PHYSICAL REVIEW B **67**, 184206 (2003)

Analytical expressions for the transport coefficients of icosahedral quasicrystals

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(Received 21 January 2003; published 30 May 2003)

We investigate by analytical means the electronic transport properties of approximants and quasicrystals. The spectral resistivity is modeled by Lorentz functions in agreement with realistic *ab initio* calculations (linear muffin-tin orbital basis, Kubo-Greenwood formula) for low-order approximants. The analytical expressions for the transport coefficients compare well with both numerical calculations and experiments. Thus, the temperature-dependent conductivity, thermopower, electronic thermal conductivity, and Lorenz number of certain approximants and quasicrystals can be consistently explained.

DOI: 10.1103/PhysRevB.67.184206 PACS number(s): 61.44.Br, 71.23.Ft, 72.15.Cz

I. INTRODUCTION

Since the discovery of the rapidly solidified Al-Mn quasicrystals (QC's) in 1984 by Shechtman *et al.*,[1] hundreds of new alloys have been observed with quasicrystalline symmetries (see, for instance, the work of Tsai[2] and references therein). The electronic behavior of QC's reveals very interesting properties. For instance, materials with abundant content of aluminum (which is a good metal) and with low transition-metal content, such as Al-Pd-Re, Al-Pd-Mn, Al-Cu-Fe, and Al-Cu-Ru, show high resistivities close to the metal-insulator transition.[3–6] This is not due to the disorder in the system, such as the Anderson transition,[7] it is rather a consequence of both the quasiperiodicity and the chemical order. Moreover, the temperature dependence of the resistivity shows a nonmetallic behavior,[4,8] the Hall coefficient is three orders of magnitude larger than for related amorphous phases,[9,10] the thermopower changes its sign with temperature,[9,10] and the thermal conductivity is two orders of magnitude lower than that in fcc Al.[11] Despite these peculiarities, the Wiedemann-Franz law is generally accepted to separate the electronic contribution of the measured thermal conductivity. However, if that is not the case, several conclusions about the phonon dynamics should also be revised. This point has received little attention.[12–14]

These *anomalous* transport properties of QC's are believed to arise from peculiar spectral features around the Fermi energy, ε_F. A wide pseudogap ($\sim$1 eV) was expected[15–18] (as a consequence of Hume-Rothery stabilization and hybridization) and confirmed experimentally.[19–23] Moreover, numerical calculations[15,17,24,25] for realistic approximant models of QC's reveal a *spiky* spectral structure throughout the valence band as a result of almost dispersionless bands. However, as yet the existence of spikes is not experimentally confirmed. It is suggested that spikes could be artifacts of the calculation[26,27] or only specific to small periodic approximants[24,28,29] (APP's). On the other hand, there is experimental evidence[30,31] for significant spectral structures around the Fermi energy down to a few 10 meV. Measurements[9,10,32,33] of the temperature-dependent conductivity and the thermopower indicate also the presence of narrow pseudogaps (width $\sim$0.1–0.2 eV) in the spectral conductivity. It is supposed that the generic properties of icosahedral high-resistive QC's arise from the special cooperation of the clusters[34] and that even low APP's should exhibit corresponding spectral signatures to be extracted and then rescaled to the appearance in the QC's.[12,13,35]

The present work shows that the temperature-dependent transport coefficients of QC's can be consistently explained employing close analytical expressions that are obtained from a realistic model for the spectral conductivity. The paper is organized as follows. In Sec. II, we present the basic concepts employed in this work, the model for the spectral conductivity of QC's, and the corresponding analytical expressions for the transport coefficients. Comparisons with exact numerical calculations and experiments in the icosahedral Al-Cu-Fe quasicrystal are presented in Sec. III. We provide a summary in Sec. IV.

II. SPECTRAL TRANSPORT MODELS OF ICOSAHEDRAL PHASES

A. Transport parameters

The temperature-dependent transport coefficients are obtained by means of the Chester-Thellung Kubo-Greenwood (CTKG) version of the linear response theory.[36–38] The central information quantities are the kinetic coefficients

$$\mathcal{L}_{ij}(T)=(-1)^{i+j}\int d\varepsilon\,\hat{\sigma}(\varepsilon)(\varepsilon-\mu)^{i+j-2}\left\{-\frac{\partial f(\varepsilon,\mu,T)}{\partial\varepsilon}\right\}, \tag{1}$$

where $f(\varepsilon,\mu,T)$ is the Fermi-Dirac distribution function, $\hat{\sigma}(\varepsilon)$ is the spectral conductivity, and

$$\mu(T)\approx\varepsilon_F-(b/2)[(d\hat{n}/d\varepsilon)/\hat{n}]_{\varepsilon_F}T^2 \tag{2}$$

is the chemical potential[39] with $b=(\pi^2/3)k_B^2$. $\hat{n}(\varepsilon)$ means the electronic density of states (DOS).

Within the above framework one obtains the conductivity

$$\sigma(T)=\mathcal{L}_{11}(T), \tag{3}$$

the thermoelectric power (or Seebeck coefficient),

$$S(T)=\frac{1}{|e|T}\frac{\mathcal{L}_{12}(T)}{\sigma(T)}, \tag{4}$$

the electronic thermal conductivity,

$$K(T)=\frac{1}{e^2T}\mathcal{L}_{22}(T)-T\sigma(T)S(T)^2, \tag{5}$$

and the Lorenz number,

$$L(T)=\frac{K(T)}{T\sigma(T)}. \tag{6}$$

Note that $\hat{\sigma}(\varepsilon)$ includes all the system-dependent features. That means the reported *anomalous* transport properties of QC's must have their origin in certain spectral features of $\hat{\sigma}(\varepsilon)$.

B. Modeling the spectral conductivity

Spectral conductivity models[40–43] have been employed to explain the temperature dependence of the transport coefficients, Eqs. (3)–(6). The idea is to find a spectral conductivity model that accounts for generic properties, and then to obtain transport parameters by means of the CTKG formalism. This procedure has been employed by Mott,[40] who proposed a simple conductivity minimum to model thermal activation near the metallic limit. Furthermore, the metal-insulator transition (MIT) and liquid semiconductors have also been discussed within this framework.[41–43]

Applications to QC's have been studied by Fujiwara,[44] who has simulated a spiky component of the spectral conductivity by a sinusoidal modulation. Thus, a qualitative explanation of the temperature-dependent thermopower was obtained. Maciá[45] has explained the conductivity of *i*-AlCuRu samples considering self-similar fine structures of the density of states (DOS) as suggested by one-dimensional QC's.

QC's and related APP's have similar local orders. It is interesting that the electronic transport properties in both systems are quite similar.[8,46] On the other hand, it is known that clusters, such as the Mackay and Bergman icosahedra, are the basic elements to build icosahedral APP's and QC's.[47,48] Hence, one can expect that these clusters, their decorations, and their arrangements on scales[46,49] of ∼10–20 Å are responsible for the spectral features that can account for the anomalous transport properties of APP's and QC's. In this sense, it should be possible to search for such spectral features in approximants with unit cells larger than ∼10 Å.

In fact, we recently have proposed a model for the spectral conductivity of icosahedral QC's based on *ab initio* calculations for small approximants,[12,13,50]

$$\hat{\sigma}(\varepsilon)=B\left\{\frac{1}{\pi}\,\frac{\gamma_1}{(\varepsilon-\delta_1)^2+\gamma_1^2}+\alpha\frac{1}{\pi}\,\frac{\gamma_2}{(\varepsilon-\delta_2)^2+\gamma_2^2}\right\}^{-1}. \tag{7}$$

Considering the spectral resistivity, $\hat{\rho}(\varepsilon)=\hat{\sigma}^{-1}(\varepsilon)$, this model is given by the sum of a wide Lorentzian (that is common with amorphous phases[12]) and a narrow Lorentzian above the self-consistently calculated Fermi energy, ε_F^{sc}, of the icosahedral Al-Cu-Fe 1/1 approximant (Cockayne *et al.* model[51]). We take ε_F^{sc} as the zero energy.[12,13,50] Each Lorentzian is characterized by its height, $1/(\pi\gamma)$, and its position, δ. The actual Fermi energy will be set to the spectral range of the narrow Lorentzian. Such shifts with respect to ε_F^{sc} are of the order of ∼100 meV and are caused by deviations in the stoichiometry or by defects in both structure and decoration.[32,52]

Note that the transport coefficients, Eqs. (3)–(6), can be obtained on integrating numerically the kinetic coefficients, Eq. (1), with the spectral conductivity model proposed above, Eq. (7). This is what we call the "exact numerical" result. In the following, we attempt to obtain approximate close analytical expressions. Both results will be compared in the next section.

C. Analytical expressions for transport coefficients

The idea is to obtain approximate analytical expressions for the kinetic coefficients, Eq. (1), as powers of the temperature, and then to replace them in the equations for the transport coefficients, Eqs. (3)–(6). We proceed as follows (see the Appendix for details). (i) We introduce the variable $x=\beta(\varepsilon-\mu)$ with $\beta=(k_BT)^{-1}$. Thus, the spectral conductivity $\hat{\sigma}(\varepsilon)\equiv\hat{\sigma}(x)$, Eq. (7), can be expressed as

$$\hat{\sigma}(x)=c_0P_4(x)/P_2(x), \tag{8}$$

where $c_0=\pi B(\gamma_1+\alpha\gamma_2)^{-1}$, and the polynomials $P_i(x)$ are defined in the Appendix. (ii) If we employ a Taylor series of $P_2^{-1}(x)$, then a polynomial form of $\hat{\sigma}(x)$ is obtained and the kinetic coefficients, Eq. (1), can be integrated term by term. We truncate the series after keeping the first four or six terms. These approximations are called here the zero approximation or the one approximation (ZA or OA). (iii) Finally, in order to simplify our results we take $\mu\simeq\varepsilon_F$ [cf. Eq. 2)]. Hence, considering the OA, one obtains for the conductivity,

$$\sigma(T)=\sigma_0[1+\xi_2bT^2+\xi_4b^2T^4+(g_1\xi_4-g_2\xi_3)b^3T^6]. \tag{9}$$

According to this expression the overall factor σ_0 appearing in Eq. (A23) can be physically interpreted as the residual electrical conductivity of the system in the zero-temperature limit.

The thermoelectric power is given by

$$S(T)=-2|e|L_0T\mathcal{D}(T), \tag{10}$$

where $L_0=\pi^2k_B^2/3e^2=2.44\times10^{-8}\ \mathrm{V}^2\,\mathrm{K}^{-2}$ is the Wiedemann-Franz Lorenz number (WFL), and we have introduced the auxiliary function

$$\mathcal{D}(T)\equiv\frac{\xi_1+\xi_3bT^2+(\frac{1}{4}q_0g_2\xi_4-g_3\xi_3)b^2T^4}{1+\xi_2bT^2+\xi_4b^2T^4+(g_1\xi_4-g_2\xi_3)b^3T^6}. \tag{11}$$

Therefore, the expression obtained for the thermoelectric power can be viewed as a product involving the factor $-2|e|L_0T$, exhibiting a linear temperature dependence, and the auxiliary function defined by Eq. (11). This function exhibits a marked nonlinear temperature dependence, which accounts for most of the Seebeck coefficient anomalies observed in QC's, as discussed in Ref. 53. We can gain some physical insight about the coefficient ξ_1 by taking the logarithmic derivative of Eq. (7) to obtain the relationship

$$\xi_1 = \frac{1}{2}\left(\frac{d \ln \hat{\sigma}(\varepsilon)}{d\varepsilon}\right)_{\varepsilon=\mu}.$$

Hence, in the low-temperature limit Eq. (10) reduces to the well-known Mott's formula $S = -|e| L_0 T [d \ln \hat{\sigma}(\varepsilon)/d\varepsilon]_{\varepsilon=\mu}$.

The electronic contribution to the thermal conductivity is given by

$$K(T) = \sigma_0 L_0 T [1 + \tfrac{21}{5}\xi_2 b T^2 + (q_0 g_3 \xi_4 - g_4 \xi_3) b^2 T^4 - 4 b T^2 \mathcal{F}(T)], \tag{12}$$

where

$$\mathcal{F}(T) \equiv \frac{[\xi_1 + \xi_3 b T^2 + (\frac{1}{4} q_0 g_2 \xi_4 - g_3 \xi_3) b^2 T^4]^2}{1 + \xi_2 b T^2 + \xi_4 b^2 T^4 + (g_1 \xi_4 - g_2 \xi_3) b^3 T^6}. \tag{13}$$

Then, making use of Eqs. (9) and (12) the Lorenz number, Eq. (6), can be written as

$$\frac{L(T)}{L_0} = \frac{1 + \dfrac{21}{5}\xi_2 b T^2 + (q_0 g_3 \xi_4 - g_4 \xi_3) b^2 T^4 - 4 b T^2 \mathcal{F}(T)}{1 + \xi_2 b T^2 + \xi_4 b^2 T^4 + (g_1 \xi_4 - g_2 \xi_3) b^3 T^6}. \tag{14}$$

In the zero-temperature limit, the Wiedemann-Franz law is satisfied $[L(T \to 0) = L_0]$. As the temperature is moderately increased the Lorenz number deviates from this ideal behavior. Thus, in the very-low-temperature range Eq. (14) can be approximated by

$$\frac{L(T)}{L_0} \simeq \frac{1 + 2\left(\dfrac{13}{5}\xi_2 - 2\xi_1^2\right) b T^2}{1 + 2\xi_2 b T^2},$$

so that the condition for the validity of the Wiedemann-Franz law depends on the particular electronic structure of the sample through the relationship $4\xi_2 = 5\xi_1^2$. As the temperature is further increased Eq. (14) indicates that the WFL will be valid as long as the coefficients ξ_2, ξ_3, and ξ_4 in $\mathcal{F}(T)$ given by Eq. (13) are negligible compared to ξ_1. Since these coefficients are multiplied by the temperature-dependent factors $b^n T^{n+2}$ it is clear that the range of validity of Eq. (14) will strongly depend on the electronic structure of the sample.

III. DISCUSSION

The analytical expressions obtained in the preceding section will be compared with the corresponding numerical calculations and with experiments by Bilušić *et al.*[54] in the polyquasicrystalline icosahedral $Al_{62}Cu_{25.5}Fe_{12.5}$ sample. The model parameters are obtained by fitting to the experimental thermopower,[54] which is closely related to $\hat{\sigma}(\varepsilon)$ [see Eq. (4)]. This procedure has proved very useful to fit the experimental transport coefficients of various icosahedral QC's.[10,12,13,35] Thus, we obtain $B = 955.11$ $(\Omega\ \mathrm{cm\ eV})^{-1}$, $\delta_1 = -0.2$ eV, $\delta_2 = 0.23$ eV, $\gamma_1 = 1.35$ eV, $\gamma_2 = 43$ meV, $\alpha = 0.98$, and ε_F is chosen 13 meV below δ_2. The analytical expressions, Eqs. (9)–(14), are evaluated employing these values.

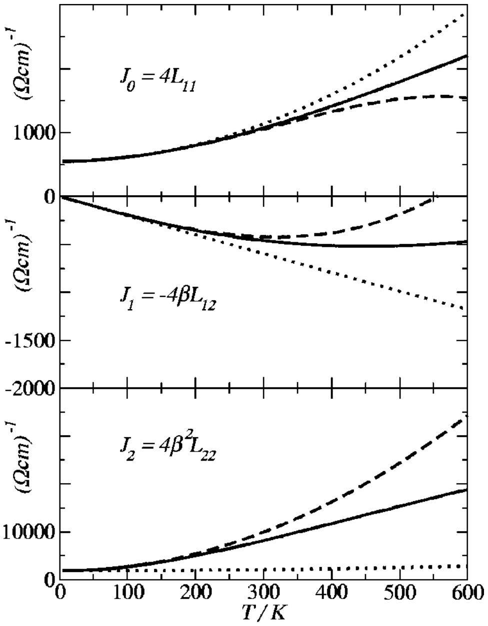

FIG. 1. Kinetic coefficients of the polyquasicrystalline icosahedral $Al_{62}Cu_{25.5}Fe_{12.5}$ sample. Numerical (solid) and analytical approaches, ZA (dots) and OA (dashes), are compared (see text for details).

Comparisons of the analytical and numerical results can be done at different levels. First, we can compare the spectral conductivity, Eq. (8), with its Taylor series. Thus, considering that $\hat{\sigma}(x)$ [or $P_2^{-1}(x)$] is weighted with the derivative of the Fermi-Dirac distribution function (thermal window) for its integration, Eq. (1) [or Eq. (A9)], we find that differences are notable only above 150 K when OA is considered. Second, we compare the numerically integrated kinetic coefficients, Eq. (1), with their analytical approaches (ZA or OA). The results are shown in Fig. 1. The differences between the numerical and analytical results increase for higher kinetic coefficients. This means the temperature range of validity of the analytical equations is reduced for higher kinetic coefficients. Hence, transport coefficients that require these higher kinetic coefficients must be most affected. This is the case for the electronic thermal conductivity and the Lorenz number, as illustrated by Fig. 2. The range of validity of the analytical equations (OA) for the conductivity increases to ~400 K (cf. Ref. 55), whereas for the Lorenz number increases to ~150 K.

In fact, considering the ZA we conclude that the Lorenz number is (nearly) temperature independent and very close to the WFL (cf. Ref. 14). A more precise result is obtained from the OA: the Lorenz number is strongly temperature dependent in agreement with numerical integrations (e.g., Fig. 2). The thermopower proves less sensitive to the improvement (ZA or OA), because the errors of the kinetic

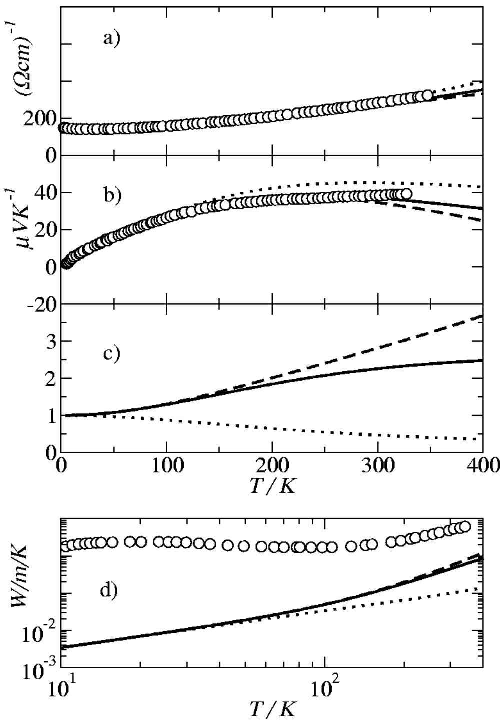

FIG. 2. Transport coefficients of the polyquasicrystalline icosahedral $Al_{62}Cu_{25.5}Fe_{12.5}$ sample. Experiment (Ref. 54) (○), numerical (solid), and analytical approaches, ZA (dots) and OA (dashes), are compared (see text for details). (a) conductivity, (b) thermopower, (c) Lorenz number $[L(T)/L_0]$, and (d) electronic (lines) and total (○) thermal conductivity.

coefficients, $\mathcal{L}_{11}$ and $\mathcal{L}_{12}$, tend to compensate one another [see Eq. (4) and Fig. 1]. Finally, it is worth noting that in some cases the approximation $\mu \simeq \varepsilon_F$ is not sufficient to explain the experiments.[13]

IV. SUMMARY

The spectral resistivity, modeled by Lorentzians, prove capable in extracting spectral features that can be scaled to account for the quasicrystal. It was shown that this model explains consistently the conductivity, thermopower, and the electronic thermal conductivity. The Lorenz number depends strongly on the temperature. The analytical expressions obtained in the present work compare well with both exact numerical calculations and experiments in the polyquasicrystalline icosahedral $Al_{62}Cu_{25.5}Fe_{12.5}$ sample.

ACKNOWLEDGMENTS

We are grateful to A. Löser, and T. Schmidt for useful discussions. This work was supported by the Deutsche Forschungsgemeinschaft.

APPENDIX

The procedure described in the following was previously employed by Maciá[14] to discuss the validity of the WFL. We have extended the procedure to be applied up to room temperatures. Thus, introducing the variable $x=\beta(\varepsilon-\mu)$ with $\beta=(k_BT)^{-1}$, the transport coefficients can be written as

$$\sigma(T)=\frac{J_0}{4}, \tag{A1}$$

$$S(T)=-\frac{k_B}{|e|}\frac{J_1}{J_0}, \tag{A2}$$

$$K(T)=\frac{k_B^2T}{4e^2}\left(J_2-\frac{J_1^2}{J_0}\right), \tag{A3}$$

$$L(T)=\frac{k_B^2}{e^2}\left(\frac{J_2J_0-J_1^2}{J_0^2}\right), \tag{A4}$$

where

$$J_n(\beta)=\int x^n\hat{\sigma}(x)\,\mathrm{sech}^2(x/2)\,dx. \tag{A5}$$

The $J_n(\beta)$ functions are called here the *reduced* kinetic coefficients. The spectral conductivity $\hat{\sigma}(\varepsilon)\equiv\hat{\sigma}(x)$, Eq. (7), can be expressed as

$$\begin{aligned}\hat{\sigma}(x)&=c_0P_4(x)/P_2(x)\\&=c_0\left\{a_2\beta^{-2}x^2+a_1\beta^{-1}x+a_0+\frac{Q_1(x)}{P_2(x)}\right\},\end{aligned} \tag{A6}$$

where

$$\begin{aligned}P_4(x)&=\beta^{-4}x^4-2\beta^{-3}n_3x^3+\beta^{-2}n_2x^2-2\beta^{-1}n_1x+n_0,\\P_2(x)&=\beta^{-2}x^2-2\beta^{-1}q_1x+q_0,\\Q_1(x)&=\beta^{-1}a_3x+a_4,\end{aligned} \tag{A7}$$

and the coefficients $n_3=\tilde{\delta}_1+\tilde{\delta}_2$, $n_2=\epsilon_1^2+\epsilon_2^2+4\tilde{\delta}_1\tilde{\delta}_2$, $n_1=\tilde{\delta}_2\epsilon_1^2+\tilde{\delta}_1\epsilon_2^2$, $n_0=\epsilon_1^2\epsilon_2^2$, $q_0=\epsilon\epsilon_1^2\epsilon_2^2(\gamma_1+\alpha\gamma_2)^{-1}$, $q_1=(\gamma_1\tilde{\delta}_2+\alpha\tilde{\delta}_1\gamma_2)(\gamma_1+\alpha\gamma_2)^{-1}$, $\epsilon_i^2=\gamma_i^2+\tilde{\delta}_i^2$, $\epsilon=\gamma_1\epsilon_1^{-2}+\alpha\gamma_2\epsilon_2^{-2}$, with $\tilde{\delta}_i=\delta_i-\mu$ and $a_0=2q_1a_1+n_2-q_0$, $a_1=2(q_1-n_3)$, $a_2=1$, $a_3=2q_1a_0-q_0a_1-2n_1$, $a_4=n_0-q_0a_0$.

Now, placing Eq. (A6) into Eq. (A5) and employing

$$\int \mathrm{sech}^2(x/2)\,dx=4,\quad \int x^2\,\mathrm{sech}^2(x/2)=4\frac{\pi^2}{3},$$

$$\int x^4\,\mathrm{sech}^2(x/2)\,dx=4\frac{7\pi^4}{15},$$

$$\int x^6\,\mathrm{sech}^2(x/2)\,dx=4\frac{31\pi^6}{21},$$

$$\int x^{2l+1}\,\mathrm{sech}^2(x/2)\,dx=0\quad\forall\quad l\geqslant 0,$$

we obtain

$$J_0 c_0^{-1} = 4\pi^2\beta^{-2}/3 + a_3\beta^{-1}H_1 + a_4H_0 + 4a_0,$$

$$J_1 c_0^{-1} = 4\pi^2 a_1\beta^{-1}/3 + a_5H_1 + a_3\beta G_0, \qquad \text{(A8)}$$

$$J_2 c_0^{-1} = 28\pi^4\beta^{-2}/15 + a_6\beta H_1 + a_5G_0\beta^2 + 4\pi^2a_0/3,$$

where $a_5 = 2a_3q_1 + a_4$, $a_6 = 2a_5q_1 - a_3q_0$, $G_0 = 4 - q_0H_0$, and

$$H_k(\beta) = \int \frac{x^k}{P_2(x)}\mathrm{sech}^2(x/2)dx. \qquad \text{(A9)}$$

To obtain close analytical expressions for the *reduced* kinetic coefficients, Eq. (A8), we expand the function $P_2^{-1}(x)$ in a Taylor series around the Fermi energy and keep the first six terms (OA approach). Thus, after taking $\mu \simeq \varepsilon_F$ we find

$$H_0 \simeq H_0^{(1)} = H_0^{(0)} + \frac{28\pi^4}{15q_0^5}(q_0^2 - 12q_0q_1^2 + 16q_1^4)\beta^{-4}, \qquad \text{(A10)}$$

$$H_1 \simeq H_1^{(1)} = H_1^{(0)} + \frac{248\pi^6}{21q_0^6}q_1(4q_1^2 - 3q_0)(4q_1^2 - q_0)\beta^{-5},$$

where,

$$H_0^{(0)} = \frac{4}{q_0}\left(1 + \frac{\pi^2}{3}\frac{4q_1^2 - q_0}{q_0^2}\beta^{-2}\right),$$

$$H_1^{(0)} = \frac{8\pi^2q_1\beta^{-1}}{3q_0^2}\left(1 + \frac{14\pi^2}{5}\frac{2q_1^2 - q_0}{q_0^2}\beta^{-2}\right). \qquad \text{(A11)}$$

Note that if we keep only the first four terms in the Taylor series of $P_2^{-1}(x)$, then Eq. (A11) will be the approximate integration of Eq. (A9) (ZA approach).

Now, inserting Eq. (A10) into Eq. (A8) we can express the reduced kinetic coefficients in the matrix form

$$c_0^{-1}\begin{pmatrix} J_0 \\ J_1 \\ J_2 \end{pmatrix} = 4\begin{pmatrix} J_{00} & 0 & J_{02} & 0 & J_{04} & 0 & J_{06} \\ 0 & J_{11} & 0 & J_{13} & 0 & J_{15} & 0 \\ (\pi^2/3)J_{20} & 0 & (\pi^2/3)J_{22} & 0 & (\pi^2/3)J_{24} & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ bT/k_B \\ bT^2 \\ b^2T^3/k_B \\ b^2T^4 \\ b^3T^5/k_B \\ b^3T^6 \end{pmatrix}, \qquad \text{(A12)}$$

where the matrix elements J_{ij} are defined by the following nested relationships:

$$J_{00} = a_0 + \frac{a_4}{q_0},$$

$$J_{02} = 1 + (J_{00} - a_0)\frac{4q_1^2 - q_0}{q_0^2} + 2a_3\frac{q_1}{q_0^2},$$

$$J_{04} = \frac{21}{5q_0^2}[a_0 - J_{00} + 2(J_{02} - 1)(2q_1^2 - q_0)],$$

$$J_{06} = \frac{279}{7q_0^4}\left[J_{02} - 1 + (a_0 - J_{00})\frac{4q_1^2 - q_0}{q_0^2}\right]\mathcal{R},$$

$$J_{11} = a_1 + 2a_5\frac{q_1}{q_0^2} - a_3\frac{4q_1^2 - q_0}{q_0^2},$$

$$J_{13} = \frac{21}{5q_0^2}[a_3 + 2(J_{11} - a_1)(2q_1^2 - q_0)],$$

$$J_{15} = \frac{279}{7q_0^4}\left[J_{11} - a_1 + a_3\frac{4q_1^2 - q_0}{q_0^2}\right]\mathcal{R},$$

$$J_{20} = a_0 + 2a_6\frac{q_1}{q_0^2} - a_5\frac{4q_1^2 - q_0}{q_0^2},$$

$$J_{22} = \frac{21}{5q_0^2}[a_5 + q_0^2 + 2(J_{20} - a_0)(2q_1^2 - q_0)],$$

$$J_{24} = \frac{279}{7q_0^4}\left[J_{20} - a_0 + a_5\frac{4q_1^2 - q_0}{q_0^2}\right]\mathcal{R},$$

where $\mathcal{R} \equiv (4q_1^2 - q_0)(4q_1^2 - 3q_0)$. By inspecting Eq. (A12) we note that the reduced kinetic coefficients J_0 and J_2 depend on even powers of the temperature only. Conversely, the reduced kinetic coefficient J_1 depends on odd powers of the temperature, instead. This is due to the even symmetry of the negative derivative of the Fermi-Dirac distribution function. From the definition of the auxiliary a_i coefficients and making use of the nested relations

$$n_0 \equiv \xi_0 q_0,$$

$$n_1=\xi_0(q_1-q_0\xi_1),$$

$$n_2=\xi_0(q_0\xi_2-4q_1\xi_1+1),$$

$$n_3=\xi_0\left(q_1\xi_2-\xi_1-\frac{5q_0}{21}\xi_3\right),$$

along with

$$\xi_4\equiv\frac{21}{5q_0}\left(\frac{1}{\xi_0}-\xi_2+\frac{20q_1}{21}\xi_3\right),$$

we obtain

$$\begin{gathered}J_{00}=J_{20}=\xi_0,\\ J_{02}=\xi_0\xi_2,\quad J_{22}=\frac{21}{5}\xi_0\xi_2,\\ J_{11}=2\xi_0\xi_1,\quad J_{13}=2\xi_0\xi_3,\\ J_{04}=\xi_0\xi_4,\quad J_{15}=2\xi_0\xi_5,\\ J_{06}=\xi_0\xi_6,\quad J_{24}=\xi_0\xi_7,\end{gathered}\tag{A13}$$

where we have introduced the phenomenological coefficients

$$\xi_0\equiv\frac{\gamma_1+\alpha\gamma_2}{\epsilon},\tag{A14}$$

$$\xi_1\equiv-\frac{\gamma_1\delta_1\epsilon_2^4+\alpha\gamma_2\delta_2\epsilon_1^4}{\epsilon\epsilon_1^4\epsilon_2^4},\tag{A15}$$

$$\xi_2\equiv4\xi_1^2+\frac{\gamma_1\epsilon_2^6(\epsilon_1^2-4\delta_1^2)+\alpha\gamma_2\epsilon_1^6(\epsilon_2^2-4\delta_2^2)}{\epsilon\epsilon_1^6\epsilon_2^6},\tag{A16}$$

$$\xi_3\equiv\frac{42}{5}\frac{\alpha\gamma_1\gamma_2\delta}{\epsilon^3\epsilon_1^4\epsilon_2^4}[\epsilon(\epsilon_2^2-\epsilon_1^2)-2\delta m_1],\tag{A17}$$

$$\xi_4\equiv\frac{21}{5}\frac{\alpha\gamma_1\gamma_2}{\epsilon^4\epsilon_1^6\epsilon_2^6}[4\delta^2\epsilon\epsilon_1^2\epsilon_2^2(\gamma_1+\alpha\gamma_2)-[4\delta m_1-\epsilon(\epsilon_2^2-\epsilon_1^2)]^2],\tag{A18}$$

$$\xi_5\equiv\frac{465q_1}{49q_0^6}(q_0\mathcal{P}\xi_4-4q_1\mathcal{R}\xi_3)\mathcal{R},\tag{A19}$$

$$\xi_6\equiv\frac{1860q_1}{49q_0^6}(2q_0q_1\mathcal{Q}\xi_4-\mathcal{P}\xi_3)\mathcal{R},\tag{A20}$$

$$\xi_7=\frac{1860q_1}{49q_0^6}(q_0q_1\mathcal{R}\xi_4-\mathcal{S}\xi_3)\mathcal{R},\tag{A21}$$

with $\delta\equiv\tilde{\delta}_1\epsilon_1^{-2}-\tilde{\delta}_2\epsilon_2^{-2}$, $m_1=\gamma_1\tilde{\delta}_2+\alpha\tilde{\delta}_1\gamma_2$, $\mathcal{P}\equiv16q_1^4-12q_0q_1^2+q_0^2$, $\mathcal{Q}\equiv2q_1^2-q_0$, and $\mathcal{S}\equiv64q_1^6-80q_0q_1^4+24q_0^2q_1^2-q_0^3$. The phenomenological coefficients given by Eqs. (A14)–(A18) are expressed in terms of the electronic model parameters. This allows us to extract relevant information about the electronic structure from a fitting analysis of the experimental transport curves at low temperatures, in the way described in previous works (Refs. 53 and 55). The remaining ones can be expressed as a linear combination of ξ_3 and ξ_4. Therefore, we can rewritte the higher-order J_{ij} matrix elements as

$$\begin{gathered}J_{06}=\xi_0(g_1\xi_4-g_2\xi_3)\equiv\xi_0 j_{06},\\ J_{15}=2\xi_0\left(\frac{q_0}{4}g_2\xi_4-g_3\xi_3\right)\equiv2\xi_0 j_{15},\\ J_{24}=\xi_0(q_0g_3\xi_4-g_4\xi_3)\equiv\xi_0 j_{24},\end{gathered}\tag{A22}$$

where

$$g_1\equiv2q_0q_1r\mathcal{Q}\mathcal{R},\quad g_3\equiv q_1r\mathcal{R}^2,$$

$$g_2\equiv r\mathcal{P}\mathcal{R},\quad g_4\equiv r\mathcal{S}\mathcal{R},$$

and $r\equiv1860q_1/49q_0^6$. Consequently, although we started with nine matrix elements we *only require five independent phenomenological coefficients* $\{\xi_0,\ldots,\xi_4\}$ in order to fully *describe all the reduced kinetic coefficients*, J_i. Making use of Eqs. (A13) and (A22), we can then express Eq. (A12) in terms of the phenomenological coefficients as

$$\begin{pmatrix}J_0\\J_1\\J_2\end{pmatrix}=4\sigma_0\begin{pmatrix}1&0&\xi_2&0&\xi_4&0&j_{06}\\0&2\xi_1&0&2\xi_3&0&2j_{15}&0\\\frac{\pi^2}{3}&0&\frac{\pi^2}{3}\frac{21}{5}\xi_2&0&\frac{\pi^2}{3}j_{24}&0&0\end{pmatrix}\begin{pmatrix}1\\bT/k_B\\bT^2\\b^2T^3/k_B\\b^2T^4\\b^3T^5/k_B\\b^3T^6\end{pmatrix},\tag{A23}$$

where $\sigma_0\equiv c_0\xi_0$. Hence, replacing the approximate kinetic coefficients J_i given by Eq. (A23) into Eqs. (A1)–(A4), one obtains close analytical expressions for the transport coefficients, Eqs. (9)–(14).

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