Role of Memory Effects on the Spreading Width of a Collective State in Extended Time-Dependent Hartree-Fock Theory

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The linearized version of the extended time-dependent Hartree-Fock theory with memory effects in the collision term is used to describe the spreading width of collective states. The retention of the memory effects is shown to enforce the energy conservation between a collective state and the more complicated states responsible for its damping.

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In this Letter we describe the damping widths of collective states in linearized extended time-dependent Hartree-Fock (TDHF) theory. The main purpose of this work is to demonstrate the effects of non-Markovian features of the collision term on the spreading widths.

Several approaches have been proposed to extend the TDHF theory by incorporation of two-body collisions which are neglected in the TDHF approximation. Various theories have been reviewed.[1-5] In all these approaches, the time-dependent single-particle density matrix, $\rho(t)$, is determined by an equation which includes a collision term in addition to the usual mean field,

$$i(\partial/\partial t)\rho(t)=[h(\rho),\rho]-iK(\rho), \tag{1}$$

where $h(\rho)$ is the self-consistent mean-field Hamiltonian, and $K(\rho)$ denotes the collision term. This collision term is derived in a weak-coupling approximation which includes two-body correlations only in the lowest order and neglects three-body and higher-order correlations. Here the specific form of the collision term which was derived in Ref. 4 [see Eq. (3.1) in the first part of Ref. 4] will be used. It is given as

$$K(\rho)=\int_0^t dt'\mathrm{Tr}'\{V(t),g(t,t')[V(t'),F(t')]g^\dagger(t,t')\}, \tag{2}$$

where $F(t)=\mathscr{A}\rho(t)\rho(t)\cdots\rho(t)$ is the uncorrelated A-particle density matrix, $g(t,t')$ is the mean-field propagator, and $V(t)=v-\mathrm{Tr}v\rho(t)$ is the residual interaction. Tr′ denotes a partial trace taken over all the degrees of freedom by $A-1$ particles, and as a result $K(\rho)$ becomes a one-body operator.

Observe that because of the non-Markovian form of collision term (2), the evolution of the single-particle density matrix depends on the previous history of the system. The purpose of this Letter is to study this memory effect on the damping widths of small-amplitude collective motion. To this end, we linearize the equation of motion (1) around the static equilibrium density matrix at finite temperature, $\rho_0(T)$,

$$\rho(t)=\rho_0(T)+\rho_1(t). \tag{3}$$

We will work in the representation in which both $h_0=h(\rho_0)$ and $\rho_0(T)$ are diagonal.

The time dependence of normal modes is sought in the form

$$\rho_1(t)=e^{-\Omega t}\delta\rho+e^{+i\Omega t}\delta\rho^\dagger, \tag{4}$$

where Ω is a complex frequency. Separating the positive and negative frequency components of the linearized form of (1), we obtain a dispersion equation for the frequencies and amplitudes of the normal modes:

$$\Omega\delta\rho=[h_0,\delta\rho]+[\delta h,\rho_0]-i\delta K(\Omega), \tag{5}$$

where small deviations in the mean field and in the collision term are given by

$$\delta h=\mathrm{Tr}v\delta\rho, \tag{6}$$

$$\delta K=\int_0^\infty d\tau\, e^{i\omega\tau}\mathrm{Tr}'[V,e^{-i\tau h_0}[V,\delta F]e^{i\tau h_0}]. \tag{7}$$

In Eq. (7) the upper limit was extended to infinity,[6] and the imaginary part of Ω is neglected in the exponent, $\omega=\mathrm{Re}\Omega$. It is important to note that the collision term in (5) depends on the collective frequency. Therefore the magnitude of the collision term can be quite different from its value in the Markovian approximation.

We will call Eq. (5) the extended random-phase-approximation (RPA) equation. The coherent solution of (5) yields the collective RPA state with complex frequency, $\Omega = \omega - i\Gamma/2$, where ω and Γ are identified with the energy and width of the collective RPA mode. This extended RPA equation can be put into a more familiar form by introducing the operators $O^\dagger$ and O (which correspond to the phonon excitation and deexcitation operators in the usual RPA theory[7]) defined as

$$\delta\rho \equiv [O^\dagger, \rho_0]. \tag{8}$$

The matrix elements of (5) yield the extended RPA equations for the amplitudes $\langle m|O^\dagger|i\rangle$ and $\langle m|O|i\rangle$. In order to obtain a closed expression for width, Γ, we multiply (5) by the operator O and take a trace over ρ_0 which gives for Γ

$$\Gamma = 2\,\mathrm{Re}[\mathrm{Tr}\,O\delta K]. \tag{9}$$

By insertion of (7) for δK and use of a cyclic permutation property of trace, (9) can be expressed as

$$\Gamma = 2\int_0^\infty d\tau\, e^{i\tau\omega}\mathrm{Tr}[D(0), D^\dagger(\tau)]F_0 + \delta\Gamma, \tag{10}$$

where

$$D^\dagger(\tau) = e^{-i\tau h_0}[V, O^\dagger]e^{+i\tau h_0}, \tag{11}$$

and δT is a small contribution and will be omitted in this Letter. The result (10) contains both the escape width due to particle emission and the spreading width due to coupling to more complicated states. Full results are discussed in a forthcoming publication,[6] and in the present Letter we will concentrate on the spreading width. To this end we consider the intermediate states of the 2p-2h nature only. Note that since we work at finite temperature T, particle (or hole) states are defined so as to be unoccupied (or occupied) when $T \to 0$, and they have Fermi-Dirac $\rho(T)$ occupation factors at finite T. After intermediate states are inserted, time integration of (10) can be performed, which leads to an energy-conserving δ function between the collective state and the 2p-2h states degenerate with it. The resulting expression for $\Gamma^\downarrow$ can be written as

$$\Gamma^\downarrow = 2\pi \sum [\,|D_I^\dagger|^2\delta(E_I - \omega) - |D_I|^2\delta(E_I + \omega)\,]S_I. \tag{12}$$

The summation I runs over 2p-2h intermediate states with energy $E_I = \epsilon_m + \epsilon_n - \epsilon_i - \epsilon_j$, and the occupation factors

$$S_I(T) = [1-\rho_m(T)][1-\rho_n(T)]\rho_i(T)\rho_j(T).$$

The strength $D_I^\dagger$ denotes 2p-2h matrix elements of $D^\dagger$ which describes the coupling between the coherent p-h mode (defined in terms of $O^\dagger$) and 2p-2h configurations and is given by

$$D_I^\dagger \equiv \langle mn|D^\dagger|ij\rangle = \sum_q (\langle mn|V|iq\rangle O_{qj}^\dagger + \langle mn|V|qj\rangle O_{qi}^\dagger) - \sum_k (O_{mk}^\dagger \langle kn|V|ij\rangle + O_{nk}^\dagger\langle mk|V|ij\rangle). \tag{13}$$

and similarly for D_I.

The expression (12) is the central result of the present work. It is not an explicit expression for the width Γ, since it contains the collective excitation operators $O^\dagger$ and O which in turn depend on the collective frequency Ω. However, it is possible to use in this expression the unperturbed collective operators corresponding to $\Omega \simeq \omega$. Observe that the width depends on temperature through the occupation factors $S_I(T)$. At zero temperature and for finite frequencies the second term of (12) vanishes identically as a result of energy conservation and the expression for $\Gamma^\downarrow$ reduces to the second RPA result of Yannouleas, Dworzecka, and Griffin.[8] The non-Markovian character of the collision term in (2) retained in our calculations enforces the energy conservation between the collective eigenmode with the frequency ω and more complicated (2p-2h) states which are responsible for its damping. On the other hand, the Markovian approximation consists of the requirement that

$$g(t,t')F(t')g^\dagger(t',t) \approx F(t) \tag{14}$$

in the collision term. In the small-amplitude limit this is equivalent to the replacement of the collective frequency ω by the unperturbed particle-hole energy $\epsilon_p - \epsilon_h$; $\omega \approx \epsilon_p - \epsilon_h$.[6] As a result, contrary to the non-Markovian expression (12), which guarantees energy conservation with respect to the actual collective energy, the Markovian approximation destroys the energy conservation. The consequence of this fact can be seen clearer in the expression described below when the spreading width is approximated in terms of single-particle widths.

Note that the expression (12) contains squares of coupling matrix elements (13) and hence, in general, will have interference effects between particles and holes. Since in the collective states particles and holes act coherently this interference effect may be quite large and typically will reduce the total width.[9] This effect is destroyed if a statistical approximation for the matrix elements of the residual interaction[10,11] is made. On the other hand, with such a statistical approximation (which retains only the squares of matrix elements of residual interaction), the expression (12) for the width can be written in the form of an independent particle-hole decay model as

$$\Gamma^{\downarrow} \approx \sum_{mi} [\Gamma_{mi}(\omega) |O_{mi}^{\dagger}|^2 - \Gamma_{mi}(-\omega) |O_{mi}|^2] \rho_i (1-\rho_m). \tag{15}$$

In addition to neglecting interference effects we have also used the fact that only p-h matrix elements of $O^{\dagger}$ are nonvanishing; hence we put the occupation factor for p (or h) states to limit the summation.

Here $\Gamma_{mi}(\omega)$ is the sum of the width for the particle (Γ_m) and hole states $(\tilde{\Gamma}_i)$ at finite temperature,

$$\Gamma_{mi} = \Gamma_m(\epsilon_i + \omega) + \tilde{\Gamma}_i(\epsilon_m - \omega). \tag{16}$$

In the expression (15) the interference effects due to coherent structure of the collective mode are destroyed by the statistical assumption introduced above. Hence, this result is clearly approximate. On the other hand, (15) is suitable for discussion of the connection (albeit approximate) between the spreading width of the collective state and the widths of individual particle and hole states comprising the collective state. As is seen in expression (15) the spreading width of the collective state is given approximately by the weighted average of the individual particle and hole widths. Contrary, however, to a naive independent-particle model, here the single-particle and hole widths have to be evaluated at shifted energies because of the requirement of energy conservation between the collective mode and the 2p-2h states into which this mode decays. This shift in single-particle energy is the consequence of the memory effects in the collision term, as discussed above. The single-particle widths strongly depend on the excitation energy[9]; hence the fact that these widths are calculated at the energy determined by the excitation energy of the system, and so shifted with respect to unperturbed p-h energy, can effect the spreading width considerably.

In conclusion, we have demonstrated that the memory effects in the collision term play an important role in determining the spreading width of the collective mode. In particular, it enforces the conservation of energy between the collective mode and the states responsible for its decay.

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