Unified Theory of Thermal Transport

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1 Unified Theory

We consider that the system of phonons are governed by the equation:

$$\frac{\partial \rho(t)}{\partial t} + \frac{i}{\hbar}\left[H_0, \rho(t)\right] = \left.\frac{\partial \rho(t)}{\partial t}\right|_{coll} \tag{1}$$

with the harmonic Hamiltonian:

$$H_0 = \sum_{q,v} \hbar\omega_{qv}\left(a^{\dagger}_{qv}a_{qv} + \frac{1}{2}\right) \tag{2}$$

The one body density matrix $\rho_1(q, q', t)$ is defined as:

$$\rho_1(q, q', t)_{v,v'} = \mathrm{Tr}[\rho(t)a^{\dagger}_{qv}a_{q'v'}] \tag{3}$$

We insert H_0 into Eq.1 and multiply on both side $a^{\dagger}_{qv}a_{q'v'}$ and take the trace:

$$\mathrm{Tr}\left[\frac{\partial \rho(t)a^{\dagger}_{qv}a_{q'v'}}{\partial t}\right] = \frac{\partial \rho_1(q, q', t)_{v,v'}}{\partial t} \tag{4}$$

$$\mathrm{Tr}\left[\left(\frac{\partial \rho(t)a^{\dagger}_{qv}a_{q'v'}}{\partial t}\right)_{coll}\right] = \left.\frac{\partial \rho_1(q, q', t)_{v,v'}}{\partial t}\right|_{coll} \tag{5}$$

For the term $\frac{i}{\hbar}\left[H_0, \rho(t)\right]$, we can derive:

$$[H_0, \rho(t)] = \hbar\omega_{q'v'}\rho_1(q, q', t)_{v,v'} - \hbar\omega_{qv}\rho_1(q, q', t)_{v,v'} \tag{6}$$

So that we obtain the equation:

$$\frac{\partial \rho_1(q, q', t)_{v,v'}}{\partial t} + i\left(\omega_{q'v'}\rho_1(q, q', t)_{v,v'} - \omega_{qv}\rho_1(q, q', t)_{v,v'}\right) = \left.\frac{\partial \rho_1(q, q', t)_{v,v'}}{\partial t}\right|_{coll} \tag{7}$$

We perform the Weyl transformation to $\partial\rho_1(q, q', t)_{v,v'}$:

$$N(R, q, t)_{v,v'} = \sum_{q''} \rho_1(q + q'', q - q'', t)_{v,v'}e^{2iq''R} \tag{8}$$

to Eq.7, we will have:

$$\frac{\partial \rho_1(q + q'', q - q'', t)_{v,v'}}{\partial t} + i\left(\omega_{q-q''v'}\rho_1(q + q'', q - q'', t)_{v,v'} - \omega_{q+q''v}\rho_1(q + q'', q - q'', t)_{v,v'}\right) \tag{9}$$

$$= \left.\frac{\partial \rho_1(q + q'', q - q'', t)_{v,v'}}{\partial t}\right|_{coll} \tag{10}$$

Assume the one particle density $\rho_1(q+q'', q-q'', t)_{v,v'}$ is sharply peaked at q, q'' will be small, we can then replace frequency $\omega_{q+q''v}$ and $\omega_{q-q''v'}$ by:

$$\omega_{q+q''v} = \omega_{qv} + \frac{\partial \omega_{qv}}{\partial q''}q'' \tag{11}$$

$$\omega_{q-q''v'} = \omega_{qv'} - \frac{\partial \omega_{qv'}}{\partial q''}q'' \tag{12}$$

Multiply both side with $e^{2iq''R}$ and integrate, we have:

$$\frac{\partial N(R,q,t)_{vv'}}{\partial t} + i\left(\omega_{qv'} N(R,q,t)_{vv'} - \omega_{qv} N(R,q,t)_{vv'}\right) + \frac{1}{2}\left(\nabla_q \omega_{qv'} \nabla_R N(R,q,t)_{vv'} + \nabla_q \omega_{qv} \nabla_R N(R,q,t)_{vv'}\right) = \left.\frac{\partial N(R,q,t)_{vv'}}{\partial t}\right|_{c} \tag{13}$$

In the form of $n_v \times n_v$ matrix, we can rewrite Eq.12 as:

$$\frac{\partial N(R,q,t)}{\partial t} + i\left[N(R,q,t), \omega_q\right] + \frac{1}{2}\left\{\nabla_R N(R,q,t), \nabla_q \omega_q\right\} = \left.\frac{\partial N(R,q,t)}{\partial t}\right|_{coll} \tag{14}$$

Appendix A. Wigner function

Define the transformation, called *Weyl transformation* from an operator A to a function $A(x,p)$:

$$\tilde{A}(x,p) = \int e^{-ipy/\hbar} \langle x + \frac{y}{2}|A|x - \frac{y}{2}\rangle dy \tag{15}$$

$$= \int e^{ixu/\hbar} \langle p + \frac{u}{2}|A|p - \frac{u}{2}\rangle du \tag{16}$$

where $\langle x|A|x'\rangle$ and $\langle p|A|p'\rangle$ denotes the matrix element of A in position or momentum base, and both integral give the same expression $\tilde{A}(x,p)$. Suppose the operator A is only a function of x, than the Weyl transformationwill give:

$$\tilde{A} = \int e^{-ipy/\hbar} \langle x + \frac{y}{2}|A|x - \frac{y}{2}\rangle dy \tag{17}$$

$$= \int e^{-ipy/\hbar} \langle x + \frac{y}{2}|A|x - \frac{y}{2}\rangle \delta_{y=0} dy \tag{18}$$

$$= \langle x|A|x\rangle = A(x) \tag{19}$$

The same will be true if an operator is purely a function of momentum p. However, this is not true if an operator is a function of x, p at the same time. It can be shown that:

$$\mathrm{Tr}[AB] = \frac{1}{\hbar} \int \int \tilde{A}(x,p)\tilde{B}(x,p) dx dp \tag{20}$$

define the density operator ρ so that $\mathrm{Tr}[\rho A] = \langle A\rangle$, we thus have:

$$\langle A\rangle = \frac{1}{\hbar} \int \int \tilde{\rho}(x,p)\tilde{A}(x,p) dx dp \tag{21}$$

It is therefore convenient to define a function:

$$W(x,p) = \frac{1}{\hbar} \int e^{-ipy/\hbar} \langle x + \frac{y}{2}|\rho|x - \frac{y}{2}\rangle dy \tag{22}$$

$$= \frac{1}{\hbar} \int e^{ixu/\hbar} \langle p + \frac{u}{2}|\rho|p - \frac{u}{2}\rangle du \tag{23}$$

This is called *Wigner function*. Now, we can find expectation value of an operator by integrating over phase space x, p, similar to classical statistic mechanics:

$$\langle A\rangle = \int \int W(x,p)\tilde{A}(x,p) dx dp \tag{24}$$

Intergrating over one phase space coordinates gives the probability distribution of another:

$$\langle A\rangle(x) = \int W(x,p)\tilde{A}(x,p) dp \tag{25}$$

Wigner function is real and normalized:

$$\int \int W(x,p) dx dp = 1 \tag{26}$$

But it is not always positive, therefore, it cannot be interpreted as a classical probability density.