Quantum diffusion: a simple, exactly solvable model

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Abstract

We propose a simple quantum mechanical model describing the time dependent diffusion current between two fermion reservoirs that were initially disconnected and characterized by different densities or chemical potentials. The exact, analytical solution of the model yields the transient behavior of the coupled fermion systems evolving to a final steady state, whereas the long-time behavior is determined by a power law rather than by exponential decay. Similar results are obtained for the entropy production which is proportional to the diffusion current.

1 Introduction

Key ingredients to the investigation of non-equilibrium features of physical systems, time irreversibility, energy dissipation and entropy production [1, 2, 3, 4, 5]
can be treated analytically only in a few cases. Providing a well-known example of the latter, the Caldeira-Leggett model [6] along with all its extensions [7, 8, 9] essentially leans on the quadratic interaction imposed to couple a huge number of harmonic oscillators. As such, the resulting equations of motion governing the dynamics of any relevant observables remain classical, in spite of the quantum mechanical nature of the density matrix, potentially representing the initial equilibrium conditions. In this light, it is tempting to conceive an exactly solvable model that reveals a signature of quantum dynamics while exhibiting at least one of the typical non-equilibrium features such as irreversibility. The model presented below describes quantum diffusion as the basic mechanism underlying the particle exchange between two fermion systems that are brought into contact at some time instant $t = 0$, while having been separated at all previous times. Section 2 introduces the model in terms of its Hamiltonian and discusses the time evolution in the framework of the Heisenberg picture. In section 3 the Heisenberg equations of motion for the fermion creation and annihilation operators are explicitly solved and the time dependent observables, including the diffusion current, are extracted by averaging the corresponding Heisenberg operators with the initial density matrix characterizing the initial equilibrium of the uncoupled fermion reservoirs. As a result, the time dependent fermion densities are calculated explicitly and the results are discussed in terms of the occurrence of time irreversibility. In particular, a direct relation between the diffusion current and the entropy production is exploited to study the time dependence of the latter. Finally, a conclusion is drawn in section 4.

2 Two coupled fermion systems: Heisenberg equations of motion

We consider two non-interacting fermion gases establishing two-dimensional reservoirs in thermal equilibrium that are completely disconnected at all times preceding $t = 0$, while being confined to two rectangular areas with sizes $L_x$ and $L_y$. The uncoupled reservoirs are at the same temperature, however with different initial densities $n_{10}$ and $n_{20}$. The Hamiltonian of the disconnected 2DEGs can be written as

$$\hat{H}_0 = \hat{H}_{01} + \hat{H}_{02} = \sum_k \epsilon_k (c_{1k}^\dagger c_{1k} + c_{2k}^\dagger c_{2k}) ,$$

(1)
where \( c_{1k}, c_{1k}^\dagger \) and \( c_{2k}, c_{2k}^\dagger \) respectively denote the fermion creation and annihilation operators for both subsystems and \( \epsilon_k \) are the single-particle eigenenergies. For the sake of simplicity, spin degrees of freedom have been ignored whereas the eigenenergies are taken to be parabolic, i.e. \( \epsilon_k = \hbar^2 k^2 / 2m \) with \( m \) denoting the fermion effective mass. As of \( t = 0 \), the two reservoirs get connected by turning on the perturbation

\[
\hat{H}' = \sum_k \Lambda_k \left( c_{1k}^\dagger c_{2k} + c_{2k}^\dagger c_{1k} \right).
\]

which initiates the exchange of fermions. \( \Lambda_k \) is the transition rate specifying the number of fermions with a given wave vector \( k \) being transferred from one reservoir to the other. Throughout this paper \( \Lambda_k \) is considered real and even in \( k \). The total Hamiltonian now reads

\[
\hat{H} = \hat{H}_0 + \theta(t) \hat{H}'.
\]

The time dependence of the observables characterizing the diffusion process will be extracted from the time dependent Heisenberg operators \( c_{1k}(t), c_{1k}^\dagger(t), c_{2k}(t), c_{2k}^\dagger(t) \). The latter are known to obey the Heisenberg equations of motion

\[
i\hbar \frac{dc_{jk}(t)}{dt} = [c_{jk}(t), \hat{H}], \quad i\hbar \frac{dc_{jk}^\dagger(t)}{dt} = [c_{jk}^\dagger(t), \hat{H}], \quad j = 1, 2.
\]

which, in the present case, reduce to

\[
i\hbar \frac{dc_{1k}(t)}{dt} = \epsilon_k c_{1k}(t) + \Lambda_k c_{2k}(t),
\]

\[
i\hbar \frac{dc_{2k}(t)}{dt} = \Lambda_k c_{1k}(t) + \epsilon_k c_{2k}(t),
\]

because the perturbation (Eq. 2) does not mix momenta during a transfer process. Consequently, we may analytically solve the equations of motion and explicitly present the solutions in terms of the Heisenberg operators at \( t = 0 \), thus yielding separately the time evolution in the form of \( 2 \times 2 \) unitary matrix for each \( k \),

\[
\begin{pmatrix}
  c_{1k}(t) \\
  c_{2k}(t)
\end{pmatrix}
= \exp \left( -\frac{i \epsilon_k t}{\hbar} \right) \begin{pmatrix}
  \cos (\frac{\Lambda_k t}{\hbar}) & -i \sin (\frac{\Lambda_k t}{\hbar}) \\
  -i \sin (\frac{\Lambda_k t}{\hbar}) & \cos (\frac{\Lambda_k t}{\hbar})
\end{pmatrix}
\begin{pmatrix}
  c_{1k}(0) \\
  c_{2k}(0)
\end{pmatrix}.
\]
In particular, the operators the average of which provides the occupation numbers of the first subsystem are given by

\[
c_{1k}(t) c_{1k}(t) = \cos^2 \left( \frac{\Lambda_k t}{\hbar} \right) c_{1k}(0) c_{1k}(0) + \sin^2 \left( \frac{\Lambda_k t}{\hbar} \right) c_{2k}(0) c_{2k}(0) \\
- i \cos \left( \frac{\Lambda_k t}{\hbar} \right) \sin \left( \frac{\Lambda_k t}{\hbar} \right) \left[ c_{1k}^+(0) c_{2k}(0) - c_{2k}^+(0) c_{1k}(0) \right]
\]

(8)

whereas a similar expression follows for \( c_{2k}(t) c_{2k}(t) \). As all time dependence is in the operators, the Heisenberg picture only requires the explicit knowledge of the initial density matrix \( \hat{\rho}_0 \) to calculate any expectation values at arbitrary later times. In general, a time dependent observable \( Y \) representing the time dependent ensemble average of a Heisenberg operator \( \hat{Y}(t) \) is to be extracted according to the recipe [10]

\[
Y_t = \langle \hat{Y}(t) \rangle = \text{Tr} \left[ \hat{\rho}_0 \hat{Y}(t) \right].
\]

(9)

As both fermion reservoirs are assumed to be uncoupled at \( t = 0 \) and before, the initial density matrix \( \hat{\rho}_0 \) reduces to the product of the two reservoir density matrices

\[
\hat{\rho}_0 = \frac{1}{Z_0} \exp \left( -\beta \left( \hat{H}_{01} - \mu_1 \hat{N}_1 \right) \right) \exp \left( -\beta \left( \hat{H}_{02} - \mu_2 \hat{N}_2 \right) \right)
= \frac{1}{Z_0} \prod_k \exp \left( -\beta \left( \epsilon_k - \mu_1 \right) c_{1k}^+ c_{1k} \right) \exp \left( -\beta \left( \epsilon_k - \mu_2 \right) c_{2k}^+ c_{2k} \right),
\]

(10)

where \( \beta = 1/k_B T \), \( Z_0 \) is the partition function and \( \mu_1, \mu_2 \) denote the reservoir chemical potentials compatible with the initial densities \( n_{10} \) and \( n_{20} \). The number operators counting the fermions in the distinguished reservoirs are given by

\[
\hat{N}_j = \sum_k c_{jk}^+ c_{jk}, \quad j = 1, 2.
\]

(11)

Obviously, the initial density matrix (10) translates to the Fermi-Dirac distribution ruling the initial occupation numbers:

\[
\langle c_{jk}^+(0) c_{jk}(0) \rangle = F_j(\epsilon_k) \delta_{i,j}, \quad F_j(E) = \frac{1}{1 + \exp \left( \beta (E - \mu_j) \right)}, \quad j, l = 1, 2.
\]

(12)

Combining Eqs. (8) and (12), we arrive at

\[
\langle c_{1k}^+(t) c_{1k}(t) \rangle = \cos^2 \left( \frac{\Lambda_k t}{\hbar} \right) F_1(\epsilon_k) + \sin^2 \left( \frac{\Lambda_k t}{\hbar} \right) F_2(\epsilon_k),
\]

(13)
In particular, we obtain the generic expression for the time dependent fermion density in the first reservoir from

\[ n_1(t) = \frac{1}{L_x L_y} \langle \hat{N}_1(t) \rangle = \frac{1}{L_x L_y} \sum_k \langle \hat{c}_{1k}^\dagger(t) \hat{c}_{1k}(t) \rangle = \frac{1}{L_x L_y} \sum_k \left[ \cos^2 \left( \frac{\Lambda_k t}{\hbar} \right) F_1(\epsilon_k) + \sin^2 \left( \frac{\Lambda_k t}{\hbar} \right) F_2(\epsilon_k) \right], \tag{14} \]

which can be rewritten as

\[ n_1(t) = \frac{1}{2} (n_{10} + n_{20}) + \frac{1}{2L_x L_y} \sum_k \cos \left( \frac{2\Lambda_k t}{\hbar} \right) [F_1(\epsilon_k) - F_2(\epsilon_k)] \] \tag{15}

3 Solution and discussion

Defining the diffusion current density \( J_D(t) \) to be the rate of change of the fermion density in the first reservoir, we may obtain the corresponding expression for the present model by simply taking the time derivative of Eq. (15),

\[ J_D(t) = \frac{dn_1(t)}{dt} = -\frac{1}{\hbar L_x L_y} \sum_k \Lambda_k \sin \left( \frac{2\Lambda_k t}{\hbar} \right) [F_1(\epsilon_k) - F_2(\epsilon_k)] \] \tag{16} \]

It is worth noting that the entropy production is unambiguously determined by the total diffusion current \( I_D = J_D L_x L_y = d \langle \hat{N}_1(t) \rangle / dt \), the initial difference of the chemical potentials \( \mu_1 - \mu_2 \) and the common, ambient temperature \( T \). Starting from the time dependent density matrix \( \hat{\rho}_t \) satisfying the quantum Liouville equation

\[ i\hbar \frac{d\hat{\rho}_t}{dt} = [\hat{H}, \hat{\rho}_t], \tag{17} \]

we first consider the relative entropy \([1, 2, 3, 4, 5]\)

\[ S[\hat{\rho}_t, \hat{\rho}_0] = -k_B \text{Tr} [\hat{\rho}_t (\ln \hat{\rho}_0 - \ln \hat{\rho}_t)]. \tag{18} \]

From Eq. (17) one may easily derive the well-known result \( \text{Tr}(\hat{\rho}_t \ln \hat{\rho}_t) = \text{Tr}(\hat{\rho}_0 \ln \hat{\rho}_0) \) which is the mathematical statement of the Shannon entropy failing to evolve in time. Substitution into Eq. (18) yields

\[ S[\hat{\rho}_t, \hat{\rho}_0] = -k_B \text{Tr} [\hat{\rho}_t (\ln \hat{\rho}_0 - \ln \hat{\rho}_0)], \tag{19} \]

5
whereas the factorized, initial density matrix in Eq. (10) leads to
\[
\text{Tr} (\hat{\rho}_t \ln \hat{\rho}_0) = -\beta \text{Tr} \left[ \hat{\rho}_t \left( \hat{H}_0 - \mu_1 \hat{N}_1 - \mu_1 \hat{N}_2 \right) \right].
\tag{20}
\]
Next, we use \(\hat{\rho}_t = \exp (-i\hat{H}t/\hbar) \hat{\rho}_0 \exp (i\hat{H}t/\hbar)\) which provides the formal solution to the Liouville equation, to eliminate the time dependence of the density matrix and recast Eq. (20) in the Heisenberg picture:
\[
\text{Tr} (\hat{\rho}_t \ln \hat{\rho}_0) = -\beta \text{Tr} \left[ \hat{\rho}_0 \left( \hat{H}_0(t) - \mu_1 \hat{N}_1(t) - \mu_1 \hat{N}_2(t) \right) \right].
\tag{21}
\]
Using Eq. (21) and bearing in mind that \(\hat{H}_0\) is a constant of motion because the diffusion process is not accompanied by energy exchange, we obtain
\[
S [\hat{\rho}_t, \hat{\rho}_0] = -\frac{1}{T} \sum_{j=1,2} \left[ \mu_j (\langle \hat{N}_j(t) \rangle - \langle \hat{N}_j(0) \rangle) \right].
\tag{22}
\]
Eq. (22) reveals that any entropy change is to be considered configurational in the sense that it is exclusively due to the redistribution of all fermions over both reservoir areas. Emerging as the time derivative of the relative entropy, the entropy production can be directly derived from Eq. (22):
\[
\frac{dS(t)}{dt} = -\frac{1}{T} \sum_{j=1,2} \left[ \mu_j \frac{d}{dt} \langle \hat{N}_j(t) \rangle \right].
\tag{23}
\]
Finally, taking into account that the total number of fermions is a constant of motion as well, we arrive at
\[
\frac{dS(t)}{dt} = -\frac{1}{T} (\mu_1 - \mu_2) I_D(t).
\tag{24}
\]
Hence, the entropy production is instantly proportional to the diffusion current while the sign of the latter depends on which of either reservoirs is being emptied into the other. In order to obtain more detailed results or numerical output based on Eq. (15), it is paramount to specify the functional dependence of \(\Lambda_k\) on the wave vector \(k\) as well as to identify the range of allowed wave vectors. A simple and straightforward model favoring the transfer of high-energy fermions corresponds to \(\Lambda_k\) being chosen proportional to \(\varepsilon_k\), say
\[
\Lambda_k = \Lambda_k = \lambda \varepsilon_k, \quad \lambda > 0
\tag{25}
\]
and will be further explored as a benchmark. Moreover, it follows from Eq. (15) emerging as a sum of trigonometric oscillations that the time evolution of the present diffusion model is bound to be reversible as long as the allowed wave vectors run through a finite, countable set. Phrased otherwise, time irreversibility is expected to occur only if the thermodynamic limit is taken with \( L_x, L_y, \langle \hat{N}_1 \rangle, \langle \hat{N}_2 \rangle \rightarrow \infty \), the densities \( n_1 \) and \( n_2 \) however remaining finite. Traditionally, this encompasses the conversion of the summation over \( k \) into a 2D integration according to
\[
\frac{1}{L_x L_y} \sum_k \rightarrow \frac{1}{4\pi^2} \int d^2 k
\]
Carrying out the latter and transforming to the “polar” coordinates \((\sqrt{E}, \phi)\) according to
\[
k_x = \frac{\sqrt{2mE}}{\hbar} \cos \phi, \quad k_y = \frac{\sqrt{2mE}}{\hbar} \sin \phi, \quad E \geq 0, \ 0 \leq \phi \leq 2\pi,
\]
we obtain
\[
n_1(t) = \frac{1}{2} (n_{10} + n_{20}) + \frac{1}{8\pi^2} \int d^2 k \cos \left( \frac{2\lambda \varepsilon_k t}{\hbar} \right) [F_1(\varepsilon_k) - F_2(\varepsilon_k)]
\]
\[
= \frac{1}{2} (n_{10} + n_{20}) + \frac{m}{8\pi^2 \hbar^2} \int_0^\infty dE \int_0^{2\pi} d\phi \cos \left( \frac{2\lambda E t}{\hbar} \right) [F_1(E) - F_2(E)]
\]
\[
= \frac{1}{2} (n_{10} + n_{20}) + \frac{m}{4\pi \hbar^2} \int_0^\infty dE \cos \left( \frac{2\lambda E t}{\hbar} \right) [F_1(E) - F_2(E)].
\]
Clearly, the damped oscillations are driven by the initial chemical potential difference \( \mu_1 - \mu_2 \). Note that the 2D geometry of the two reservoirs enables us to extract analytically the relation between \( \mu_1, \mu_2 \) and the corresponding initial densities from
\[
\mu_j = k_B T \ln \left[ \exp \left( \frac{2\pi \hbar^2 n_{j0}}{mk_B T} \right) - 1 \right], \quad j = 1, 2.
\]
Any further analytical treatment of Eq. (28) amounts to either a series expansion of the Fermi-Dirac distribution function when it comes to keep track of the temperature dependence, or to studying the extreme quantum limit at zero temperature. In the latter case, the Fermi-Dirac functions reduce to step functions respectively
imposing integration boundaries at $E = \mu_1 > 0$ and $E = \mu_2 > 0$, yielding

$$n_1(t) = \frac{1}{2} (n_{10} + n_{20}) + \frac{m}{4\pi\hbar^2} \int_{\mu_2}^{\mu_1} dE \cos \left( \frac{2\lambda E t}{\hbar} \right)$$

$$= \frac{1}{2} (n_{10} + n_{20}) + \frac{m}{8\pi\hbar} \cdot \frac{1}{t} \left[ \sin \left( \frac{2\lambda \mu_1 t}{\hbar} \right) - \sin \left( \frac{2\lambda \mu_2 t}{\hbar} \right) \right]$$  \hspace{1cm} (30)

On the other hand, in the classical limit corresponding to $k_B T \gg \pi \hbar^2 n_{j0}/m$ and $\mu_1, \mu_2 < 0$ we may replace the Fermi-Dirac functions with bare exponentials to arrive at

$$n_1(t) = \frac{1}{2} (n_{10} + n_{20}) + \frac{m}{4\pi\hbar^2} \int_0^\infty dE \cos \left( \frac{2\lambda E t}{\hbar} \right) e^{-\beta E}$$

$$= \frac{1}{2} (n_{10} + n_{20}) + \frac{\beta m}{4\pi} \left( e^{\beta \mu_1} - e^{\beta \mu_2} \right) \frac{1}{\beta^2\hbar^2 + 4\lambda^2 t^2}$$

$$= \frac{1}{2} (n_{10} + n_{20}) + \frac{1}{2} \frac{(n_{10} - n_{20})}{\beta^2\hbar^2 + 4\lambda^2 t^2}$$  \hspace{1cm} (31)

This time, the evolution of $n_1(t)$ towards its steady-state value $n_s = 1/2(n_{10} + n_{20})$ is governed by a $t^{-2}$ power law, while no oscillations are observed during the transient regime. Note that, whenever irreversibility is established, the evolution from the original equilibrium state to the final steady state corresponds to an entropy increase because $n_{10}$, the original density in reservoir 1, decreases (increases) towards $n_s$ provided that $\mu_1 > (\mu_2)$, as can also be seen from the entropy change per particle,

$$\Delta s \equiv \lim_{t \to \infty} \frac{S[\hat{\rho}_t, \hat{\rho}_0]}{\langle \hat{N}_1(t) \rangle + \langle \hat{N}_2(t) \rangle} = \frac{\mu_1 - \mu_2}{T} \cdot \frac{n_{10} - n_{20}}{n_{10} + n_{20}}.$$  \hspace{1cm} (32)

4 Conclusion

The quantum diffusion model presented in this paper can be solved analytically to obtain a closed-form integral representation of the time dependent observables, such as the fermion density in the reservoirs. The long-time behavior is governed by a power law $t^{-\alpha}$ where $\alpha = 1$ and $\alpha = 2$ respectively characterize the extreme quantum regime and the classical regime. The time dependent entropy production is proportional to the diffusion current while the irreversibility of the latter in the case of the thermodynamic limit corresponds to a net increase of the (configurational) entropy when the steady-state is attained.
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