Nuclear Response Function in the Mori Formalism

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The Mori formalism is used to study the nuclear response function at finite temperatures. This formalism rather naturally leads to an extension of the zero-temperature random-phase approximation for finite temperatures, and it provides a prescription for the calculation of the damping widths of vibrational states at finite temperatures.

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Time-correlation functions of dynamical variables play an important role in the description of many-body systems, such as liquids and plasmas.[1] It is well known that the transport parameters which characterize the irreversible behavior of such thermodynamical systems can be expressed in terms of time-correlation functions calculated under equilibrium conditions. Observables can often be related to appropriate correlation functions. For example, the density-correlation function characterizes the linear response of the system to an external perturbation. The transition strengths from ground state to excited states induced by an external field and inelastic scattering in the Born approximation can be directly related to the nuclear response function, that is, the Fourier transform of the density-correlation function.[2]

In statistical mechanics very powerful formalisms are developed for the description of irreversible properties of many-body systems. In particular, the Mori formalism provides a rather convenient framework for calculating time-correlation functions of dynamical variables. This formalism can be used to describe a broad range of relaxation processes observed in nuclear collisions and to compute transport parameters which characterize the approach to thermal or chemical equilibrium. In the present work, as an illustrative example, we study the density-correlation function (nuclear response function) in the framework of the Mori formalism. In particular, we focus our attention on the damping of the density-correlation function and calculate the spreading widths of vibrational states at finite temperature.[3]

There has been considerable interest in the application of projection-operator techniques developed by Zwanzig[4] for the study of irreversible processes. This approach was subsequently generalized and extended by Mori[5] who, utilizing projection operators similar to those of Zwanzig, derived an exact "generalized Langevin equation" (GLE), describing the time evolution of an arbitrary vector of observables, $A(t)$, whose components, $A_a(t)$, are dynamical variables of a many-body system:

$$dA(t)/dt - i\Omega \cdot A(t) + \int_0^t d\tau\, \phi(\tau) \cdot A(t-\tau) = f(t). \quad (1)$$

Here the dynamical variables are defined such that they have no time-invariant part, $A(t) = \mathcal{A}(t) - \langle \mathcal{A}(t) \rangle$, where (and also in the rest of the paper) $\langle \ldots \rangle$ denotes an average over the equilibrium canonical ensemble $\rho = \exp(-\beta H)/Z$, characterized by a temperature, $\beta = 1/T$. Notice that Eq. (1) is a generalized form of the Langevin equation familiar from the stochastic theory of Brownian motion. However, it is an exact equation for $A(t)$, and hence equivalent to the equations of motion for the many-body system. In the Mori formalism, the choice of the set of dynamical variables is essentially left arbitrary. For any given set of dynamical variables, the "frequency matrix" Ω, the "damping term" $\phi(\tau)$, and the "random force" $f(t)$ are precisely defined in the GLE. Since we are concerned, in the present work, with the density-correlation function, we choose the dynamical variables as the set of particle-hole (p-h) excitation operators, $A = \{a_k^\dagger a_l,\ k < l\}$, which satisfies a normalization condition

$$\langle [A_a,\ A_b^\dagger] \rangle = \delta_{ab}. \quad (2)$$

Here $A_a = A_a(0)$ and $A_b^\dagger = A_b^\dagger(0)$ denote the initial values of dynamical variables, e.g., Heisenberg operators. Unless otherwise indicated, we use the notation $A_a = a_k^\dagger a_l$ for an ordered p-h excitation operator with a single index $a = (k,l)$.

For the set of p-h operators obeying the normalization condition (2), the frequency matrix in GLE is given by

$$\Omega_{ab} = \langle [[H, A_a], A_b^\dagger] \rangle \quad (3)$$

and the damping term is given by the time-correlation function of the random force as

$$\phi_{ab}(t) = \langle [f_a(t), f_b^\dagger(0)] \rangle. \quad (4)$$

The random force on the dynamical variable A_a is expressed as

$$f_a(t) = \exp[it(1-P)L]\, i(1-P)LA_a, \quad (5)$$

where $L = i[H, \cdot\,]$ is the Liouville operator, and P denotes a projection operator on the p-h subspace and is defined by its action on an arbitrary dynamical variable G as

$$PG = \sum_a \{\langle [G, A_a^\dagger] \rangle A_a - \langle [G, A_a] \rangle A_a^\dagger\}. \quad (6)$$

The GLE can be used either to study correlations among the variables in the set A or to obtain equations of motion for the mean values and the variances of the dynamical variables. In the first case, one proceeds by noting that $\langle [f_a(t), A_b^\dagger] \rangle = 0$ for $\tau \geq 0$. Hence, multiplying Eq. (1) by $A_b^\dagger$ and averaging over the equilibrium canonical ensemble, we can derive an equation for the density-correlation function,

$$R_{ab}(t) = \langle [A_a(t), A_b^\dagger] \rangle, \tag{7}$$

which takes the form

$$\frac{d}{dt} R(t) - i\Omega \cdot R(t) + \int_0^t d\tau\, \phi(\tau) \cdot R(t-\tau) = 0. \tag{8}$$

If one wishes, instead, to obtain an equation of motion for the mean values of $A_a(t)$, then the GLE can be averaged over a constrained equilibrium ensemble (the initial state) to find an equation for the averaged single-particle density matrix. In a similar fashion, an equation of motion for the variances of the variables $A_a(t)$, which describes the density fluctuations, can be obtained by considering a larger set of dynamical variables including $\{A_a^\dagger A_b\}$ in addition to $\{A_a\}$.

Since Eq. (8) for the density-correlation function and the equations obtained for the averages and the variances of the variables $A_a(t)$ are still exact, and hence only formal identities with the equation of motion for the many-body system, one must eventually introduce approximations. However, the attractive feature of these equations is that the damping terms are quite convenient for approximation or modeling.[6] That is, the GLE is of value primarily because it reexpresses the relevant quantities in forms involving damping terms which are then easily approximated.

A study of the average single-particle density matrix [averages of $A_a(t)$] and the density fluctuations [variances of $A_a(t)$] will be discussed elsewhere.[7] Here, we discuss the density-correlation function given by Eq. (7). The Fourier transform of the density-correlation function is referred to as the response function,

$$R_{ab}(w) = \int_0^\infty dt\, e^{-iwt} \langle [A_a(t), A_b^\dagger] \rangle. \tag{9}$$

Taking the one-sided Fourier transform of Eq. (8) leads to a matrix equation for the response function,

$$[w - \Omega - i\phi(w)] \cdot R(w) = -iI, \tag{10}$$

where I denotes a unit matrix and $\phi(w)$ is the Fourier transform of the damping term,

$$\phi_{ab}(w) = \int_0^\infty dt\, e^{-iwt} \langle [f_a(t), f_b^\dagger(0)] \rangle. \tag{11}$$

The frequency matrix, Ω, has a structure similar to the matrix appearing in the formalism of the random-phase approximation (RPA).[8,9] The essential difference here is that the core state is not the ground state but it is an ensemble characterized by a temperature T. Hence, the Mori formalism provides, rather naturally, an extension of the zero-temperature RPA to finite temperatures and furthermore it provides a prescription for the damping widths of RPA modes. The frequencies, Ω_λ, and the amplitudes, C^λ, of the finite-temperature RPA modes can be determined by diagonalization of the frequency matrix Ω,[8,9]

$$\langle [Q_\lambda, [H, Q_\mu^\dagger]] \rangle = \Omega_\lambda \langle [Q_\lambda, Q_\mu^\dagger] \rangle = \Omega_\lambda \delta_{\lambda\mu}. \tag{12}$$

The RPA mode creation and destruction operators are given by a superposition of p-h excitation operators,

$$Q_\lambda^\dagger = \sum_a \{C_a^\lambda A_a - \tilde{C}_a^\lambda A_a^\dagger\}, \tag{13}$$

where $C_a^\lambda = C_{kl}^\lambda$ and $\tilde{C}_a^\lambda = C_{lk}^\lambda$ denote the p-h excitation and deexcitation amplitudes, respectively. At zero temperature, because of the sharp Fermi surface, the sum over a in Eq. (13) is restricted to p-h states, only. As a result, the only nonvanishing amplitudes are p-h and h-p amplitudes and in terms of the usual notation they are given by $C_{\rm ph}^\lambda = X_{\rm ph}^\lambda$ and $\tilde{C}_{\rm ph}^\lambda = Y_{\rm ph}^\lambda$. However, at finite temperatures, the Fermi surface is not sharp any more and, in principle, there is no restriction on the summation over a in Eq. (13).

By inversion of the matrix Eq. (10), the response function can be expressed in terms of the RPA representation,[8] and we obtain

$$R_{ab}(w) = \sum_\lambda \left[\frac{C_a^\lambda C_b^{\lambda *}}{w - \Omega_\lambda - i\phi_\lambda(w)} - \frac{\tilde{C}_b^\lambda \tilde{C}_a^{\lambda *}}{w + \Omega_\lambda + i\phi_\lambda(w)} \right], \tag{14}$$

where $\phi_\lambda(w)$ is the damping term for the RPA mode with multipolarity λ. It is given by Eq. (11) with the random forces in Eq. (11) replaced by the random force on the RPA mode,

$$f_\lambda(t) = \exp[it(1-P)L]_I (1-P) L Q_\lambda^\dagger = \exp[it(1-P)L]_I [V, Q_\lambda^\dagger], \tag{15}$$

where $V = H - H_0$ is the coupling interaction which is the part of the total Hamiltonian not contained in the RPA Hamiltonian H_0. If we neglect the damping term in Eq. (14) completely, we obtain the response function in the random-phase approximation. The RPA provides a good description for both the mean energies and the detailed structure of the vibrational states. However, it does not give any description for the damping of the vibrational states. These simple RPA modes are embedded in a complex spectrum and consequently mix with the nearby states. As a result of this mixing the observed strength function spreads over many configurations. This spreading is described

by the damping term $\phi_\lambda(w)$ in the response function.

An exact calculation of the damping term (and hence the response function), is not possible, because of the fact that it contains the modified propagator, $\exp[it(1-P)L]$. A study of the modified propagator would involve solving the many-body problem, directly. We have to introduce approximations to obtain useful results. A systematic approach to approximating the damping term consists of applying standard perturbative methods.[4-6] This provides a consistent evaluation of the damping term to a given order of perturbation of the coupling V. Here we consider it in a weak-coupling approximation and calculate the damping width up to second order by taking into account only the coupling of simple RPA modes with the states of the next level of complexity (doorway approximation).[3,10] Hence, in the weak-coupling approximation, the modified propagator $\exp[it(1-P)L]$ is replaced by the free propagator, $\exp[it(1-P)L_0] = \exp[itL_0]$. Performing the time integration in Eq. (11), we obtain

$$i\phi_\lambda(w) = \Delta\Omega_\lambda(w) + \tfrac{1}{2}i\Gamma_\lambda(w). \tag{16}$$

Here $\Delta\Omega_\lambda$ denotes the energy shift due to the coupling and the width Γ_λ is given

$$\Gamma_\lambda(w) = 2\pi\sum_{n,I}\{|D_{nI}^\lambda|^2\delta(w-E_{In}) - |D_{In}^\lambda|^2\delta(w+E_{In})\}e^{-\beta E_n}/Z, \tag{17}$$

where $D_{nI}^\lambda = \langle n|[V,Q_\lambda]|I\rangle$ is the coupling matrix element between the RPA mode λ and the intermediate doorway states, I, while the $E_{In} = E_I - E_n$ are the excitation energies of the intermediate states with respect to the core energies. The first term in Eq. (17) describes the loss of energy from the RPA mode by emission of a phonon of frequency w. At finite temperatures, as a result of thermal fluctuations, the inverse process is also possible. The RPA mode can absorb a phonon of frequency w from the heat bath and be reexcited again. This is described by the second term in the expression (17). Consequently the damping width of an RPA mode at a finite temperature is determined by the net effect of the emission width and the absorption width. The result of (17) can be written in a more convenient form as

$$\Gamma_\lambda(w) = \Gamma_\lambda^e(w)(1-e^{-\beta w}), \tag{18}$$

where Γ_λ^e is the emission width only, and is given by the first term on the right-hand side of Eq. (17).

In a further evaluation of the damping term, we should specify the structure of the intermediate states contributing to Eq. (17). At low energies, the nucleon mean free path is much larger than the size of the nucleus. As a result the volume dissipation caused by two-body collisions is not important. Consequently, the phase space for the uncorrelated 2p-2h intermediate states in Eq. (17) is strongly diminished. At low energies, the single-particle motion is damped predominantly by inelastic collisions of nucleons with the surface of the mean field and by excitation of the low-energy vibrational modes. The same mechanism is also responsible for the damping of the RPA modes. Then, at low energies, the dominant contributions to the damping term arise from the low-lying correlated 2p-2h intermediate states. Bortignon, Broglia, and Dasso have calculated the damping widths of vibrational states at zero temperature, considering a particle-vibration model with a coupling of the form[10]

$$V = \sum_\lambda F^\lambda Q_\lambda^\dagger + \text{H.c.}, \tag{19}$$

where F^λ is a single-particle field with the multipolarity λ, and $Q_\lambda^\dagger$ is an RPA excitation operator. At finite but not too high temperatures, the RPA modes are damped mainly by the same mechanism, e.g., by the excitation of a low-lying vibrational mode and a p-h pair. Hence we can use the same model for the calculation of the damping widths at finite temperatures. Using the particle-vibration coupling given by Eq. (19), we can evaluate the thermal average in Eq. (17) and find that the damping width due to emission processes is given by

$$\Gamma_\lambda^e(w) = 2\,\mathrm{Im}\sum|D_{kl}^{\lambda\mu}|^2\left\{\frac{(1+\bar n_\mu)n_l(1-n_k)}{w-\epsilon_{kl}-\Omega_\mu-i\eta} + \frac{\bar n_\mu n_l(1-n_k)}{w-\epsilon_{kl}+\Omega_\mu-i\eta}\right\}. \tag{20}$$

Here the recombined coupling amplitude is

$$D_{kl}^{\lambda\mu} = \sum_r(C_{kr}^\lambda F_{rl}^\mu - F_{rk}^\mu C_{rl}^\lambda) \tag{21}$$

and

$$\bar n_\lambda = [\exp(\beta\Omega_\lambda)-1]^{-1},$$

$$n_k = [\exp\beta(\epsilon_k-\mu)+1]^{-1}$$

are the occupation factors for phonons and nucleons, respectively. The first term in Eq. (20) describes the decay of an RPA state by the excitation of a phonon together with a p-h pair, while the second term describes the excitation of a p-h pair accompanied by the simultaneous absorption of a phonon of frequency Ω_μ such that $w+\Omega_\mu = \epsilon_{kl}$. The total damping width is determined by Eq. (18). The damping width is suppressed by a factor $1-\exp(-\beta w)$ as a result of the inverse processes due to thermal fluctuations. At low temperatures or for high frequencies, $\beta w \gg 1$, the thermal fluctuations are small, and hence the inverse processes are not important. Consequently, to a

good approximation, the damping widths of vibrational states are described by the emission widths, Eq. (20), alone. In this case the temperature dependence of the damping widths is mainly determined by the occupation factors, n_μ, of the low-lying vibrational states with $\Omega_\mu \sim T$.

Recently, Bortignon *et al.* have extended their calculations for finite temperature by using a different formalism and obtained similar results for the damping widths.[11]

At higher energies, $w \geq 15$ MeV, and also at larger temperatures, the volume dissipation becomes increasingly more important, because of the shorter nucleon mean free path and the increase in the phase space for the uncorrelated 2p-2h states. Consequently, at higher energies, the damping widths of vibrational states are predominantly determined by the decay into the uncorrelated 2p-2h intermediate states in Eq. (17). This can be calculated and we obtain for the emission width,[12,13]

$$\Gamma^e_\lambda(w) = 2\,\mathrm{Im}\sum_{}|D^\lambda_{pk,ql}|^2 \frac{n_q n_l (1-n_p)(1-n_k)}{w - \epsilon_{pq} - \epsilon_{kl} - i\eta}, \tag{22}$$

where the transition amplitudes are given by the 2p-2h matrix elements of the effective coupling, $D^\lambda_{pk,ql} = \langle pk|[V,Q_\lambda]|ql\rangle$. Again, the total damping width is determined by Eq. (18) which includes a suppression factor due to the inverse processes.

This projection formalism of the statistical mechanics provides two alternative approaches: The Mori formalism, which is followed in this work, deals with the time evolution of observables. On the other hand, the Zwanzig formalism seeks an effective equation for the projected density matrix. The latter approach was already applied to the nuclear many-body problem and was shown to give an extended time-dependent Hartree-Fock equation.[14–16]. The damping width of the vibrational states can be evaluated by linearization of this equation around a finite-temperature Hartree-Fock solution as it was done in Ref. 13. However, this approach can only account for the volume damping given by Eq. (22), because of the fact that the intermediate states occurring in the collision term of the extended time-dependent Hartree-Fock equation consist of the uncorrelated 2p-2h states. It cannot account for the surface damping given by Eq. (20) which arises from the particle-vibration coupling.

In conclusion, a broad range of relaxation processes observed in nuclear collisions can be studied in the framework of the Mori formalism. In the present work, we studied the nuclear response function using the Mori formalism. This naturally leads to an extension of the zero-temperature RPA formalism to finite temperatures and also provides a prescription for the calculation of the damping widths of vibrational states at finite temperatures.

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