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Density-Matrix For An Ideal Driven Current Cylinder

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We consider an ideal mesoscopic cylinder in which a steady azimuthal current is generated. We show that the closed interacting-electron system in the presence of the current is described by a density matrix which is that of an equilibrium system without current but with a constrained Hamiltonian.

Two recent papers present new approaches to nonequilibrium steady-state systems. The important common point made in both papers is that steady-state mesoscopic systems can be described by a density matrix which has the form of an *equilibrium* density matrix, but with a constrained Hamiltonian. In the first paper, Hershfield[1] demonstrated that the density matrix $\hat{\rho}$ of a steady-state nonequilibrium quantum system has the general form

$$\hat{\rho} = e^{-\beta(\hat{H}-\hat{Y})}, \tag{1}$$

where $\hat{H}$ is the Hamiltonian, β is the inverse temperature (we will use units in which $k_B = \hbar = e = m_e = 1$), and $\hat{Y}$ is an operator which depends on how the system is driven out of equilibrium. This operator is defined implicitly in terms of a nontrivial infinite set of differential equations. In the other paper (Ref. 2, hereafter referred to as HJ), we formulated an approach to steady-state mesoscopic transport based on the maximum entropy principle of nonequilibrium statistical mechanics.[3] Using the maximum entropy principle, we derived the following density matrix for a multiterminal steady-state mesoscopic system:

$$\hat{\rho} = \exp\left[-\beta\left(\hat{H} - \mu\hat{N} - \sum_{\alpha}\xi_{\alpha}\hat{I}_{\alpha}\right)\right], \tag{2}$$

where $\hat{I}_{\alpha}$ is the current incoming from terminal α and the Lagrangian multipliers ξ_{α} are adjusted to give the applied source-drain current and zero current at all other terminals. This density matrix, like that in Eq. (1), has the form of an equilibrium density matrix of a constrained Hamiltonian. It can also be argued on general grounds using Galilean invariance that distributions of the form obtained from Eq. (2) can be expected in an infinitely long ideal mesoscopic wire.[2,4]

One important point to be noted is that the single-particle distributions obtained in HJ (see also Ref. 5) differ, even when linearized with respect to the currents, from the local-equilibrium distributions typically used in the Landauer-Büttiker[6] formalism of mesoscopic transport. In the linear-response regime, one would not expect that measurements of, for example, conductivity directly probe the electron distributions, since it can in the linear-response approximation be expressed as the trace over the equilibrium density matrix and two-point correlation functions. However, experiments conducted beyond the linear-response regime should be sensitive to the nonequilibrium steady-state electron distributions. This should be the case for precision measurements of the integer quantum Hall effect, where the measured Hall voltage exceeds $16\hbar\omega_c/e$, with ω_c the cyclotron frequency. We demonstrated in HJ that a transport theory based on Eq. (2) can explain the quantization of the integer quantum Hall effect at such large, but experimentally typical, currents, while the Landauer-Büttiker formalism fails to do so.

In deriving the density matrix Eq. (2) using the maximum entropy principle, it was necessary to make assumptions about which are the relevant observables, the expectation values of which are taken to be known. While this is a standard procedure of the maximum entropy approach to statistical mechanics, it is also the source of some controversy about this approach, since no unambiguous procedure for choosing the observables exists.[7] It is therefore desirable to inquire whether such steady-state distributions in mesoscopic systems can be obtained by other means. The purpose of the present paper is to present one such example. We will show by an explicit calculation that the exact density matrix in the presence of a steady current is precisely that of HJ for a simple specific case: a closed system of interacting (spinless) electrons in an ideal, mesoscopic, two-dimensional cylinder. Here we obtain this result by considerations of equilibrium thermodynamics in a rotating reference frame, plus adiabatic switching on, without appeal to the maximum entropy principle. By an ideal system we mean that there are no elastic or inelastic scattering processes other than those resulting from electron-electron interactions. A current is generated in the electron system by adiabatically threading the cylinder with an integral number of flux quanta. In this case, there is then a one-to-one correspondence between the many-body eigenstates in the presence and in the absence of the current. This allows us to demonstrate that the density matrix in the presence of the current can be directly related to the density matrix in the absence of current and has the form of an equilibrium density matrix with a constrained Hamiltonian. While we draw no conclusions about *open* systems here, we provide an explicit example of a system which by an independent calculation proves to be described by the density matrix obtained by HJ.

While the system studied here resembles those con-

sidered in investigations of persistent currents[8] in mesoscopic rings, there are important differences. In those investigations the current as a function of an applied dc magnetic flux is typically calculated for a non-interacting system in the presence of elastic scatterers. (The role of interactions in the presence of disorder is complicated and unclear.[9]) Great care has to be taken to ensemble-average correctly and to account correctly for the magnetic field penetrating the ring itself in an experiment. Also, in the presence of scatterers which break the rotational invariance there is no adiabatic curve crossing as the magnetic flux is increased adiabatically. Here we are considering a closed impurity-free *interacting* electron system and the flux is used only as a device[10] to generate the electric field and the resulting current. Our ultimate goal is to obtain the exact density matrix in the presence of a steady current.

We take the system to be a two-dimensional interacting electron gas confined to a cylindrical shell of radius R. Positions on the shell are described by cylindrical coordinates (r,θ,z), with $r=R$. A uniform azimuthal electric field $E\hat{\theta}$ is generated by piercing the bore of the cylinder with adiabatically increasing magnetic flux. The electric field is described by a time-dependent vector potential

$$\mathbf{A}(r,\theta;t)=\frac{\Phi}{2\pi r}f(t)\hat{\theta}, \tag{3}$$

where Φf is the magnetic flux piercing the cylinder's bore. The monotonically non-decreasing function $f(t)$ describes the adiabatic turning on of the vector potential, with $f(t\to-\infty)=0$ and $f(t\to\infty)=1$. We will assume that $\Phi=p\Phi_0$ with p an integer and $\Phi_0=2\pi c$ the flux quantum, so that the cylinder contains an integral number of flux quanta as $t\to\infty$. From

$$\mathbf{E}=-\frac{1}{c}\frac{\partial\mathbf{A}}{\partial t} \tag{4}$$

the electric field then vanishes for $t\to\pm\infty$ but is finite during the time that f is changing. This finite electric field sets up an azimuthal current which persists as the electric field vanishes, since the system is dissipationless.

With the vector potential given by Eq. (3), the first-quantized many-body Hamiltonian is

$$H=\sum_i\frac{1}{2m^*}\left[-\frac{\partial^2}{\partial z_i^2}+\frac{1}{R^2}\left[L_{z,i}+pf(t)\right]^2\right]+\sum_i V_c(z_i)+\frac{1}{2}\sum_{i\neq j}V(r_{ij}), \tag{5}$$

where the sums are over the N particles of the system, $V_c(z)$ is a confining potential, $r_{ij}=|\mathbf{r}_i-\mathbf{r}_j|$, and $V(r)$ is the electron-electron interaction. Note that $L_{z,i}=-i\partial/\partial\theta_i$ is the canonical angular momentum operator, which is independent of $\mathbf{A}$. The eigenstates of H are given by N-particle wave functions $\Psi=\Psi(z_1\theta_1,z_2\theta_2,\ldots,z_N\theta_N)$. To proceed, we second-quantize the Hamiltonian Eq. (5) using the field operators

$$\hat{\psi}(z,\theta)=\sum_{m,n}c_{mn}\psi_{mn}(z,\theta)\ , \tag{6}$$

where the single-particle wave functions $\psi_{mn}(z,\theta)=\frac{1}{\sqrt{2\pi R}}e^{im\theta}\phi_{mn}(z)$ (normalized to give probability per unit area) satisfy

$$\left[-\frac{1}{2m^*}\nabla^2+V_c(z)\right]\psi_{mn}(z,\theta)=\epsilon_{mn}\psi_{mn}(z,\theta). \tag{7}$$

Here n is a subband index and m an angular momentum index. The second-quantized Hamiltonian is

$$\hat{H}=\sum_{m,n}\epsilon_{mn}c^\dagger_{mn}c_{mn}+\sum_{m,n}\frac{[pf(t)]^2+2mpf(t)}{2m^*R^2}c^\dagger_{mn}c_{mn}+\frac{1}{2}\sum_{\substack{m,m',k\\ n_1,n_2,n_3,n_4}}V_{k;n_1,n_2,n_3,n_4}c^\dagger_{m,n_1}c^\dagger_{m'-k,n_2}\times c_{m',n_3}c_{m-k,n_4}, \tag{8}$$

with $V_{k;n_1,n_2,n_3,n_4}$ the matrix elements of the particle interaction. The total angular momentum operator $L_z=\sum_i L_{z,i}$ becomes

$$\hat{L}_z=\sum_{m,n}mc^\dagger_{mn}c_{mn}. \tag{9}$$

The azimuthal current density operator is $\hat{j}_\theta(z,\theta)=\frac{1}{2}[\hat{\psi}^\dagger v_\theta\hat{\psi}+(v_\theta\hat{\psi})^\dagger\hat{\psi}]$, where $v_\theta=\frac{1}{2m^*R}(L_z+pf)$ is the speed in the azimuthal direction. This can be written

$$\hat{j}_\theta(z,\theta)=\frac{1}{2\pi m^*R^2}\sum_{m,m',n,n'}\left[\frac{m'+m}{2}+pf(t)\right]\times e^{-i(m-m')\theta}\phi^*_{mn}(z)\phi_{m'n'}(z)c^\dagger_{mn}c_{m'n'}. \tag{10}$$

We also introduce an azimuthal current operator $\hat{I}$ by integrating $\hat{j}_\theta(z,\theta)$ over z and averaging over θ, which yields

$$\hat{I}=\frac{1}{2\pi m^*R^2}\sum_{m,n}[m+pf(t)]c^\dagger_{mn}c_{mn}. \tag{11}$$

It is straightforward to show that $\hat{H}$, $\hat{I}$, $\hat{L}_z$, and the number operator $\hat{N}=\sum_{mn}c^\dagger_{mn}c_{mn}$ all commute, so we choose a basis in which all are diagonal. In fact,

$$\hat{I}=\frac{1}{2\pi m^*R^2}(\hat{L}_z+pf\hat{N}), \tag{12}$$

so a basis diagonal in $\hat{L}_z$ and $\hat{N}$ is automatically diagonal in $\hat{I}$, and the eigenvalues I and M of $\hat{I}$ and $\hat{L}_z$ are simply related.

Let us consider next the adiabatic evolution of some N-electron wave function Ψ. Suppose that Ψ is an eigenstate of $H_0\equiv H(f=0)$ with energy E and total angular momentum M. From Eq. (5), the Hamiltonian in the presence of the flux tube can be written

$$H=H_0+\frac{pf}{m^*R^2}\left(L_z+\frac{1}{2}pfN\right). \tag{13}$$

As long as the field is switched on adiabatically (i.e., df/dt is much smaller than electron-electron scattering rates), Ψ remains an eigenstate of H when $f \neq 0$. Although its (canonical) total angular momentum is unchanged, its energy and current change with f. Since p is an integer, the vector potential as $f \to 1$ can be removed by a unitary gauge transformation:

$$\widetilde{\Psi} = \exp\left(ip\sum_i \theta_i\Psi\right),$$
$$\widetilde{H} = \exp\left(ip\sum_i \theta_i\right) H \exp\left(-ip\sum_i \theta_i\right) = H_0. \tag{14}$$

The transformed state $\widetilde{\Psi}$ has total angular momentum $M + pN$ and is an eigenstate of H_0. Thus the spectrum of the Hamiltonian for $t \to \infty$ is identical to the spectrum for $t \to -\infty$. In addition, when $f = 1$ the energy and current of a state with angular momentum M are precisely those of an eigenstate of H_0 with angular momentum $M + pN$. It is clear from this and Eq. (13) that as f grows from 0 to 1 the subset of the spectrum consisting of eigenvalues of states with angular momentum M evolves to the subset of eigenvalues of eigenstates of H_0 with angular momentum $M + pN$. This occurs with no level crossings between states in this subspace (although crossings occur between states with different M).

In particular, suppose we start at $t \to -\infty$ with the system in the interacting ground state (with $M = 0$) and adiabatically turn on the vector potential. Then at $t \to \infty$ the system's energy and current will be that of the lowest-energy eigenstate of H_0 with angular momentum pN. Thus the final energy and current are obtained by finding the lowest-energy eigenstate of H_0 in the subspace with $\langle \hat{L}_z \rangle = pN$. In other words, the final state when a current has been turned on can be found by extremizing H_0 subject to the constraint that $\langle \hat{L}_z \rangle = pN$. Using Eq. (12), we can instead constrain the current to be $\langle \hat{I}_0 \rangle = pN/2\pi m^* R^2$ (where $\hat{I}_0$ is the current operator with $f = 0$). In practice, a convenient way to satisfy the constraint is to introduce a Langrangian multiplier and to look for stationary states of

$$\hat{H}_0 - \xi \hat{I}_0, \tag{15}$$

where ξ is chosen so that $\hat{I}_0$ has the required eigenvalue.

We next turn to finite temperatures and consider a system initially in contact with a particle reservoir, which maintains the average number of particles at N, and in thermal contact with a heat reservoir at temperature T. Initially ($t \to -\infty$) the density matrix is

$$\hat{\rho}_0 = e^{-\beta(\hat{H}_0 - \mu_0 \hat{N})}, \tag{16}$$

and the system has zero average current $\langle \hat{I}_0 \rangle_T \equiv \mathrm{Tr}(\hat{I}_0\hat{\rho}_0)/\mathrm{Tr}(\hat{\rho}_0) = 0$. We then insulate the system thermally from the heat reservoir and adiabatically turn on the vector potential while keeping the average number N fixed. There are two ways to understand what then happens. First, notice that when the system is isolated thermally each subspace of states with a given total angular momentum M becomes a separate subsystem. Although electron-electron interactions could cause reequilibration within a subset, these interactions conserve total angular momentum and so cannot, e.g., transfer energy from one angular momentum subspace to another. Moreover, as explained above, the energy of each state in a given subset changes by exactly the same amount when f varies [see Eq. (13)]. That is, the spacings in energy between the states in each subspace remain constant and consequently the occupancies of these states will not change. Then the occupancy of a state at $t \to \infty$ is given precisely by its initial occupancy at $t \to -\infty$. Consider an N-electron state with initial energy E and angular momentum M. Initially the occupancy of this state is $e^{-\beta(E-\mu_0 N)}$. At $t \to \infty$, this energy and current of this state become

$$E' = E + \frac{p}{m^* R^2}(M + \tfrac{1}{2}pN),$$
$$I' = \frac{1}{2\pi m^* R^2}(M + pN). \tag{17}$$

The occupancy of this state is still $e^{-\beta(E-\mu_0 N)}$. That is, the occupancy is determined not by its energy E', but by E, which can be related to E' and I' using the above. Since the initial and final sets of states are identical (for p an integer), the density matrix can be written in terms of the $f = 0$ operators H_0 and I_0. As $t \to \infty$, the density matrix evolves to

$$\hat{\rho} = \exp\left\{-\beta\left[\hat{H}_0 - \frac{p}{m^* R^2}\left(\hat{L}_z + \frac{1}{2}p\hat{N}\right) - \mu_0\hat{N}\right]\right\}$$
$$= \exp\left\{-\beta\left(\hat{H}_0 - \xi\hat{I}_0 - \mu\hat{N}\right)\right\}, \tag{18}$$

where the final equality defines $\xi = 2\pi p$ and $\mu = \mu_0 + p^2/2m^* R^2$.

A second way to understand this result is to consider equilibrium in a rotating reference frame. As the vector potential is turned on, the system evolves adiabatically as $t \to \infty$ to a state with average current $\langle \hat{I} \rangle_T = I$. After the electric field has returned to zero (as $t \to \infty$), we transform to a coordinate frame rotating with an angular velocity Ω relative to the laboratory frame, where Ω is chosen so that the azimuthal current is zero in the rotating frame. The Hamiltonian $\tilde{H}$ in the rotating frame and the Hamiltonian $\hat{H}$ in the original frame are related by[11]

$$\tilde{H} = \hat{H} - \Omega\hat{L}_z, \tag{19}$$

where

$$\Omega = \frac{p}{m^* R^2}. \tag{20}$$

In the rotating frame, the system consists of an isolated interacting electron gas at zero net current. In this frame, one should expect the electron-electron interactions to equilibrate the system. (This equilibration is at the same temperature T that the system was in at $t \to -\infty$ in the laboratory frame, since the center-of-mass motion of a system does not change the temperature.[12]) Thus, in the

rotating frame, the system has an equilibrium density matrix

$$\tilde{\rho} = e^{-\beta(\tilde{H}-\tilde{\mu}\hat{N})}. \tag{21}$$

We express this density operator in terms of the Hamiltonian $\hat{H}_0$ of the stationary frame at zero flux by first using Eq. (19) and then gauging away the vector potential as above. With the operators in their first-quantized form, this gauge transformation gives

$$\begin{aligned} e^{-\beta(H-\Omega\hat{L}-\tilde{\mu}N)} &\to \exp\left(ip\sum_i \theta_i e^{-\beta(H-\Omega L-\tilde{\mu}N)}\right) \\ &\quad \times \exp\left(-ip\sum_i \theta_i\right) \\ &= \exp\left[-\beta(H_0 - \mu N - \Omega L)\right], \end{aligned} \tag{22}$$

where $\mu = \tilde{\mu} + p^2/m^*R^2$. Thus the system is described by the density matrix

$$\hat{\rho} = e^{-\beta(\hat{H}_0-\xi\hat{I}_0-\mu\hat{N})}, \tag{23}$$

where we have used Eq. (12) [with $\hat{I}_0 = I(f=0)$], and as before $\xi = 2\pi p$. In practice one can regard μ and ξ as parameters which are adjusted to give the required thermal averages of particle number and current. Thus the density matrix is that of an equilibrium systems described by a *constrained* Hamiltonian and is identical to that [Eq. (2)] obtained in HJ by maximizing the entropy subject to constraints on internal energy, particle number, and total current.

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