Quantum Boltzmann equation and Kubo formula for electronic transport in solids

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We present a derivation of the quantum Boltzmann equation for linear dc transport with a correction term to the Mahan-Hansch equations and derive a formal solution to it. Based on this formal solution, we find the electric conductivity can be expressed as the retarded current-current correlation. Therefore we explicitly demonstrate the equivalence of the two most important theoretical methods: the quantum Boltzmann equation and the Kubo formula.

Because of its practical importance, the investigation of electronic transport in solids has received much attention. Of the theoretical methods for the linear transport process, the Kubo current-current correlation formula[1] is generally regarded as an exact formalism for quantum many-body systems. The other general method, e.g., the Boltzmann equation, however, has often been treated with classical or semiclassical approximations.[2] Recently, Mahan[3] and Hansch and Mahan[4] proposed a set of quantum Boltzmann equations (QBE) for the linear transport of many-electron systems. Their QBE is derived from the Dyson equation of the nonequilibrium Green's function.[5-10] In the Born approximation, the Mahan-Hansch QBE produces the same results for dc conductivity of electron-phonon-impurity systems as those derived from the Kubo formula in the ladder diagram approximation. Then it is natural to raise the question of whether the two general methods, the QBE and the Kubo formula, are exactly equivalent or not. Although the equivalence between them could be physically expected, it is not actually obvious because their forms are quite different. The Kubo formula relates the conductivity to an equilibrium current-current correlation function which is a kind of two-particle (four-point) Green's function. While the QBE provides a kinetic equation for the nonequilibrium quantum distribution function which is a kind of one-particle (two-point) Green's function. In this Brief Report:

(i) We present first a new derivation of QBE for linear transport. Because electric field enters into and complicates the functional dependence of self-energy upon the Green's function, the expansion with respect to electric field for obtaining the correct linear QBE has to be performed very carefully. In this derivation, we find a correction term due to electric field modification of the scattering effect, which has not been considered in Refs. 3 and 4. Only when this correction term is included could the QBE be equivalent to the Kubo formula for dc transport.

(ii) We derive an integral equation satisfied by the four-point (two-particle) Green's function, of which the kernel is the functional derivative of the two-point (one-particle) self-energy with respect to the two-point (one-particle) Green's function. With the help of this equation, we find a formal solution of the linear QBE.

(iii) We show that the dc conductivity calculated from this formal solution is exactly the retarded current-current correlation. Therefore, we prove the exact equivalence of the QBE and the Kubo formula.

In the presence of a uniform constant electric field (E field) $\mathbf{E}$, the Hamiltonian of the electron system can be written as

$$H=H_A+H_{\text{int}}=\frac{(\mathbf{p}-e\mathbf{A})^2}{2m}+H_{\text{int}}\,, \tag{1}$$

where H_{int} is the interaction between electrons and phonons or impurities, etc., and $\mathbf{A}(t)=-\mathbf{E}t$ is the vector potential. This system is typically nonequilibrium for which the nonequilibrium Green's function (GF) provides a convenient description. The retarded (advanced) GF, G_r (G_a), characterizes the spectrum and the dissipation for the system and the distribution GF, G_{+-} ($\equiv G^<$ of the Kadanoff-Baym notation[3,4,7]), which is similar to the Wigner distribution function, carries the distribution information. In fact, G_r, G_a, and G_{+-} are three independent components of the nonequilibrium closed-time-path Green's function (CTPGF).[5-10] A more symmetrical form of CTPGF, $G=(G_{\alpha\beta})$, which has four components: $G_{\alpha\beta}=-i\langle T_p\psi_\alpha\psi_\beta^\dagger\rangle$ where $\alpha,\beta=+$ or $-$, is much easier to manage. They are defined on the closed-time path, which runs from $-\infty$ to $+\infty$ (positive "+" branch) and then returns back from $+\infty$ to $-\infty$ (negative "−" branch), with T_p being the generalized time-ordering operator:[8,9]

$$iG_{++}(x,x')=\langle T_p\psi_+(x)\psi_+^\dagger(x')\rangle=\langle T\psi(x)\psi^\dagger(x')\rangle\,, \tag{2}$$

$$iG_{+-}(x,x')=\langle T_p\psi_+(x)\psi_-^\dagger(x')\rangle=-\langle\psi^\dagger(x')\psi(x)\rangle\,, \tag{3}$$

$$iG_{-+}(x,x')=\langle T_p\psi_-(x)\psi_+^\dagger(x')\rangle=\langle\psi(x)\psi^\dagger(x')\rangle\,, \tag{4}$$

$$iG_{--}(x,x')=\langle T_p\psi_-(x)\psi_-^\dagger(x')\rangle=\langle\tilde{T}\psi(x)\psi^\dagger(x')\rangle\,, \tag{5}$$

where $x=(\mathbf{x},t)$ and $\langle\cdots\rangle$ means the statistical ensemble average (generally nonequilibrium) $\text{Tr}(\rho\cdots)$. It is easy to verify $G_r=\frac{1}{2}\xi_\alpha\eta_\beta G_{\alpha\beta}$ and $G_a=\frac{1}{2}\eta_\alpha\xi_\beta G_{\alpha\beta}$. Here and in the following context the repeated time branch indices are summed over "+" and "−" branches, $\xi_+=\xi_-=1$ and

$\eta_+ = 1 = -\eta_-$. $G_{\alpha\beta}$ satisfies the following Dyson equation:[3–10]

$$\int dz[\Gamma_{0A}(x_1,z)_{\alpha\mu} - \Sigma_A(x_1,z)_{\alpha\mu}]\eta_\mu G_A(z,x_2)_{\mu\beta} = \delta_{\alpha\beta}(x_1-x_2), \quad (6)$$

$$\Gamma_{0A}(x_1,x_2)_{\alpha\beta} = \left[i\frac{\partial}{\partial t_1} - H_A(t_1)\right]\delta_{\alpha\beta}(x_1-x_2), \quad (7)$$

where the generalized δ function $\delta_{++}(\cdot) = \delta(\cdot) = -\delta_{--}(\cdot)$ and $\delta_{+-} = \delta_{-+} = 0$. Because the interaction $H_{\rm int}$ is independent of the vector potential, the self-energy Σ_A depends on the E field only through its functional dependence upon the G_A, i.e.,

$$\Sigma_A = \Sigma[G_A], \quad (8)$$

where $\Sigma[G]$ becomes the equilibrium self-energy if G_A is replaced with G. In order to avoid confusion, we use G,Σ to denote the equilibrium Green's functions to distinguish them from all the nonequilibrium ones. From the Dyson equation [Eq. (6)], we will deduce the QBE, the kinetic equations for G_{Ar}, G_{Aa}, and G_{A+-} for linear transport.

In a static E field, one would physically expect that there is a constant current and the properties of the system are space-time translationally invariant. However, the Dyson equation [Eq. (6)] for the Green's function G_A is not translation invariant. Nevertheless, we could derive a translation invariant description for the system from it by making use of the following transformation (which has been utilized by Mahan[3] and Hansch and Mahan[4] in the momentum space):

$$G_A(x_1,x_2) = \exp[-ie\mathbf{E}(t_1+t_2)\cdot(\mathbf{x}_1-\mathbf{x}_2)/2]\tilde{g}(x_1,x_2), \quad (9)$$

$$\Sigma_A(x_1,x_2) = \exp[-ie\mathbf{E}(t_1+t_2)\cdot(\mathbf{x}_1-\mathbf{x}_2)/2]\tilde{\sigma}(x_1,x_2), \quad (10)$$

$\tilde{g}$ and $\tilde{\sigma}$ here are introduced as the reduced Green's function and self-energy, respectively. For linear transport in weak E field, the nonequilibrium GF can be expanded as the equilibrium part plus a linear response term: $\tilde{g}_{\alpha\beta} = G_{\alpha\beta} + \delta g_{\alpha\beta}$. Utilizing the transformation in Eqs. (9) and (10) and the expansion to the linear order in E, we obtain the following translation invariant kinetic equation, the QBE for the reduced GF's:

$$\left[i\frac{\partial}{\partial t_1} - \frac{\hat{\mathbf{p}}_1^2}{2m}\right]\tilde{g}_{\alpha\beta}(x_1,x_2) - \int dz\tilde{\sigma}_{\alpha\mu}(x_1,z)\eta_\mu\tilde{g}_{\mu\beta}(z,x_2) = \delta_{\alpha\beta}(x_1-x_2) - \tfrac{1}{2}e\mathbf{E}\cdot\left[(\mathbf{x}_1-\mathbf{x}_2) + \frac{\mathbf{p}_1}{m}(t_1-t_2)\right]G_{\alpha\beta}(x_1-x_2)$$
$$- \frac{i}{2}e\mathbf{E}\cdot\int dx'[(\mathbf{x}_1-\mathbf{x}')(t'-t_2) - (\mathbf{x}'-\mathbf{x}_2)(t_1-t')]$$
$$\times\,\Sigma_{\alpha\nu}(x_1-x')\eta_\nu G_{\nu\beta}(x'-x_2), \quad (11)$$

in which each function is only dependent upon the coordinate differences $(x-x') = (\mathbf{x}-\mathbf{x}', t-t')$. The self-energy $\tilde{\sigma} = \Sigma + \delta\sigma$ and [using Eqs. (8)–(10) and making linear expansion]

$$\delta\sigma = \Sigma[G+\delta g] - \Sigma[G] + \delta_A\sigma, \quad (12)$$

in which

$$\delta_A\sigma_{\alpha\beta}(x_1-x_2) = \int dy_1 dy_2 \frac{\delta\Sigma_{\alpha\beta}(x_1,x_2)}{\delta G_{\mu\nu}(y_1,y_2)}\eta_\mu\eta_\nu\frac{i}{2}e\mathbf{E}(t_{y1}+t_{y2}-t_{x1}-t_{x2})\cdot(\mathbf{y}_1-\mathbf{y}_2)G_{\mu\nu}(y_1,y_2), \quad (13)$$

is a new term describing the E field modification of the scattering effect, which has been ignored in Refs. 3 and 4. This correction term vanishes only in the Born approximation where the self-energy Σ is a linear functional of G.

Since Eq. (11) is space-time translation invariant, it could be easily transferred into the momentum-energy $(\mathbf{p},\omega)$ space. Using the linear relation between $\tilde{g}_r$, $\tilde{g}_a$, and $\tilde{g}_{\alpha\beta}$, we arrive at the QBE, i.e., the quantum kinetic equation, for the spectrum and distribution

$$\left[\omega - \frac{\mathbf{p}^2}{2m}\right]\tilde{g}_r - \tilde{\sigma}_r\tilde{g}_r = 1, \quad \left[\omega - \frac{\mathbf{p}^2}{2m}\right]\tilde{g}_a - \tilde{\sigma}_a\tilde{g}_a = 1, \quad (14)$$

$$\tilde{\sigma}_{+-}(p)[\tilde{g}_r(p) - \tilde{g}_a(p)] - [\tilde{\sigma}_r(p) - \tilde{\sigma}_a(p)]\tilde{g}_{+-}(p) = ie\mathbf{E}\cdot\left[\left[1 - \frac{\partial}{\partial\omega}{\rm Re}\Sigma_r(p)\right]\frac{\partial}{\partial\mathbf{p}} + \left[\frac{\mathbf{p}}{m} + \frac{\partial}{\partial\mathbf{p}}{\rm Re}\Sigma_r(p)\right]\frac{\partial}{\partial\omega}\right]G_{+-}(p)$$
$$- ie\mathbf{E}\cdot\left[\frac{\partial}{\partial\mathbf{p}}{\rm Re}G_r(p)\frac{\partial}{\partial\omega}\Sigma_{+-}(p) - \frac{\partial}{\partial\mathbf{p}}\Sigma_{+-}(p)\frac{\partial}{\partial\omega}{\rm Re}G_r(p)\right]. \quad (15)$$

Equations (14) and (15) derived here exactly agree with Mahan-Hansch's equations [Eqs. (70) and (75) of Ref. 3] if the self-energy correction term $\delta_A\sigma$ in Eq. (13) could be set zero. This self-energy correction term indeed vanishes in the Born approximation which corresponds to the ladder diagram approximation for the current-current correlation in the Kubo formula. If one goes beyond the Born approximation, the self-energy is no longer linear in the full Green's function and then the correction term has a nonvanishing contribution to the QBE. In order to show the exact equivalence between the QBE and the Kubo formula it is necessary to include this correction term.

For the linear response term δg of GF: $\tilde{g}=G+\delta g$, we could derive the following integral equation from Eq. (11):

$$\delta g_{\alpha\beta}(x_1,x_2)-\int dy_1dy_2\Pi_{\alpha\beta\mu\nu}(x_1,x_2,y_1,y_2)\eta_\mu\eta_\nu\delta g_{\mu\nu}(y_1,y_2)$$
$$=e\mathbf{E}\cdot\left[\int dz G_{\alpha\mu}(x_1,z)\eta_\mu G_{\mu\beta}(z,x_2)\frac{\hat{p}_z}{2m}(2t_z-t_{x_1}-t_{x_2})\right.$$
$$\left.-\int dy_1dy_2\Pi_{\alpha\beta\mu\nu}(x_1,x_2,y_1,y_2)(t_{x_1}+t_{x_2}-t_{y_1}-t_{y_2})\frac{i}{2}(\mathbf{y}_1-\mathbf{y}_2)\eta_\mu\eta_\nu G_{\mu\nu}(y_1,y_2)\right], \quad (16)$$

$$\Pi_{\alpha\beta\mu\nu}(x_1,x_2,z_1,z_2)=\int dy_1dy_2G_{\alpha\delta}(x_1,y_1)\eta_\delta\frac{\delta\Sigma_{\delta\gamma}(y_1,y_2)}{\delta G_{\mu\nu}(z_1,z_2)}\eta_\gamma G_{\gamma\beta}(y_2,x_2)\,, \quad (17)$$

where the momentum operator $\hat{\mathbf{p}}=(\overleftarrow{\nabla}-\overrightarrow{\nabla})/2i$. It is interesting to verify that the solution of Eq. (16) can be expressed in terms of the two-particle (four-point) CTPGF:

$$G^{(2)}_{\alpha\beta\mu\nu}(x_1,x_2,x_3,x_4)=\langle T_p\psi_\alpha(x_1)\psi^\dagger_\beta(x_2)\psi_\mu(x_3)\psi^\dagger_\nu(x_4)\rangle\,. \quad (18)$$

And $G^{(2)}$ satisfies the following integral equation:[11]

$$G^{(2)}_{\alpha\beta\mu\nu}(x_1,x_2,x_3,x_4)-\int dz_1dz_2\Pi_{\alpha\beta\delta\gamma}(x_1,x_2,z_1,z_2)\eta_\delta\eta_\gamma G^{(2)}_{\delta\gamma\mu\nu}(z_1,z_2,x_3,x_4)=G_{\alpha\nu}(x_1,x_4)G_{\mu\beta}(x_3,x_2)\,. \quad (19)$$

Utilizing this integral equation, we find the formal solution of Eq. (16) as follows:

$$\delta g_{\alpha\beta}(x_1,x_2)=e\mathbf{E}\cdot\int dz G^{(2)}_{\alpha\beta\mu\mu}(x_1,x_2,z,z)\eta_\mu\frac{\hat{p}_z}{2m}(2t_z-t_{x_1}-t_{x_2})\,. \quad (20)$$

Actually, the proof for Eq. (20) being the solution to Eq. (16) can also be achieved directly by the Feynman diagram expansion method. The perturbative solution of Eq. (16) can be obtained, without much difficulty, to show that the Feynman diagrams for it and those for Eq. (20) coincide graph by graph, order by order.

According to the transformation in Eq. (9), the electric current $\mathbf{j}=(-ie/m)(\hat{p}_x-e\mathbf{A})G_{A+-}(x,x)$ can be expressed as $(-ie/m)\hat{p}_x\delta g_{+-}(x,x)$. From Eq. (20) and after some management concerning the closed time path time ordering definition [see Eqs. (2)–(5)], the conductivity $\sigma(\mathbf{j}=\sigma\cdot\mathbf{E})$ takes the following form

$$\sigma=-ie^2\int dz(t_z-t_x)\frac{\hat{p}_z}{m}\frac{\hat{p}_x}{m}G^{(2)}_{+-\mu\mu}(x,x,z,z)\eta_\mu=\int dz(-i)\Theta(x-z)\left\langle\left[\psi^\dagger(x)\frac{e\hat{p}_x}{m}\psi(x),\psi^\dagger(z)\frac{e\hat{p}_z}{m}\psi(z)\right]\right\rangle. \quad (21)$$

Obviously, our result for dc conductivity, Eq. (21) derived from QBE does exactly coincide with the Kubo formula. Therefore, we prove the equivalence between the kinetic equation approach (QBE) and the Kubo formula for linear transport in weak static uniform electric field.

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