Generalized-master-equation theory for heavy ion collisions

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We apply nonequilibrium quantum statistical mechanics to the description of heavy ion collisions. Starting from the Liouville-Von Neumann equation we derive via the generalized master equation, the drift and diffusion coefficients.

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Recently[1-3] transport equations in general and the Fokker-Planck equation in particular have been used with considerable success in explaining the experimental data in heavy ion collisions with energies up to several MeV per particle. Consequently, the drift and diffusion coefficients which characterize the solution of the Fokker-Planck equation are of considerable importance. Thus a justification of these coefficients, from first principle in terms of the dynamics of the system, is very much warranted. In a recent publication, Randrup[4] has attempted to find the expressions of these coefficients. Taking the Fokker-Planck equation for granted, he has tried to obtain the expressions using a time-dependent perturbation theory in the framework of quantum mechanics. Here, we present a simple and straightforward derivation of these coefficients starting from the Liouville-Von Neumann equation and following the basis of nonequilibrium statistical mechanics. At the outset we must emphasize that the basic quantity in our formalism is the memory function [Eq. (10)] which is kept completely general in the present communication. By assigning different forms and shapes to memory functions one arrives at different types of transport equations. This is very interesting. However, we defer its discussion at present and shall elaborate on it elsewhere.

The details of the formalism using the memory functions are discussed elsewhere[5] and hence will not be repeated. However, with the help of a few essential steps we define our notations. The Liouville-Von Neumann equation for the density matrix ρ is

$$i\hbar \frac{\partial \rho}{\partial t} = [H, \rho] = L\rho , \tag{1}$$

where L is the Liouville operator and H is the Hamiltonian of the system which can be written as

$$H = H_0 + V . \tag{2}$$

Let $i, j, \ldots$ and $\epsilon_i, \epsilon_j, \ldots$ refer to the eigenstates and energy eigenvalues of H_0. The occupation probability P_i in the state i is given by the diagonal element of the density matrix

$$P_i = \langle i|\rho|i\rangle . \tag{3}$$

Following Zwanzig[5] one introduces a projection operator defined through the relation

$$(\mathcal{P}O)_{ij} = O_{ii}\delta_{ij} \tag{4}$$

for any operator O and then one obtains from Eq. (1)

$$\frac{\partial P_i(t)}{\partial t} = \int_0^t ds \sum_j [W_{ij}(t-s)P_j(s) - W_{ji}(t-s)P_i(s)] + \mathcal{g}_i(t) , \tag{5}$$

where

$$W_{ij}(t) = -\{\mathcal{P}Le^{-it(1-\mathcal{P})L}(1-\mathcal{P})L\}_{iijj} \tag{6}$$

and

$$\mathcal{g}_i(t) = i\{\mathcal{P}Le^{-it(1-\mathcal{P})L}(1-\mathcal{P})\rho(0)\}_{ii} . \tag{7}$$

Under the initial diagonality condition

$$\rho(0) = \rho_d(0) , \tag{8}$$

$\mathcal{g}_i(t)$ becomes zero in Eq. (5) and one obtains the generalized master equation (GME) as

$$\frac{\partial P_i(t)}{\partial t} = \int_0^t ds \sum_j [W_{ij}(t-s)P_j(s) - W_{ji}(t-s)P_i(s)] , \tag{9}$$

where W's are called the memory functions. Under the weak coupling approximation, Zwanzig has obtained the expression for W as

$$W_{ij}(t) = 2|\langle i|V|j\rangle|^2 \cos(\epsilon_i - \epsilon_j)t . \tag{10}$$

Equation (8) is an exact consequence of quantum mechanics and describes the time evolution of the microscopic state $|i\rangle$. However, to use the GME for macroscopic description, one introduces

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coarse graining by labeling a group of eigenstates of H_0 as a single coarse grained state $|I\rangle$ and then makes the identification

$$P_I = \sum_{i \in I} \langle i|\rho|i\rangle . \tag{11}$$

The resulting GME has exactly the same form as (9)

$$\frac{\partial P_I(t)}{\partial t} = \int_0^t ds \Big\{ \sum_J [W_{IJ}(t-s)P_J(s) - W_{JI}(t-s)P_I(s)] \Big\} . \tag{12}$$

The coarse grained memory function also assumes the form

$$W_{IJ}(t) = 2 \sum_{\substack{i \in I \\ j \in J}} |\langle i|V|j\rangle|^2 \cos(\epsilon_i - \epsilon_j)t . \tag{13}$$

We make nearest neighbor approximation on W in (12) and obtain

$$\frac{\partial P_I(t)}{\partial t} = \int_0^t ds [W_{I,I-1}(t-s)P_{I-1} + W_{I,I+1}(t-s)P_{I+1} - W_{I-1,I}P_I - W_{I+1,I}P_I] . \tag{14}$$

Taking the continuum limit and assuming W to be symmetric we obtain from Eq. (14)

$$\frac{\partial P_I(t)}{\partial t} = \int_0^t ds \Big[W_V \frac{\partial P_I}{\partial I} + \frac{1}{2!} W_D \frac{\partial^2 P_I}{\partial I^2} \Big], \tag{15}$$

where

$$W_V = W_{I,I+1} - W_{I,I-1}$$

and (16)

$$W_D = W_{I,I+1} + W_{I,I-1} .$$

It is easy to see that the Marcoffion approximation on W_D and W_V would lead to the usual Fokker-Planck equation.

Now we consider two isolated systems A and B, the projectile and target, respectively, consisting of many noninteracting fermions. Assuming a single-particle picture for both, the Hamiltonian H_0 in Eq. (2) could be written as

$$H_0 = H_A + H_B = \sum_\alpha e_\alpha a_\alpha^\dagger a_\alpha + \sum_\beta e_\beta b_\beta^\dagger b_\beta , \tag{17}$$

where a_α, $a_\alpha^\dagger$ and b_β, $b_\beta^\dagger$ are the destruction and creation operators satisfying the usual anticommutation rule. The two systems are allowed to interact by way of exchanging particles. This interaction is represented by one-particle transfer operator V given by

$$V = \sum_{\alpha\beta} \langle \alpha|V|\beta\rangle [a_\alpha^\dagger b_\beta + b_\beta^\dagger a_\alpha] , \tag{18}$$

which transfers particles from target B to projectile A and vice versa. The microscopic states i, $i-1$, and $i+1$ can be written as

$$i = \phi_p(N_A)\phi_T(N_B) ,$$
$$i-1 = \phi_p(N_A - 1)\phi_T(N_B + 1) ,$$
$$i+1 = \phi_p(N_A + 1)\phi_T(N_B - 1) ,$$

where

$$\phi_p(N_A) = \prod_{\alpha=1}^{N_A} a_\alpha^\dagger |0\rangle ,$$
$$\phi_T(N_B) = \prod_{\beta=1}^{N_B} b_\beta^\dagger |0\rangle .$$

Thus we assume that successive macrostates differ by the configuration of only one microscopic state. It is straightforward to obtain from Eq. (13) the expression for $W_{I,I-1}$ and $W_{I,I+1}$ as

$$\begin{aligned} W_{I,I+1} &= 2 \sum_{\alpha\beta} \{\langle \alpha|V|\beta\rangle [(1 - f_\alpha^A)^{1/2} (f_\beta^B)^{1/2}]\}^2 \\ &\quad \times \cos(e_\alpha - e_\beta)t , \\ W_{I,I-1} &= 2 \sum_{\alpha\beta} \{\langle \alpha|V|\beta\rangle [(f_\alpha^A)^{1/2} (1 - f_\beta^B)^{1/2}]\}^2 \\ &\quad \times \cos(e_\alpha - e_\beta)t , \end{aligned} \tag{19}$$

where f_α^A and f_β^B are the occupation probability of the single-particle states α and β in the nuclei A and B, respectively.

Following Munn[6] it is easy to show that the memory is related to the diffusion constant D as

$$2D = \int_0^\infty W_D(t)dt . \tag{20}$$

Straightforward analogy gives the drift coefficient V_D as

$$V_D = \int_0^\infty W_V(t)dt . \tag{21}$$

Using (16), (19), (20), and (21) we arrive at

$$\begin{aligned} 2D &= 2\pi \sum_{\alpha\beta} [f_\alpha^A(1 - f_\beta^B) + f_\beta^B(1 - f_\alpha^A)] \\ &\quad \times |\langle \alpha|V|\beta\rangle|^2 \delta(e_\alpha - e_\beta) , \\ V_D &= 2\pi \sum_{\alpha\beta} [f_\alpha^A - f_\beta^B] |\langle \alpha|V|\beta\rangle|^2 \delta(e_\alpha - e_\beta) . \end{aligned}$$

Considering the two systems to be large, we replace the sums over the states as integrations over energy

$$\sum_\alpha \to \int de_A \rho_A(e_A) ,$$
$$\sum_\beta \to \int de_B \rho_B(e_B) ,$$

where $\rho_A(e_A)$ and $\rho_B(e_B)$ are the density of single-particle states in A and B, respectively. This leads to

$$2D = 2\pi \int de[(1 - f^A(e)) f^B(e) + f^A(e)(1 - f^B(e))] \times |V(e)|^2 \rho_A(e)\rho_B(e),$$

$$V_D = 2\pi \int de[f^B(e) - f^A(e)] |V(e)|^2 \rho_A(e)\rho_B(e).$$

These expressions for drift and diffusion coefficients match up exactly with the expressions obtained by Randrup.[4] Using a model heavy ion potential he has applied these expressions to specific cases of physical interest. Consequently, we do not elaborate on their applications here. It is gratifying to note that using quantum statistical mechanics and via GME one arrives at the expressions of drift and diffusion coefficient without making a Marcoffion approximation which have been obtained by Randrup following the time-dependent perturbation theory in the framework of quantum mechanics. It is worth emphasizing here that the present work links in a straightforward manner the dynamics of the system with the nonequilibrium statistical aspects of the transfer phenomena in heavy ion collision.

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