The Tamm-Dancoff, random-phase approximation (RPA), and linear response theory

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Outline

Introduction

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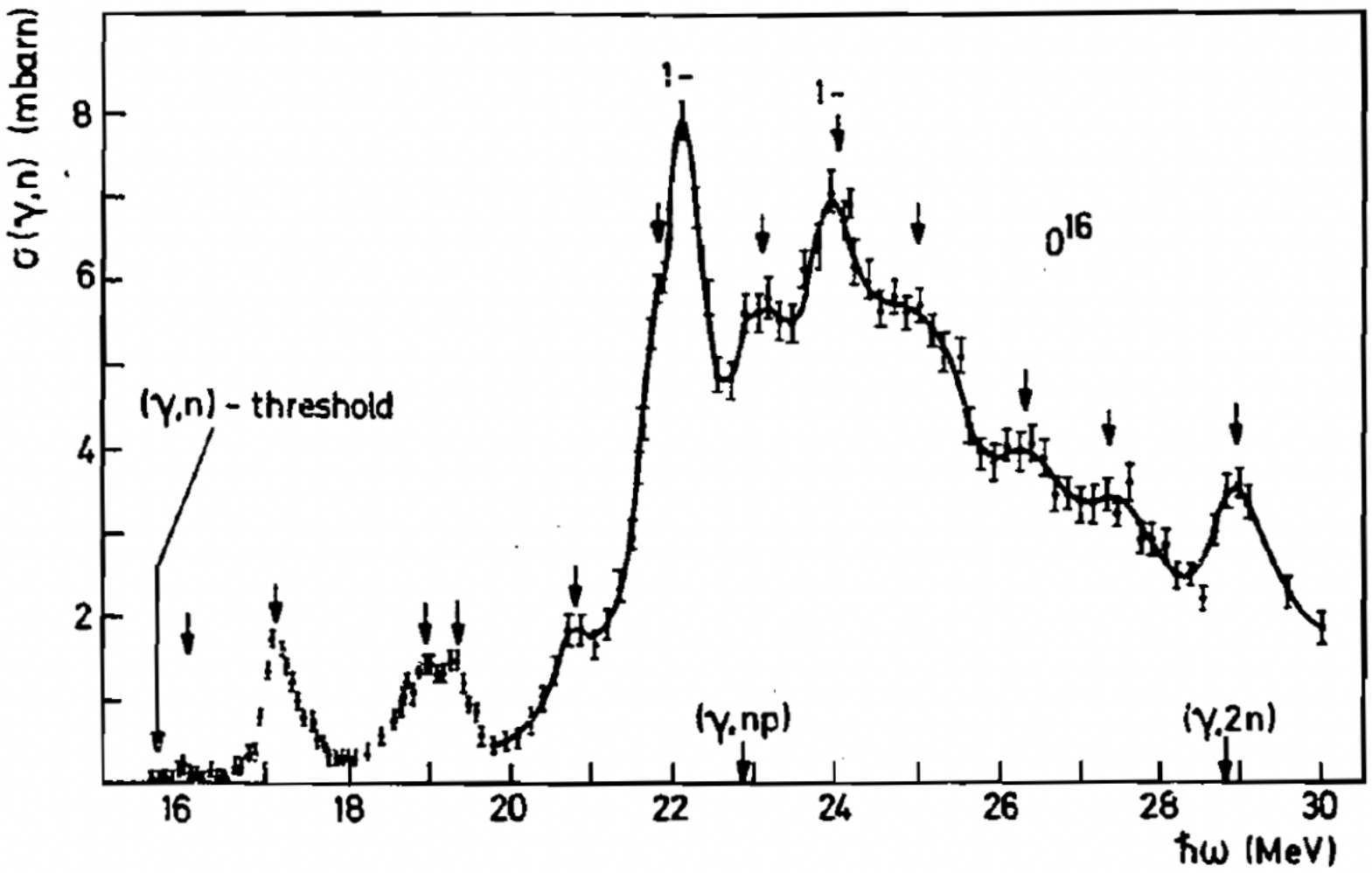
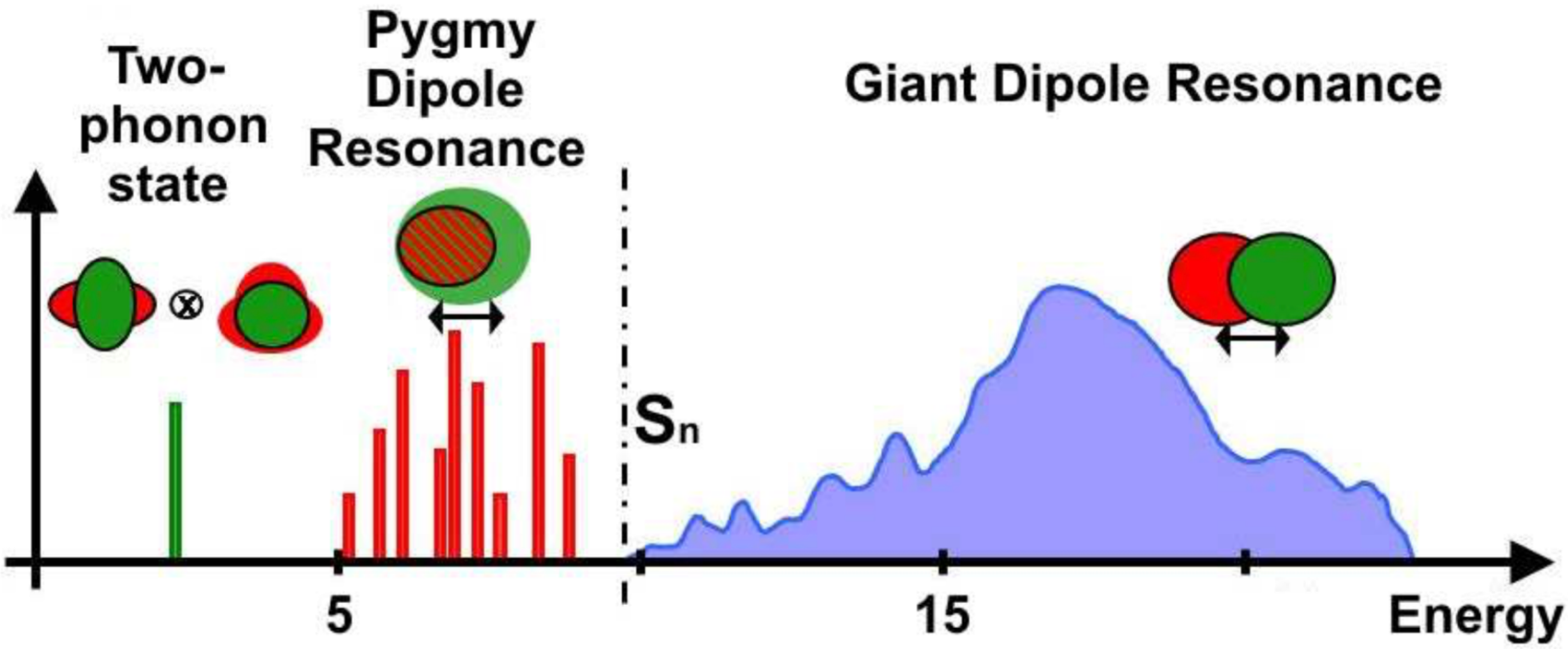


Introduction

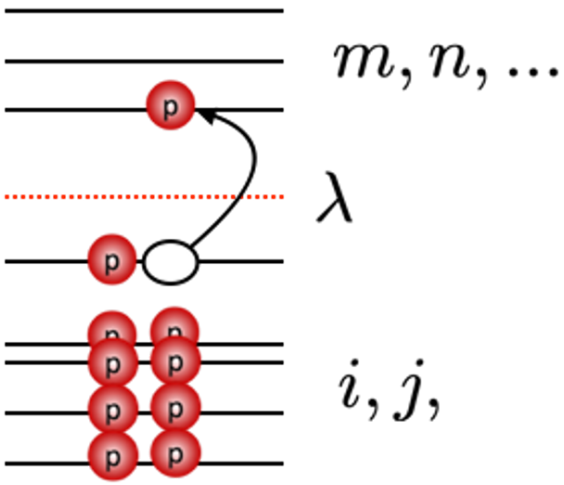
$E1$ strength in (spherical) atomic nuclei



- The Pygmy Dipole Resonance (PDR) might play an important role in nuclear astrophysics.
- The pygmy $E1$ strength provides information on the symmetry energy term of the nuclear equation of state, relevant for the modeling of neutron stars. C. J. Horowitz and J. Piekarewicz, PRL86, 5647 (2001).

The Tamm-Dancoff approximation

The Tamm-Dancoff approximation



- The ground-state wave function

$$|\Psi_0\rangle = C_0^0|\mathrm{HF}\rangle + \sum_{mi} C_{mi}^0 a_m^+ a_i|\mathrm{HF}\rangle + \frac{1}{4}\sum_{mnij} C_{mn,ij}^0 a_m^+ a_n^+ a_i a_j|\mathrm{HF}\rangle + \cdots$$

- The excited-state wave function

$$|\Psi_\nu\rangle = C_0^\nu|\mathrm{HF}\rangle + \sum_{mi} C_{mi}^\nu a_m^+ a_i|\mathrm{HF}\rangle + \frac{1}{4}\sum_{mnij} C_{mn,ij}^\nu a_m^+ a_n^+ a_i a_j|\mathrm{HF}\rangle + \cdots$$

The Tamm-Dancoff approximation

- The ground-state wave function

$$|\Psi_0\rangle \simeq C_0^0|\mathrm{HF}\rangle$$

- The excited-state wave function

$$|\Psi_\nu\rangle \simeq \sum_{mi} C_{mi}^\nu a_m^+ a_i|\mathrm{HF}\rangle$$

The ground state is still a HF state without many-body correlations. Correlations are only taken into account in the excited states which are approximated as a linear combination of 1p-1h excitation configurations.

The Tamm-Dancoff approximation

- The unknown coefficients in the excited-state wave function are determined by the variational principles

$$|\delta\nu\rangle = \sum_{mi} a_m^+ a_i |\mathrm{HF}\rangle \delta C_{mi}^{\nu}$$

which leads to the following eigenvalue equation

$$\sum_{nj} \left\{ \left\langle \mathrm{HF} \left| a_i^+ a_m H a_n^+ a_j \right| \mathrm{HF} \right\rangle - E_\nu \left\langle \mathrm{HF} \left| a_i^+ a_m a_n^+ a_j \right| \mathrm{HF} \right\rangle \right\} C_{nj}^{\nu} = 0$$

Namely,

$$\sum_{nj} \left\langle \mathrm{HF} \left| a_i^+ a_m \left[H, a_n^+ a_j \right] \right| \mathrm{HF} \right\rangle C_{nj}^{\nu} = \left(E_\nu - E_0^{\mathrm{HF}} \right) C_{mi}^{\nu}$$

where

$$\left[H, a_n^+ a_j \right] = \sum_r \left(t_{rn} a_r^+ a_j - t_{jr} a_n^+ a_r \right) + \frac{1}{2} \sum_{rst} \bar{v}_{rsnt} a_r^+ a_s^+ a_t a_j - \frac{1}{2} \sum_{rst} \bar{v}_{jrst} a_n^+ a_r^+ a_t a_s$$

The Tamm-Dancoff approximation

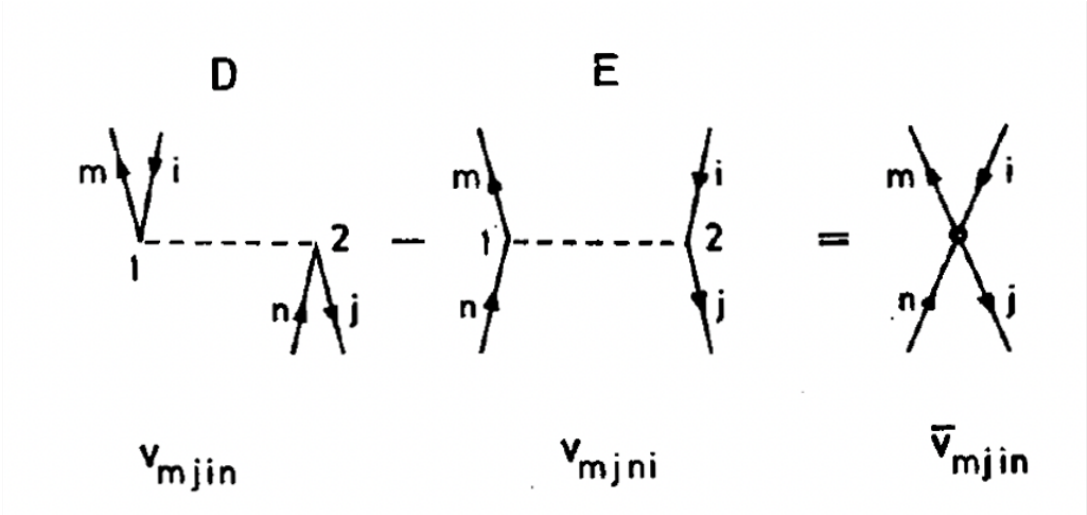
Substituting the single-particle energy

$$h_{kk'} = t_{kk'} + \sum_{i=1}^{A} \bar{v}_{kik'i} = \epsilon_k \delta_{kk'}$$

the above equations becomes,

$$\sum_{nj} \left[(\epsilon_m - \epsilon_i)\, \delta_{mn}\delta_{ij} + \bar{v}_{mjin} \right] C^{\nu}_{nj} = E^{\mathrm{TDA}}_{\nu} C^{\nu}_{mi}$$

The ground-state energy E^{HF}_0 has been set to zero by a suitable choice of the energy scale and E^{TDA}_{ν} is the excitation energy of $|\nu\rangle$ in Tamm-Dancoff approximation (TDA).



The particle-hole TDA

A separable QQ interaction

- The separable particle-hole residual interaction

$$\bar{v}_{mjin} = \lambda \cdot D_{mi} D^*_{nj}$$

Further, it is assumed that the D_{mi} are matrix elements of a multipole operator as, for example, the quadrupole operator

$$D_{mi} = \left\langle m \left| r^2 Y_{2\mu} \right| i \right\rangle$$

The multipolarity agrees, of course, with the angular momentum to which the particle-hole pair (m, i) is coupled. The matrix element is certainly not antisymmetric as it should be. However, it turns out that the exchange term is small and neglecting it is a good approximation.

A separable ph interaction

- With the ansatz, the secular equation has the following form.

$$\left(E_\nu^{\mathrm{TDA}} - \epsilon_m + \epsilon_i\right) C_{mi}^\nu = \lambda D_{mi} \sum_{nj} D_{nj}^* C_{nj}^\nu \tag{1}$$

The states $|\nu\rangle$ should be normalized. We therefore have:

$$\sum_{mi} C_{mi}^{\nu\,*} C_{mi}^{\nu'} = \delta_{\nu\nu'}$$

With $\sum_{nj} D_{nj}^* C_{nj}^\nu = \mathrm{const.}$, the coefficients C_{mi}^ν are determined by

$$C_{mi}^\nu = N \cdot \frac{D_{mi}}{E_\nu^{\mathrm{TDA}} - \epsilon_m + \epsilon_i} \tag{2}$$

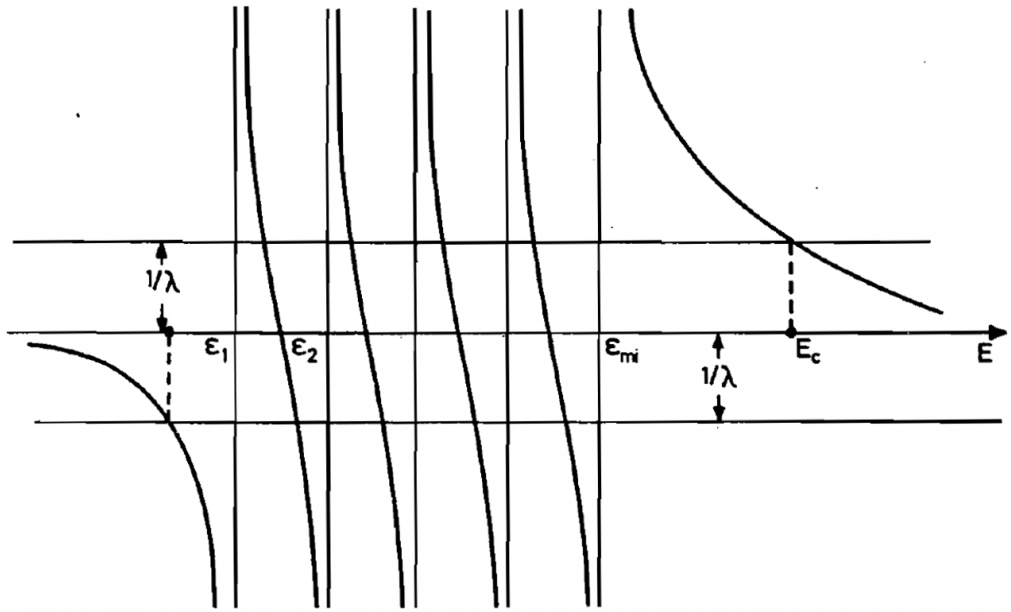
$$N^{-2} = \sum_{mi} \frac{|D_{mi}|^2}{\left(E_\nu^{\mathrm{TDA}} - \epsilon_m + \epsilon_i\right)^2} \tag{3}$$

A separable ph interaction

Multiplying (1) by $D^*_{mi}\left(E_\nu^{\rm TDA}-\epsilon_m+\epsilon_i\right)^{-1}$ and summing over m, i, we obtain an eigenvalue equation for the excitation energies $E_\nu^{\rm TDA}$:

$$\frac{1}{\lambda}=\sum_{mi}\frac{|D_{mi}|^2}{E_\nu^{\rm TDA}-\epsilon_{mi}},\qquad \epsilon_{mi}=\epsilon_m-\epsilon_i \tag{4}$$

We can solve it graphically by plotting the r.h.s. as a function of $E_\nu^{\rm TDA}$. We thus obtain the eigenvalues from the intersection of this function with the straight line $1/\lambda$.



A separable ph interaction

- For the degenerate case $\epsilon_{mi} = \epsilon$. Substituting into (2) and (3), one finds

$$C_{mi} = \left(\sum_{mi} |D_{mi}|^2 \right)^{-1/2} \cdot D_{mi}$$

and from (4)

$$E_c^{\mathrm{TDA}} = \epsilon + \lambda \sum_{mi} |D_{mi}|^2$$

which means the collective states are pushed up by the sum of all the diagonal elements of the interaction.

A separable ph interaction

- The collective state

$$|\nu_c\rangle = \left(\sum_{mi} |D_{mi}|^2\right)^{-1/2} \sum_{mi} D_{mi} a_m^+ a_i |\mathrm{HF}\rangle$$

from which one finds the transition probability of the operator $D = \sum_{kk'} D_{kk'} a_k^\dagger a_{k'}$,

$$|\langle \nu_c | D | \mathrm{HF} \rangle|^2 = \sum_{mi} |D_{mi}|^2 .$$

A separable ph interaction

The sum rule:

$$\begin{aligned}\sum_{\nu}|\langle\nu|D|\mathrm{HF}\rangle|^2 &= \sum_{\nu\neq\nu_c}\cdots+|\langle\nu_c|D|\mathrm{HF}\rangle|^2\\ &=\sum_{\nu}\left\langle\mathrm{HF}\left|D^+\right|\nu\right\rangle\langle\nu|D|\mathrm{HF}\rangle\\ &=\sum_{mi}\left\langle\mathrm{HF}\left|D^+\right|mi\right\rangle\langle mi|D|\mathrm{HF}\rangle=\sum_{mi}|D_{mi}|^2\end{aligned}\tag{5}$$

Here we replaced the complete set $|\nu\rangle$ in the *ph* space by the complete set $|mi\rangle$. It is seen that the total sum rule is exhausted by the collective state. This means that in the degenerate case there is no transition probability from the ground state to any non-collective state. On the other hand, the transition probability to the collective state is drastically enhanced. We thus have a qualitative explanation for the strong 1^- resonance shown in ^{16}O.

The particle-particle TDA

The pp-TDA

- For the closed-shell plus two-nucleon systems: the wave function

$$|\tau, A+2\rangle = \sum_{m<n} C^{\tau}_{mn} a^{+}_{m} a^{+}_{n} |\mathbf{HF}\rangle$$

The coefficients C^{τ}_{mn} are supposed to be antisymmetric, that is, $C^{\tau}_{mn} = -C^{\tau}_{nm}$. In complete analogy to the ph-DA case, we obtain the pp-TDA secular equation:

$$\left(E^{\mathrm{TDA}}_{\tau} - \epsilon_m - \epsilon_n\right) C^{\tau}_{mn} = \sum_{m'<n'} \bar{v}_{mnm'n} C^{\tau}_{m'n'}$$

The pp-TDA

This is a linear Hermitian eigenvalue problem. The eigenvectors have to fulfill the nor m and closure relations ($n < m, n' < m'$)

$$\sum_{m<n} C^{\tau *}_{mn} C^{\tau'}_{mn} = \delta_{\tau\tau'}$$
$$\sum_{\tau} C^{\tau}_{mn} C^{\tau *}_{m'n'} = \delta_{mm'}\delta_{nn'}$$

As indicated, the sum in principle runs over all levels above Fermi energy and therefore includes bound and continuum states. Since this generally gives rise to matrices too big for present day computers, we usually work in a restricted subspace, taking into account one or two major shells above the Fermi level. In order to account for the levels not included, we must take a suitably "renormalized" interaction.

The pp-TDA for pairing vibration

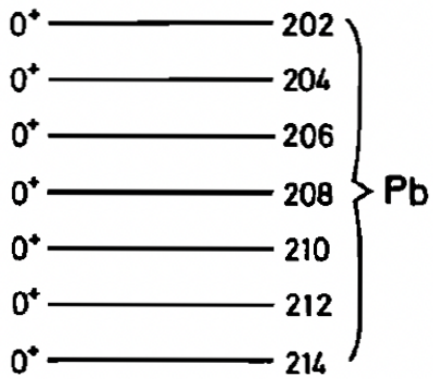


Figure 8.9. Schematic representation of the ground state energies in the even Pb isotopes.

- Two particles form such a stable entity that they can be multiplied, added to, or removed from a nucleus (like, for example, ^{208}Pb).
- The spectrum should therefore be approximately harmonic. This harmonic spectrum is what has been termed the spectrum of "pairing vibrations."
- Removing from ^{208}Pb a 0^+ pairing phonon leads us to ^{206}Pb and adding a phonon leading to the ^{210}Pb.

The Random-Phase-Approximation (RPA)

The derivation of RPA equation

- The TDA equation can be derived also by the equation-of-motion technique:

$$H|\nu\rangle = E_\nu|\nu\rangle.$$

It is possible to define operators ${Q_\nu}^+$ and Q_ν in such a way that

$$|\nu\rangle = {Q_\nu}^+|0\rangle \quad \text{and} \quad Q_\nu|0\rangle = 0$$

where the Q_ν^+ can be chosen as

$${Q_\nu}^+ = |\nu\rangle\langle 0|$$

From the Schrödinger equation we get the equation of motion

$$\left[H, {Q_\nu}^+\right]|0\rangle = (E_\nu - E_0)\,{Q_\nu}^+|0\rangle.$$

The derivation of RPA equation

Multiplying from the left with an arbitrary state of the form $\langle 0|\delta Q$ we get

$$\left\langle 0 \left| \left[\delta Q, \left[H, Q_\nu^+\right]\right] \right| 0 \right\rangle = (E_\nu - E_0) \left\langle 0 \left| \left[\delta Q, Q_\nu^+\right] \right| 0 \right\rangle$$

We can use the commutator, because $\langle 0|Q_\nu^+ = \langle 0|HQ_\nu^+ = 0$. Until now we were exact and, since the variation of $\delta Q|0\rangle$ exhausts the whole Hilbert space. First we re-derive the TDA equation by approximating the exact ground state $|0\rangle$ by the HF state $|\mathrm{HF}\rangle$ and the operator Q_ν by the collective ph-operator

$$Q_\nu{}^+ = \sum_{mi} C_{mi}^\nu a_m^+ a_i$$

By this approximation, we restrict ourselves to the space of $1p-1h$ excitations, that is, we set, $\delta Q|0\rangle = \sum_{mi} a_m^+ a_i |\mathrm{HF}\rangle \delta C_{mi}$,

$$\sum_{nj} \left\langle \mathrm{HF} \left| \left[a_i^+ a_m, \left[H, a_n^+ a_j\right]\right] \right| \mathrm{HF} \right\rangle C_{nj}^\nu = E_\nu^{\mathrm{TDA}} C_{mi}^\nu$$

where E_ν^{TDA} is the excitation energy in TDA approximation.

The derivation of RPA equation

- The RPA equation: a more general vibration creation operator

$$Q_\nu^+ = \sum_{mi} X_{mi}^\nu a_m^+ a_i - \sum_{mi} Y_{ni}^\nu a_i^+ a_m$$

where the minus sign has been chosen for convenience. The RPA ground state $|RPA\rangle$ is defined by analogy by

$$Q_\nu |\mathrm{RPA}\rangle = 0$$

We will later on deduce from this condition an explicit expression for the ground state. Instead of only one matrix C_{mi}^ν we now have two matrices X_{mi}^ν and Y_{mi}^ν. We also have two kinds of variations $\delta Q|0\rangle$, namely $a_m^+ a_i|0\rangle$ and $a_i^+ a_m|0\rangle$.

$$\left\langle \mathrm{RPA} \left| \left[a_i^+ a_m, \left[H, Q_\nu^+ \right] \right] \right| \mathrm{RPA} \right\rangle = \hbar\Omega_\nu \left\langle \mathrm{RPA} \left| \left[a_i^+ a_m, Q_\nu^+ \right] \right| \mathrm{RPA} \right\rangle$$
$$\left\langle \mathrm{RPA} \left| \left[a_m^+ a_i, \left[H, Q_\nu^+ \right] \right] \right| \mathrm{RPA} \right\rangle = \hbar\Omega_\nu \left\langle \mathrm{RPA} \left| \left[a_m^+ a_i, Q_\nu^+ \right] \right| \mathrm{RPA} \right\rangle$$

where $\hbar\Omega_\nu$ is the excitation energy of the state $|\nu\rangle$. These equations contain only expectation values of four Fermion operators, which are still very complicated to calculate, because we do not as yet know the ground state $|\mathrm{RPA}\rangle$.

The derivation of RPA equation

- The quasi-boson approximation: If we assume that the correlated ground state does not differ very much from the HF ground state, we can calculate all expectation values in the HF approximation,

$$\begin{aligned}\left\langle \mathrm{RPA}\left|\left[a_i^+ a_m, a_n^+ a_j\right]\right|\mathrm{RPA}\right\rangle =& \delta_{ij}\delta_{mn} - \delta_{mn}\left\langle \mathrm{RPA}\left|a_j a_i^+\right|\mathrm{RPA}\right\rangle \\ & - \delta_{ij}\left\langle \mathrm{RPA}\left|a_n^+ a_m\right|\mathrm{RPA}\right\rangle \\ \simeq & \left\langle \mathrm{HF}\left|\left[a_i^+ a_m, a_n^+ a_j\right]\right|\mathrm{HF}\right\rangle = \delta_{ij}\delta_{mn} \end{aligned} \tag{6}$$

The name "quasi-boson" approximation comes from the fact that the equation would be an exact relation if the ph creation and annihilation operators obeyed the commutation relations for boson field operators. The above equation however, violates the Pauli principle because we have neglected terms coming from the commutator.

The derivation of RPA equation

Within the quasi-boson approximation, the amplitudes X^{ν}_{mi} and Y^{ν}_{mi} have a very direct meaning: their absolute squares give the probability of finding the states $a^{+}_{m}a_{i}|\Psi_0\rangle$ and $a^{+}_{i}a_{m}|\Psi_0\rangle$ in the excited state $|\nu\rangle$,

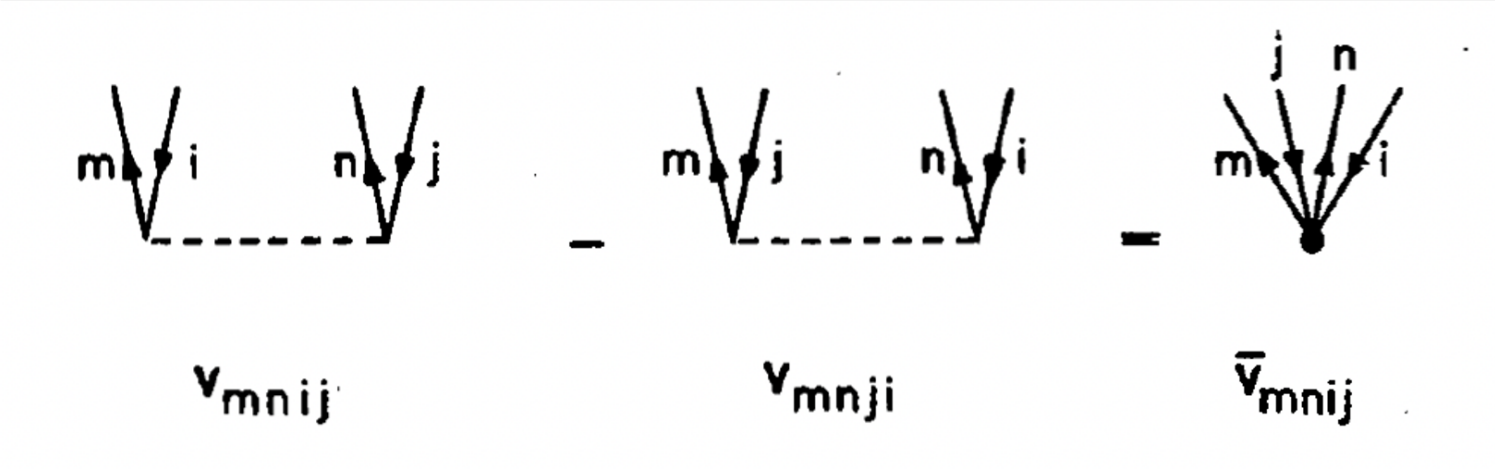
$$\begin{aligned}\rho^{(1)^{\nu}}_{mi} &= \left\langle \Psi_0 \left| a^{+}_{i}a_{m} \right| \Psi_{\nu} \right\rangle \simeq \left\langle \mathrm{HF} \left| \left[a^{+}_{i}a_{m}, Q^{+}_{\nu} \right] \right| \mathrm{HF} \right\rangle = X^{\nu}_{mi} \\ \rho^{(1)^{\nu}}_{im} &= \left\langle \Psi_0 \left| a^{+}_{m}a_{i} \right| \Psi_{\nu} \right\rangle \simeq \left\langle \mathrm{HF} \left| \left[a^{+}_{m}a_{i}, Q^{+}_{\nu} \right] \right| \mathrm{HF} \right\rangle = Y^{\nu}_{mi}\end{aligned} \tag{7}$$

In a compact from, one obtains the RPA equation

$$\begin{pmatrix} A & B \\ B^{*} & A^{*} \end{pmatrix} \begin{pmatrix} X^{\nu} \\ Y^{\nu} \end{pmatrix} = \hbar\Omega_{\nu} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} X^{\nu} \\ Y^{\nu} \end{pmatrix} \tag{8}$$

with $(X^{\nu})_{mi} = X^{\nu}_{mi}$ and $(Y^{\nu})_{mi} = Y^{\nu}_{mi}$.

The derivation of RPA equation



The matrix elements

$$
\begin{aligned}
A_{\text{minj}} &= \left\langle \text{HF} \left| \left[a_i^+ a_m \left[H, a_n^+ a_j \right] \right] \right| \text{HF} \right\rangle = \left(\epsilon_m - \epsilon_i \right) \delta_{mn} \delta_{ij} + \bar{v}_{mjin} \\
B_{minj} &= - \left\langle \text{HF} \left| \left[a_i^+ a_m \left[H, a_j^+ a_n \right] \right] \right| \text{HF} \right\rangle = \bar{v}_{mnij}
\end{aligned}
\tag{9}
$$

The matrix A is hermitian and B is symmetric. The RPA equation reduces to the TDA equation by setting $Y_{mi}^{\nu} = 0$.

The validity of RPA

- The quasi-boson approximation is valid for very collective states with many X^{ν}_{mi} of the same order of magnitude, in which case the violation of Pauli princinple can be neglected.
- The amplitude Y^{ν}_{mi} should be small compared to X^{ν}_{mi} because it describes the ground-state correlation. If it is large, then the replacement of $|\mathrm{RPA}\rangle$ with $|\mathrm{HF}\rangle$ is not justified.

The RPA for transition strengths

- To calculate transition probabilities between the excited state $|\Psi_\nu\rangle$ and the ground state $|\Psi_0\rangle$ we only need matrix elements of the type $\langle\Psi_0|F|\Psi_\nu\rangle$ for a Hermitian one-body operator F. In the RPA approximation they are given by

$$\langle\Psi_0|F|\Psi\nu\rangle = \sum_{kk'} F_{kk'}\rho^{(1)'}_{k'k} = \sum_{mi} F_{im}X^\nu_{mi} + F_{mi}Y^\nu_{mi}$$

In the following sections we will frequently use the notation

$$\langle\Psi_0|F|\Psi_\nu\rangle = f^+\mathcal{X}^\nu$$

with the column vectors

$$f = \begin{pmatrix} F_{mi} \\ F^*_{mi} \end{pmatrix} \quad \text{and} \quad \mathcal{X}^\nu = \begin{pmatrix} X^\nu_{mi} \\ Y^\nu_{mi} \end{pmatrix} \tag{10}$$

The normalization and closure relations

- The normalization of the RPA excited state,

$$\Psi_\nu = Q_\nu^+ |\mathrm{RPA}\rangle, \quad Q|\mathrm{RPA}\rangle = 0,$$

is given by

$$\delta_{\nu\nu'} = \left\langle \mathrm{RPA} \left| \left[Q_\nu, Q_{\nu'}^+ \right] \right| \mathrm{RPA} \right\rangle \simeq \left\langle \mathrm{HF} \left| \left[Q_\nu, Q_{\nu'}^+ \right] \right| \mathrm{HF} \right\rangle \tag{11}$$

$$\delta_{\nu\nu'} = \sum_{mi} \left(X_{mi}^{\nu^*} X_{mi}^{\nu'} - Y_{mi}^{\nu^*} Y_{mi}^{\nu'} \right) \tag{12}$$

The quasiparticle RPA

- In the case that atomic nucleus has pairing correlation, the H can be written as

$$H = H^{0} + H^{11} + H^{31} + H^{40} + H^{22}$$

The Q operator becomes

$$Q^{+}_{\nu} = \frac{1}{2}\sum_{kk'}\left(X^{\nu}_{kk'}\alpha^{+}_{k}\alpha^{+}_{k'} - Y^{\nu}_{kk'}\alpha_{k'}\alpha_{k}\right)$$

The quasiparticle RPA

The matrices A and B are now given by $(k < k', l < l')^*$

$$
\begin{aligned}
A_{kk'll'} &= \left\langle \mathrm{HFB} \left| \left[\alpha_{k'} \alpha_k, \left[H, \alpha_l^+ \alpha_{l'}^+ \right] \right] \right| \mathrm{HFB} \right\rangle \\
&= \left(E_k + E_{k'} \right) \delta_{kl} \delta_{k'l'} + H^{22}_{kk'll'} \\
B_{kk'll'} &= - \left\langle \mathrm{HFB} \left| \left[\alpha_{k'} \alpha_k, \left[H, \alpha_l, \alpha_l \right] \right] \right| \mathrm{HFB} \right\rangle = 4! \cdot H^{40}_{kk'll'}
\end{aligned}
$$

Low-Energy Electric Dipole Response of ^{120}Sn

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Microscopic Structure of the Low-Energy Electric Dipole Response of ^{120}Sn

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The microscopic structure of the low-energy electric dipole response, commonly denoted as pygmy dipole resonance (PDR), was studied for ^{120}Sn in a ^{119}Sn$(d, p\gamma)^{120}$Sn experiment. Unprecedented access to the single-particle structure of excited 1^- states below and around the neutron-separation threshold was obtained by comparing experimental data to predictions from a novel theoretical approach. The novel approach combines detailed structure input from energy-density functional plus quasiparticle-phonon model theory with reaction theory to obtain a consistent description of both the structure and reaction aspects of the process. The presented results show that the understanding of one-particle–one-hole structures of the 1^- states in the PDR region is crucial to reliably predict properties of the PDR and its contribution to nucleosynthesis processes.

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Low-Energy Electric Dipole Response of ^{120}Sn

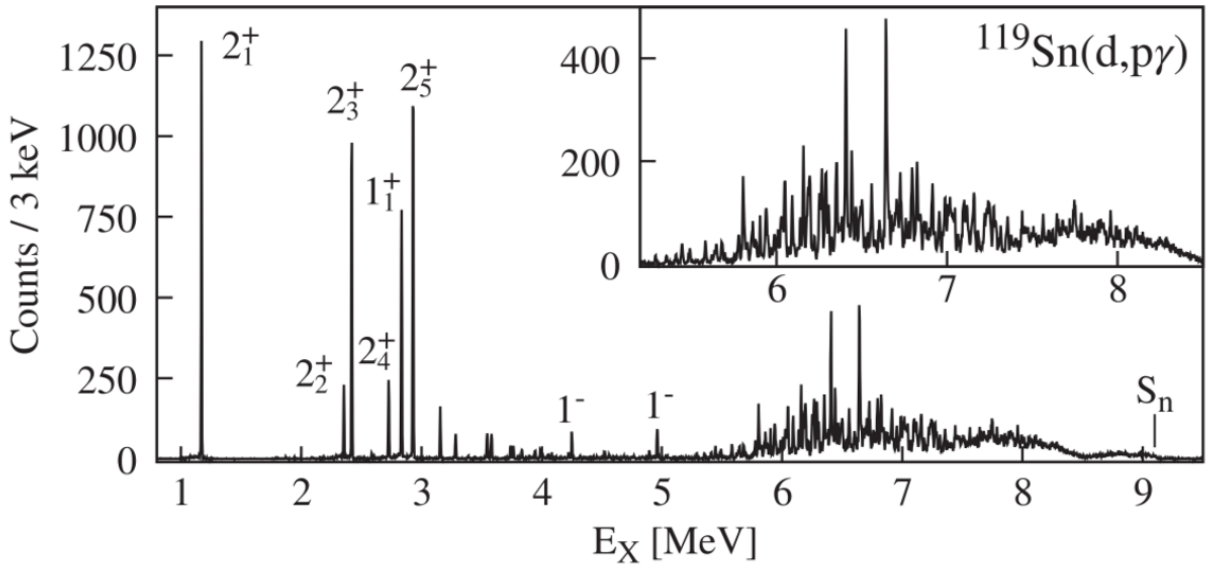
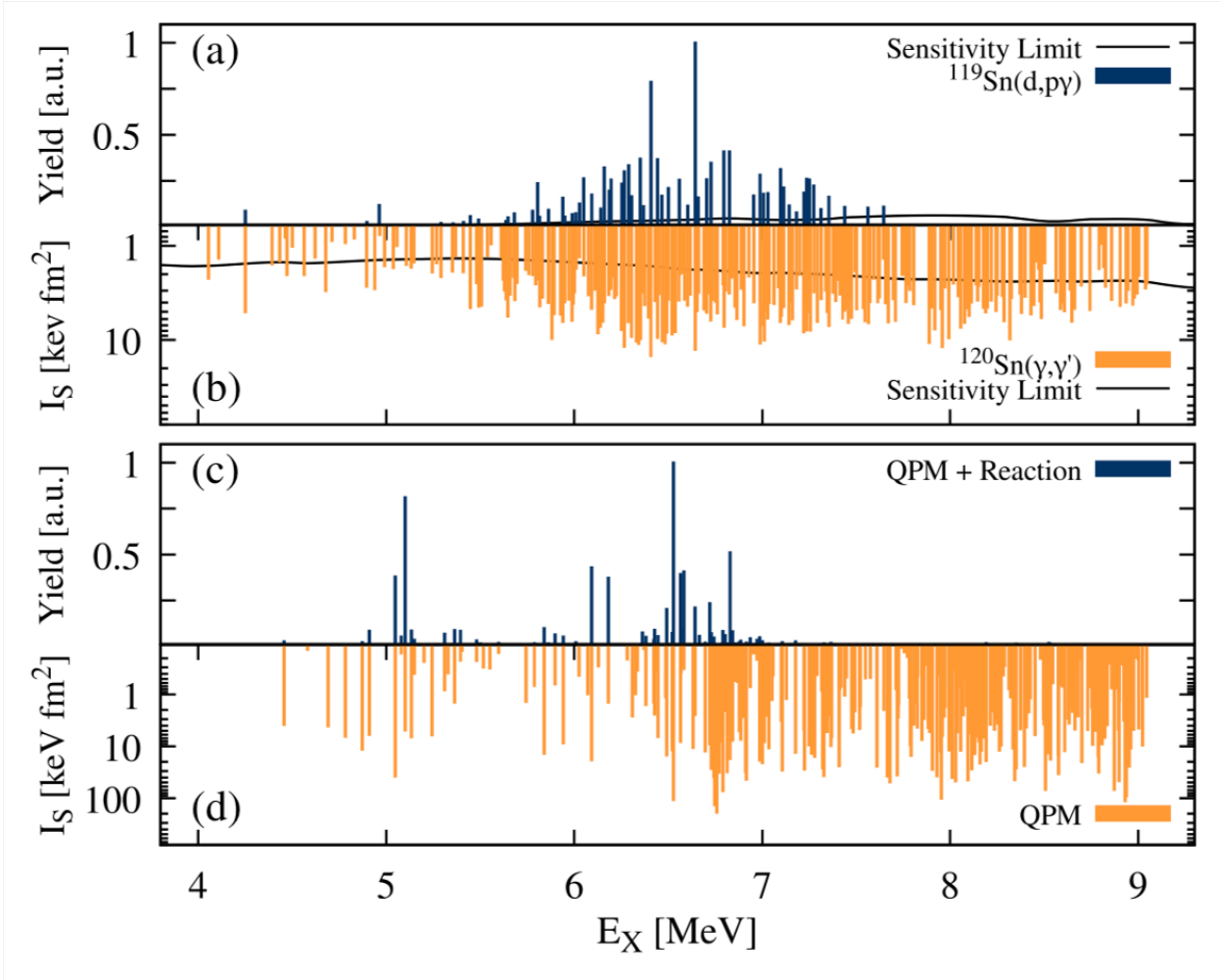


FIG. 1. Ground-state γ-decay spectrum for excited states in ^{120}Sn. Because of selective gates, the spectrum is free of any contaminants. Marked are ground-state decays from several known states in ^{120}Sn and the neutron separation energy S_n. The inset shows the energy region of interest, where the low-energy dipole response is concentrated. Note the clear gap between the discrete transitions at lower energies and the resonancelike structure starting at around 6 MeV possibly corresponding to the gap between the $3\hbar\omega$ and $4\hbar\omega$ harmonic oscillator shells.

Low-Energy Electric Dipole Response of ^{120}Sn



Low-Energy Electric Dipole Response of ^{120}Sn

Theoretical approach.—In this novel approach, the nuclear excitations are expressed in terms of quasiparticle-random-phase-approximation (QRPA) phonons,

$$Q^{+}_{\lambda\mu i} = \frac{1}{2}\sum_{jj'}[\psi^{\lambda i}_{jj'}A^{+}_{\lambda\mu}(jj') - \varphi^{\lambda i}_{jj'}\tilde{A}_{\lambda\mu}(jj')], \qquad (1)$$

where the set of quantum numbers $j \equiv (nljm\tau)$ labels single-nucleon states, and $A^{+}_{\lambda\mu}$ and $\tilde{A}_{\lambda\mu}$ are the time-forward and time-backward two-quasiparticle operators, creating or annihilating two quasiparticles coupled to a total angular

Ref. [43]. The wave functions Ψ_ν of the excited QPM 1^- states ν of an even-even nucleus contain contributions from one-, two-, and three-phonon configurations,

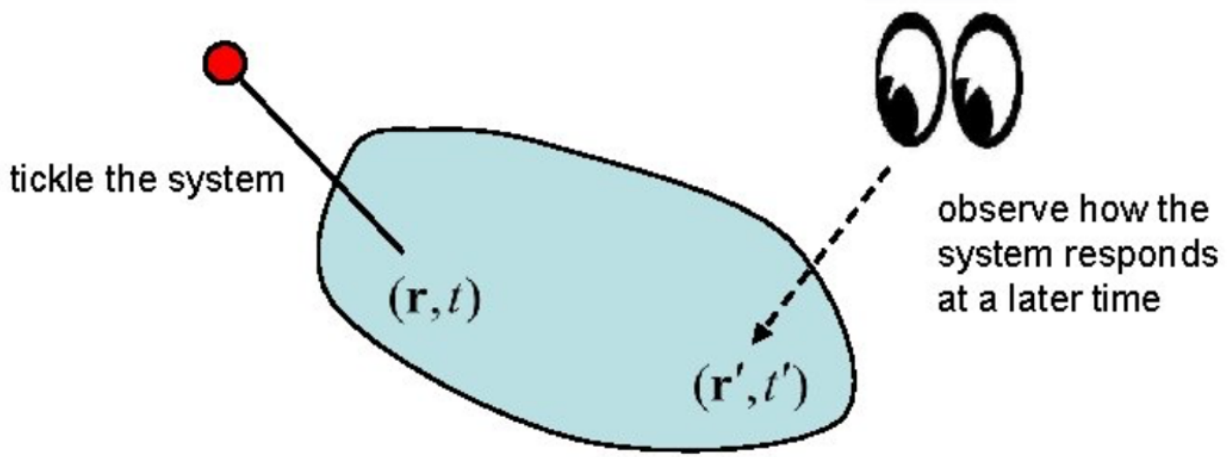
$$\Psi_\nu = \Bigg\{\sum_i R_i(\nu)Q^{+}_{1Mi} + \sum_{\substack{\lambda_1 i_1\\ \lambda_2 i_2}} P^{\lambda_q i_1}_{\lambda_2 i_2}(\nu)[Q^{+}_{\lambda_1\mu_1 i_1}\times Q^{+}_{\lambda_2\mu_2 i_2}]_{1M}$$
$$+ \sum_{\substack{\lambda_1 i_1\lambda_2 i_2\\ \lambda_3 i_3 I}} T^{\lambda_1 i_1\lambda_2 i_2 I}_{\lambda_3 i_3}(\nu)\Bigg[[Q^{+}_{\lambda_1\mu_1 i_1}\times Q^{+}_{\lambda_2\mu_2 i_2}]_{IK}$$
$$\times Q^{+}_{\lambda_3\mu_3 i_3}\Bigg]_{1M}\Bigg\}\Psi_0, \qquad (2)$$

[43] N. Tsoneva and H. Lenske, Phys. At. Nucl. 79, 885 (2016)

where the R, P, and T coefficients are the one-, two-, and three-phonon amplitudes, respectively, and Ψ_0 is the ground-state wave function of the even-even nucleus ^{120}Sn (phonon vacuum). The QPM model space includes two- and three-phonon configurations resulting from the coupling of $J^\pi = 1^\pm - 6^\pm$ QRPA phonons up to $E_x = 9$ MeV. For the dipole excitations, one-phonon states up to $E_x = 35$ MeV are taken into account, so that the isovector giant dipole resonance core polarization contributions to the $E1$ transitions of the low-lying 1^- states are taken into account explicitly and without effective charges. Since ground-state correlations are predicted to be small, i.e., the QRPA backward amplitudes are small, the ^{119}Sn target is assumed to be a pure $3s_{1/2}$ hole relative to the ^{120}Sn "core." Experimental data from ^{118}Sn$(t,d)^{119}$Sn support that the ground state of ^{119}Sn is indeed dominated by a hole (particle) in the neutron $3s_{1/2}$ orbital [44,45]. Within this approximation, the ^{119}Sn$(d,p)^{120}$Sn reaction populates QPM 1^- states that contain $3p_{1/2}$ and $3p_{3/2}$ one-quasiparticle states, i.e., states with neutron $(3s_{1/2})^{-1}(3p_{1/2})^{+1}$ and $(3s_{1/2})^{-1}(3p_{3/2})^{+1}$ $1p$-$1h$ components. The corresponding angular differential

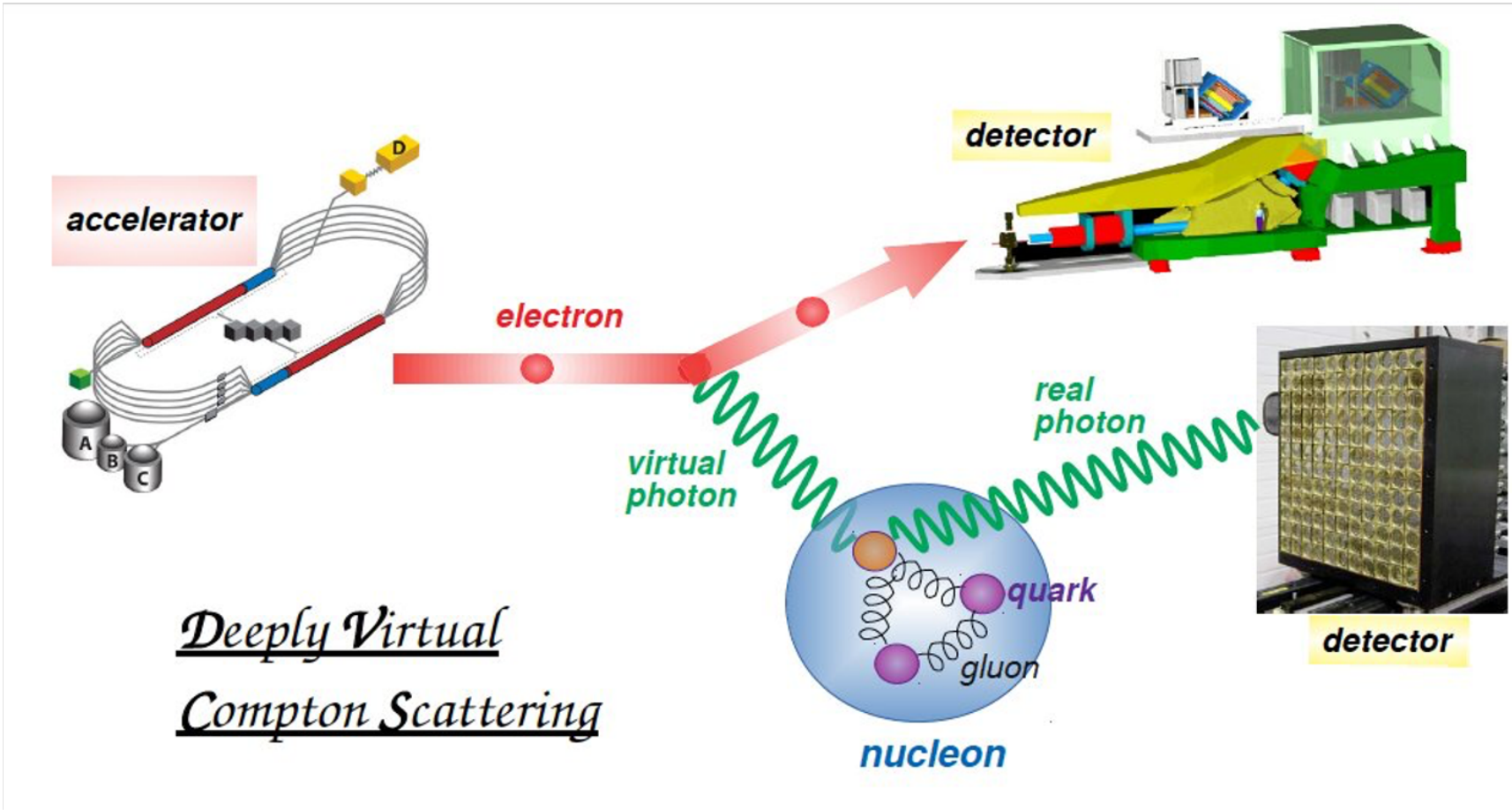
The Linear Response Theory

Linear Response Theory



The formal framework to describe the behavior of a system under weak perturbations is called **Linear Response Theory.**

Linear Response Theory



Linear Response Theory: the external field

- the influence of an external time-dependent field

$$F(t) = Fe^{-i\omega t} + F^{+}e^{i\omega t}$$

Assuming that F is a one-body operator,

$$F(t) = \sum_{kl} f_{kl}(t) a_k^{+} a_l,$$

and that the field is weak, that is, it introduces only small changes of the nuclear density, which we can treat in linear order.

Linear Response Theory: density matrix

The wave function $|\Phi(t)\rangle$ of a nuclear system in an external $F(r)$ field is no longer stationary. The corresponding one-body density

$$\rho_{kl}(t) = \left\langle \Phi(t) \left| a_l{}^+ a_k \right| \Phi(t) \right\rangle$$

is now time dependent.

1. Assume that at any time $\rho(t)$ corresponds to a Slater determinant (i.e., $\rho^2 = \rho$). Then ρ obeys the following equation of motion.

$$i\hbar\dot{\rho} = \Big[h[\rho] + f(t), \rho \Big].$$

   This is the time-dependent Hartree-Fock (TDHF) equation.

Linear Response Theory: density matrix

2. Assume that the external field $f(t)$ is weak, that is, it introduces only oscillations with small amplitudes around the stationary density $\rho^{(0)}$, which is itself a solution of the stationary Hartree-Fock equation, $\left[h\left[\rho^{(0)}\right], \rho^{(0)}\right] = 0$. Therefore, the density has the form

$$\rho(t) = \rho^{(0)} + \delta\rho(t)$$

where

$$\delta\rho = \rho^{(1)} e^{-i\omega t} + \rho^{(1)^+} e^{i\omega t}$$

is linear in the field f.
In the basis in which $\rho^{(0)}$ and $h\left[\rho^{(0)}\right]$ are diagonal, that is, in the HF-basis:

$$\rho^{(0)}_{kl} = \delta_{kl} \cdot \rho^{(0)}_{k} = \begin{cases} 0 & \text{for particles,} \\ 1 & \text{for holes,} \end{cases}$$

and

$$(h_0)_{kl} = \left(h\left[\rho^{(0)}\right]\right)_{kl} = \delta_{kl} \cdot \epsilon_k.$$

Linear Response Theory: linear response equation

3. The condition $\rho^2 = \rho$ implies that the only non-vanishing matrix elements of $\rho^{(1)}$ are *ph* and *hp* matrix elements $\rho^{(1)}_{mi}$ and $\rho^{(1)}_{im}$. They are determined by the solution of the TDHF equation.
   Expand up to linear order in the external field f,

$$i\hbar\delta\dot{\rho} = [h_0, \delta\rho] + \left[\frac{\delta h}{\delta\rho}\cdot\delta\rho, \rho^{(0)}\right] + \left[f, \rho^{(0)}\right]$$

   where $\delta h/\delta\rho\cdot\delta\rho$ is a shorthand notation for

$$\sum_{im}\left(\left.\frac{\partial h}{\partial\rho_{mi}}\right|_{\rho=\rho^{(0)}}\cdot\delta\rho_{mi} + \left.\frac{\partial h}{\partial\rho_{im}}\right|_{\rho=\rho^{(0)}}\cdot\delta\rho_{im}\right).$$

   Using the rules for the calculation with HF densities, one finds that the *pp* and the *hh* matrix elements vanish identically. For the *ph* and *hp* elements the linear response equation

$$\left\{\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} - \hbar\omega\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\right\}\begin{pmatrix} \rho^{(1)ph} \\ \rho^{(1)hp} \end{pmatrix} = -\begin{pmatrix} f^{ph} \\ f^{hp} \end{pmatrix}$$

   with

$$A_{minj} = (\epsilon_m - \epsilon_i)\,\delta_{mn}\delta_{ij} + \frac{\partial h_{mi}}{\partial\rho_{nj}}; \quad B_{minj} = \frac{\partial h_{mi}}{\partial\rho_{jn}}$$

Linear Response Theory: interaction

These matrices correspond exactly to the matrices A and B of the RPA method, if we use as a residual interaction

$$\tilde{v}_{psqr} = \frac{\partial h_{pq}}{\partial \rho_{rs}} = \frac{\partial^2 E}{\partial \rho_{qp} \partial \rho_{rs}}.$$

In the case of HF theory without density dependent forces, we can use the expression for the energy and thus we get back the RPA matrices. However, the above derivation is more general. It can also be applied to theories with density dependent forces. In this case, for the calculation of excited states we have to use the force as the second derivative of the ground state energy with respect to the density. In particular, this force is no longer necessarily antisymmetric in the indices q and r.

Linear Response Theory: response function

- The linear response equation can be solved by inverting the matrix on the left-hand side. We then find a linear connection between the external field f and the change in the nuclear density (i.e., the response of the system):

$$\rho^{(1)}_{kl} = \sum_{pq} R_{klpq}(\omega) f_{pq}.$$

The function $R_{klpq}(\omega)$ is called the response function.

Linear Response Theory

The response function R depends on the frequency of the external field. It has poles at the eigenfrequencies of the system, where already an infinitesimal field f is sufficient to excite the corresponding eigenmode. To find these resonances ($\omega = \Omega_\nu$), we have to look for the solutions of the homogeneous equation with vanishing external field.

$$(\mathcal{M} - \hbar\Omega_\nu \mathcal{N})\, \rho^{(1)\nu} = 0.$$

where

$$\mathcal{M} = \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix}, \quad \mathcal{N} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

This is exactly the RPA equation. Its solution gives the transition densities

$$\rho^{(1)}_{pq}(\Omega_\nu) = \left\langle 0 \left| a^+_q a_p \right| \nu \right\rangle$$

The average nuclear potential oscillates around its stationary value, which corresponds to a minimum in the energy surface of all possible product wave functions. In the limit of small amplitudes we thus get a linear eigenvalue problem for the determination of the normal modes of the system. The RPA approximation is therefore nothing but the small amplitude limit of the time-dependent mean field approach.

Linear Response Theory

Knowing the eigenmodes of the system, that is, the frequencies Ω_ν and the RPA amplitudes X and Y, makes it possible to solve the linear response equation

$$\mathcal{M} - \hbar\omega\mathcal{N} = \hbar\mathcal{N}\mathcal{X}(\omega - \Omega)\mathcal{N}\mathcal{X}f$$

which can easily be inverted:

$$\rho^{(1)} = \frac{1}{\hbar}\mathcal{X}(\omega - \Omega)^{-1}\mathcal{N}\mathcal{X}^{+}\mathcal{N}$$

We have now an explicit expression for the response function, namely its spectral representation:

$$R_{pqp'q'}(\omega) = \frac{1}{\hbar}\sum_{\nu>0}\left(\frac{\left\langle 0\left|a_q^{+}a_p\right|\nu\right\rangle\left\langle\nu\left|a_{p'}^{+}a_{q'}\right|0\right\rangle}{\omega - \Omega_\nu + i\eta} - \frac{\left\langle 0\left|a_{p'}^{+}a_{q'}\right|\nu\right\rangle\left\langle\nu\left|a_q^{+}a_p\right|0\right\rangle}{\omega + \Omega_\nu + i\eta}\right).$$

Again, the index pairs pq and $p'q'$ run only over ph and hp pairs. All other matrix elements of R vanish in RPA order. The form is more general. If we use exact eigenfunctions $|\nu\rangle$ and exact energies $\hbar\Omega_\nu$ of the system, $R_{pqp'q'}(\omega)$ is just the exact response function.

Linear Response Theory

If we introduce the response function R^0 of the free system (without residual interaction $\tilde{v}$),

$$R^0_{pqp'q'}(\omega) = \frac{\rho^{(0)}_q - \rho^{(0)}_p}{\hbar\omega - \epsilon_p + \epsilon_q + i\eta}\delta_{pp'}\delta_{qq'},$$

we can finally, in RPA approximation, derive another equation for $R(\omega)$, the so-called linearized Bethe-Salpeter equation

$$R_{pqp'q'} = R^0_{pqp'q'} + \sum_{\substack{p_1 q_1 \\ p_2 q_2}} R^0_{pqp_1 q_1}\,\tilde{v}_{p_1 q_2 q_1 p_2}\,R_{p_2 q_2 p'q'}.$$

The correctness of this equation can be verified simply by multiplying by $(\hbar\omega - \epsilon_p + \epsilon_q)$ and using the definition of R^0, the spectral representation for R and the RPA equation.

Linear Response Theory

Another useful property of the linear response function lies in the fact that its imaginary part is related to the total transition probability. We define

$$R_F(\omega) := \mathrm{Tr}\left(f^+\rho^{(1)}(\omega)\right) = \sum_{pqp'q'} f^*_{pq} R^{(\omega)}_{pqp'q'} f_{p'q'}$$

and use the relation $1/(\omega + i\eta) = P(1/\omega) - i\pi\delta(\omega)$ to obtain

$$\mathrm{Im}\, R_F(\omega) = -\pi \sum_{\nu>0} |\langle\nu|F|0\rangle|^2 \delta\left(\hbar\omega - \hbar\Omega_\nu\right), \quad \omega > 0.$$

We get the energy-weighted sum rule by integrating this function,

$$S_1 = \sum_\nu \hbar\Omega_\nu |\langle\nu|F|0\rangle|^2 = -\frac{\hbar^2}{\pi}\int_0^\infty \omega ImR(\omega) d\omega$$

and the transition matrix element $|\langle\nu|F|0\rangle|^2$ as the residue of $R_F(\omega)$ at the pole $\omega = \Omega_\nu$.

Linear Response Theory: a simple example

A separable ansatz for the ground state correlation matrix element

$$\tilde{v}_{mjin} = \lambda D_{mi} D^*_{nj}, \quad \tilde{v}_{mnij} = \lambda D_{mi} D_{nj}$$

where D is identical with the external field operator F. From the Bethe-Salpeter equation, we get

$$R_D(\omega) = R^0_D(\omega)\left[1 + \lambda R_D(\omega)\right]$$

with

$$R^0_D(\omega) = \sum_{pqp'q'} D^*_{pq} R^0_{pqp'q'} D_{p'q'} = \sum_{mi} |D_{mi}|^2 \left(\frac{1}{\hbar\omega - \epsilon_m + \epsilon_i + i\eta} - \frac{1}{\hbar\omega + \epsilon_m - \epsilon_i + i\eta} \right)$$

Solving for $R_D(\omega)$ yields

$$R_D(\omega) = \frac{R^0_D}{1 - \lambda R^0_D}$$

The poles of $R_D(\omega)$ give the excitation energies Ω_ν and thus in the schematic model

Linear Response Theory: a simple example

We have the following dispersion relation.

$$\frac{1}{\lambda} = R_D^0(\Omega_\nu) = \sum_{mi} |D_{mi}|^2 \frac{2\epsilon_{mi}}{\hbar^2\Omega_p^2 - \epsilon_{mi}^2}; \quad \epsilon_{mi} = \epsilon_m - \epsilon_i$$

We can drop the infinitessimal η because we are only interested in bound states for which $\Omega_\nu \neq \epsilon_{mi}$.)
Compared to the TDA, two qualitative differences which are due to the RPA ground state correlations:

- In the case where the residual interaction becomes stronger than the critical value (i.e., $\lambda < \lambda_{\text{crit}}$) the energy of the low-lying collective state becomes imaginary.
- The ($T = 0$)-RPA state is shifted further down than its corresponding TDA state for a comparable interaction strength λ.

Linear Response Theory: a simple example

We can study this more closely in the degenerate case. If we put all ϵ_{mi} equal to ϵ we have

$$E^2_{\text{coll}} = \epsilon^2 + 2\epsilon\lambda \sum_{mi} |D_{mi}|^2$$

In the degenerate case, therefore, we have for λ_{crit}

$$\lambda_{\text{crit}} = -\frac{\epsilon}{2\sum_{mi} |D_{\text{mi}}|^2}$$

This is the point where the chosen HF-basis no longer gives the minimum for the ground state energy. The true minimum now occurs in a different HF-solution, which turns out to be deformed. We therefore of call λ_{crit} the point at which a phase transition from spherical state into a deformed shape of the nucleus occurs.

Linear Response Theory: a simple example

We now want to turn to the calculation of transition matrix elements. We have to calculate the residue of $R_D(\omega)$ at the pole $\omega = \Omega_\nu$. In the vicinity of Ω_ν, $R_D(\omega)$ has the form:

$$R_D(\omega) = \frac{R_D^0(\Omega_\nu)}{-\lambda \left(dR^0/d\omega\right)\big|_{\omega=\Omega 2} \cdot (\omega - \Omega_\nu)}$$

We therefore get

$$|\langle\nu|D|0\rangle|^2 = -\frac{\hbar}{\lambda^2}\left(\frac{dR^0}{d\omega}\right)^{-1}_{\Omega_r} = \left(\lambda^2 \sum_{mi} |D_{mi}|^2 \frac{4\epsilon_{mi}\hbar\Omega_\nu}{\left(\hbar^2\Omega_\nu^2 - \epsilon_{mi}^2\right)^2}\right)^{-1}$$

In the degenerate case this yields

$$|\langle\nu|D|0\rangle|^2 = \frac{\epsilon}{E_{\text{coll}}} \sum_{mi} |D_{mi}|^2$$

We see that for the low-lying states the transition probability is enhanced as compared to the TDA value by a factor $\epsilon/E_{\text{coll.}}$. For the collective octupole and quadrupole states this factor can be as large as two. Similar but less pronounced results are found in realistic calculations.