_{kn}(t)=c_{kn}\exp\{-it[(\boldsymbol{k}+m^*\boldsymbol{v}_e)^2/2m^*+\varepsilon_{0n}]\},$$

and

$$b_{Q\lambda}(t)=b_{Q\lambda}\exp\{-it\Omega_{Q\lambda}\}. \tag{13}$$

Replacing A in (12) by $\dot{P}_x$, and using the steady-state condition (11), we obtain

$$NeE_x=\int_{-\infty}^{0}dt\sum_{k,Q,\lambda,n}q_x\{|M_{nn}(Q,\lambda)|^2[\Lambda_{nn}(\boldsymbol{k},\boldsymbol{q},t)+\Lambda_{nn}(\boldsymbol{k},\boldsymbol{q},-t)]$$

$$+2|M_{n,n+1}(Q,\lambda)|^2[\Lambda_{n,n+1}(\boldsymbol{k},\boldsymbol{q},t)+\Lambda_{n,n+1}(\boldsymbol{k},\boldsymbol{q},-t)]\}, \tag{14}$$

where

$$\Lambda_{nm}(\boldsymbol{k}, \boldsymbol{q}, t) = \langle [c^+_{k+q,n} c_{km} b_{Q\lambda}, c^+_{km}(t) c_{k+q,n}(t) b^+_{Q\lambda}(t)] \rangle_0. \tag{15}$$

With the relations (13), equation (15) becomes

$$\Lambda_{nm}(\boldsymbol{k}, \boldsymbol{q}, t) = \exp\{-it(\varepsilon_{k+q} - \varepsilon_k + q_x v_e - \Omega_Q) \langle [c^+_{k+q,n} c_{km} b_{Q\lambda}, c^+_{km} c_{k+q,n} b^+_{Q\lambda}] \rangle_0, \tag{16}$$

in which

$$\begin{aligned}
&\langle [c^+_{k+q,n} c_{km} b_{Q\lambda}, c^+_{km} c_{k+q,n} b^+_{Q\lambda}] \rangle_0 \\
&\quad = \langle c^+_{k+q,n} c_{k+q,n} \rangle_0 \langle c_{km} c^+_{km} \rangle_0 \langle b_{Q\lambda} b^+_{Q\lambda} \rangle_0 - \langle c_{k+q,n} c^+_{k+q,n} \rangle_0 \langle c^+_{km} c_{km} \rangle_0 \langle b^+_{Q\lambda} b_{Q\lambda} \rangle_0 \\
&\quad = f(\varepsilon_{k+q})[1 - f(\varepsilon_k)][1 + n(\Omega_Q)] - [1 - f(\varepsilon_{k+q})] f(\varepsilon_k) n(\Omega_Q) \\
&\quad = [f(\varepsilon_{k+q}) - f(\varepsilon_k)][n(\Omega_Q) - n(\varepsilon_{k+q} - \varepsilon_k)].
\end{aligned} \tag{17}$$

It is easy to see from (16) and (17) that $\Lambda_{nm}(\boldsymbol{k}, \boldsymbol{q}, t)$ is independent of the plane indices n and m since the electric field is assumed to be in the in-plane directions in this section. Here $f(\varepsilon_k)$ is the usual Fermi function and $n(\Omega_Q)$ the phonon distribution function. Substituting (16) and (17) into (14) and performing the integration over t, we obtain the force-balance equation as

$$NeE_x = F(v_e, T), \tag{18}$$

$$\begin{aligned}
F(v_e, T) = 2 \sum_{n,\boldsymbol{Q},\lambda} &\{|M_{nn}(\boldsymbol{Q}, \lambda)|^2 + 2|M_{n,n+1}(\boldsymbol{Q}, \lambda)|^2\} q_x \\
&\times \Pi_2(\boldsymbol{q}, q_x v_e + \Omega_Q)[n(\Omega_Q) - n(q_x v_e + \Omega_Q)],
\end{aligned} \tag{19}$$

where

$$\Pi_2(\boldsymbol{q}, \omega) = 2\pi \sum_k [f(\varepsilon_k) - f(\varepsilon_{k+q})] \delta(\omega - \varepsilon_{k+q} + \varepsilon_k), \tag{20}$$

is the imaginary part of the carrier density–density retarded correlation function. For a two-dimensional electron gas the summation over $\boldsymbol{k}$ in equation (20) is replaced by $\int d\boldsymbol{k}^2/(2\pi)^2$. After performing the integration over the angle between $\boldsymbol{k}$ and $\boldsymbol{q}$, we have

$$\Pi_2(q, \omega) = (m/\pi q) \int_0^\infty dk\, [df(\varepsilon_k)/dk] \zeta(k, q, \omega), \tag{21}$$

where

$$\zeta(k, q, \omega) = \theta(z_-)(z_-)^{1/2} - \theta(z_+)(z_+)^{1/2}, \; Z_\pm = k^2 - (q/2 \pm m\omega/q)^2, \tag{22}$$

with $\theta(x)$ the unit step function. Since the current of the carriers is $J = nev_e$ with n as the number of carriers per unit volume, the in-plane resistivity is $\rho_{ab} = E_x/nev_e = F(v_e, T)/n^2e^2v_e$. In the zero-field limit: $E \to 0$ and $v_e \to 0$, $F(v_e, T)$ can be expanded to the lowest order in v_e so that ρ_{ab} is given by

$$\begin{aligned}
\rho_{ab} = (2m/\pi T n^2 e^2 d) &\sum_{\boldsymbol{Q},\lambda} |\tilde{M}(\boldsymbol{Q}, \lambda)|^2 q_x^2 n(\Omega_Q)[1 + n(\Omega_Q)]/q \\
&\times \int_0^\infty dk\, [-df(\varepsilon_k)/dk) \zeta(k, q, \Omega_Q).
\end{aligned} \tag{23}$$

It seems to be the same as the expression for ρ_{ab} in Ref. [14], but $|\tilde{M}(\boldsymbol{Q}, \lambda)|^2$ in (23) is a renormalisation matrix element:

$$|\tilde{M}(Q, \lambda)|^2 = [C_0(q_z) + 2C_1(q_z)]\,|M(Q, \lambda)|^2,$$
$$C_I(q_z) = \left| \int \mathrm{d}z \exp(q_z z)\varphi^*(z)\varphi(z - Id) \right|^2, \tag{24}$$

with $I = 0, 1$. The normalisation matrix element of the electron–phonon interaction contains the phonon scattering processes not only within plane but also between adjacent planes.

4. Out-of-plane conductivity and thermopower

We now turn our attention to the out-of-plane conductivity perpendicular to the Cu–O plane. From the following calculation we shall see that this conductivity originates from phonon-assisted hopping processes in which electrons hop from plane to plane via phonon emission and absorption. We choose the $\boldsymbol{E}$ direction parallel to the c-axis. Following Ref. [17], the current operator J_c for the tight binding model in the c-direction can be defined as

$$J_c = e\frac{\mathrm{d}}{\mathrm{d}t}\left(\sum_{k,n} ndc^+_{kn}c_{kn}\right) = ied\left[H, \sum_{k,n} nc^+_{kn}c_{kn}\right], \tag{25}$$

where nd is the position of the nth Cu–O plane along the c-axis. Using the model Hamiltonian (2), we find that only the Hamiltonian $H_{e\text{-}ph}$ contributes to the commutator in equation (25), yielding

$$J_c = ied \sum_{k,Q,\lambda,n} M_{n,n+1}(\boldsymbol{Q}, \lambda)(c^+_{k+q,n}c_{k,n+1} - c^+_{k+q,n+1}c_{k,n})\varphi_{Q\lambda}. \tag{26}$$

In terms of the linear response formula (12) and the equilibrium statistical operator (9), we obtain for the ensemble average of J_c:

$$\langle J_c\rangle = \int_{-\infty}^{\infty} \mathrm{d}t \sum_{k,Q,\lambda,n} |M_{n,n+1}(Q, \lambda)|^2 \{\Lambda_{n,n+1}(\boldsymbol{k}, \boldsymbol{q}, t) - \Lambda_{n+1,n}(\boldsymbol{k}, \boldsymbol{q}, t)\}, \tag{27}$$

where

$$\Lambda_{n,n+1}(\boldsymbol{k}, \boldsymbol{q}, t) = \exp\{-it(\varepsilon_{k+q} - \varepsilon_k - \Omega_Q + \varepsilon_{0n} - \varepsilon_{0,n+1})\}$$
$$\times \langle [c^+_{k+q,n}c_{k,n+1}b_{Q\lambda}, c^+_{k,n+1}c_{k+q,n}b^+_{Q\lambda}]\rangle_0. \tag{28}$$

Since the electric field E applied in the c-axis leads to $\varepsilon_{0n} - \varepsilon_{0,n+1} = eEd$, $\Lambda_{n,n+1}(\boldsymbol{k}, \boldsymbol{q}, t)$ and $\Lambda_{n+1,n}(\boldsymbol{k}, \boldsymbol{q}, t)$ are different from each other. Substituting (17) and (28) into (27), and performing the integration over t, we obtain

$$\langle J_c\rangle = 2e\sum_{Q,\lambda} C_1(q_2)|M(\boldsymbol{Q}, \lambda)|^2\{\Pi_2(\boldsymbol{q}, eEd + \Omega_Q)[n(\Omega_Q) - n(eEd + \Omega_Q)]$$
$$- \Pi_2(\boldsymbol{q}, \Omega_Q - eEd)[n(\Omega_q) - n(\Omega_Q - eEd)]\}. \tag{29}$$

The out-of-plane conductivity is defined as $\sigma_c = \lim_{E\to 0}(\langle J_c\rangle/E)$. In this limit we obtain from (29),

$$\sigma_c = (4e^2md/\pi T)\sum_{Q,\lambda} c_1(q_z)\,|M(Q,\lambda)|^2 n(\Omega_Q)[1+n(\Omega_Q)]/q \times \int_0^\infty \mathrm{d}k[-\mathrm{d}f(\varepsilon_k)/\mathrm{d}k]\zeta(k,q,\Omega_Q), \tag{30}$$

which is similar to equation (16) for σ_c of Ref. [14] in which the electron hopping via phonons is assumed to be the origin of the out-of-plane conductivity. The present expression (30) for σ_c is microscopically derived from the electron–phonon Hamiltonian (2)–(6), and the explicit expressions for $C_0(q_z)$ and $C_1(q_z)$ have been given, while in Ref. [14] an anisotropic factor of the electron–phonon interaction is phenomenologically introduced.

Then, we discuss the thermopower S_c along the c-axis. It is straightforward to extend the calculation for the ensemble average of the current operator J_c to the case in the presence of both a weak electric field and a small temperature gradient ∇T in the c-direction. In the limits of both $E\to 0$ and $\nabla T\to 0$, the result for $\langle J_c\rangle$ is

$$\langle J_c\rangle = (4em/\pi)\sum_{Q,\lambda} C_1(q_z)\,|M(Q,\lambda)|^2 n(\Omega_Q)[1+n(\Omega_Q)]/q \times \int_0^\infty \mathrm{d}k[-\mathrm{d}f(\varepsilon_k)/\mathrm{d}k]\zeta(k,q,\Omega_Q)\{edE/T-(\varepsilon_k-\mu)d\nabla T/T^2\}. \tag{31}$$

Comparing (31) with the definition for the thermopower $E = S_c\nabla T$ with $\langle J_c\rangle = 0$, we obtain

$$S_c = (\pi^2 T/3e)[\mathrm{d}\ln\sigma_c(\varepsilon)/\mathrm{d}\varepsilon]_{\varepsilon=\mu}, \tag{32}$$

provided the degenerate condition $\mu \gg T$ is satisfied. Here the expression (32) for S_c is similar in form to that for the diffusion thermopower in metals [20] in spite of their different transport mechanisms. In deriving equation (32) we have used the approximation relation $\mathrm{d}f(\varepsilon_k)/\mathrm{d}\varepsilon_k \simeq -\delta(\varepsilon_k-\mu)$ for $\mu \gg T$, whose physical meaning is that the only electrons in a narrow energy region around the Fermi level make contributions to the hopping conduction. Under this approximation equation (30) becomes

$$\sigma_c = (4e^2md/\pi T)\sum_{Q,\lambda} Y(Q,\lambda)\zeta(k,q,\Omega_Q)|_{k=k_F}, \tag{33}$$

with

$$Y(Q,\lambda) = C_1(q_z)\,|M(Q,\lambda)|^2 n(\Omega_Q)[1+n(\Omega_Q)]/q, \tag{34}$$

and $k_F = (2m^*\mu)^{1/2}$. It then follows that

$$[\mathrm{d}\ln\sigma_c(\varepsilon)/\mathrm{d}\varepsilon]_{\varepsilon=\mu} = m\sum_{Q,\lambda} Y(Q,\lambda)\zeta'(k_F,q,\Omega_Q)\Big/\sum_{Q,\lambda} Y(Q,\lambda)\zeta(k_F,q,\Omega_Q), \tag{35}$$

where

$$\zeta'(k,q,\omega) = \theta(z_-)(z_-)^{-1/2} - \theta(z_+)(z_+)^{-1/2}, \tag{36}$$

and the expression for $\zeta(k,q,\omega)$ has been given by equation (22).

5. Discussion and conclusion

In the previous sections we have derived the explicit expressions for ρ_{ab}, σ_c, and S_c. Let us now study their temperature dependences. First, we demonstrate that the three linear temperature laws hold within a temperature range of $\mu \gg T > T^*$ where $T^* = 2v_s k_F$, (v_s denoting the sound velocity), is a characteristic temperature introduced in Ref. [12]. As discussed in the last section, when the condition $\mu \gg T$ is satisfied, the expression (30) for σ_c reduces to (33) in which the upper limit on the summation over q is put by the step functions $\theta(z_-)$ and $\theta(z_+)$ that appears in $\zeta(k_F, q, \Omega_Q)$. Considering the dispersion relation $\Omega_Q = v_s q$ for the longitudinal acoustic phonon, one follows from equation (22) for $\theta(z_-)$ and $\theta(z_+)$ that $k_F^2 - (q/2 \pm m^* v_s)^2 \geqslant 0$, yielding the upper limit: $q_D = 2(k_F \pm m^* v_s)$, or $q_D \simeq 2k_F$ due to $k_F \gg m^* v_s$. Thus, the upper limit of the phonon energy $v_s q$ is $T^* = 2v_s k_F$ which may be well below the Debye temperature Θ_D [12], and for $T > T^*$ we can make the following approximation:

$$n(\Omega_Q)[1 + n(\Omega_Q)] = \operatorname{sech}^2(v_s q/2T)/4 \simeq T^2/(v_s q)^2. \tag{37}$$

Substituting (37) and (34) into (33), we obtain the linearity of the T dependence of σ_c. It is easy to see that the expression (23) for ρ_{ab} is quite similar in form to (30) for σ_c. It then follows that both ρ_{ab} and σ_c have the same linear temperature dependence. Under the approximation (37), the renormalisation matrix element $|\tilde{M}(\boldsymbol{Q}, \lambda)|^2$ in (23) will not alter the linear temperature dependence of ρ_{ab} but make a few changes in the magnitude of ρ_{ab}. At the same time, it is easily seen from (35) that if the condition $\mu \gg T > T^*$ is satisfied, $[\mathrm{d} \ln \sigma_c(\varepsilon)/\mathrm{d}\varepsilon]_{\varepsilon=\mu}$ is independent of temperature so that S_c given by (32) is also a linear function of temperature.

For YBCO compounds, we estimate [14] $\mu(T = 0) \simeq 1080$ K and $T^* \simeq 266$ K by taking typical values of parameters [12]: the hole density $n = 5 \times 10^{21}$ cm^{-3}, the effective mass $m^* = 5m_e$, and the sound velocity $v_s = 5 \times 10^5$ cm/s. In view of these parameters the condition $\mu \gg T$ is not strictly satisfied at room temperature. Moreover, for YBCO $T_c = 93$ K, is much lower than T^*, and the approximation (37) can not be used generally below T^*. Thus, to study the T dependences of ρ_{ab} and σ_c, a numerical evaluation for equations (23) and (30) is necessary. Using a set of parameters extracted from the experimental data we have calculated the in-plane resistivity and out-of-plane conductivity [14]. The obtained results show that both ρ_{ab} and σ_c have nearly linear T dependences from T_c to room temperature with $\mathrm{d}\rho_{ab}/\mathrm{d}T$ and $\mathrm{d}\sigma_c/\mathrm{d}T$ only slowly varying functions of temperature. This feature is consistent with that observed in many experimental measurements on single-crystal YBCO [5, 8]. It is interesting to notice that the nearly linear temperature laws still hold within the range from T^* down to T_c. This is similar to the situation of a typical metal in which the resistivity due to phonon scattering exhibits well linear T behaviour from high temperatures down to $\Theta_D/5$ [20]. The origin of this effect may be that owing to the factor $n(\Omega_Q)[1 + n(\Omega_Q)]$ included in equations (23) and (30), the main contributions to the summations (or integrations) over q comes from small phonon momenta q for which the approximation (37) still holds below T^* provided that $v_s q < 2T$.

Very recently it was pointed out [21] that the out-of-plane resistivity seems to depend very much on the way the single-crystal YBCO is grown. When Al_2O_3 is used for the crucible, the described $1/T$ behaviour of ρ_c is observed, while when ZrO_2 is used, a linear behaviour of ρ_c is obtained [21]. The present phonon-assisted hopping mechanism is used to explain $\rho_c \propto 1/T$ behaviour. The linear T dependence of ρ_c observed on a few samples [21, 22] implies that both ρ_{ab} and ρ_c come from the electron–phonon scattering

mechanism. Which behaviour of ρ_c represents the intrinsic property of YBCO is a pending question and remains to be studied still further.

Finally, we wish to ascertain the sign of S_c in equation (32). The variation of $\sigma(\varepsilon)$ with energy will mainly depend on the change of the effective carrier mobility $\mu(\varepsilon)$ of each electron as its energy changes. In usual metals and semiconductors, the thermopower S and carrier charge e have the same sign, S being negative for electrons ($e<0$) and positive for holes ($e>0$). This is because faster electrons are scattered less easily so that $\mu(\varepsilon)$ tends to increase with ε and the derivative of $\ln \sigma(\varepsilon)$ is positive. In the present hopping transport along the c-axis, however, the conclusion is quite the contrary. It is easy to see from (22) and (36) that $z_- > z_+$ for all q so that $\zeta(k_F, q, \Omega_Q)$ is always positive, but

$$\zeta'(k_F, q, \Omega_Q) = \begin{cases} (z_-)^{-1/2} - (z_+)^{-1/2} < 0 & \text{if } 0 \leqslant q \leqslant 2(k_F - m^* v_s), \\ (z_-)^{-1/2} > 0 & \text{if } 2(k_F - m^* v_s) < q \leqslant 2(k_F + m^* v_s). \end{cases}$$

As mentioned above, due to the factor $n(\Omega_Q)[1 + n(\Omega_Q)]$, the main contributions to the summations in equation (35) come from those small q. Moreover, in equation (35) the summating range, $0 \leqslant q \leqslant 2(k_F - m^* v_s)$, for $\zeta'(k, q, \Omega_Q) < 0$ is much larger than that for $\zeta'(k, q, \Omega_Q) > 0$ because of $k_F \gg m^* v_s$. It then follows that the summation in the numerator of equation (35) is less than zero so that $[\mathrm{d} \ln \sigma_c(\varepsilon)/\mathrm{d}\varepsilon]_{\varepsilon=\mu}$ is negative. Thus, it is concluded that the sign of S_c given by (32) is opposite from that of the carrier charge e. This result may arise from the hopping conduction mechanism for which the electron–phonon interaction does help the conduction of electrons, and faster electrons hop more difficultly from plane to plane. Recent measurements for S_c on single-crystal YBCO have reported [6, 7] that the out-of-plane thermopower S_c is positive, from which one could deduce that the carriers dominating the out-of-plane transport are the electrons rather than holes. This deduction is also consistent with the measured data for the Hall coefficient on single-crystal YBCO [5, 9], which show that the Hall coefficient is negative or electron-type when the magnetic field is applied parallel to the Cu–O planes. It has been reported [9] that the Hall constant on single-crystal YBCO, for the magnetic field parallel to c-axis, is positive (hole-like) and inversely proportional to temperature. This latter behaviour is very unusual. A possible two-band model [16] has been suggested to explain the unusual behaviour of the Hall constant, as well as of the in-plane thermopower in YBCO.

In conclusion, we have shown that the electron–phonon model with quasi-two-dimensional character of the electron dynamics can be used to explain the strong anisotropies and unusual temperature dependences of the transport coefficients in YBCO, including the in-plane resistivity ρ_{ab}, the out-of-plane conductivity σ_c and thermopower S_c.

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