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Normalization for the random phase approximation with energy-dependent interactions

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Different normalization conditions for random phase approximation amplitudes have been obtained recently for use with energy-dependent interactions. These conditions are shown to be equivalent. A third method, which has a wider applicability, is also discussed.

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The random phase approximation (RPA) [1, 2] is a well-known method to describe the excitation of many-body systems. As such it has also frequently been applied in nuclear structure theory. In these applications [2], one often adopted phenomenological interactions with a few parameters adjusted so as to reproduce the energies of the most collective excitations. More recently it has been realized that this approach can only yield reasonable results in a unified description of both low-energy excitations and those at higher energies, e.g., giant resonances, if the interaction is allowed to be energy dependent. The main physical origin of this energy dependence of the effective interaction in the RPA is the induced interaction via medium polarization as well as the dispersive contributions to the particle and hole propagators. These effects are explicitly treated to some extent in the extended RPA (ERPA) method, utilized recently by various authors [3–6].

One of the features of the ERPA method, and of the use of energy-dependent interactions in the RPA in general, is that this energy dependence yields an extra term in the normalization condition for the RPA amplitudes. In Ref. [6], this normalization condition was expressed in the form

$$\sum_{ph}|X^n_{ph}|^2-\sum_{hp}|X^n_{hp}|^2\equiv\sum_{\alpha\beta}|X^n_{\alpha\beta}|^2/Q_{\alpha\beta} = 1+\sum_{\alpha\beta\gamma\delta}X^{n*}_{\alpha\beta}X^n_{\gamma\delta} \times \left.\frac{dV^{ph}_{\alpha\beta\gamma\delta}(\omega)}{d\omega}\right|_{\omega=E^n}, \tag{1}$$

where X^n_{ph} and X^n_{hp} are the ERPA excitation amplitudes of the nth excited state with excitation energy E^n. In this equation the operator

$$Q_{12}=\theta(1-F)\theta(F-2)-\theta(F-1)\theta(2-F) \tag{2}$$

is introduced, where $\theta(1-F)$ is 1 (0) if orbital 1 is unoccupied (occupied) in the Fermi sea, etc. Thus Q_{12} gives a plus or minus sign depending on whether it refers to a particle-hole or hole-particle index. The energy-dependent particle-hole interaction $V^{ph}(\omega)$ is

$$V^{ph}_{\alpha\beta\gamma\delta}(\omega)=\langle\alpha\beta^{-1}|V(\omega)|\gamma\delta^{-1}\rangle\ . \tag{3}$$

Now it can be shown that in a proper conserving theory [6] the last term on the right in Eq. (1) is always negative. Even for low-energy excitations it may be as large as several tens of percent, thereby contributing to the explanation of observed quenching phenomena in, e.g., low-lying magnetic excitations as well as giant resonances [5, 6].

The observation that the normalization condition of the RPA amplitudes is affected by the energy dependence of the interaction was also made in a paper by Yang and Kuo [7]. These authors gave the normalization condition, using here the notation of Eq. (1):

$$\sum_{\alpha\beta}|X^n_{\alpha\beta}|^2/Q_{\alpha\beta}=\left(1-\left.\frac{d\Delta_n(\omega)}{d\omega}\right|_{\omega=E^n}\right)^{-1}, \tag{4}$$

which at first sight seems completely different from Eq. (1). In this expression $\Delta_n(\omega)$ is the eigenvalue of the RPA equation with an energy-dependent interaction

$$\sum_{56}\left[(\varepsilon_1-\varepsilon_2)\delta_{15}\delta_{26}+Q_{12}V^{ph}_{1256}(\omega)\right]X^{n*}_{56}(\omega) = \Delta_n(\omega)X^{n*}_{12}(\omega)\ . \tag{5}$$

In the ERPA, and in any theory which obeys conservation laws according to the Baym-Kadanoff prescriptions [8], $\Delta_n(\omega)$ is a monotonically decreasing function of ω and therefore also in Eq. (4) the normalization of the RPA amplitudes is less than unity. We shall now demonstrate that Eqs. (1) and (4) are equivalent.

For a clear exposition of the problem, it is useful to go back to the Bethe-Salpeter (BS) equation

$$\Pi_{1234}(\omega) = \Pi^0_{1212}(\omega)+\sum_{56}\Pi^0_{1212}(\omega)V^{ph}_{1256}(\omega)\Pi_{5634}(\omega) \tag{6}$$

that is adopted in the ERPA for the particle-hole propagator Π. The spectral representation of Π is

$$\Pi_{1234}(\omega) = \sum_{n\neq 0}\left[\frac{X^{n*}_{12}X^n_{34}}{\omega - E^n + i\eta} - \frac{X^n_{21}X^{n*}_{43}}{\omega + E^n - i\eta}\right] , \tag{7}$$

with η a positive infinitesimal.

The philosophy of the ERPA is to adopt for Π^0 the free particle-hole propagator

$$\Pi^0_{1234}(\omega) = \left[\frac{\theta(1-F)\theta(F-2)}{\omega - (\varepsilon_1 - \varepsilon_2) + i\eta} - \frac{\theta(F-1)\theta(2-F)}{\omega - (\varepsilon_1 - \varepsilon_2) - i\eta}\right] \times\delta_{13}\delta_{24} , \tag{8}$$

without the dressing of the particle or hole lines that is assumed in the usual form of the full BS equation [9]. This dressing of the particle and hole lines, as well as induced forces, are included in the effective, energy-dependent, particle-hole interaction $V^{ph}(\omega)$. If the poles E^n of the propagator Π, which represent the excitation energies of the system, are well separated, one may solve the BS equation (6) by considering the residues of both sides of the equation at a pole E^n. Then the first term of the right-hand side (rhs) drops out, as it has no pole at E^n, and the homogeneous equation (5) for the amplitudes is obtained. This derivation implies that a solution of Eq. (5) is only a physical solution, i.e., a solution of Eq. (6), if an eigenvalue coincides with the ω parameter of the interaction $V^{ph}(\omega)$ and this is then the excitation energy

$$E^n = \Delta_n(E^n) . \tag{9}$$

These solutions must then be obtained by solving Eq. (5) for many values of the energy parameter ω and searching for the crossing points of the eigenvalue curves Δ with the line $\omega = E$; see, e.g., Ref. [6].

Since Eq. (5) is a homogeneous equation, it cannot provide the normalization of the amplitudes. For this purpose one has to return to the inhomogeneous equation (6), which holds for all values of ω and consider a value of ω that differs by a small quantity δ from the eigenvalue E^n, so that the contribution of the inhomogeneous term cannot be neglected. A useful expression is that for the inverse of the propagator Π, which follows immediately from Eq. (6) by multiplication with Π^{-1} from the left and $(\Pi^0)^{-1}$ from the right

$$\Pi^{-1}_{1234}(\omega) = [\Pi^0_{1212}(\omega)]^{-1}\delta_{13}\delta_{24} - V^{ph}_{1234}(\omega) . \tag{10}$$

Now consider the identity

$$\delta_{13}\delta_{24} = \sum_{56}\{[\Pi^0_{1212}(\omega = E^n+\delta)]^{-1}\delta_{15}\delta_{26} - V^{ph}_{1256}(\omega = E^n+\delta)\}\Pi_{5634}(\omega = E^n+\delta) . \tag{11}$$

The factor in curly brackets is regular at $\omega = E^n$ and may be Taylor expanded. The propagator Π may be split into a part $\Pi^R(\omega = E^n + \delta)$ that is regular at $\omega = E^n$ and a pole term. Neglecting terms of order δ one then obtains from Eq. (11):

$$\begin{aligned}\delta_{13}\delta_{24} = \sum_{56}\Bigg[&\left\{[\Pi^0_{1212}(\omega = E^n)]^{-1}\delta_{15}\delta_{26} - V^{ph}_{1256}(\omega = E^n)\right\}\frac{X^{n*}_{56}X^n_{34}}{\delta}\\ &+\left\{[\Pi^0_{1212}(\omega = E^n)]^{-1}\delta_{15}\delta_{26} - V^{ph}_{1256}(\omega = E^n)\right\}\Pi^R_{5634}(\omega = E^n+\delta)\\ &+\left\{Q^{-1}_{12}\delta_{15}\delta_{26} - \left.\frac{dV^{ph}_{1256}(\omega)}{d\omega}\right|_{\omega=E^n}\right\}X^{n*}_{56}X^n_{34}\Bigg] .\end{aligned} \tag{12}$$

Now the first term on the rhs vanishes because $\omega = E^n$ is a physical solution of Eq. (5). For the same reason the second term will vanish upon multiplication from the left with X_{12} and summation over indices 1 and 2. In this way one is left with the equation

$$X^n_{34} = \sum_{1256}X^n_{12}\left(Q^{-1}_{12}\delta_{15}\delta_{26} - \left.\frac{dV^{ph}_{1256}(\omega)}{d\omega}\right|_{\omega=E^n}\right)X^{n*}_{56}X^n_{34} , \tag{13}$$

from which the normalization condition (1) is immediately obtained on division by X^n_{34}.

Also the normalization condition (4) is now readily obtained by using Eq. (5) for $\omega = E^n + \delta$ and making a Taylor expansion. The terms to zero order in δ then just satisfy Eq. (5) for $\omega = E^n$ and therefore one is left with the terms to first order in δ, which yield

$$\sum_{56}\left[\left\{(\varepsilon_1-\varepsilon_2)\delta_{15}\delta_{26}+Q_{12}V^{ph}_{1256}(E^n)\right\}\left.\frac{dX^{n*}_{56}(\omega)}{d\omega}\right|_{\omega=E^n}+Q_{12}\left.\frac{dV^{ph}_{1256}(\omega)}{d\omega}\right|_{\omega=E^n}X^{n*}_{56}(E^n)\right]$$
$$=\left.\frac{d\Delta_n(\omega)}{d\omega}\right|_{\omega=E^n}X^{n*}_{12}(E^n)+E^n\left.\frac{dX^{n*}_{12}(\omega)}{d\omega}\right|_{\omega=E^n}. \quad (14)$$

Multiplication by $X^n_{12}(E_n)Q^{-1}_{12}$ from the left and summation over its indices eliminates the terms which contain the derivatives of the vectors X, because of the relation

$$\sum_{12}X^n_{12}Q^{-1}_{12}\left[(\varepsilon_1-\varepsilon_2-E^n)\delta_{15}\delta_{26}+Q_{12}V^{ph}_{1256}(E^n)\right]=0\,, \quad (15)$$

which follows from the transpose of (5). In this way Eq. (14) therefore yields the relation

$$\sum_{1256}X^n_{12}\left.\frac{dV^{ph}_{1256}(\omega)}{d\omega}\right|_{\omega=E^n}X^{n*}_{56}=\left.\frac{d\Delta_n(\omega)}{d\omega}\right|_{\omega=E^n}\sum_{12}X^n_{12}Q^{-1}_{12}X^{n*}_{12}\,. \quad (16)$$

If this is substituted in the normalization condition (1), condition (4) is obtained immediately.

From the derivation presented here, it is clear that these methods are only applicable if the excitation energy E^n is well separated from the other solutions. In the ERPA the use of Eq. (1) does not require much more computational work than Eq. (4) because the matrix elements of $\frac{dV^{ph}}{d\omega}$ differ only by simple energy denominators from those of V which are required anyway. However, Eq. (4) has the advantage of being more transparent when the ERPA equations are solved graphically, as, e.g., in Fig. 8 of Ref. [6]. In such a plot the normalization is directly related to the steepness of the eigenvalue curve $\Delta_n(\omega)$ at the physical point $\omega=\Delta_n(\omega)=E^n$.

We have focused here on the particle-hole RPA; however, the same argument may be carried through for the particle-particle, hole-hole RPA, where $Q_{12}=\Theta(1-F)\Theta(2-F)-\Theta(F-1)\Theta(F-2)$. One may also generalize to finite temperature where the respective Q operators are

$$Q^{ph}_{12}=\bar f_1 f_2-f_1\bar f_2,\quad Q^{pphh}_{12}=\bar f_1\bar f_2-f_1 f_2\,, \quad (17)$$

with $\bar f=1-f$ and the occupation probability $f=[1+\exp(\frac{\epsilon-\mu}{T})]^{-1}$ in an obvious notation; note that in this case Q is no longer of magnitude unity.

At higher excitation energy, i.e., in the region of two-particle–two-hole states, the interaction $V(\omega)$ will begin to exhibit many close-lying singularities and consequently many close-lying physical eigenvalues E^n will be found. The procedure sketched here, i.e., the search for the physical solutions of Eq. (5), then becomes rather impractical. For this reason one applies another method [6] to calculate excitation strengths directly after solving Eq. (6) by means of Eq. (10). Here we apply this method to derive the normalized ERPA amplitudes for discrete states and we remark that it is in fact more widely applicable than Eqs. (1) and (4). For this purpose consider the response matrix

$$R_{\alpha\beta\gamma\delta}(\omega)=-\tfrac{1}{\pi}\mathrm{Im}\,\Pi_{\alpha\beta\gamma\delta}(\omega)=\sum_{n\neq0}[\delta(\omega-E^n)X^{n*}_{\alpha\beta}X^n_{\gamma\delta}-\delta(\omega+E^n)X^n_{\beta\alpha}X^{n*}_{\delta\gamma}]\,. \quad (18)$$

Clearly $R(\omega)$ as well as $\Pi(\omega)$ is singular at $\omega=E^n$ and therefore the matrix (10) cannot be inverted. This problem is circumvented by keeping a finite value for η in Eq. (7). Then

$$R_{\alpha\beta\gamma\delta}(\omega,\eta)=\tfrac{1}{\pi}\sum_{n\neq0}\left[X^{n*}_{\alpha\beta}X^n_{\gamma\delta}\frac{\eta}{(\omega-E^n)^2+\eta^2}+X^n_{\beta\alpha}X^{n*}_{\delta\gamma}\frac{\eta}{(\omega+E^n)^2+\eta^2}\right]. \quad (19)$$

The response function for a one-body probe

$$\mathcal{O}=\sum_{\alpha\beta}\langle\alpha|\mathcal{O}|\beta\rangle a^\dagger_\alpha a_\beta \quad (20)$$

is then immediately obtained as [6]

$$S_{\mathcal{O}}(\omega,\eta)=\sum_{\alpha\beta\gamma\delta}\langle\alpha|\mathcal{O}|\beta\rangle^*R_{\alpha\beta\gamma\delta}(\omega,\eta)\langle\gamma|\mathcal{O}|\delta\rangle\,, \quad (21)$$

i.e., as a sum of Lorentzians. If the value of η is taken sufficiently small these Lorentzian distributions may be separated off for well isolated physical excitation energies E^n. In this case the ERPA amplitudes, including their normalization, may be directly deduced from the matrix

$$X^{n*}_{\alpha\beta}X^n_{\gamma\delta}=-\eta\mathrm{Im}\,\Pi_{\alpha\beta\gamma\delta}(\omega=E^n,\eta) \quad (22)$$

after $\Pi(\omega,\eta)$ is obtained from the inverse of the rhs of Eq. (10). Of course Eq. (22) holds formally only in the limit that η tends to zero. This method has the advantage that it can also be applied in cases where one does not use Π^0 in the BS equation (6), but a free propagator which includes already the dressing of the particle and hole lines, as in the standard BS equation [9]. In such cases one cannot derive an ERPA equation of the form (5), but one can still use Eq. (10). So this method is generally applicable to solve equations of the form (6) with any chosen Π^0, e.g., to systems at finite temperature. One may note that instead of using Eq. (22), $X^{n*}_{\alpha\beta}X^n_{\gamma\delta}$ may also be obtained by contour integration of $\Pi(\omega)$ around the pole $\omega=E^n$, excluding all other poles of (7). Such a procedure is numerically more involved and therefore the use of (22) is more practical.

In summary, we have discussed several apparently different expressions for the normalization of the RPA transition amplitudes and shown the equivalence among them. We would like to emphasize that the magnitude of this normalization is in general smaller than unity when a realistic energy dependent vertex function is employed. This is in contrast to a number of early calculations where this normalization was taken to be either $+1$ or -1. This reduction of normalization has been found to be important in determining nuclear transition rates [5,6]. It has also been found to be important for nuclear matter saturation properties, as indicated by a recent ring-diagram nuclear matter calculation [10].

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