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Electron–phonon scattering rates in impure metals

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Abstract

We study the electron–phonon scattering rate $1/\tau_{ep}$ in impure metals in the dirty limit. We show that, if all impurities are substitutional, the previous Reizer–Sergeyev result, $1/\tau_{ep} \sim T^4$, holds even when discreteness of the lattice structure is taken into account, where T = temperature. However, the result is modified when we also allow for random positional shift of impurities, in which case the result $1/\tau_{ep} \sim T^2$, is obtained.

1. Introduction

Electron–phonon (e–ph) interaction in clean metals is well understood. However, for dirty systems, it is still a subject of investigation. The primary issue of concern is whether the presence of disorder weakens or enhances the e–ph interaction in the so-called dirty limit, i.e. $q_T l \ll 1$, where $q_T = k_B T/\hbar c_s$, with l = electron mean free path, T = temperature and c_s = the velocity of sound. This limit occurs when the temperature is sufficiently low or when the disorder is strong enough, and theoretical calculations performed by Schmid and co-workers [1, 2] and later by Reizer and Sergeyev [3] (referred to as RS in below) in the limit obtain the e–ph scattering rate $1/\tau_{ep} \propto T^4$. This rate is a reduction compared with the result for clean systems (characterized by the condition $q_T l \gg 1$), where $1/\tau_{ep}^{(0)} \propto T^3$ [4]. On the other hand, in the dirty limit, various T-dependences of the rate have been observed, including that of the theoretical prediction, $1/\tau_{ep} \propto T^4$ [5]. But it is widely reported to have observed the deviating behaviour, $1/\tau_{ep} \propto T^2$, which is an enhancement over the clean-limit result [6, 7]. The deviation from the theoretical prediction presents an interesting question and has been a subject of long-term study.

Since Schmid *et al* and RS obtain the same T^4-dependence with different theoretical approaches, the consensus among the theorists has been that the T^4-dependence is somewhat firmly established and, to explain the observed T^2-dependence, attention should turn to model assumptions. For example, Beltz *et al* [8] have introduced strong phonon damping, and

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demonstrated that it can modify $1/\tau_{ep}$ and lead to agreement with experiment. Sergeev *et al* [9] have invoked static random potentials which do not move with lattice vibrations, and obtained an enhanced $1/\tau_{ep}$, too.

In this paper, we shall address the role played by the 'geometric symmetry'[4] of impure systems in the issue of e–ph scattering rate. We shall show that, if the geometric translational symmetry of a metal is preserved in the presence of impurities, the e–ph scattering rate has the T^4-dependence. On the other hand, if the impurity destroys the symmetry, it results in the enhanced T^2-dependence.

2. Theoretical model

Since our calculation below is based on an extension of the RS treatment of e–ph scattering, our presentation shall avoid repeating details which can be found in RS. Let us firstly summarize their work. It contains an extensive analysis of Feynman diagrams, and it shows, for the calculation of the e–ph scattering rate, that there are two important classes of diagrams designated as A and B, respectively. Class A makes to $1/\tau_{ep}$ the contribution which is of the order of T^4, while class B contains basically two types of diagrams, each consisting of a leading-order T^2-term and a next-order T^4-term. RS show that the T^2-terms from the two types of diagrams in class B cancel exactly with each other but the higher-order T^4-terms do not. Upon summing classes A and B, therefore, it is the T^4-dependence that finally dominates the scattering rate.

A fact worth noticing is that, concerning the cancellation of T^2-terms as well as the non-cancellation of T^4-terms, there is a familiar parallel in the modelling of optical properties of a system. There, recall that, if inversion symmetry is present in the system, electric dipole transitions are zero between states of the same parity, while higher-order transitions, for example, magnetic dipole or electric quadrupole ones, can still be finite between them. Therefore, it may not be unreasonable to conjecture a similar symmetry-related reason for the fact noted above of the simultaneous occurrences of T^2-cancellation and T^4-non-cancellation. In other words, some specific symmetry may have been present in the RS model and results in a weakened scattering rate with theT^4-dependence. If the symmetry is removed, one may obtain the much stronger T^2-dependence.

We are thereby motivated to examine the geometric symmetry incorporated in the RS model. In particular, we shall focus on if there are any 'symmetry-introducing' approximations in the RS model. One candidate is the approximation of replacing the discrete lattice structure of a metal by a continuum. The approximation is not worded explicitly in their work but is implied by the fact that they use, in place of crystal waves containing cell-periodic Bloch functions, plane waves as unperturbed electronic eigenstates. This is a popular approximation in solid-state theory and generally valid. However, this approximation needs attention when impurities are present. Let us now consider a discrete lattice. When the lattice is doped with one impurity, two consequences can result depending on the location of the impurity. If the impurity substitutes for a host atom, then the translational symmetry of lattice is preserved (assuming we disregard the difference between the atomic potentials of an impurity and a host atom); whereas, if it precipitates to an interstitial place, the symmetry is broken. In contrast, within the continuum approximation of a lattice, it always results in the same situation irrespective of the impurity site, i.e. the translational symmetry is always preserved. In particular, in the case of a metal doped with non-substitutional impurities, the foregoing discussion implies that the

[4] We define a geometric symmetry to be a symmetry present in the system when impurities and host atoms are both regarded as simple geometric objects undistinguishable from one another. This is somewhat different from the usual notion of symmetry in physics.

continuum approximation would *over-impose* translational symmetry on the metal where, as a matter of fact, such a symmetry should be absent.

Apart from the above concern about a possible interplay between the symmetry and scattering rate, another reason why, in the present context, it is worthwhile considering the discrete nature of a metal is the following. The e–ph scattering is a wave phenomenon, and it depends on the interference between various scattering paths. To accurately account for the interference, especially that between scatterings of an electron off moving impurities and those off moving host atoms, one must consider the exact positions of impurities relative to the host lattice. Thereby, it suggests that one should take into account the discrete nature of a lattice.

In what follows, we shall provide evidence for our conjecture of a relation existing between the translational symmetry and the e–ph scattering rate. In particular, we shall carry out two calculations, all in the limit of dilute impurity concentration. Firstly, we shall show that, when one considers a discrete lattice with only substitutional impurities (in which case the translational symmetry is preserved) the cancellation of T^2-terms shown in the RS calculation still holds and, so, the scattering rate still scales as T^4. Secondly, we shall show that, when one considers a discrete lattice with non-substitutional impurities (in which case the translational symmetry is destroyed), the T^2-terms do not cancel, leading to a T^2-behaviour of the rate.

2.1. A discrete lattice with only substitutional impurities

To facilitate the calculation, the lattice is taken to have inversion symmetry. (We shall constantly assume so for a clean lattice throughout this work, valid for most metals.) We carry out a calculation where both impurity and interaction effects on electrons are treated within perturbation theory. We write the total perturbation as $H_{\rm int} = H_{\rm e-e} + H_{\rm e-i} + H_{\rm e-ph} + H_{\rm e-mi}$, where $H_{\rm e-e}$ is the e–e interaction, $H_{\rm e-i}$ the electron–impurity (e–i) interaction, $H_{\rm e-ph}$ the e–ph interaction, and $H_{\rm e-mi}$ the electron–moving impurity (e–mi) interaction. In the work of RS, unperturbed electron states are approximated with plane waves, and the perturbation is evaluated within the usual impurity-diagrammatic technique [10]. The present calculation differs from latter mainly in that we take into account the discrete lattice structure and use, in place of plane waves, the crystal wave function $\psi_p = |p\rangle = \exp(\mathrm{i}p\cdot r)u_p(r)$, where u_p is the cell-periodic Bloch function. We discuss how it modifies, for example, the RS e–i and e–mi vertices. For scattering of an electron off the impurity at lattice site R_i, we obtain the following scattering matrix element (assuming the system volume is unity):

$$\langle p{+}k|V_{\rm imp}(r-R_i)|p\rangle = \sum_{\rm G} V_{\rm imp}(k-G)C(G;\,p+k,\,p)\exp[-\mathrm{i}(k-G)\cdot R_i]$$

where G is a reciprocal lattice vector and $C(G;\,p+k,\,p) \equiv \int \exp(-\mathrm{i}G\cdot r)u^*_{p+k}u_p\,\mathrm{d}r$. In contrast, in the RS calculation, $C(G;\,p+k,\,p) = \delta_{G,0}$, and the element is $\langle p+k|V_{\rm imp}(r-R_i)|p\rangle = V_{\rm imp}(k)\exp(-\mathrm{i}k\cdot R_i)$. To adapt the diagrammatic technique to the present calculation, we replace the RS e–i vertex, $V_{\rm imp}(k)\exp(-\mathrm{i}k\cdot R_i)$, with ours. To modify the e–mi vertex, we write (with $\hbar = 1$)

$$H_{\rm e-mi} = \sum_{p,\sigma}\sum_{k\neq 0}\sum_{q\neq 0,\lambda}\sum_{G} C(G;\,p,\,p-k)\;\gamma(k-G,q,\lambda)c^+_{p,\sigma}c_{p-k,\sigma}(b_{q,\lambda}+b^+_{-q,\lambda}) \times\sum_{R_i}\exp[-\mathrm{i}(k-G-q)\,R_i]$$

where $\gamma(k-G,q,\lambda) = -\mathrm{i}V_{\rm imp}(k-G)\,(k-G)\cdot e_{q\lambda}/(2MN\omega_{q\lambda})^{1/2}$. In the above, c and c^+ are electron operators, b and b^+ phonon operators, $e_{q\lambda}$ a unit vector along the phonon polarization,

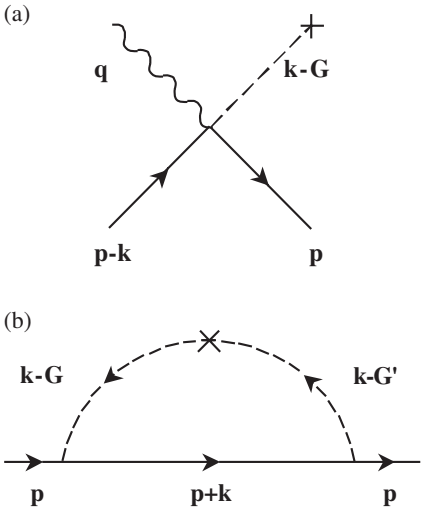

Figure 1. (a) The diagram of an e–mi interaction vertex. (b) The self-energy diagram due to the e–i interaction. Solid line—electron line, wavy line—phonon line, dashed line—impurity line, 'x'—impurity.

λ the phonon branch index, M = mass of a unit cell, N = number density of unit cells, and $\omega_{q\lambda}$ = phonon energy. In figure 1 (a), we show the diagram for an e–mi interaction vertex. The vertex is proportional to[5] $\mathrm{i}(k-G)\cdot e_{q\lambda}V_{\mathrm{imp}}(k-G)/\varepsilon(k-G,\omega)$. Here, we have included the dynamic screening of the e–mi vertex by the e–e interaction, with $\varepsilon(k-G,\omega)$ the dielectric function. For comparison, the corresponding RS vertex is proportional to $\mathrm{i}\,k\cdot e_{q\lambda}V_{\mathrm{imp}}(k)/\varepsilon(k,\omega)$.

We now examine how the RS result of scattering rates is modified. Let us firstly calculate the impurity scattering rate, which is the imaginary part of the self-energy[6] in figure 1 (b). We note a few facts which shall be used in the calculation. Firstly, there are two useful identities involving C:

$$\sum_G C(G;\,p+k,\,p)=\psi^*_{p+k}(r=0)\,\psi_p(r=0) \tag{1}$$

$$\sum_G C(G;\,p+k,\,p)(k-G)=\mathrm{i}\times\nabla[\psi^*_{p+k}(r)\psi_p(r)]_{r=0} \tag{2}$$

$$C(G;\,p+k,\,p)=\text{real} \tag{3}$$

$$\psi^*_p(r)=\psi_{-p}(r)\qquad\text{and}\qquad|\psi_p(r)|=|\psi_p(-r)|. \tag{4}$$

Equations (1) and (2) follow from the definition of $C(G;\,p+k,\,p)$, (3) from inversion symmetry[7], and (4) from time reversal and inversion symmetries of the system, respectively. In accordance with RS, we take, for simplification, the impurity potential screened by conduction

[5] We have adopted the convention where a momentum is associated with an impurity line. Let the impurity momentum be $k-G$, we then associate $\mathrm{i}(k-G)\cdot e_{q\lambda}V_{\mathrm{imp}}(k-G)/\varepsilon(k-G,\omega)$ with the e–mi vertex, and weigh each vertex with the factor $C(G;\,p,\,p-k)$, where $p-k$ = incoming electron momentum and p = outgoing electron momentum, and sum the result over G.

[6] Similar to the case of e–mi vertex, the e–i vertices are to be weighted by $C(G;\,p+k,\,p)$ and $C^*(G';\,p+k,\,p)$ and summed over G and G'.

[7] We write $u_{\mathrm{p}}(\mathrm{r})=\sum_G \mathrm{d}(G;\,p)\,\exp(\mathrm{i}G\cdot r)$, and note that $\mathrm{d}(G;\,p)$ satisfies the Hamiltonian matrix equation

$$[\hbar^2(p+G)^2/2m-\xi_p]\,\mathrm{d}(G;\,p)+\sum_{G'}V(G-G')\,\mathrm{d}(G';\,p)=0$$

where $V(G-G')$ is the Fourier transform of $V(r)$, the crystal potential. Using the property $V(r)=V(-r)$, $V(G-G')$ is real. Therefore, the solution $\mathrm{d}(G;\,p)$ to the Hamiltonian equation can be chosen to be real. Using such u_p and u_{p+k} to evaluate $C(G;\,p+k,\,p)\equiv\int\exp(-\mathrm{i}G\cdot r)u^*_{p+k}u_p\,\mathrm{d}r$, one sees that $C(G;\,p+k,\,p)$ is real.

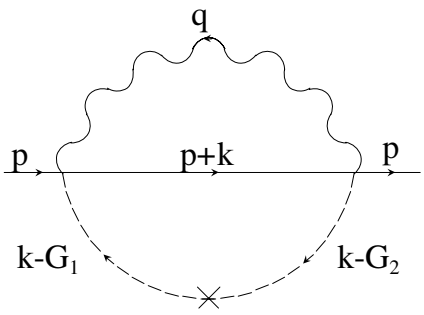

Figure 2. The diagram for I_7.

electrons to be a δ-function with strength V_0 and obtain the impurity scattering rate of the state $|p\rangle$ at the Fermi level

$$\begin{aligned}\frac{1}{\tau_p} &= 2\pi \sum_k N_{\rm imp}|V_0|^2 \delta(\xi_{p+k}-\xi_p) \sum_{G,G'} C(G;\, p+k,\, p)\, C^*(G';\, p+k,\, p) \\ &= 2\pi |\psi_p(r=0)|^2 \sum_k N_{\rm imp}|V_0|^2 \delta(\xi_{p+k}-\xi_p)|\psi_{p+k}(r=0)|^2 \\ &= \frac{1}{\tau_0}|\psi_p(r=0)|^2 \int \frac{{\rm d}\Omega_{p+k}}{4\pi}\,|\psi_{p+k}(r=0)|^2 \end{aligned} \tag{5}$$

where $N_{\rm imp}$ = impurity density, ξ_p = electronic energy, and $\frac{1}{\tau_0} \equiv \pi \nu\, N_{\rm imp}\, |V_0|^2$ with ν = electronic density of states at the Fermi level. The second line of equation (5) is obtained from the first line with C and C^* replaced according to equations (1)–(4). We note, incidentally, that $1/\tau_0$ is the impurity scattering rate in the RS calculation. Therefore, equation (5) shows how the RS result of impurity scattering is modified when discreteness of the lattice structure is taken into account.

Next, we calculate the e–ph scattering rate. We shall consider mainly the dominant diagrams (of class B) in figures 2 and 3, each of which involves the e–mi interaction and gives rise to an integral (designated by RS as I_7 and I_8, respectively) making an order of T^2 contribution to the rate. Other diagrams, i.e. those of class A, have been shown by RS to result in an integral, designated as I_A, which is of the order of T^4. With the integrals, the rate is determined as $\frac{1}{\tau_{\rm ep}(\xi)} = -\frac{\delta(I_7+I_8+I_A)}{\delta n_\xi}$, where n_ξ is the Fermi–Dirac distribution function at energy ξ. For the diagram in figure 2, we have the integral

$$\begin{aligned} I_7 = \frac{\rm i}{\pi\nu}\frac{N_{\rm imp}|V_0|^2}{2MN}\int \frac{{\rm d}^3p\,{\rm d}^3(p+k)\,{\rm d}^3q\,{\rm d}\omega}{(2\pi)^{10}}\,\frac{J_7 R(\xi,\omega)}{\omega_{q,\lambda}}[G^A(p,\xi)-G^R(p,\xi)] \\ \times[G^A(p+k,\xi+\omega)-G^R(p+k,\xi+\omega)]\,[D^R(q,\omega)-D^A(q,\omega)] \end{aligned} \tag{I.1}$$

where

$$\begin{aligned} J_7 &= \sum_{G_1,G_2} C(G_1;\, p+k,\, p)\, C^*(G_2;\, p+k,\, p)\,[e_{q\lambda}\cdot(k-G_1)]\,[e_{q\lambda}\cdot(k-G_2)] \\ &= |e_{q\lambda}\cdot\nabla[\psi^*_{p+k}(r)\,\psi_p(r)]_{r=0}|^2. \end{aligned} \tag{I.2}$$

The second line of (I.2) is obtained with the help of equations (1)–(4). For comparison, we also list the corresponding J_7 of RS here

$$J_7^{RS} = (e_{q\lambda}\cdot k)^2.$$

In I_7, the expression R is given as

$$R(\xi,\omega) = N_\omega n_\xi (1-n_{\xi+\omega}) - (1+N_\omega)(1-n_\xi)n_{\xi+\omega}$$

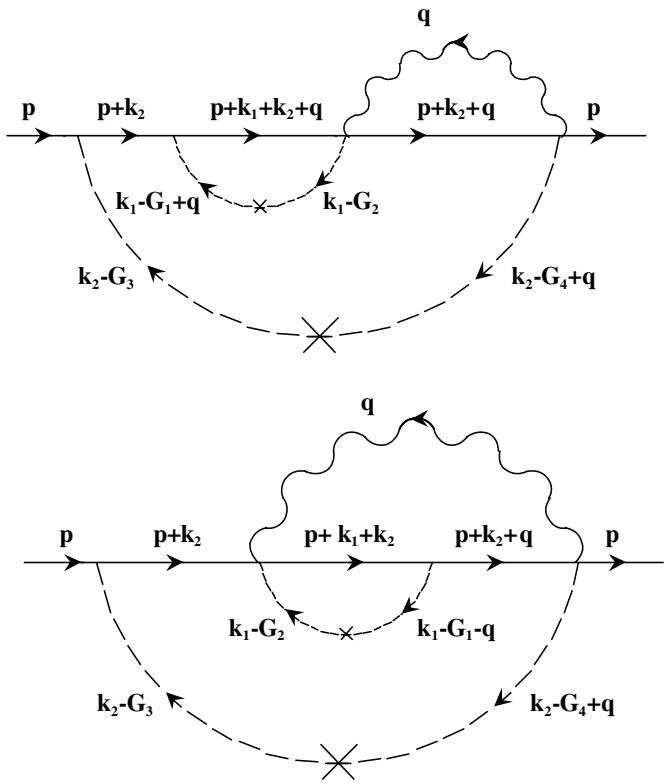

Figure 3. The diagram for I_8. Each diagram here actually has a symmetric counterpart not shown in the figure.

with N_ω the Bose–Einstein distribution. G^R and G^A are retarded and advanced Green functions, respectively, with

$$G^R(p,\xi) = [G^A(p,\xi)]^* = (\xi - \xi_p + \mathrm{i}/2\tau_p)^{-1}.$$

D^R and D^A are retarded and advanced phonon propagators, respectively, with

$$D^R(q,\omega) = [D^A(q,\omega)]^* = (\omega - \omega_{q\lambda} + \mathrm{i}0)^{-1} - (\omega + \omega_{q\lambda} + \mathrm{i}0)^{-1}.$$

Using the properties, equations (1)–(4), we obtain

$$I_7 = -\frac{\pi\nu N_{\mathrm{imp}}|V_0|^2}{MN}\int\frac{\mathrm{d}^3q}{(2\pi)^3}\frac{R(\xi,\omega_{q\lambda})}{\omega_{q\lambda}}\int\frac{\mathrm{d}\Omega_p}{4\pi}|\psi_p(r=0)|^2 \times\int\frac{\mathrm{d}\Omega_{p''}}{4\pi}\left|e_{q\lambda}\cdot[\nabla\psi_{p''}(r)]_{r=0}\right|^2. \tag{6}$$

Next, we calculate the contribution from the diagrams in figure 3. Each diagram here actually has a symmetric counterpart not explicitly shown in the figure. With all these diagrams, we have the integral

$$I_8 = \frac{\mathrm{i}}{\pi\nu}\frac{N_{\mathrm{imp}}^2|V_0|^4}{2MN}\int\frac{\mathrm{d}^3p\,\mathrm{d}^3(p+k_1+k_2)\,\mathrm{d}^3(p+k_2)\,\mathrm{d}^3q\,\mathrm{d}\omega}{(2\pi)^{13}}\;\frac{J_8R(\xi,\omega)}{\omega_{q\lambda}} \times[G^A(p,\xi) - G^R(p,\xi)]$$

$$\times[G^A(p+k_1+k_2,\xi+\omega)-G^R(p+k_1+k_2+q,\xi)]$$
$$\times[G^R(p+k_2,\xi)\,G^A(p+k_2+q,\xi+\omega)+\text{c.c.}]$$
$$[D^R(q,\omega)-D^A(q,\omega)] \tag{I.3}$$

where

$$J_8=\sum_{G_1G_2G_3G_4} C(G_1;\,p+k_1+k_2,\,p+k_2)C^*(G_2;\,p+k_1+k_2,\,p+k_2\,)C(G_3;\,p+k_2,\,p\,)$$
$$\times C^*(G_4;\,p+k_2,\,p\,)\,[(k_2-G_4)\cdot e_{q\lambda}][(k_1-G_2)\cdot e_{q\lambda}]. \tag{I.4}$$

For comparison, in the RS calculation,

$$J_8^{RS}=(k_2\cdot e_{q\lambda})(k_1\cdot e_{q\lambda}).$$

To proceed, we note that the major contribution to the integral I_8 comes, when integrated with respect to q, from $q\sim q_T$, the thermal phonon wavevector. Since q_T is small at low temperatures, we can regard the phonon wavevector q as also being small, and Taylor-expand the integrand of I_8 around $q=0$. We retain only the leading-order term, which, because $q\sim q_T=k_{\rm B}T/\hbar c_s$, corresponds to the dominant T-dependence. With the approximation, we obtain

$$J_8\approx-|\psi_p(r=0)|^2|\psi_{p+k_1+k_2}(r=0)|^2|\psi_{p+k_2}(r=0)|^2|e_{q\lambda}\cdot[\nabla\psi_{p+k_2}(r)]_{r=0}|^2$$

and

$$I_8\approx\frac{\pi\nu N_{\rm imp}|V_0|^2}{MN}\int\frac{{\rm d}^3q}{(2\pi)^3}\,\frac{R(\xi,\omega_{q\lambda})}{\omega_{q\lambda}}\int\frac{{\rm d}\Omega_p}{4\pi}\,|\psi_p(r=0)|^2\int\frac{{\rm d}\Omega_{p'}}{4\pi}|\psi_{p'}(r=0)|^2$$
$$\times\int\frac{{\rm d}\Omega_{p''}}{4\pi}\,\frac{\tau_{p''}}{\tau_0}|\psi_{p''}(r=0)|^2|e_{q\lambda}\cdot[\nabla\psi_{p''}(r)]_{r=0}|^2 \tag{7}$$

correct to the order of q_T^2. The next-order term corresponds to the order[8] of q_T^4 (or T^4). Now, we sum integrals I_7 and I_8, and obtain

$$I_7+I_8\approx\frac{\pi\nu N_{\rm imp}|V_0|^2}{MN}\int\frac{{\rm d}^3q}{(2\pi)^3}\,\frac{R(\xi,\omega_{q\lambda})}{\omega_{q\lambda}}\int\frac{{\rm d}\Omega_p}{4\pi}|\psi_p(r=0)|^2$$
$$\times\int\frac{{\rm d}\Omega_{p''}}{4\pi}\left\{|e_{q\lambda}\cdot[\nabla\psi_{p''}(r)]_{r=0}|^2\right.$$
$$\left.\times\left[-1+|\psi_{p''}(r=0)|^2\frac{\tau_{p''}}{\tau_0}\int\frac{{\rm d}\Omega_{p'}}{4\pi}|\psi_{p'}(r=0)|^2\right]\right\}=0+{\rm o}(T^4)$$

where equation (5) has been used to obtain the last line. It then follows that $\frac{1}{\tau_{\rm ep}(\xi)}=-\frac{\delta(I_7+I_8+I_A)}{\delta n_\xi}={\rm o}(T^4)$. In summary, in the present case where a discrete lattice with substitutional impurities is considered, the e–ph scattering rates varies as T^4.

2.2. A discrete lattice with non-substitutional impurities

In a previous paper by Jan, Wu and Wei (referred to as JWW in what follows) we studied the particular case of polycrystalline systems with grain boundary defects, where a T^2-behaviour of the e–ph scattering rate is derived [11]. In this work, we shall consider impurities with positional shift. Although such a case is perhaps not easy to realize in experiments, the purpose here is to demonstrate, from a theoretical point of view, that destruction of translational symmetry can enhance the scattering rate. We study two cases, in particular. In case 2.1, deviation of impurity sites from lattice points is completely random. In case 2.2, the deviation is small in magnitude. The calculation proceeds in a manner similar to that in JWW.

[8] This can be seen by carrying out the q expansion to higher order.

Case 2.1. Note firstly the following important fact. In the impurity-diagrammatic technique, results have to be averaged over all impurity configurations. With the random positional shift of impurities, the diagrams surviving the configuration average are those such as that of figure 1(*b*) *with* $G = G'$. This particular diagram, for example, contains the factor $\sum_{R_i} \exp[-\mathrm{i}(G' - G) \cdot R_i]$, a sum over the random distribution of impurity position R_i, and is finite only when $G = G'$. A similar derivation shows that, for the present calculation of the e–ph scattering rate, the earlier expressions, (I.1)–(I.4), should be used with the modification that[9] $G_1 = G_2$ and $G_3 = G_4$.

We discuss the functional dependence of $1/\tau_{\mathrm{ep}}$ in the following way. Firstly, note that, in the mathematical expressions I_7 and I_8, we can regard the Fermi wavevector k_f as a continuous variable and I_7 and I_8 as functions of k_f. For technical purposes, we require their domain of k_f to be the interval $(k_f^-, k_f^+ \sim \mathrm{o}(G/2))$, with k_f^- small but still large enough to satisfy the condition $k_f^- l \gg 1$. For example, if $l = 100a/\pi$, we take k_f^- to be $0.1\pi/a$. The enforcement of the foregoing inequality is to make sure that we are always in the limit of dilute impurity concentration, so the expressions I_7 and I_8 obtained in the limit can be consistently used throughout the interval (k_f^-, k_f^+).

We now evaluate $1/\tau_{\mathrm{ep}}$ for the case where k_f is small, i.e. near k_f^-. In this case, our argument against the cancellation of T^2-terms in $1/\tau_{\mathrm{ep}}$ is made in two steps. (A) First we make the approximation that $u_{kf} \sim u_0$, where u_{kf} and u_0 are the Bloch cell-periodic functions at k_f and at the zone centre, respectively. The validity of this approximation follows from the $k \cdot p$ theory of band structures in which one expands u_{kf} in a perturbation series with u_0 being the leading-order term. Moreover, we assume reasonably that u_0 has the full symmetry of the lattice, for example, u_0 is S-like in the case of a crystal with cubic symmetry. With the approximation that $u_{kf} \sim u_0$, we have $C(G; p_1, p_2) \sim C(G; 0, 0)$ when p_1 and p_2 both are restricted to the Fermi surface. Moreover, it is obvious that $|C(G; 0, 0)| = |\int \exp(-\mathrm{i}G \cdot r) u_0^* u_0 \, \mathrm{d}r| = |C(|G|; 0, 0)|$, independent of the G direction, which follows from the, for example, S-like symmetry of u_0. (B) Next, we note that, in J_7 and J_8, the phonon wavevector $q \sim 0$, and, moreover, the electron wavevectors p, $p + k$, $p + k_2$ and $p + k_1 + k_2$ which appear as arguments in various $C(G)$ there are all restricted to the Fermi surface, both due to the fact that contributions to the integrals I_7 and I_8 mainly come from the region with $q \sim 0$ and with the foregoing electron wavevectors $\sim k_f$. So, we can take all $C(G)$ in J_7 and J_8 as $C(G; k_f, k_f)$, which can be replaced with $C(G; 0, 0)$, according to (A). With this, we expand J_7 and obtain the cross term

$$2\sum_G |C(G; 0, 0)|^2 (k \cdot e_{q\lambda})(G \cdot e_{q\lambda}) = 2\sum_{|G|} |C(|G|; 0, 0)|^2 (k \cdot e_{q\lambda}) \left(e_{q\lambda} \cdot \sum_{\Omega_G} G \right)$$

where $\sum_{\Omega_G} G$ denotes the summation of G over the direction of G with the magnitude $|G|$ fixed. Since $\sum_{\Omega_G} G = 0$ with G distributing symmetrically for a crystal of, say, cubic symmetry, the cross term vanishes. We are then left with only the squared terms in J_7 and, so,

$$J_7 = \sum_G |C(|G|; 0, 0)|^2 [(k \cdot e_{q\lambda})^2 + (G \cdot e_{q\lambda})^2]. \tag{8}$$

Similarly, we have

$$J_8 = \sum_{G,G'} |C(|G|; 0, 0)|^2 |C(|G'|; 0, 0)|^2 (k_1 \cdot e_{q\lambda}) \, (k_2 \cdot e_{q\lambda}). \tag{9}$$

[9] Sums of the type $\sum_{R_i} \exp[-\mathrm{i}(G' - G) \cdot R_i]$ represent interference among various scattering events. The modification with $G_1 = G_2$ and $G_3 = G_4$ means that the random positional shift of impurities bears a certain effect on the interference.

We note that the $(k \cdot e_{q\lambda})^2$-term in J_7 and the whole J_8 are of the same forms as those of J_7^{RS} and J_8^{RS}, respectively. When put back in the integrals I_7 and I_8, they both result in the order of T^2 contributions to $1/\tau_{\mathrm{ep}}$ that cancel with each other just as in the RS calculation. This leaves us the $(G \cdot e_{q\lambda})^2$-term in J_7. It is easy to see that the $(G \cdot e_{q\lambda})^2$-term, when integrated, makes a T^2-order contribution to $1/\tau_{\mathrm{ep}}$, comparable to that from the $(k \cdot e_{q\lambda})^2$-term. Therefore, after summing I_7 and I_8, we obtain $1/\tau_{\mathrm{ep}} \sim \mathrm{o}(T^2)$.

(A) together with (B) is a rigorous argument in the case of small k_f. This result is significant and distinct from that of RS, since theirs always gives T^4-dependence regardless of the value of k_f.

Now, we discuss the functional dependence of $1/\tau_{\mathrm{ep}}$ when k_f increases towards $\mathrm{o}(G/2)$, which is the case for a practical metal. Generally speaking, cancellation among terms is less likely to occur than non-cancellation, unless there is certain symmetry-dictated reason behind it. A good example is the earlier-discussed electric dipole transition between two states, which is usually finite unless there is inversion symmetry and the two states are of the same parity. In our case, if there should be a symmetry-caused cancellation, it would have shown up in the foregoing calculation for a small k_f, since such symmetry is not likely to depend on the value of k_f. The fact that the cancellation does not occur there strongly suggests lack of such symmetry. Moreover, if we write $1/\tau_{\mathrm{ep}} = f(k_f)T^2$ and regard $f(k_f)$ as an analytic function of k_f, with $f(k_f) \geqslant 0$, it is hardly likely that the coefficient $f(k_f)$ should vary from being non-vanishing in the domain of small k_f, proved earlier, to being *identically zero* for all large values of k_f. Therefore, we can conclude convincingly against the vanishing of $f(k_f)$ for a general value of k_f. In other words, the e–ph scattering rate varies as T^2 in the general case of a discrete lattice with non-substitutional impurities.

Case 2.2. We now turn to the case where impurity sites deviate only slightly from lattice points. We write the impurity position $R_i = R_{i0} + s_i$, where R_{i0} is the corresponding lattice vector and s_i = deviation. We take $|s_i| = s_0 =$ constant, with $s_0 \ll a$, and the orientation of s_i to be random. Moreover, we take k_f to be small, just as in case 2.1, and continue to make use of the properties of $C(G)$ discussed there in this regime. These properties allow us to obtain analytical result in the present case. Since the calculation proceeds in much the same way as in case 2.1, we shall only sketch the major difference between this one and that in case 2.1.

Recall that, in case 2.1, because of the fact that $\sum_{R_i} \exp[-\mathrm{i}(G' - G) \cdot R_i] \propto \delta_{G,G'}$, only diagonal terms (such as those with $G_1 = G_2$ and $G_3 = G_4$) in the diagrams contribute. But in the present case, this is no longer true and we have to use the full expression instead. For example, we need to insert $(1/N_{\mathrm{imp}})\sum_{R_i} \exp[\mathrm{i}(G - G') \cdot R_i]$ in (5) and write

$$\frac{1}{\tau_p} = 2\pi \sum_k N_{\mathrm{imp}} |V_0|^2 \delta(\xi_{p+k} - \xi_p) \sum_{G,G'} \left\{ C(G;\, p+k,\, p)\, C^*(G';\, p+k,\, p) \times \left[\frac{1}{N_{\mathrm{imp}}} \sum_{R_i} \exp[\mathrm{i}(G - G') \cdot R_i] \right] \right\}.$$

Similarly, we need to insert, respectively, $(1/N_{\mathrm{imp}})\sum_{R_i} \exp[\mathrm{i}(G_1 - G_2) \cdot R_i]$ in (I.2) and $(1/N_{\mathrm{imp}})\sum_{R_i} \exp[\mathrm{i}(G_1 - G_2) \cdot R_i](1/N_{\mathrm{imp}})\sum_{R_j} \exp[\mathrm{i}(G_3 - G_4) \cdot R_j]$ in (I.4). We then Taylor-expand these additional factors to the order of s_0^2. This leads to

$$I_7 + I_8 = -\frac{2\pi s_0^2}{3} \frac{\pi \nu N_{\mathrm{imp}} |V_0|^2}{MN} \int \mathrm{d}^3 q \, \frac{R(\xi, \omega_{q,\lambda})}{\omega_{q,\lambda}} \left| \sum_G C(|G|;\, 0,\, 0)\, (G \cdot e_{q\lambda})^2 \right|^2.$$

From it, we obtain $1/\tau_{\rm ep}(s_0) \sim {\rm o}(s_0^2/a^2)\, 1/\tau_{\rm ep,\ case\,2.1}$ to the order of T^2, where $1/\tau_{\rm ep}(s_0)$ is the e–ph scattering rate in the present case and $1/\tau_{\rm ep,\ case\,2.1}$ is the scattering rate obtained in the case of a random positional shift of impurities, i.e. case 2.1.

It is interesting to examine the last scattering rate result in various limits. Firstly, if we increase the deviation parameter and extrapolate the expression to $s_0 \sim {\rm o}(a)$, the result is in agreement with that obtained in case 2.1, where the deviation is large. Secondly, in the limit of vanishing deviation, it gives $1/\tau_{\rm ep}(s_0 \to 0) \to 0$ to the order of T^2, in agreement with our earlier 'substitutional' result. If we further take the limit $a \to 0$, we obtain $\lim_{a\to 0} \lim_{s_0 \to 0} 1/\tau_{\rm ep}(s_0) = 0$ to the order of T^2, which is the 'continuum' result of RS.

3. Conclusion

In summary, we have discussed the temperature dependence of $1/\tau_{\rm ep}$ in the dirty limit for impurity-doped metals. Discreteness of the lattice structure has been taken into account in the calculation. We show, in the case of substitutional impurities, that the previous RS result, $1/\tau_{\rm ep} \sim T^4$, holds. However, the result is modified when we allow for destruction of the translational symmetry by random positional shift of impurities, and an enhanced rate, $1/\tau_{\rm ep} \sim T^2$, is obtained.

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