

Current Carrying States in Quantum Statistics of an Open System

W. Schattke

Institut für Theoretische Physik und Sternwarte der Universität Kiel

Z. Naturforsch. **35a**, 665–671 (1980); received March 1, 1980

The current as a thermodynamic variable of an open system is investigated in the context of the nonlinear response to a static field. Starting from a closed system it is shown that usual ensemble statistics can be applied to the open system. The case of two weakly coupled systems is considered for illustration.

A great deal of the success perturbation theory gained in treating the many body problem consists in the systematic way the expansion with respect to a small parameter is carried out in the perturbation of both the stationary state and the statistical distribution. When practising this approach, however, one often leaves the systematic path and partially sums the series up to infinite order, more or less justified by the underlying physical ideas. One of the most fruitful considerations in the context of transport properties, the fluctuation-dissipation theorem, bases on a first order perturbation expansion with respect to the applied potential [1]. Thus the validity of this linear response is confined to small potentials. In some conduction phenomena one is rather interested in a nonlinear current-voltage relation, specifically if the static energy of the space charge in the external potential is considerable whereas the energy of the currents is almost negligible. In this case a linear response with respect to the current is more adequate. The static energy should be retained and its dominant contribution treated exactly. This contrasts with a systematic perturbation expansion, where the small parameter, the current itself, is only the final result. In this respect some generalization of the fluctuation-dissipation relation would be useful. This will be one aspect of the subsequent considerations.

Another point is associated with the choice of thermodynamic variables in an open system. Generally the entropy production is determined by the product of the flux with the respective force and is positive in irreversible processes. Considering a sit-

uation where matter is transported through the system with vanishing entropy production the external force has to be balanced by a gradient in the chemical potential. Such a situation may be described within equilibrium statistics. The flux passing through the system is a conserved quantity and can be incorporated in the construction of a canonical ensemble by adding it with a Lagrange multiplier, which represents the respective statistical potential, to the hamiltonian of the statistical operator. Thus the constraint of a fixed quantity is released leaving a fluctuating variable, the average of which is determined by the statistical potential [2]. This result arises in a natural way in the procedure under consideration. The transition to the open system is achieved by putting the boundary walls to infinity. States normalized on a finite box then change into current states which yield macroscopic stationary currents. During the transition the free energy and its time rate decreases according to an irreversible process. The corresponding calculation yields an expression for the hamiltonian associated with the currents.

A further object of interest consists in exploiting symmetry properties with respect to time reversal. The asymptotic form in the time evolution of the statistical operator may be simplified considerably if only those contributions are picked up which lead to a nonvanishing current. They are characterized by antisymmetry against time reversal.

On the following pages some simple manipulations with the statistical operator (I) will be followed by the derivation of a nonlinear response formula (II). A subsequent Sect. III is concerned with the transition to an open system. In the last Sect. IV the application is illustrated by an example for a nonlinear transport between weakly

Reprint requests to Dr. W. Schattke, Institut für Theoretische Physik der Universität Kiel, Olshausenstrasse, D-2300 Kiel.

0340-4811 / 08 / 0700-0665 \$ 01.00/0. — Please order a reprint rather than making your own copy.



Dieses Werk wurde im Jahr 2013 vom Verlag Zeitschrift für Naturforschung in Zusammenarbeit mit der Max-Planck-Gesellschaft zur Förderung der Wissenschaften e.V. digitalisiert und unter folgender Lizenz veröffentlicht: Creative Commons Namensnennung-Keine Bearbeitung 3.0 Deutschland Lizenz.

Zum 01.01.2015 ist eine Anpassung der Lizenzbedingungen (Entfall der Creative Commons Lizenzbedingung „Keine Bearbeitung“) beabsichtigt, um eine Nachnutzung auch im Rahmen zukünftiger wissenschaftlicher Nutzungsformen zu ermöglichen.

This work has been digitalized and published in 2013 by Verlag Zeitschrift für Naturforschung in cooperation with the Max Planck Society for the Advancement of Science under a Creative Commons Attribution-NoDerivs 3.0 Germany License.

On 01.01.2015 it is planned to change the License Conditions (the removal of the Creative Commons License condition “no derivative works”). This is to allow reuse in the area of future scientific usage.

coupled systems. As regards a former investigation of solid state tunneling some approximations with respect to the smallness of the transmission coefficient are avoided, thereby leading to a more transparent interpretation and a slight generalization of the tunneling theory.

I. Evolution of the Statistical Operator

As we are interested in the time development of an arbitrary observable after an external potential \hat{V} has been switched on, we begin at $t=0$ with a distribution of states given by the statistical operator

$$t=0: \quad \hat{\rho}_0 = e^{-\beta \hat{H}_0} / \text{Trace } e^{-\beta \hat{H}_0} \quad (1)$$

with the hamiltonian \hat{H}_0 . The system is initially in equilibrium defined by \hat{H}_0 . The sudden rise of a potential will be described by an operator $\hat{V}\theta(t)$, with a step function $\theta(t)$ and a time independent operator \hat{V} , such as to get for later times

$$t>0: \quad \hat{H} = \hat{H}_0 + \hat{V}. \quad (2)$$

This hamiltonian characterizes the time development of an initial state $|\psi_n\rangle$ via the unitary transformation

$$|\psi_n(t)\rangle = e^{(-i/\hbar)\hat{H}t} |\psi_n\rangle. \quad (3)$$

The density operator (1) is transformed correspondingly

$$\begin{aligned} \hat{\rho}(t) &= e^{(-i/\hbar)\hat{H}t} e^{-\beta \hat{H}_0} e^{(i/\hbar)\hat{H}t} / \text{Trace } e^{-\beta \hat{H}_0} \\ &= e^{-\beta \hat{H}} / Z_t. \end{aligned} \quad (4)$$

In the last equation the transformation has been pushed in the exponent on the operator \hat{H}_0 ,

$$\hat{H}_t \equiv e^{(-i/\hbar)\hat{H}t} \hat{H}_0 e^{(i/\hbar)\hat{H}t} \quad (5)$$

defining a time dependent hamiltonian \hat{H}_t of a fictive equilibrium. By cyclic invariance of the trace the sum over states, Z_t , may be written alternatively

$$Z_t = \text{Tr } e^{-\beta \hat{H}_t} = \text{Tr } e^{-\beta \hat{H}_0} \quad (6)$$

from which follows that the free energy

$$F = -kT \log Z_t$$

and its derivatives do not depend on time. The system is closed. Using (2) we get

$$\begin{aligned} \hat{H}_t &= \hat{H} - e^{(-i/\hbar)t\hat{H}} \hat{V} e^{(i/\hbar)t\hat{H}} \\ &= \hat{H}_0 - \int_0^t d\tau' \frac{d}{d\tau'} \hat{V}(-\tau'), \end{aligned} \quad (7)$$

where the time dependence is defined by

$$\hat{V}(t) \equiv e^{(i/\hbar)t\hat{H}} \hat{V} e^{(-i/\hbar)t\hat{H}}. \quad (8)$$

Let the external potential be given by a volume integral over a density

$$\hat{V}(t) = \int_{\Omega} d\nu \hat{v}(t). \quad (9)$$

Then we can establish a continuity equation, which reflects the conservation of particle number,

$$\frac{d\hat{v}(t)}{dt} = \frac{i}{\hbar} [\hat{H}, \hat{v}(t)]. \quad (10)$$

We may express the one particle potential, (9), with fermi field operators $\hat{\psi}^{(+)}(\mathbf{r})$

$$\hat{v}(t) = v(\mathbf{r}) \hat{\psi}^+(\mathbf{r}, t) \hat{\psi}(\mathbf{r}, t), \quad (11)$$

where the time dependence of (8) is incorporated. The commutator of (10) may be evaluated, leading in the case of a velocity independent interaction to the usual quantum mechanical expression for the current density operator

$$-\frac{d\hat{v}(t)}{dt} = \frac{1}{e} v(\mathbf{r}) \text{div} \hat{\mathbf{j}}(\mathbf{r}, t) \quad (12)$$

with

$$\begin{aligned} \hat{\mathbf{j}}(\mathbf{r}, t) &= \frac{ie\hbar}{2m} \{ (\nabla \hat{\psi}^+(\mathbf{r}, t)) \hat{\psi}(\mathbf{r}, t) - \hat{\psi}^+(\mathbf{r}, t) \\ &\quad \cdot (\nabla \hat{\psi}(\mathbf{r}, t)) \}. \end{aligned}$$

Inserting in (7) we get

$$\hat{H}_t = \hat{H}_0 - \frac{1}{e} \int_0^t d\tau' \int_{\Omega} d\nu v(\mathbf{r}) \text{div} \hat{\mathbf{j}}(\mathbf{r}, -\tau')$$

and using Gauss' law with electrostatic field $\mathbf{E} = -(1/e)\nabla v$

$$\hat{H}_t = \hat{H}_0 - \int_0^t d\tau' \int_{\Omega} d\nu (\hat{\mathbf{j}}(\mathbf{r}, -\tau') \mathbf{E}(\mathbf{r})), \quad (13)$$

where the surface term has been dropped according to the boundary conditions. Because of its time dependence the current operator is scarcely manageable for interacting particles. Thus it is the starting point of various approximations for the exponent of the statistical operator. One way to escape the problem is to treat $\hat{\mathbf{j}}(\mathbf{r}, -\tau')$ by a perturbation expansion with respect to some parameter characterizing the many-body interaction. The essential fact, however, in this derivation is that we expand the exponent of the statistical operator (4) and not

the exponential function itself, as is usually done in linear response theory. With this step we certainly depart from a consequent perturbation theory. Trying to get some approximate expression for \hat{H}_t which does not neglect the driving force we may arrive at a nonlinear response theory. As the time dependent statistical operator has the form of equilibrium thermodynamics it is suggestive to interpret the operator \hat{H}_t as that observable, which replaces the energy, the hamiltonian \hat{H} , in the canonical ensemble. From the view of an instantaneous micro-canonical ensemble it is the eigenvalue of \hat{H}_t which would remain constant during the system moving in phase space. Current and potential appear in (13) as conjugate variables in thermodynamical sense and represent the operator equivalent of the time integral of a "dissipated" power. As the system is closed, the expression "dissipation" should here be used with caution, justified only by formal similarity.

II. Nonlinear Response

If we neglect the external potential within the time dependence of the current density operator (13) we can derive a nonlinear response formula for the considered case of a static field. The field is still present, however, in the hamiltonian \hat{H}_t describing the statistical operator. Therefore we get a current which is nonlinear in the field being calculated via

$$\langle \hat{\mathbf{j}}(\mathbf{r}) \rangle = (Z_t)^{-1} \text{Tr } e^{-\beta \hat{H}_t} \hat{\mathbf{j}}(\mathbf{r}) \quad (14)$$

with \hat{H}_t as in (13) and with the approximation

$$\hat{\mathbf{j}}(\mathbf{r}, -t') = e^{(-i/\hbar)t' \hat{H}_0} \hat{\mathbf{j}}(\mathbf{r}) e^{(i/\hbar)t' \hat{H}_0}. \quad (15)$$

The latter is related to the case where the electrostatic energy as represented in \hat{H} is small in comparison with the energy of the currents in \hat{H}_t which may be rather important as a consequence of a high conductivity. Using the Fourier representation for

$$\hat{\mathbf{j}}(\mathbf{r}, t) = \frac{1}{\sqrt{\Omega}} \sum_{\mathbf{k}} e^{i(\mathbf{k} \cdot \mathbf{r})} \hat{\mathbf{j}}(\mathbf{k}, t) \quad (16)$$

and similarly for $\mathbf{E}(\mathbf{r})$ we introduce the static conductivity tensor by

$$\frac{\partial \langle \hat{\mathbf{j}}_n(\mathbf{k}) \rangle}{\partial E_m(\mathbf{k})} = \sigma_{nm}(\mathbf{k}). \quad (17)$$

For simplicity we neglect the difference between the driving field, which determines the experimental

conductivity, and the external field. Differentiating (14) with respect to $E_m(\mathbf{k})$ we use the identity

$$\frac{\partial}{\partial E_m(\mathbf{k})} e^{-\beta \hat{H}_t} = - \int_0^\beta d\beta' e^{-(\beta-\beta') \hat{H}_t} \frac{\partial \hat{H}_t}{\partial E_m(\mathbf{k})} e^{-\beta' \hat{H}_t}$$

with

$$\frac{\partial \hat{H}_t}{\partial E_m(\mathbf{k})} = - \int_0^t d\tau' \hat{\mathbf{j}}_m(-\mathbf{k}, \tau')$$

and get

$$\sigma_{nm}(\mathbf{k}, t) = \int_0^t d\tau' \int_0^\beta d\beta' \langle \{ e^{\beta' \hat{H}_t} \hat{\mathbf{j}}_n(\mathbf{k}) e^{-\beta' \hat{H}_t} - \langle \hat{\mathbf{j}}_n(\mathbf{k}) \rangle \} \hat{\mathbf{j}}_m(-\mathbf{k}, \tau') \rangle. \quad (18)$$

This expression agrees with the result of linear response theory, if one replaces \hat{H}_t by the hamiltonian \hat{H}_0 of initial equilibrium, i.e. if one neglects the nonlinear field contributions. It states a nonlinear generalization of the static fluctuation-dissipation theorem. The rather simple manipulations in deriving (18) suggest that the complications in calculating the physical quantities will not decrease when using (18). However, if the difference $(\hat{H}_t - \hat{H}_0)$ arising in the statistical operator is approximated by a one body potential it may be diagonalized together with a starting unperturbed hamiltonian. At a first glance, for an electron system this term merely displaces the fermi sphere. \hat{H} changes expectation values but will not seriously affect fluctuations except of the case that the displacement touches some structure in momentum space. In that case, e.g. a fermi surface near the boundary of a Brillouin zone, the conductivity could alter remarkably.

III. Steady State Current

So far the time evolution governed by a unitary transformation is reversible and the free energy is constant in time. The system is closed within a finite volume, open only to particle and energy transfer referring to a given chemical potential and temperature. The particle flow through the boundaries vanishes because of the boundary conditions imposed on the wave function.

To put irreversibility into the equations the usual "adiabatic" trick is applied. Extending first the boundaries of the volume to infinity and proceeding then to the infinite time limit one avoids the recurrence by Poincaré cycles. The perturbation of the electron gas introduced by the potential at $t = 0$ will

thus irreversibly spread over the whole infinite volume without the quasi periodicity caused by finite boundaries. One arrives at an open system as will be outlined below. Surely the result depends on the stage at which the going to limits is performed because the boundary conditions roughly speaking implicitly change during the adiabatic switch-off. The choice preferred in this contribution is only a possible one, however it matches with some physical situations.

Let $|n\rangle$ be the stationary states of the finite system for $t > 0$

$$\hat{H}|n\rangle = \varepsilon_n |n\rangle \quad (19)$$

then the time dependence in (13) can be written

$$\hat{\mathbf{j}}(\mathbf{r}, -t') = \sum_{n, n'} e^{(-i/\hbar)t'(\varepsilon_n - \varepsilon_{n'})} \cdot |n\rangle \langle n| \hat{\mathbf{j}}(\mathbf{r}, 0) |n'\rangle \langle n'|. \quad (20)$$

The intended limit in the integral over t' leads to

$$\begin{aligned} \int_0^t e^{-i\omega t'} dt' &\rightarrow \frac{1}{i} \frac{1}{\omega - i\delta} \\ &= \frac{1}{i} P\left(\frac{1}{\omega}\right) + \pi\delta(\omega) \end{aligned} \quad (21)$$

with δ an arbitrary small positive quantity and ω to be replaced by $1/\hbar(\varepsilon_n - \varepsilon_{n'})$. In the case of a discrete spectrum only the first term, the principal part at the pole in (21), appears. But as the volume tends to infinity before the time limit is performed, the energies become continuously distributed and the additional contribution $\pi\delta(\omega)$ must be taken into account. It is merely this quantity we are interested in.

Combining (13), (20), and (21) the final system is described by the statistical operator of an equilibrium ensemble with the hamiltonian

$$\hat{H}_\infty = \hat{H}_0 + \hat{H}_v + \hat{H}_c, \quad (22)$$

$$\begin{aligned} \hat{H}_v &= -\frac{\hbar}{i} \sum_{n, n'} P\left(\frac{1}{\varepsilon_n - \varepsilon_{n'}}\right) |n\rangle \langle n| \\ &\quad \cdot \int d\mathbf{v} (\hat{\mathbf{j}}(\mathbf{r}, 0) \mathbf{E}(\mathbf{r})) |n'\rangle \langle n'|, \\ \hat{H}_c &= -\pi\hbar \sum_{n, n'} \delta(\varepsilon_n - \varepsilon_{n'}) |n\rangle \langle n| \\ &\quad \cdot \int d\mathbf{v} (\hat{\mathbf{j}}(\mathbf{r}, 0) \mathbf{E}(\mathbf{r})) |n'\rangle \langle n'|. \end{aligned}$$

The states of the continuous spectral representation implied in (22) are not distinguished by a special notation from a discrete representation. The first

two terms are invariant with respect to complex conjugation, whereas \hat{H}_c changes sign because \mathbf{j} does so. Therefore only the last term guarantees a non-vanishing average current. The boundaries of the volume integral approach to infinity. In \hat{H}_c a surface integral remains

$$\int_{\Omega_\infty} d\mathbf{v} (\hat{\mathbf{j}} \mathbf{E}) = -\frac{1}{e} \int_{S_\infty} (d\mathcal{S} \hat{\mathbf{j}}(\mathbf{r}, 0)) v(\mathbf{r}) + \dots \quad (23)$$

and recalling (10) and (12) the matrix elements of the omitted terms give no contribution because of the commutator in (10) and the energy δ -function in \hat{H}_c . Thus the macroscopic current is associated in the hamiltonian \hat{H}_∞ with the energy of a flux leaving the system through an infinite surface. As the surface integral could be dropped in the finite system, the stage at which the going to limits is performed is seen to be essential.

The invariant part $\hat{H}_0 + \hat{H}_v$ determines the final equilibrium independently of the external current. Applying Gauss' law to \hat{H}_v the surface term now will be neglected in comparison with the volume term. Then (10) and (12) show that \hat{H}_v is equal to $\hat{V}(0)$, thus

$$\hat{H}_\infty = \hat{H} + \hat{H}_c. \quad (24)$$

Clearly \hat{H}_c commutes with \hat{H} . Therefore the flux is a conserved quantity under the hamiltonian \hat{H}_∞ of the statistical operator. Definite values may be assigned to it thus representing a thermodynamic variable controlled by the surroundings of this open system [3].

The ideas leading to (24) have to be modified if dissipation is included because the infinitesimal quantity, δ , of (21) becomes finite.

In the context of the uniqueness of the limits mainly two questions arise. In the first place the unitary invariance of the trace (6) contrasts with the result of (24). However, the time evolution equals no longer a unitary transformation in view of the adiabatic trick in (21). In the second place differentiation of the statistical operator with respect to time does not seem to commute with the time limiting at first glance. The derivative of a quantity which becomes asymptotically constant, clearly vanishes asymptotically. If e.g. the free energy is examined

$$\frac{d}{dt} F = - \int_{\Omega_\infty} d\mathbf{v} \langle \hat{\mathbf{j}}(\mathbf{r}, -t) \rangle \mathbf{E}(\mathbf{r}) \quad (25)$$

the current is seen to decay exponentially with lifetime $1/\delta$ from (21). Similar to irreversible thermodynamics, where from the second law the right hand side of (25) must be negative, the free energy decreases saturating in the stationary system with “least-namely zero-dissipation of energy” [4].

(24) yields a convenient description of an open system via the statistical operator of a canonical ensemble. The internal energy follows from averaging \hat{H}_∞ which differs from the mechanical energy given in the average of the dynamical hamiltonian \hat{H} by the energy of the penetrating flux. It is shown that the result can be obtained by a simple, specific limit procedure.

IV. Weakly Coupled Systems

The results of the last section are illustrated by applying them with a slight modification to a system consisting of two subsystems which are weakly coupled. We are interested in the current flowing between the subsystems, whereas we disregard the dynamics of a single subsystem.

The systems defined by the hamiltonians \hat{A} and \hat{B} shall be weakly coupled if a perturbation expansion according to the interaction energy, $\delta\hat{H}_0$, leads in low order to a good approximation of the equilibrium situation.

$$\hat{H}_0 = \hat{A} + \hat{B} + \delta\hat{H}_0. \quad (26)$$

We assume that the operator of the external potential may be decomposed in a similar way

$$\hat{V} = \hat{V}_A + \hat{V}_B + \delta\hat{V} \quad (27)$$

with a small perturbation $\delta\hat{V}$.

To be specific we choose as an example a tunnel-junction in which the two sides separated by a high barrier potential represent the weakly interacting subsystems. The voltage, say on the right hand side, is suddenly set on a higher level and we look at the resulting current flowing from right to left [5].

We denote the sides by an index $\alpha = \pm$ and introduce creation and annihilation operators, $\hat{c}_{k\alpha}^{(\pm)}$ representing oneparticle states which belong to one complete set of real wave functions localized either on the left ($\alpha = -$) or right hand side ($\alpha = +$) for energies ε_k below the top of the barrier potential. These are clearly not eigenstates of the initial equilibrium hamiltonian because those should by symmetrical or antisymmetrical in the case of a sym-

metrical barrier potential. Nevertheless we may use them as a basis for representing all operators

$$\begin{aligned} \hat{H}_0 = & \sum \varepsilon_k \hat{c}_{k\alpha}^+ \hat{c}_{k\alpha} \\ & + \sum W_{k\alpha, k'\alpha'} \hat{c}_{k\alpha}^+ \hat{c}_{k'\alpha'}, \end{aligned} \quad (28)$$

$$\begin{aligned} \hat{V} = & \hat{V}_A + \delta\hat{V} = V_0 \sum \hat{c}_{k+}^+ \hat{c}_{k+} \\ & + \sum Q_{k\alpha, k'\alpha'} \hat{c}_{k\alpha}^+ \hat{c}_{k'\alpha'}. \end{aligned} \quad (29)$$

In the last equation the fact is expressed that the main contribution to the energy of a constant potential V_0 applied to the right hand side arises from the particle number of that side multiplied by V_0 . The last terms in (28) and (29) couple both sides and are assumed to be small. Returning to (7) we write

$$\begin{aligned} \hat{H}_t = & \hat{H}_0 + \frac{i}{\hbar} \int_0^t d\ell' e^{(-i/\hbar)\ell'\hat{H}} [\hat{H}, \hat{V}] e^{(i/\hbar)\ell'\hat{H}} \\ = & \hat{H}_0 + \frac{i}{\hbar} \int_0^t d\ell' e^{(-i/\hbar)\ell'\hat{H}} \\ & \cdot \{[\hat{A} + \hat{B}, \delta\hat{V}] + [\delta\hat{H}_0, \hat{V}_A] + [\delta\hat{H}_0, \delta\hat{V}]\} e^{(i/\hbar)\ell'\hat{H}}. \end{aligned} \quad (30)$$

The coupling terms $\delta\hat{H}_0$ and $\delta\hat{V}$ will be treated as a perturbation and retained only in lowest order. The time dependence thus may be simplified in replacing \hat{H} by $\hat{A} + \hat{B} + \hat{V}_A$, e.g.

$$\begin{aligned} e^{(-i/\hbar)\ell'\hat{H}} \delta\hat{V} e^{(i/\hbar)\ell'\hat{H}} = & \sum Q_{k\alpha, k'\alpha'} \cdot \exp \\ & \cdot \{(-i/\hbar)\ell'(\varepsilon_k - \varepsilon_{k'} + V_0\delta_{\alpha+} - V_0\delta_{\alpha'+})\} \hat{c}_{k\alpha}^+ \hat{c}_{k'\alpha'}. \end{aligned}$$

From (30) we get within this approximation

$$\begin{aligned} \hat{H}_t = & \hat{H}_0 + \frac{i}{\hbar} \int_0^t d\ell' \sum \exp \{(-i/\hbar)\ell' \\ & \cdot (\varepsilon_k - \varepsilon_{k'} + V_0\delta_{\alpha+} - V_0\delta_{\alpha'+})\} \\ & \cdot \{Q_{k\alpha, k'\alpha'}(\varepsilon_k - \varepsilon_{k'}) - W_{k\alpha, k'\alpha'} \\ & \cdot V_0(\delta_{\alpha+} - \delta_{\alpha'+})\} \hat{c}_{k\alpha}^+ \hat{c}_{k'\alpha'}. \end{aligned}$$

The time integral is performed as in (21):

$$\begin{aligned} \hat{H}_\infty = & \hat{H}_0 + \delta\hat{V} - \sum \frac{V_0(\delta_{\alpha+} - \delta_{\alpha'+})}{\varepsilon_k - \varepsilon_{k'} + V_0\delta_{\alpha+} - V_0\delta_{\alpha'+} - i\varepsilon} \\ & \cdot (Q_{k\alpha, k'\alpha'} + W_{k\alpha, k'\alpha'}) \hat{c}_{k\alpha}^+ \hat{c}_{k'\alpha'}. \end{aligned} \quad (31)$$

As we are interested in contributions to \hat{H}_∞ which are not invariant under time reversal, we retain only the δ -function part of (31):

$$\begin{aligned} \hat{H}_\infty = & \hat{H}_0 - i\pi V_0 \sum \{Q_{k+, k'-} + W_{k+, k'-} \\ & \cdot \delta(\varepsilon_k - \varepsilon_{k'} + V_0) \hat{c}_{k+}^+ \hat{c}_{k'-} - \text{h.c.}\}. \end{aligned} \quad (32)$$

We gain some insight in the second term of the last equation if we calculate the current operator which

is the time derivative of the particle number of one side.

$$\begin{aligned}\frac{d}{dt} \hat{N}_+ &\equiv \frac{d}{dt} \sum \hat{c}_{k+}^+ \hat{c}_{k+} = \frac{i}{\hbar} [\hat{H}_0 + \hat{V}, \hat{N}_+] \\ &= -\frac{i}{\hbar} \sum \{Q_{k+, k'-} + W_{k+, k'-}\} \cdot \hat{c}_{k+}^+ \hat{c}_{k'-} - \text{h.c.}\} = -\frac{1}{e} \hat{J}.\end{aligned}\quad (33)$$

From a comparison with (32) we conclude that the hamiltonian incorporates matrix elements which coincide with the matrix elements of the current operator \hat{J} taken on the energy shell. The coefficients $Q_{k+, k'-}$ lead to the direct tunneling current through the barrier whereas $W_{k+, k'-}$ represents the so called "assisted" tunneling caused by some potential which is not related to the driving field and may be in addition some perturbation like an impurity.

In a rough estimate we evaluate the k' -sum in (32) for free electrons. In the assumed onedimensional configuration we have translational invariance in two directions, say in the yz -plane, and the matrix elements contain Kronecker deltas $\delta_{k_y, k_{y'}} \delta_{k_z, k_{z'}}$. Only the k_x' -sum is affected by the δ -function of energy conservation. Because of the additional counting by the "side" index α the component k_x runs over positive values:

$$\hat{H}_\infty = \hat{H}_0 - i\pi V_0 \sum \frac{Lm}{2\pi\hbar^2 k_x'} \cdot \{(Q_{k+, k'-} + W_{k+, k'-}) \hat{c}_{k+}^+ \hat{c}_{k'-} - \text{h.c.}\} \quad (34)$$

with

$$k_x' = \sqrt{k_x^2 + \frac{2mV_0}{\hbar^2}}, \quad k_y' = k_y, \quad k_z' = k_z.$$

Only a fraction of the total sum in the current operator of (33) appears in (34) according to energy conservation. It is known that electrons with k_x near the Fermi momentum k_F and $k_y, k_z \approx 0$ dominantly contribute to the current. We replace k_x' by k_F , define

$$\hat{J}_d \equiv \frac{ie}{\hbar} \sum \{(Q_{k+, k'-} + W_{k+, k'-}) \hat{c}_{k+}^+ \hat{c}_{k'-} - \text{h.c.}\} \quad (35)$$

and get

$$\hat{H}_\infty = \hat{H}_0 - \tau \frac{1}{e} V_0 \hat{J}_d \quad (36)$$

with $\tau \equiv Lm/2\hbar k_F$ as the time an electron with Fermi velocity needs to travel through the distance $\frac{1}{2}L$ from the barrier to the boundary of the normaliz-

ing box. The signs of V_0 and $\langle \hat{J}_d \rangle$ will be equal so that the average contribution to the energy is negative as already mentioned. Thus it may be considered as the energy transferred to the currents by the power $(1/e) V_0 \langle \hat{J}_d \rangle$ during the time τ . The current system has completely developed and the final state is reached when the time τ has elapsed. As a consequence of the special procedure to take the limits $L \rightarrow \infty, t \rightarrow \infty$ no reflection at the boundary and therefore no finite recurrence time occurs.

The current can be calculated by from (32) in combination with (14). As long as we refer to weakly coupled systems the same result could be obtained by an expansion of the exponential function in (14) with respect to the second term in (32) as is extensively done in a tunneling theory [5]. There is no approximation involved in treating the potential difference V_0 , first term of (29), which therefore arises nonlinear to all orders in the final formulae e.g. as an argument in the δ -function of (32). The original intention was, however, to consider also some nonlinear aspects of the second term in (29) and similarly in (28) by retaining the whole current contribution in the exponent of the statistical operator. From the view of practical use this treatment may offer an extension as soon as we go beyond weak coupling. If we expect the tunneling current not to be governed by an exponential small transmission coefficient as produced by a thick insulating barrier, i.e. if some resonant mechanism leads to a high conducting channel, this treatment will be more adequate, though an approximation with respect to weak coupling is still further involved. The latter consists in approximating the time dependence of the current operator, once established as a part of the statistical operator \hat{H}_t , by a hamiltonian less complicated than \hat{H} . Surely some dynamical features are thereby neglected, but one may expect an improvement beyond that approximating the statistical operator itself, which is quite another thing.

A rough estimate of the current is obtained by neglecting the second term in \hat{H}_0 , (28), because of its time reversal invariance, and diagonalizing the resulting hamiltonian \hat{H}_∞ , (34), which leads to a 2×2 matrix in the two momenta k_x and k_x' . The unitary transformation

$$\tilde{c}_{k+} = \frac{1}{\sqrt{|\alpha|^2 + \gamma^2}} (\gamma \hat{c}_{k+} + \alpha \hat{c}_{k'-}),$$

$$\tilde{c}_{k-} = \frac{1}{\sqrt{|\alpha|^2 + \gamma^2}} \alpha^* \hat{c}_{k+} - \gamma \hat{c}_{k'-}$$

results in

$$H_\infty = \sum \lambda_{k\sigma} \tilde{c}_{k\sigma}^+ \tilde{c}_{k\sigma}$$

with

$$\lambda_{k\pm} = \varepsilon_{k+} + \frac{1}{2} V_0 (1 \mp \sqrt{1 + |\alpha|^2}),$$

$$\gamma = 1 + \sqrt{1 + |\alpha|^2},$$

$$\alpha = i \frac{Lm}{\hbar^2 k_x'} (Q_{k+, k'-} + W_{k+, k'-}).$$

The new particle operators represent wave functions which contain a current carrying part in form of the pure imaginary admixtures with coefficients α and α^* . Electrons of both states are travelling in opposite directions, whereas the initial wavefunctions were real and consequently carried no current. The energy $\lambda_{k\sigma}$ is different in both states and we get a nonvanishing thermal average of the current.

$$\begin{aligned} \langle j \rangle &= \text{Tr } e^{-\beta \hat{H}_\infty} \hat{j} / \text{Tr } e^{-\beta \hat{H}_\infty} \\ &= \sum \frac{\hbar e k_x'}{Lm} \frac{|\alpha|^2}{\sqrt{1 + |\alpha|^2}} (f(\lambda_{k+}) - f(\lambda_{k-})). \end{aligned}$$

The matrix elements which reflect the structure of

the potential barrier and step appear via $|\alpha|^2$ in the argument of the fermi distribution $f(\lambda_{k\pm})$. This feature is absent in the ordinary theory of independent particle tunneling [6]. The result corresponds to a picture where the electrons are put along a fermi distribution into some sort of scattering — not box normalized — states, which are solutions of the tunneling hamiltonian with the external potential thereby included. These states are individually current carrying states. The current increases with increasing transition matrix elements through both, the prefactor and the difference of fermi functions. The former saturates with $|\alpha|^2$ whereas the latter grows until all electrons take part in the current. Near $T=0$ the denominator of the prefactor is reduced by the fermi functions and the conventional result linear in the transparency, i.e. in the squared tunneling matrix element, appears.

The advantage of the procedure is now again the possibility of applying well known approximation techniques to a statistical operator in a form of equilibrium thermodynamics in order to calculate a transport quantity like the current. This is attractive in the case of electron tunneling with many body interactions which may be included as well [5].

[1] R. Kubo, Rep. Prog. Phys. **29**, 255 (1966).

[2] E. T. Jaynes, Phys. Rev. **106**, 620 (1957).

[3] D. N. Zubarev, Dokl. Akad. Nauk SSSR **140**, 92 (1962).

[4] J. Gyarmati, Non-equilibrium Thermodynamics, Springer-Verlag, Berlin 1970.

[5] W. Schattke and G. K. Birkner, Z. Physik **252**, 12 (1972).

[6] C. B. Duke, Tunneling in Solids, Suppl. 10, Solid State Physics, Acad. Press. (1969).