Quantum Scattering Theoretical Description of Thermodynamical Transport Phenomena

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We give a method of describing thermodynamical transport phenomena, based on a quantum scattering theoretical approach. We consider a quantum system of particles connected to thermodynamical reservoirs by leads. The effects of the reservoirs are imposed as an asymptotic condition at the end of the leads. We derive an expression for a current of a conserved quantity, which is independent of the details of the Hamiltonian operator. The Landauer formula and its generalizations are derived from this method.

1. Introduction

Statistical mechanical description of thermodynamical responses has been one of the important subjects of nonequilibrium statistical mechanics. Some methods have been proposed for this purpose (for example, see Ref. [1]). Of special interest is a method pioneered by Landauer [2], who heuristically derived an expression for an electric current, employing a scattering theoretical approach. His method was generalized to some cases; for example, a multichannel case [3-5], a case of a finite temperature [4,6], a case of a heat current [6,7] and a case of an inelastic scattering process caused by a random potential [8]. These methods describe linear responses of a system to thermodynamical gaps of reservoirs which induce Fermi distributions in the system. However, these have not explicitly treated an effect of inelastic scattering processes caused by scatterers, and applications of these methods have been mainly restricted to mesoscopic phenomena. Moreover, there have not existed a unified statistical mechanical derivation of all the generalizations of Landauer formula [9].

The purpose of the present Letter is to give a statistical mechanical method for descriptions of thermodynamical responses, based on a quantum scattering theoretical approach. We show that Landauer formula and its generalizations are derived by this method. This method covers all the cases which have been contained in the generalizations of Landauer formula. Moreover, it can be ap-
plied to some new cases; nonlinear responses to thermodynamical gaps of more
general reservoirs inducing non-Fermi distributions in a system, inelastic pro-
cesses caused by scatterers, and currents other than an electric or a heat current,
etc. So, this method can give new generalizations of Landauer formula.

\[ \text{2. Set-up} \] We consider a quantum system of particles in a three-
dimensional region \( \Omega \). The system consists of two kinds of particles, which
we call ‘transport particles’ and ‘scatterers’. The transport particles are in a
scattering state, and the scatterers are in a bound state. The region \( \Omega \) consists
of a finite region \( \Omega_0 \) and \( N \) semi-infinite columned regions \( \Omega_j, j = 1, 2, \ldots, N \).
The semi-infinite columned region \( \Omega_j \) connects the region \( \Omega_0 \) to infinity. We
call the columned region the ‘lead’.

For simplicity, we treat a system of only two particles; one transport particle
and one scatterer. We assume the Hamiltonian operator \( \hat{H} \) of this system to be
of the form

\[ \hat{H} = \frac{1}{2m} \left( \hat{p} - \frac{q}{c} A(\hat{x}) \right)^2 + \frac{1}{2M} \left( \hat{P} - \frac{Q}{c} A(\hat{X}) \right)^2 + U(\hat{x}, \hat{X}) \] (1)

where \( c \) is the velocity of light, \( m \) and \( M \) are the masses of the transport particle
and the scatterer, respectively, \( q \) and \( Q \) are the charges of the transport particle
and the scatterer, respectively, \( \hat{x} \) and \( \hat{X} \) are the coordinate operators of the
transport particle and the scatterer, respectively, \( \hat{p} \) and \( \hat{P} \) are the momentum
operators of the transport particle and the scatterer, respectively, \( A(\hat{x}) \) and
\( A(\hat{X}) \) are the vector potential operators acting on the transport particle and
the scatterer, respectively, \( U(\hat{x}, \hat{X}) \) is the potential operator of the transport
particle and the scatterer. Here the square of a vector means the inner product
of the vector with itself.

The state of this system at time \( t \) is described by a density operator \( \hat{\rho}(t) \)
which obeys the Liouville-von Neuman equation

\[ i\hbar \frac{d\hat{\rho}(t)}{dt} = [\hat{H}, \hat{\rho}(t)] \] (2)

where \( 2\pi\hbar \) is the Planck constant.

We introduce \( |x, X \rangle \) as the eigenstate of the operators \( \hat{x} \) and \( \hat{X} \) with
eigenvalues \( x \) and \( X \), respectively. We introduce the unit vectors \( e_i^{(j)} \), \( k = 1, 2, 3 \)
as a basis of \( \mathbb{R}^3 \) such that \( e_1^{(j)} \) is parallel to the \( j \)-th columned region and is
pointing to the finite region $\Omega_0$. We define $\hat{x}_k^{(j)}$ by $\hat{x}_k^{(j)} \equiv e_k^{(j)} \cdot \hat{x}$, and introduce $x_k^{(j)}$ as an eigenvalue of $\hat{x}_k^{(j)}$ ($j = 1, 2, \cdots, N, k = 1, 2, 3$). We assume the functions $A(x)$ and $U(x, X)$ to have the asymptotic forms satisfying

$$A(x) \sim e^{x_3^{(j)}} A^{(1, \infty)}(x_2^{(j)}, x_3^{(j)}), \quad \text{in } x \in \Omega_j,$$

$$U(x, X) \sim e^{x_3^{(j)}} U^{(1, \infty)}(x_2^{(j)}, x_3^{(j)}, X), \quad \text{in } x \in \Omega_j,$$

where $A^{(1, \infty)}(x_2^{(j)}, x_3^{(j)})$ is a function of $x_2^{(j)}$ and $x_3^{(j)}$, and $U^{(1, \infty)}(x_2^{(j)}, x_3^{(j)}, X)$ is a function of $x_2^{(j)}$, $x_3^{(j)}$ and $X$ only. We consider the operator $\hat{H}^{(1, \infty)}$ defined by

$$\hat{H}^{(1, \infty)} \equiv \frac{1}{2m} \left\{ \hat{p} - \frac{q}{c} A^{(1, \infty)}(\hat{x}_2^{(j)}, \hat{x}_3^{(j)}) \right\}^2 + \frac{1}{2M} \left\{ \hat{P} - \frac{Q}{c} A(X) \right\}^2 + U^{(1, \infty)}(\hat{x}_2^{(j)}, \hat{x}_3^{(j)}, X)$$

The eigenstate $| \Phi^{(1, \infty)}_{kn} \rangle$ of the operator $\hat{H}^{(1, \infty)}$ can be represented as

$$| \Phi^{(1, \infty)}_{kn} \rangle = | \phi^{(j)}_k \rangle \otimes | \varphi^{(1, \infty)}_{kn} \rangle.$$

Here, $| \phi^{(j)}_k \rangle$ is the eigenstate of the operator $e_k^{(j)} \cdot \hat{p}$ with the eigenvalue $hk$ and have an orthonormality

$$\langle \phi^{(j)}_k | \phi^{(j)}_{k'} \rangle = 2\pi \delta(k - k').$$

And $| \varphi^{(1, \infty)}_{kn} \rangle$ is introduced as the eigenstate of the operator $\hat{H}^{(1, \infty)}_{kn}$ which is defined by $\langle \phi^{(j)}_k | \hat{H}^{(1, \infty)} | \phi^{(j)}_{k'} \rangle \equiv \hat{H}^{(1, \infty)}_{kn} \langle \phi^{(j)}_k | \phi^{(j)}_{k'} \rangle$. We introduce $E_{kn}$ as the eigenvalue of the operator $\hat{H}^{(1, \infty)}_{kn}$ corresponding to the eigenstate $| \Phi^{(1, \infty)}_{kn} \rangle$. And $| x_2^{(j)}, x_3^{(j)}, X \rangle$ is introduced as the eigenstate of the operators $\hat{x}_2^{(j)}$, $\hat{x}_3^{(j)}$ and $\hat{X}$ with eigenvalues $x_2^{(j)}$, $x_3^{(j)}$ and $X$, respectively. We assume an orthonormality

$$\int_{S_j} dx_2^{(j)} dx_3^{(j)} \int_{\Omega} dX \langle \varphi^{(1, \infty)}_{kn} | x_2^{(j)}, x_3^{(j)}, X \rangle \langle x_2^{(j)}, x_3^{(j)}, X | \varphi^{(1, \infty)}_{kn'} \rangle = \delta_{nn'}$$

of the states $\{| \varphi^{(1, \infty)}_{kn} \rangle \}_n$, where $S_j$ represents the projection of the cross section of the $j$-th columned region onto the $x_2^{(j)} x_3^{(j)}$ plane.
We assume that there exists an eigenstate \( | \Psi_{kn}^{(j)} \rangle \) of the Hamiltonian operator \( \hat{H} \) with the eigenvalue \( E_{kn}^{(j)} \). Here, the eigenstate \( | \Psi_{kn}^{(j)} \rangle \) satisfies the following asymptotic condition:

\[
\langle x, X | \Psi_{kn}^{(j)} \rangle \big|_{x \to \infty} \sim \begin{cases} 
( x, X | \Phi_{kn}^{(j, \infty)} ) + \sum_{k' n'} r_{(k', n', k, n)}^{(j)} ( x, X | \Phi_{k' n'}^{(j, \infty)} ), & \text{in } x \in \Omega_j \\
\sum_{k' n'} t_{(k', n', k, n)}^{(j, l)} ( x, X | \Phi_{k' n'}^{(l, \infty)} ), & \text{in } x \in \Omega_l, \ l \neq j 
\end{cases}
\]

where \( r_{(k', n', k, n)}^{(j)} \) and \( t_{(k', n', k, n)}^{(j, l)} \) are constants determined by the fact that \( | \Psi_{kn}^{(j)} \rangle \) is an eigenstate of the operator \( \hat{H} \). It should be noted that the eigenstate \( | \Psi_{kn}^{(j)} \rangle \) may not be determined uniquely by the asymptotic condition (9). So we should introduce a new suffix in order to distinguish the eigenstates having the same asymptotic form. But in order to avoid a complicated notation we do not write such a suffix explicitly, but distinguish such degenerate states by different values of \( n \) from now on.

We assume that the condition

\[
\lim_{|X| \to \infty} \langle x, X | \hat{\rho}(t) | X \rangle = 0
\]

is satisfied for an arbitrary state \( | X \rangle \). The condition (10) may be satisfied by the assumption that the scatterer is in a bound state. The transport particle is assumed to be in a scattering state which satisfies the asymptotic condition

\[
\langle x, X | \hat{\rho}(t) | x', X' \rangle \big|_{|x| \to \infty, |x'| \to \infty} = \sum_{j=1}^{N} \sum_{k n} F_{j}(k, n) \langle x, X | \Psi_{kn}^{(j)} \rangle \langle \Psi_{kn}^{(j)} | x', X' \rangle
\]

(11)
where $F_j(k,n)$ is a positive function of $k$ and $n$. We interpret that the function $F_j(k,n)$ represents a distribution induced in the system by an interaction with the reservoir at the end of the $j$-th lead.

(3. Current of a Conserved Quantity) We consider a conserved quantity. This quantity corresponds to a Hermitian operator $\hat{G}$, which satisfies the relation $[\hat{H},\hat{G}] = 0$.

We introduce the symmetrized product $\hat{X} \star \hat{Y}$ of two arbitrary operators $\hat{X}$ and $\hat{Y}$ as

$$\hat{X} \star \hat{Y} \equiv \{\hat{X}\hat{Y} + (\hat{X}\hat{Y})^\dagger\}/2$$

where $(\hat{X}\hat{Y})^\dagger$ means the Hermitian conjugate operator of the operator $\hat{X}\hat{Y}$.

By Eqs. (2), (10), (12) and Gauss’ divergence theorem we obtain an equation of continuity

$$\partial \partial_t \int_\Omega d\mathbf{X} \langle \mathbf{x}, \mathbf{X} | (\hat{\rho}(t) \star \hat{G}) | \mathbf{x}, \mathbf{X} \rangle + \partial \partial_x \cdot \int_\Omega d\mathbf{X} \langle \mathbf{x}, \mathbf{X} | ((\hat{\rho}(t) \star \hat{G}) \star \hat{v}) | \mathbf{x}, \mathbf{X} \rangle = 0$$

where $\hat{v}$ is defined by $\hat{v} \equiv -[\hat{H},\hat{x}]/(i\hbar)$. By Eq. (13) we interpret the quantity

$$\int_\Omega d\mathbf{X} \langle \mathbf{x}, \mathbf{X} | ((\hat{\rho}(t) \star \hat{G}) \star \hat{v}) | \mathbf{x}, \mathbf{X} \rangle$$

as a current density of the conserved quantity due to the transport particle at time $t$.

We consider the current $J_j$ in the $j$-th lead, defined by

$$J_j \equiv \lim_{x_1^{(j)} \to -\infty} \int_{S_j} dx_2^{(j)} dx_3^{(j)} e_1^{(j)} \int_{\Omega} d\mathbf{X} \langle \mathbf{x}, \mathbf{X} | ((\hat{\rho}(t) \star \hat{G}) \star \hat{v}) | \mathbf{x}, \mathbf{X} \rangle.$$

We assume that the eigenstate $|\Psi_{kn}^{(j)}\rangle$ is also the eigenstate of the operator $\hat{G}$ [14]. And we introduce $G_{kn}^{(j)}$ as the eigenvalue of the operator $\hat{G}$ corresponding to the eigenstate $|\Psi_{kn}^{(j)}\rangle$. From Eqs. (11) and (14) we derive

$$J_j = \frac{1}{\hbar} \sum_{k,n} F_j(k,n) G_{kn}^{(j)} \left\{ \frac{\partial E_{kn}^{(j)}}{\partial k} - \sum_{k',n'} |\psi_{(-k',n',k,n)}^{(j)}\rangle^2 \frac{\partial E_{-k'n'}^{(j)}}{\partial k'} \right\}$$
By the equation of continuity (13), the current of the quantity $G$
where we used the following fact [15]:

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scattered wave has the same wave number as its incident wave, that is, when

As a special case, we consider a case satisfying the following conditio ns: (A) The

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and $E$

$\langle e^{(j)}_{k',n'} | \hat{\Phi}_{k,n}^{(j,\infty)} \rangle$

$\langle \hat{\Phi}_{k,n}^{(j,\infty)} \rangle$

$\langle \Phi_{k,n}^{(j,\infty)} \rangle$

$|x\rangle_{\frac{1}{2}} \rightarrow \infty \frac{1}{\hbar} \frac{\delta E_{kn}^{(j)}}{\delta k} \delta_{n'n'} \delta_{kk'}, \quad \text{in } x \in \Omega_j. \quad (16)$

By the equation of continuity (13), the current of the quantity $G$ which flows through any cross section of the $j$-th columned region takes the value $J_j$ in any steady state. It is important to note that the effect of interference among the incident wave, its reflective waves and its transmitted waves does not appear in the quantity $J_j$, because of Eq. (16). Eq. (17) is one of the main results in the present Letter.

(4. Derivation of Landauer Formula and its Generalizations)

As a special case, we consider a case satisfying the following conditions: (A) The scattered wave has the same wave number as its incident wave, that is, when $r_{(j'),(n',k,n)}^{(j)} \neq 0$, $kk' > 0$ and $E_{(j')_{k'n'}}^{(j)} = E_{kn}^{(j)}$ in $n'$, $k$, $n$ on $\mathcal{F}_j$, or $t_{(j),(-k',n',k,n)}^{(j)} \neq 0$, $kk' > 0$ and $E_{(j')_{k'n'}}^{(j)} = E_{kn}^{(j)}$ in $n'$ on $\mathcal{F}_j$ and in $n'$ on $\mathcal{F}_i$, the relation $k' = k$ is satisfied, where $\mathcal{F}_j$ is the support of the function $F_j(k,n)$. It implies that the scattering processes are almost elastic. (B) The distribution function $F_j(k,n)$ is a function only of the energy eigenvalue $E_{kn}^{(j)}$. So we put a function $\tilde{F}_j(E_{kn}^{(j)})$ of $E_{kn}^{(j)}$ instead of $F_j(k,n)$. (C) The operator $\hat{G}$ is a function only of the operator $\hat{H}$. So we put an operator $\hat{G}(\hat{H})$, which is a function of $\hat{H}$, instead of $\hat{G}$. (D) The coefficients $r_{(j),(-k',n',k,n)}^{(j)}$ and $t_{(j),(-k',n',k,n)}^{(j)}$ are dependent on the suffixes $k$ and $n$ on $\mathcal{F}_j$ only through the energy eigenstate $E_{kn}^{(j)}$. So we put the coefficients $r_{(j'),(n',k,n)}^{(j)}(E_{kn}^{(j)})$ and $t_{(j'),(n',k,n)}^{(j)}(E_{kn}^{(j)})$ instead of the coefficients $r_{(j'),(n',k,n)}^{(j)}$ and $t_{(j'),(n',k,n)}^{(j)}$, respectively. (E) The function $E_{kn}^{(j)}$ of the variable $k$ projects the domain $(0, \infty)$ of the variable $k$ to the domain $\Lambda_j$ of the variable $\varepsilon$. The domain $\Lambda_j$ is independent of the value
of the suffix \( n \). (F) The suffix \( n \) takes \( \tilde{n} \) of values on \( F_j \). Under the conditions (A)-(F), Eq. (15) becomes

\[
J_j = \frac{\tilde{n}}{2\pi \hbar} \left\{ \int_{\Lambda_j} d\varepsilon \, \tilde{F}_j(\varepsilon) \tilde{G}(\varepsilon) (1 - R_j(\varepsilon)) - \sum_{l=1}^{N} \int_{\Lambda_l} d\varepsilon \tilde{F}_l(\varepsilon) \tilde{G}(\varepsilon) T_{jl}(\varepsilon) \right\} .
\]

(17)

Here \( R_j(\varepsilon) \) and \( T_{jl}(\varepsilon) \) are defined by

\[
R_j(\varepsilon) \equiv \sum_{k'n'} | r_{k'n'}^{(j)}(\varepsilon) |^2 \quad \text{and} \quad T_{jl}(\varepsilon) \equiv \sum_{k'n'} | t_{k'n'}^{(j,l)}(\varepsilon) |^2,
\]

respectively where the sums over the suffixes \( k' \) and \( n' \) are taken only over values satisfying the condition \( E_{k'n'} = \varepsilon \) and \( E_{k'n'} = \varepsilon \), respectively. And we used the fact that the sum over the suffixes \( k > 0 \) in \( k > 0 \) corresponds to the integral over the suffix \( k \) in \( k > 0 \) multiplied the factor \( 1/(2\pi) \).

From Eq. (17) we can derive Landauer formula and its generalizations which have already been proposed. For example, if \( \tilde{G}(\tilde{H}) = q, \tilde{F}_j(\varepsilon) = \lim_{T \to 0} \{ \exp \{ (\varepsilon - \mu_j)/k_B T \} + 1 \}^{-1} = \theta(\varepsilon - \mu_j) \) (where \( k_B, T \) and \( \mu_j \) are positive constants), \( (\mu_j - \tilde{\mu})/\tilde{\mu} \ll 1 \) (where \( \tilde{\mu} \equiv (\mu_1 + \mu_2 + \cdots + \mu_N)/N \), \( \tilde{n} = 2 \) and \( \Lambda_j = (0, \infty) \), then Eq. (17) become

\[
J_j \approx \frac{q}{\pi \hbar} \left\{ (1 - R_j(\tilde{\mu})) \mu_j + \sum_{l=1}^{N} T_{jl}(\tilde{\mu}) \mu_l \right\} .
\]

(18)

in the first approximation of \( (\mu_j - \tilde{\mu})/\tilde{\mu} \). Eq. (18) is one of the generalizations of Landauer formula, and was proposed by M. Büttiker [5].

\[ 5. \text{Conclusion and Remarks} \] In the present Letter, we have described thermodynamical nonlinear responses of a quantum system to thermodynamical gaps of reservoirs. Here, the thermodynamical reservoirs were connected to the system with leads, and effects of the reservoirs were introduced as an asymptotic condition at the ends of the leads. Thermodynamical gaps of the reservoirs cause thermodynamical transport phenomena. We derived an expression of a current of a conserved quantity, which is independent of the details of the Hamiltonian operator. For example, this method can describe
an energy current which is caused inside a system connected to heat reservoirs having different temperatures.

This method leads to Landauer formula and its generalizations which have already been proposed. Moreover, we can also give further generalizations of Landauer formula by this method. For example, in this method we can deal with nonlinear responses, reservoirs inducing non-Fermi distribution in a system, inelastic processes caused by scatterers and currents other than an electric or a heat current, etc., which have not been treated earlier. The method in the present Letter can be generalized to the case of many transport particles and many scatterers [16]. (However the two-particles system, which we discussed in the present Letter, can be interpreted as a mean field approximation for a system consisting of many transport particles and many scatterers.) This method can also be generalized to the case where interactions of the particles are given by a complex potential only in a finite region.

We interpreted that the function $F_j(k, n)$ of $k$ and $n$ represents a distribution induced in the system by an interaction with thermodynamical reservoir at the end of the $j$-th lead, because it represents a distribution of the incident wave at the end of the $j$-th lead, and we can use an equilibrium distribution function as the stationary distribution function $F_j(k, n)$. But these reservoirs do not cause a dissipation of the system in this method. And as the distribution function $F_j(k, n)$ we can select a distribution function which is not an equilibrium distribution function. In this sense, we can describe non-thermodynamical transport phenomena by this method.

One may notice that this method does not treat distributions of thermodynamic quantities inside a system, because we do not assume the local equilibrium assumption, etc. in this method. For example, this method does not treat temperature distribution inside a system connected to heat reservoirs having different temperatures. To treat such a distribution by a generalization of this method remains as a future problem.

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[14] The exchangeable operators $\hat{H}$ and $\hat{G}$ have a common eigenstate, and the state $|\Psi^{(j)}_{kn}\rangle$ is an eigenstate of the operator $\hat{H}$. But the common eigenstate of operators $\hat{H}$ and $\hat{G}$ may not have the asymptotic form $|\Psi^{(j)}_{kn}\rangle$. So, this is a new assumption.
[15] The outline of the derivation of Eq. (16) is as follows. We first note that the divergence of the integrated function of $x^{(j)}_2$ and $x^{(j)}_3$ in the left hand side of Eq. (16) must be zero when $E^{(j)}_{kn} = E^{(j)}_{k'n'}$. So the left hand side of Eq. (16) must be zero except for the case $k = k'$ in $|x^{(j)}_1| \to \infty$, $x \in \Omega_j$ when $E^{(j)}_{kn} = E^{(j)}_{k'n'}$. Besides, we have $\langle x, X | e^{(j)}_1 \cdot \hat{v} \rangle |\Phi^{(j)}_{kn}(s)\rangle \sim \langle x, X | \left(\frac{1}{\hbar} \partial \hat{H}^{(j)}_{k'n'} / \partial k\right) |\Phi^{(j)}_{kn}(s)\rangle$ as $|x^{(j)}_1| \to \infty$ in $x \in \Omega_j$. By these and Eq. (8), we obtain Eq. (16).
[16] For such a generalization we must deal with energy eigenstates of the system consisting of the many transport particles and many scatterers, which must be required to satisfy the Pauli principle.