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The energy loss rate and dynamical resistivity of hot electrons in semiconductors

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Abstract. Among many proposed field theories for thermal phenomena, thermo-field dynamics (TFD) is a very useful and simple tool to study non-equilibrium many-body systems, especially for a complicated system composed of several subsystems at different thermal equilibria. A complete perturbative calculation scheme in TFD for such systems will be presented. In the TFD method, explicit investigation will be made of the energy loss rate (ELR) and resistivity of hot electrons in semiconductors. Our ELR formula is shown to be different from that obtained by the Keldysh method. The possible ambiguity in the Keldysh method is discussed.

1. Introduction

The present paper is to address the following questions: when the electrons in semiconductors are heated up by a very short laser beam pulse, what will be (1) the dynamical resistivity, and (2) the energy loss rate (ELR) of the hot electrons?

The study of hot-electron energy relaxation and dynamical resistivity has been of great interest among experimentalists in the past [1]. An early theoretical description of the ELR in the hot-electron system is that of Kogan [2] who used Fermi-golden-rule theory. Recently, the Keldysh Green-function method was used by Dharma-wardana [3, 4] to study the ELR of hot electrons in semiconductors, in order to study the effect of the coupled optical mode. His results did not agree with the earlier results claimed by Das Sarma *et al* [5], who found that the coupled mode is responsible for a significant increase of ELR at low electron temperatures. Upon inspection, however, I found that the Keldysh method might need some modification in order to be applied to the hot-electron problem in the wide range of electron temperatures concerned [6].

This paper is a theoretical study of the dynamical properties of hot-electron system. I try to provide an alternative Green-function method, *thermo-field dynamics* (TFD), to study the dynamical resistivity and ELR of hot electrons in condensed matter. I shall derive the mathematical formulae for the resistivity and ELR in the TFD framework. I show that my expression for ELR is somewhat different from that derived from the Keldysh method. In order to facilitate the readers' judgement of the discrepancy between the Keldysh and TFD methods, I shall first briefly discuss some important aspects of the Keldysh method, followed by a detailed formulation of TFD general non-equilibrium problems. My calculation of the dynamical resistivity and ELR will be carried out based on the formulation presented. The possible limitation of the Keldysh method will also be pointed out. Here I would like to mention that in his recent NATO report [6] and in [4], Dharma-wardana also noted the discrepancy between the TFD approach and the Keldysh approach.

The present paper thus has the following structure. In this section I try to make a few comments on the Keldysh method. Then I shall discuss different representations (denoted by different α values) of TFD in the next section, followed by the detailed formulation of $\alpha = \frac{1}{2}$ TFD for non-equilibrium situations in section 3. The application to hot-electron problems will be presented in section 4. A final summary concludes the paper. Those who are already familiar with the Keldysh method and the basic concepts of the TFD method can start reading from section 3. I choose to separate section 3 from section 4 simply because I hope that the general formulation in section 3 can also be applied to other non-equilibrium many-body problems.

An early attempt to study many-body systems at finite temperature by using quantum-field theory was made by Matsubara in 1955 [7]. In his method, the temperature is regarded as an imaginary time resulting in a discrete summation over frequencies. However, the applicability of Feynman rules in momentum space in the Matsubara method was not clarified until two independent works by Abrikosov *et al* [8] and Umezawa *et al* [9]. The possible application of the quantum-field theory to non-equilibrium thermal systems in the linear-response approximation was later pursued by many scientists, Martin and Schwinger [10], Kadanoff and Baym [11], Keldysh [12] and Takahashi and Umezawa [13], to name just a few. Among the theories proposed by these physicists, the Keldysh method (also called the closed-path integral method) [12] is most widely used. It has been applied to transport phenomena, superconductivity, spin systems, laser systems [14], hot-electron systems [3, 15], quantum wires and so on. In contrast, TFD invented by Umezawa and his collaborators in the early 1970s [13, 16, 17] is less well known to condensed matter physicists. In the present paper I will show general readers that TFD is a very simple and useful tool not only in dealing with equilibrium states [18, 19], but in the study of non-equilibrium many-body problems.

In order to appreciate the simplicity of the TFD approach, let us first discuss briefly the Keldysh method. A good review of this method can be found in [20]. The core of the application of quantum-field theory to condensed matter is to calculate the Green function as follows:

$$\mathbf{G}(x_1 - x_2) = -i\langle T(A(x_1)B(x_2)) \rangle \quad (1.1)$$

where $\langle A \rangle = \text{Tr}[\rho A]$ with ρ being the thermal density operator, i.e. $\rho = \exp(-\beta\mathbf{H})$. All quantities are in the Heisenberg representation. T represents the usual time ordering. After choosing a proper time contour, the above Green function can be rewritten as a closed-path Green function which can be put into a 2×2 matrix form,

$$\mathbf{G} = \begin{pmatrix} G^R & G^K \\ 0 & G^A \end{pmatrix}$$

where G^R and G^A are the retarded and advanced Green functions respectively, and $G^K(x_1, x_2) = -i\langle [A(x_1)B(x_2)]_{\pm} \rangle$. Two main difficulties may be associated with this approach. First, the calculation of the Dyson equation is non-trivial for general non-equilibrium cases. For example, the off-diagonal term in the Dyson equation reads $G^K = G^R G^A [(G_0^K / G_0^R G_0^A) - \Sigma^K]$, which is not easy to calculate. Second, the choice of the time path depends on the thermal parameter β (please note that in the equilibrium case only, $\beta = 1/k_B T$). This is a crucial point with regard to the transform of the density matrix from the starting one $\rho (= \exp(-\beta\mathbf{H}))$ to that in the interaction picture, i.e. $\rho_0 = \exp(-\beta\mathbf{H}^I)$. Here \mathbf{H} is the total Hamiltonian in the Heisenberg picture, and \mathbf{H}^I is the free Hamiltonian in the interaction picture. In a multi-temperature system this transformation may become ambiguous. We will come back to this point later.

2. TFD and its different representations

Although there are many papers and books on TFD, I choose to describe TFD heuristically in this section so that general readers could have some primitive ideas about TFD and will not have to read references back and forth. Those who want to know the details of the foundation of TFD are referred to the book by Umezawa [17].

Suppose a_k and a_k^\dagger are annihilation and creation operators respectively of a particle with momentum k on a vacuum $|0\rangle$ at zero temperature: $a_k|0\rangle = 0$ and $\langle 0|a_k^\dagger a_k|0\rangle = 0$. At finite temperature the thermal population of the particle makes $\langle a_k^\dagger a_k \rangle \neq 0$. In the Matsubara or Keldysh methods, these brackets denote thermal averaging. When we compare this with the calculation of the order parameter in superconductivity, it is suggestive to define a thermal vacuum, $|0(\beta)\rangle$, and its conjugate $\langle 0(\beta)|$ and we hope that the thermal occupation can be calculated from a simple operator algebra, i.e. $n_k = \langle 0(\beta)|a_k^\dagger a_k|0(\beta)\rangle$. At equilibrium, as is well known, $n_k = 1/(\exp(\beta\epsilon_k) \pm 1)$ (the sign depends on whether the particle is a fermion or a boson). If we can define the thermal vacuum $|0(\beta)\rangle$, then obviously a_k, a_k^\dagger are not the annihilation and creation operators for this thermal vacuum, but experience with superconductivity gives us a hint that we may define a new set of annihilation and creation operators $\alpha_k, \alpha_k^\dagger$ on the thermal vacuum, i.e.

$$\alpha_k|0(\beta)\rangle = 0 \quad \langle 0(\beta)|\alpha_k^\dagger = 0.$$

The relation between (a_k, a_k^\dagger) and $(\alpha_k, \alpha_k^\dagger)$ should bear a similarity to the Bogoliubov transformation in the superconductivity. This idea is accomplished by introducing the 'ghost' operators or tilde operators, i.e. double-degree freedom. For any operator A , there is a tilde operator \tilde{A} to associate with it. Then the total Hamiltonian is $\hat{H} = \mathbf{H} - \tilde{\mathbf{H}}$. Thus in TFD, thermal averaging is replaced by a simple operator calculation. For the multi-temperature many-body system, the thermal vacuum is defined as $|0(\beta_1, \beta_2, \dots)\rangle \equiv |0(\beta_1)\rangle \otimes |0(\beta_2)\rangle \dots$, and the annihilation and creation operators of different subsystems can be defined in the different thermal vacuum states. In TFD, the thermal vacuum can be described as follows. In the equilibrium state, it was characterized by the given temperature ($\beta = 1/k_B T$) and usual equilibrium statistics; however in the non-equilibrium state, the parameter β does not usually correspond to a specific temperature. In the latter case, the thermal vacuum is characterized by the thermal occupation number n_k which may differ from either the usual bosonic or fermionic distributions.

The tilde operation can be summarized as

$$(AB)^\sim = \tilde{A}\tilde{B}, (cA)^\sim = c^*\tilde{A}, \tilde{\tilde{A}} = \sigma A \\ \langle\langle 0(\beta)|, |0(\beta)\rangle\rangle^\sim = (\langle 0(\beta)|, |0(\beta)\rangle).$$

In the above c is a c -number and $\sigma = 1, -1$ for fermions and bosons respectively. The relation between (a_k, a_k^\dagger) and $(\alpha_k, \alpha_k^\dagger)$ is through a so-called thermal Bogoliubov transformation. Without any specification, we write this relation conveniently as

$$\begin{pmatrix} \alpha_k \\ \tilde{\alpha}_k^\dagger \end{pmatrix} = \mathbf{B}(k, \alpha) \begin{pmatrix} a_k \\ \tilde{a}_k^\dagger \end{pmatrix}. \quad (2.1)$$

\mathbf{B} is the thermal Bogoliubov transformation matrix, which should be determined by the condition $n_k = \langle 0(\beta)|a_k^\dagger a_k|0(\beta)\rangle$. Because TFD is virtually an operator formalism, we can

have different representations with different rotation in the Fock space. Generally matrix \mathbf{B} is written as

$$\mathbf{B} = (1 + \sigma n_k)^{1/2} \begin{pmatrix} 1 & -f^\alpha(k) \\ -\sigma f^{1-\alpha}(k) & 1 \end{pmatrix} \quad (2.2)$$

with $f(k) = n_k/(1 + \sigma n_k)$. Therefore different representations of TFD can be classified by the factor α ($1 \geq \alpha \geq 0$). There are two commonly used representations of TFD: $\alpha = 1$ and $\alpha = \frac{1}{2}$. The $\alpha = 1$ TFD has the merit that it does not need the Gell-Mann-Low theorem as in the Keldysh method [17].

It is believed that the $\alpha = 1$ representation is the most convenient one in handling non-equilibrium many-body system. However, in my opinion, it has some difficulties. The prominent drawback in the $\alpha = 1$ representation is that the corrected phonon propagator *cannot* be easily calculated. To be more specific, I first write out the bare Green function for the phonon field ϕ , i.e. $i\mathbf{D}(x - y) = \langle 0(\beta) | T[\Phi(x)\bar{\Phi}(x)] | 0(\beta) \rangle$

$$\mathbf{D}_0(k) = (1/\omega_k) \left\{ \left[\mathbf{B}^{-1}(k_0)(k_0 - \omega_k + i\delta\tau) \right] \mathbf{B}(k_0) - \left[\tau \mathbf{B}^{-1}(-k_0)(k_0 + \omega_k - i\delta\tau) \right] \mathbf{B}(-k_0) \tau \right\}^T \quad (2.3)$$

where the superscript T means the transpose operation. In this paper I use the following convention: $k = (\mathbf{k}, k_0)$; $\delta = 0^+$; τ is the third Pauli matrix. We reserve ω_k for the phonon energy spectrum, and ϵ_k for the electron energy spectrum. The Green function of the phonon is denoted by \mathbf{D} and that of the electron is denoted by \mathbf{G} . We ignore the electron spin index whenever appropriate. In the $\alpha = 1$ representation, the thermal doublets Φ , $\bar{\Phi}$ are defined as

$$\Phi = \begin{pmatrix} \phi \\ \phi^\dagger \end{pmatrix} \quad \bar{\Phi} = \begin{pmatrix} \phi^\dagger \\ -\sigma\bar{\phi} \end{pmatrix}$$

so the (1,1) component of the Green function corresponds to the usual causal Green function as in other methods. The Dyson equation is written as

$$\mathbf{D} = 1/(\mathbf{D}_0^{-1} + \Sigma).$$

It will not be difficult to see that the calculation of \mathbf{D}_0^{-1} , i.e. the inverse of the bare-phonon Green function matrix in (2.3), is not at all easy to achieve. This makes practical application of $\alpha = 1$ TFD in solid-state problems rather difficult. Therefore we use the $\alpha = \frac{1}{2}$ representation. We will formulate TFD in the $\alpha = \frac{1}{2}$ representation so that it is applicable to non-equilibrium situations.

3. TFD in $\alpha = \frac{1}{2}$ for non-equilibrium states

In this section I will formulate the Green-function method in TFD in such a general way that it can be used in the next section to study the ELR and dynamical resistivity of hot electrons in semiconductors. Due to the practical problem with the $\alpha = 1$ representation mentioned earlier, I shall use the $\alpha = \frac{1}{2}$ representation. This representation of TFD was actually the original TFD when it was first proposed for *equilibrium* states. The details of TFD at *equilibrium* are described in the previous paper [18]. It has been used in many

areas, such as high- T_c superconductivity [21] and surface infrared absorption [22, 23]. In this section, I extend our discussions to the general case, which may be either equilibrium or non-equilibrium.

In the $\alpha = \frac{1}{2}$ representation, the thermal Bogoliubov transformation reads

$$\begin{pmatrix} \alpha \\ \bar{\alpha}^\dagger \end{pmatrix} = \begin{pmatrix} c_B & -d_B \\ -d_B & c_B \end{pmatrix} \begin{pmatrix} a \\ \bar{a}^\dagger \end{pmatrix} \quad (3.1)$$

for bosons and

$$\begin{pmatrix} \alpha \\ \bar{\alpha}^\dagger \end{pmatrix} = \begin{pmatrix} c_F & -d_F \\ d_F & c_F \end{pmatrix} \begin{pmatrix} a \\ \bar{a}^\dagger \end{pmatrix} \quad (3.2)$$

for fermions. Although there are four operators a , a^\dagger , \bar{a} and \bar{a}^\dagger in the above, we only need to write out two since the other two can be obtained easily from either complex conjugation or tilde operation. Here

$$c_B^2 = 1 + d_B^2$$

$$d_B^2 = n_B$$

$$c_F^2 = 1 - d_F^2$$

$$d_F^2 = n_F$$

in which n_B , n_F can be any boson and fermion thermal occupation functions. For the equilibrium state only, we have $n_B = 1/[\exp(\beta\omega_k) - 1]$ and $n_F = 1/[\exp(\beta\epsilon_k) + 1]$.

The two-point Green function is

$$\begin{aligned} iG^{ij}(x-y) &= \langle 0(\beta) | T[\psi^i(x)\psi^{j\dagger}(y)] | 0(\beta) \rangle \\ m\mathbf{s}iD^{ij}(x-y) &= \langle 0(\beta) | T[\phi^i(x)\phi^{j\dagger}(y)] | 0(\beta) \rangle \end{aligned} \quad (3.3)$$

where ψ and ϕ are electron and phonon fields. The thermal doublet is defined as

$$\begin{aligned} \psi^1 &= \psi & \psi^2 &= \bar{\psi}^\dagger \\ \phi^1 &= \phi & \phi^2 &= \bar{\phi}^\dagger. \end{aligned}$$

In TFD, it is quite convenient to start with the time-ordered Green function. The retarded or advanced Green function is easily obtained by the following substitution:

$$G^R(k) = \mathbf{G}(k, k_0 + i\delta)$$

$$G^A(k) = \mathbf{G}(k, k_0 - i\delta)$$

etc.

Using the relation in (3.1) and (3.2), one can easily obtain bare Green functions

$$D_0^{ij}(k) = \left\{ \mathbf{u}_B(k) \tau [k_0^2 - (\omega - i\delta\tau)^2]^{-1} \mathbf{u}_B(k) \right\}^{ij} \quad (3.4)$$

$$G_0^{aj}(k) = \left\{ \mathbf{u}_F(k) [k_0 - \epsilon_k + i\delta\tau]^{-1} \mathbf{u}_F^\dagger(k) \right\}^{ij} \quad (3.5)$$

where

$$\mathbf{u}_B = \begin{pmatrix} c_B & d_B \\ d_B & c_B \end{pmatrix}$$

$$\mathbf{u}_F = \begin{pmatrix} c_F & d_F \\ -d_F & c_F \end{pmatrix}.$$

To make our argument applicable, we need to prove that the corrected Green function takes the same form as the bare one. We start with the phonon's propagator. The Dyson equation reads

$$\mathbf{D}(k) = 1/[\mathbf{D}_0^{-1}(k) + \Sigma(k)]. \quad (3.6)$$

We ignore the superscript index of thermal doublets. All the quantities are in 2×2 matrices unless otherwise indicated. The wonderful thing in TFD is that the form of the matrix plays a very important role in simplifying the calculation. If we observe the following facts: the effect of electrons (fermions) on phonon propagators originates only from electron-hole bubbles, the symmetric properties of matrices \mathbf{u}_B , \mathbf{u}_F , it is easy to see that no matter what order or what type of Feynman diagram we are calculating, the self-energy always takes the following matrix form:

$$\Sigma = \begin{pmatrix} \Sigma_R & 0 \\ 0 & -\Sigma_R \end{pmatrix} + i \begin{pmatrix} \Sigma_1 & -\Sigma_2 \\ -\Sigma_2 & \Sigma_1 \end{pmatrix} \quad (3.7)$$

where Σ_R is a real quantity that contributes to the energy renormalization. Then the simple calculation leads to

$$\mathbf{D}(k) = \mathbf{u}_B(k)\tau \left[k_0^2 - \{\omega_R(k) - i[\gamma(k)/2\omega_R(k)]\tau\}^2 \right]^{-1} \mathbf{u}_B(k) \quad (3.8)$$

where the 'super' matrix \mathbf{u}_B is calculated as

$$\mathbf{u}_B = \begin{pmatrix} C_B & D_B \\ D_B & C_B \end{pmatrix}$$

and $C_B^2 = D_B^2 + 1$ with

$$D_B^2 = \frac{1}{2} \left(\Sigma_1/\gamma - 1 \right)$$

in which

$$\gamma^2 = (\Sigma_1)^2 - (\Sigma_2)^2. \quad (3.9)$$

The renormalized phonon energy is $\omega_k^2(k) = \omega_k^2 - \Sigma_R(k)$. So the relaxation of phonons, i.e. γ , is represented in (3.9). The physical meaning of the minus sign can be found, for example, on page 36 of [11].

For the electron causal Green function, we perform a similar calculation to obtain the matrix form for the self-energy

$$\Sigma = \begin{pmatrix} \Sigma_R & 0 \\ 0 & \Sigma_R \end{pmatrix} + i \begin{pmatrix} \Sigma_1 & \Sigma_2 \\ -\Sigma_2 & \Sigma_1 \end{pmatrix} \quad (3.10)$$

and the corrected Green function is

$$\mathbf{G}(k) = \mathbf{U}_F(k) [k_0 - \epsilon_R(k) - i\gamma(k)\tau]^{-1} \mathbf{U}_F^\dagger(k) \quad (3.11)$$

with $\epsilon_R(k) = \epsilon_k - \Sigma_R(k)$ and the super-matrix \mathbf{U}_F is

$$\mathbf{U}_F = \begin{pmatrix} C_F & D_F \\ -D_F & C_F \end{pmatrix}$$

where $C_F^2 = 1 - D_F^2$ and

$$D_F^2 = \frac{1}{2} \left(1 - \Sigma_1 / \gamma \right)$$

with

$$\gamma^2 = (\Sigma_1)^2 + (\Sigma_2)^2.$$

It is easy to check that at the one-temperature equilibrium case, the present Dyson equations recover those equations described in the previous paper [18].

It is interesting to notice that the corrected Green functions in (3.8) or (3.11) share the same structure as the bare Green functions in (3.4) and (3.5). This is unique for the TFD method.

Finally, I shall emphasize that TFD does not require that all the propagators in a Feynman diagram be at the same temperature. The different propagators may be defined in the different sub-thermal vacuum states. The bare Green function takes a sandwich form, i.e. ud_0u or ud_0u^\dagger , depending on whether it is bosonic or fermionic with d_0 being diagonalized. In order to calculate the *corrected* Green functions, one needs simply to cast (or renormalize) the corrected Green functions into the sandwich forms as in (3.8) or (3.11). Please note that the so called supermatrices \mathbf{U}_B and \mathbf{U}_F , functions of \mathbf{u}_B and \mathbf{u}_F , are determined by imaginary parts of the self-energy, which means that the quasi-particle is subject to thermal dissipation at finite temperature [17].

4. ELR and resistivity of hot electrons

Now we consider the practical applications of the formalism established in the last section. A very good application is short-laser-pulse-heated metals in which the electrons can be heated to a higher temperature (T_e) while the ions remain at a low-temperature (T_i). Much experimental [1] and theoretical [2, 5, 3, 24] work has been done in the field to understand the ELR and the resistivity of hot electrons in a relatively cold medium. The scenario is quite simple: due to the intense short laser beam, the electrons are heated up to a quasi-thermal equilibrium state characterized by temperature T_e because of the strong Coulomb interactions; because the impulse is so short we can be fairly safe in assuming a slow change of temperature, i.e. we assume the steady-state approximation; due to the weak electron-phonon interaction in most metals, linear-response theory is applicable. After these considerations, such a laser-heated system can be pictured as a system composed of two subsystems at different quasi-equilibria. In our previous papers [18, 25] we discussed the resistivity and ELR in such a system to the zeroth order, i.e. the bare phonon and electron Green functions were used. In [25], we provide a Boltzmann kinetic equation

approach to the ELR problem. In this paper, in order to compare with other work we shall demonstrate how to include the correction to the phonon Green function due to the creation of electron-hole pairs. The correction to the electron propagator (relatively unimportant) will be left for future work, because it requires self-consistent calculations of both phonon and electron propagators if we try to consider both corrections at the same time, which is beyond the scope of this paper. The thermal vacuum $|0(\beta)\rangle$ in this case is defined as $|0(\beta)\rangle = |0(\beta_e)\rangle \otimes |0(\beta_i)\rangle$ with $\beta_i = 1/k_B T_i$, $\beta_e = 1/k_B T_e$.

4.1. Resistivity

The electron-phonon interaction Hamiltonian is written as

$$H_{e-p} = \int d^2x [\psi^\dagger \psi - n_e] g(\delta) \phi \tag{4.1}$$

with coupling constant $g(\delta) \exp(ikx) = g_k \exp(ikx)$ and $n_e = \langle 0(\beta) | \psi^\dagger \psi | 0(\beta) \rangle$.

The detailed formulation for the problem was presented in [18] and [25], where the calculation was performed only to zeroth order. The dynamical resistivity $R(\omega)$ is related to the relaxation time $\tau^{-1}(\omega)$ as [26]

$$R(\omega) = (m_e/e^2) n_e \tau(\omega). \tag{4.2}$$

$\tau(\omega)$ is calculated as

$$\tau^{-1} = (m_e \omega / n_e e^2) \text{Im} \pi_R^{11}(\omega) \tag{4.3}$$

where π_R^{11} is the (1,1) component of the retarded current-current correlation function

$$i\pi^{11}(\omega) = \int dt \exp(i\omega t) \langle 0(\beta) | T [j_z(t) j_z(0)] | 0(\beta) \rangle.$$

Simple calculation leads to

$$\pi^{11}(\omega) = -i \frac{e^2}{m_e^2 (i\omega)^2} \sum_q g_q^2 q_z^2 \int \frac{d\omega_1}{2\pi} D^{11}(q, \omega_1) \chi^{11}(q, \omega + \omega_1) \tag{4.4}$$

where $i\chi^{11}(t) = \langle 0(\beta) | T [\rho(t) \rho(0)] | 0(\beta) \rangle$ is the (1,1) component of the density-density correlation function (response function).

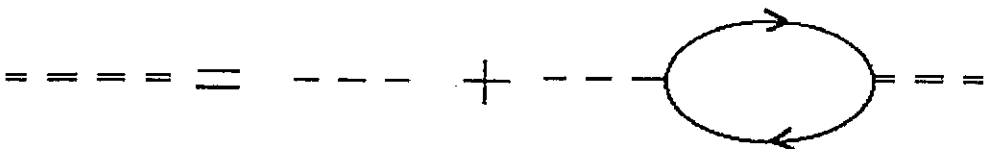


Figure 1. The correction to the phonon propagator. The double broken lines are the corrected phonon Green function. The single broken line is the bare phonon propagator including γ_p , while the full curve is the electron Green function. This corrected phonon is often referred to as the coupled mode.

We now take into account the electron-hole pair bubble effect on the phonon propagator (figure 1). Then the Green function of the phonon becomes

$$\mathbf{D}(k) = \mathbf{U}_B(k) \left(\tau / \left[k_0^2 - \{ \omega_k - i[\gamma(k)/2\omega_k] \tau \}^2 \right] \right) \mathbf{U}_B(k) \quad (4.5)$$

with

$$\begin{aligned} (U_B^{12}(k))^2 &= (U_B^{21}(k))^2 \\ &= \frac{1}{2} \left[\left\{ \gamma_p(k)[1 + 2n_B(k_0, \beta_i)] + \gamma_e(k)[1 + 2n_B(k_0, \beta_e)] \right\} / \gamma(k) - 1 \right] \end{aligned}$$

and

$$(U_B^{11}(k))^2 = (U_B^{22}(k))^2 = (U_B^{12}(k))^2 + 1$$

and

$$\gamma^2(k) = \gamma_p^2(k) + \gamma_e^2(k) + 2Q(k_0)\gamma_e(k)\gamma_p(k) \quad (4.6)$$

in which

$$Q(k_0) \equiv 1 + 2n_B(k_0, \beta_e)n_B(k_0, \beta_i) [\exp(\beta_i k_0/2) - \exp(\beta_e k_0/2)]^2. \quad (4.7)$$

So Q is a factor characterizing the effects of different thermal equilibria on the relaxation of phonons. Clearly when $\beta_i = \beta_e$, Q becomes unity. Dharma-wardana [27] suggested that this factor may be due to the renormalization of thermal baths at two different temperatures. In the above equation, γ_p^{-1} , responsible for the hot-phonon effect, is the lift-time of phonons contributed from the phonon-phonon interaction. $\gamma_e(k) = 2g_k^2 \text{Im } \chi(k)$. To derive (4.5), one simply needs to diagonalize the Dyson equation.

If we only consider the modification on the phonon propagator and take χ as the bare density-density Green function, then we derive that

$$\begin{aligned} \tau^{-1}(\omega) &= \frac{1}{2\pi n_e^2 m_e \omega} \sum_q g_q^2 q_x^2 q^2 \int d\omega' \sigma_p(q, \omega') \text{Im} \frac{1}{\epsilon(q, \omega + \omega')} [n'_B(\beta_i, \beta_e; \omega, q) \\ &\quad - n_B(\beta_e, \omega + \omega')]. \end{aligned} \quad (4.8)$$

This equation has not been derived previously in the Green-function approach. Here $\epsilon(k)$ is the dielectric function and

$$n'_B(\beta_i, \beta_e; k) = (U_B^{12}(k))^2.$$

In the above $n_B(k_0, \beta) = 1/[\exp(\beta k_0) - 1]$. $\sigma_p(\omega, q)$ is the spectral function of the phonon

$$\sigma_p(k) = \text{Im}(\mathbf{D}(k)) = (1/\pi) [\gamma(k)/2\omega_k] / [(k_0^2 - \omega_k^2)^2 + (\gamma(k)/2\omega_k)^2].$$

If we take $\gamma_e = 0$ then $U_B^{11}(k) = n_B(k_0, \beta_i)$. (4.8) recovers the equation given in [18] and [24]. It is also obvious that when $\beta_i = \beta_e$, it recovers that obtained by Mahan [26].

4.2. ELR of hot electrons

Theoretical study of the ELR of hot electrons in semiconductors is quite controversial. The phenomenological formula was first given by Kogan [2]. It was used to interpret the experimental data on the hot-electron relaxation in polar semiconductors by Das Sarma and his co-workers [5]. However as demonstrated by Dharma-wardana [3], the Keldysh method does not produce the results claimed by Das Sarma *et al*.

Now we shall use the formulation established in the last section to investigate the problem. The ELR can be formulated in linear-response theory as [28]

$$\text{ELR} = \sum_q \int \frac{d\omega}{\pi} \omega g_q^2 D^{11}(q, \omega) \chi^{11}(q, \omega). \quad (4.9)$$

If we ignore the modification of the electron Green function from the phonon-electron interaction and consider the bubble diagram (figure 1) for the phonon field, then we can derive easily

$$\text{ELR} = \sum_q \int \frac{d\omega}{\pi} \sigma_p(q, \omega) \text{Im} \frac{1}{\epsilon(q, \omega)} [n'_B(\beta_i, \beta_e; q, \omega) - n_B(\beta_e, \omega)] \quad (4.10)$$

where σ_p is the full phonon spectral function that was given in the last subsection. Write out $n'_B(\beta_i, \beta_e; q, \omega)$ repetitively:

$$\begin{aligned} n'_B(\beta_i, \beta_e; k) &= [1/2\gamma(k)] \{ \gamma_p(k) [1 + 2n_B(\beta_i, k_0)] \\ &\quad + \gamma_e(k) [1 + 2n_B(\beta_e, k_0)] - \gamma(k) \}. \end{aligned} \quad (4.11)$$

It is worth noting that when we take the limit $\gamma_p \rightarrow \infty$, the above ELR formula recovers exactly that obtained by Kogan. On the other hand, if $\gamma_p \ll \gamma_e$, the electron-phonon interactions will quickly thermalize the phonons and electrons to the same temperature, i.e. $n'_B(\beta_i, \beta_e; k) \simeq n_B(\beta_e, k)$. Therefore $\text{ELR} \simeq 0$. In this case, our steady-state approximation of ELR is not valid.

A simple calculation shows that $-\Delta N_{\text{cm}} \equiv n'_B(\beta_i, \beta_e; q, \omega) - n_B(\beta_e, \omega)$ in our approach is different from that obtained by the Keldysh method [3] from (5) in [29]. In our approach, the quantity $-\Delta N_{\text{cm}}$ cannot be put into the following form as declared by several authors [29, 30]:

$$\Delta N_{\text{cm}} = [\gamma_p / (\gamma_p + \gamma_e)] [n_B(\beta_e, \omega) - n_B(\beta_i, \omega)]. \quad (4.12)$$

This form can be only valid if we take Q as unity, or ignore the negative branch of the phonon energy spectrum in our theory.

I also used the Keldysh method to inspect the controversy. I was convinced that the renormalization of the thermal reservoir was ignored in the Keldysh method. To specify my argument, I briefly repeat the Keldysh-method approach. The Keldysh method starts with a density matrix $\rho = \exp(-\beta\mathbf{H})$ with \mathbf{H} being a total Hamiltonian. Then one can simply choose a proper time contour in the interaction picture, and then obtains a thermal-density matrix $\rho_0 = \exp(-\beta\mathbf{H}_0)$. In the two-temperature case, the calculation in the Keldysh method [30] starts with the density matrix $\rho_0 = \exp(-\beta_e\mathbf{H}_e - \beta_i\mathbf{H}_i)$, which has two thermal parameters. Here \mathbf{H}_e and \mathbf{H}_i are the free Hamiltonians for electrons and ions respectively. However the original density matrix is $\rho = \exp(-\beta\mathbf{H})$, which bears a single thermal parameter β . The transformation from the original density matrix ρ to the new density matrix

ρ_0 is not clear in the Keldysh method. In the Keldysh method the phonon relaxation γ is simply the sum of γ_e and γ_p , i.e. $\gamma = \gamma_e + \gamma_p$ while the TFD result is $\gamma^2 = \gamma_e^2 + \gamma_p^2 + 2Q\gamma_e\gamma_p$, see (4.6). To make the result in the Keldysh method equal to the TFD result, one has to assume $Q = 1$, which is approximately true at $T_e \simeq T_i$. Therefore in my view, the Keldysh method may be only approximately valid for the case $\beta_i \simeq \beta_e$. Considering the parameters chosen by Dharma-wardana, the conclusion in [3] is qualitatively valid.

5. Summary

In the present paper, I have described the TFD method in dealing with many-body problems. For comparison, I discussed the Keldysh method and pointed out its possible difficulty and limitation. Differing from the Keldysh or Matsubara methods, TFD is an operator method which does not rely on a density matrix. TFD offers an alternative way of calculating thermal properties, which is especially helpful when the thermal averaging is not clear. A general structure of the Green functions in TFD was formulated in such a way that it can be readily used to study both equilibrium and non-equilibrium many-body problems. Application to hot-electron ELR and dynamical resistivity was detailed. Our ELR formula differs from that derived by the Keldysh method. A comparison was given in the text.

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