

Notes on Siemens Ch. 8.4

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Harmonic Vibrations in the Random Phase Approximation

- We are going to look at small vibrations around equilibrium (Q^0).
- Follow the cranking model which says that $Q_\alpha = Q_\alpha(t)$, and then solve for the equations of motion for $Q_\alpha(t)$.
- He says that this chapter treats Q_α as the main dynamic variable. Elevating it above \mathbf{r}_i and \mathbf{p}_i comes at the expense of a classical treatment of Q_α .

Harmonic Vibrations in the Random Phase Approximation

Constructing the Single-particle Hamiltonian

- The HF mean field expectation value double counts the two-body potential terms so we can't use those.

$$\sum_{j=1}^A \varepsilon_j = \langle \psi_{HF} | \sum_{i=1}^A \frac{p_i^2}{2m_N} | \psi_{HF} \rangle + \langle \psi_{HF} | \sum_{ij} V(\mathbf{r}_i - \mathbf{r}_j) | \psi_{HF} \rangle \quad (1)$$

where

$$\begin{aligned} \langle \psi_{HF} | H | \psi_{HF} \rangle &= \langle \psi_{HF} | \sum_{i=1}^A \frac{p_i^2}{2m_N} | \psi_{HF} \rangle \\ &\quad + \frac{1}{2} \langle \psi_{HF} | \sum_{ij} V(\mathbf{r}_i - \mathbf{r}_j) | \psi_{HF} \rangle \end{aligned} \quad (2)$$

Harmonic Vibrations in the Random Phase Approximation

Constructing the Single-particle Hamiltonian

- The (incorrect) independent-particle model (ipm) energy is given by

$$\hat{\mathcal{E}} = \sum_{i=1}^A \hat{\varepsilon}_i.$$

- Strutinsky, in chapter 5, found a correction to the ipm energy in terms of the liquid-drop energy and the smoothed single-particle energy $\tilde{\mathcal{E}}$.

$$\langle \psi_{HF} | H | \psi_{HF} \rangle = \hat{\mathcal{E}} + \delta\tilde{\mathcal{E}} \quad (3)$$

$$\delta\tilde{\mathcal{E}}(Q_\alpha) = \tilde{E} - \tilde{\mathcal{E}} = -B_{LD} - \tilde{\mathcal{E}} \quad (4)$$

- Which gives us the single-particle hamiltonian

$$H_{sp} = \sum_{i=1}^A H^{sp}(\mathbf{r}_i, \mathbf{p}_I, \{Q_\alpha\}) = \delta\tilde{\mathcal{E}}(\{Q_\alpha\}) + \sum_{i=1}^A H^{ipm}(\mathbf{r}_i, \mathbf{p}_I, \{Q_\alpha\}) \quad (5)$$

- Notice that the additional term doesn't depend on the intrinsic coordinates, \mathbf{r} and \mathbf{p} .

Harmonic Vibrations in the Random Phase Approximation

Constructing the Single-particle Hamiltonian

- Equations 8.2.3 and 8.2.15 are then just changed by a constant value

$$H_0^{sp} = H^{ipm}(\mathbf{r}, \mathbf{p}, \{Q_\alpha^0\}) + \delta\tilde{\mathcal{E}}(\{Q_\alpha^0\})/A \quad (6)$$

$$F_\mu^{sp} = \frac{\partial H^{sp}}{\partial Q_\mu} \Big|_{\{Q_\alpha = Q_\alpha^0\}} = F_\mu^{ipm} + \frac{\partial}{\partial A_\mu^0} \frac{\delta\tilde{\mathcal{E}}(\{Q_\alpha^0\})}{A} \quad (7)$$

Where the F is the form factor

- This will shift F_μ and the single-particle energies by a uniform amount, but will not effect the response function because it does not depend on the diagonal elements.

Harmonic Vibrations in the Random Phase Approximation

Constructing the Equation of Motion

- We now use this single-particle hamiltonian, the fact that $\langle H_{sp} \rangle$ is conserved, and Ehrenfest's theorem to get the equations of motion.
- Ehrenfest's theorem: $\frac{d}{dt} \langle A \rangle = \frac{1}{i\hbar} \langle [A, H] \rangle + \langle \frac{\partial A}{\partial t} \rangle$

$$0 = \frac{d}{dt} \langle \psi(t) | H_{sp} | \psi(t) \rangle = \left\langle \psi(t) \left| \frac{\partial}{\partial t} H_{sp}(\{Q_\alpha(t)\}) \right| \psi(t) \right\rangle \quad (8)$$

$$= \sum_\mu \frac{dQ_\mu}{dt} \left\langle \psi(t) \left| \frac{\partial H_{sp}}{\partial t} \right| \psi(t) \right\rangle \quad (9)$$

- The solution to this for any dynamic Q_α implies that

$$\left\langle \psi(t) \left| \frac{\partial H_{sp}}{\partial Q_\mu} \right| \psi(t) \right\rangle = 0 \quad (10)$$

Harmonic Vibrations in the Random Phase Approximation

Constructing the Equation of Motion

- Now remember that we are doing this for small oscillations around Q_μ^0 . So let's expand to second order in $Q_\mu - Q_\mu^0$.

$$H_{sp} \approx \sum_i H_0^{sp}(\mathbf{r}_i, \mathbf{p}_i) + \sum_\mu (Q_\mu - Q_\mu^0) \sum_i F_\mu^{sp}(\mathbf{r}_i, \mathbf{p}_i, \{Q_\alpha^0\}) \\ + \frac{1}{2} \sum_{\mu, \nu} (Q_\mu - Q_\mu^0)(Q_\nu - Q_\nu^0) \sum_i \frac{\partial^2 H^{sp}}{\partial Q_\mu \partial Q_\nu}(\mathbf{r}_i, \mathbf{p}_i, \{Q_\alpha^0\}) \quad (11)$$

- Now let's force equation 10 to be zero.

$$-\left\langle \psi(t) \left| \frac{\partial H_{sp}}{\partial Q_\mu} \right| \psi(t) \right\rangle = 0 \approx -\left\langle \psi(t) \left| \sum_i F_\mu^{sp}(\mathbf{r}_i, \mathbf{p}_i, \{Q_\alpha^0\}) \right| \psi(t) \right\rangle \\ - \sum_\nu (Q_\nu(t) - Q_\nu(t)^0) \left\langle \psi(t) \left| \sum_i \frac{\partial^2 H^{sp}}{\partial Q_\mu \partial Q_\nu}(\mathbf{r}_i, \mathbf{p}_i, \{Q_\alpha^0\}) \right| \psi(t) \right\rangle \quad (12)$$

Harmonic Vibrations in the Random Phase Approximation

Constructing the Equation of Motion

- Now using equation 8.4.12 and adding the linear term from above we get can find the equation of motion for Q_ν .

$$0 = \int_{-\infty}^{\infty} dt' \sum_{\nu} \tilde{\chi}_{\mu\nu}^{ipm}(t - t') (Q_{\nu}(t') - Q_{\nu}^0) - \left\langle gs \left| \sum_i F_{\mu}^{sp} \right| gs \right\rangle \quad (13)$$
$$+ \sum_{\nu} \kappa_{\mu\nu} (Q_{\nu}(t) - Q_{\nu}^0)$$

where

$$\kappa_{\mu\nu} = \left\langle gs \left| \sum_i \frac{\partial^2 H^{sp}}{\partial Q_{\mu} \partial Q_{\nu}}(\mathbf{r}_i, \mathbf{p}_i, \{Q_{\alpha}^0\}) \right| gs \right\rangle. \quad (14)$$

Harmonic Vibrations in the Random Phase Approximation

Small-amplitude Vibrational Solutions

- How are we going to solve this?
- Let's assume small-vibrations around the equilibrium $\{Q_\alpha^0\}$, where

$$\left\langle gs \left| \sum_i F_\mu^{sp}(\{Q_\alpha^0\}) \right| gs \right\rangle = 0. \quad (15)$$

- Now let's try a solution of the form $Q_\nu(t) = Q_\nu^0 + A_\nu^n e^{-i\omega_n t + \phi}$.
- This is a solution given the condition (eigenvalue equation)

$$\sum_\nu [\kappa_{\mu\nu} + \chi_{\mu\nu}^{ipm}(\omega_n)] A_\nu^n = 0 \quad (16)$$

- This is a solution given the condition

$$\det |\kappa_{\mu\nu} + \chi_{\mu\nu}^{ipm}(\omega_n)| = 0 \quad (17)$$

- This is called the characteristic equation of the RPA (Random Phase Approximation).

Harmonic Vibrations in the Random Phase Approximation

Small-amplitude Vibrational Solutions

- Let's try to understand the RPA eigenvalue equation by assuming that both $\kappa_{\mu\nu}$ and $\chi_{\mu\nu}^{ipm}$ are diagonal.
- If we do this we get solutions when $\chi_{\mu}^{ipm} = -\kappa_{\mu}$, where these are the μ^{th} diagonal elements.
- From the previous equations of the ipm (8.2.10, 8.2.11, 8.1.18) we get

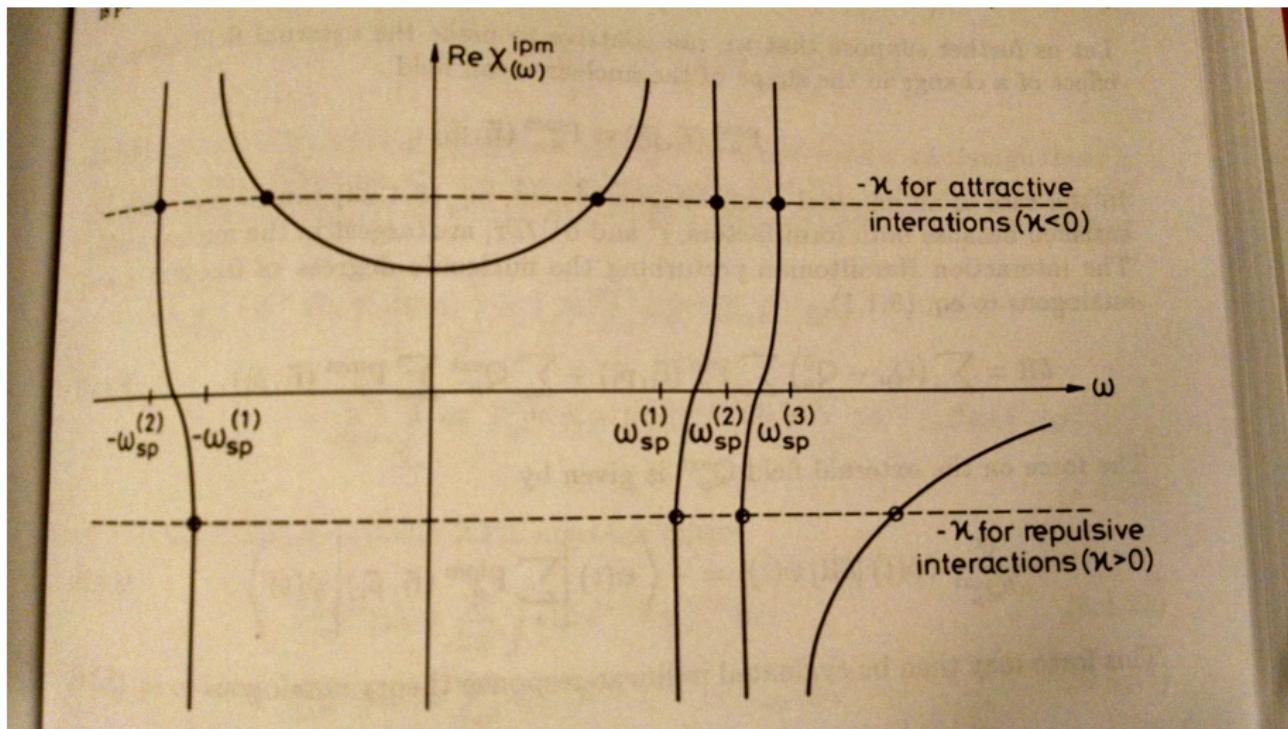
$$\chi_{\mu}^{ipm}(\omega) = \sum_{jk} \frac{N_{jk}}{\hbar} |\langle j | F_{\mu}^{ipm} | k \rangle|^2 \left[\frac{2\omega_{kj}P}{\omega_{kj}^2 - \omega^2} + i\pi [\delta(\omega - \omega_{kj}) - \delta(\omega - \omega_{kj})] \right]. \quad (18)$$

- Since $\chi_{\mu}^{ipm'}$ is the real part, when κ_{μ} is real we get

$$\chi_{\mu}^{ipm'}(\omega_n) = \sum_{jk} \frac{N_{jk}}{\hbar} |\langle j | F_{\mu}^{ipm} | k \rangle|^2 \left[\frac{2\omega_{kj}}{\omega_{kj}^2 - \omega_n^2} \right] = -\kappa_{\mu} \quad (19)$$

Harmonic Vibrations in the Random Phase Approximation

Small-amplitude Vibrational Solutions



Harmonic Vibrations in the Random Phase Approximation

RPA Response to an External Field

- Let's add in a weak external field with parameters $Q_\mu^{ext}(t)$ and see how the nucleus responds.

$$H = \sum_i H^{sp}(\mathbf{r}_i, \mathbf{p}_i, \{Q_\alpha(t)\}) + H^{ext}(\mathbf{r}_i, \mathbf{p}_i, \{Q_\mu^{ext}(t)\}) \quad (20)$$

$$H^{ext} = \sum_\mu F_\mu^{ext}(\mathbf{r}_i, \mathbf{p}_i) Q_\mu^{ext}(t) \quad (21)$$

- Not to simplify things let's assume we can make the external field look like the mean field.

$$F_\mu^{ext}(\mathbf{r}_i, \mathbf{p}_i) \approx F_\mu^{ipm}(\mathbf{r}_i, \mathbf{p}_i) \quad (22)$$

Harmonic Vibrations in the Random Phase Approximation

RPA Response to an External Field

- Now we can write the perturbing hamiltonian as

$$\delta H = \sum_{\mu} (Q_{\mu} - Q_{\mu}^0) \sum_i F_{\mu}^{sp}(\mathbf{r}_i, \mathbf{p}_i) + \sum_{\mu} Q_{\mu}^{ext} \sum_i F_{\mu}^{ipm}(\mathbf{r}_i, \mathbf{p}_i) \quad (23)$$

- Then the force on the external field is

$$-\frac{\partial}{\partial Q_{\mu}^{ext}} \langle \psi(t) | \delta H | \psi(t) \rangle = -\left\langle \psi(t) \left| \sum_i F_{\mu}^{ipm}(\mathbf{r}_i, \mathbf{p}_i) \right| \psi(t) \right\rangle \quad (24)$$

- With linear-response theory (see eq. 8.1.6) this becomes

$$\begin{aligned} \left\langle \psi(t) \left| \sum_i F_{\mu}^{ipm}(\mathbf{r}_i, \mathbf{p}_i) \right| \psi(t) \right\rangle &= \left\langle gs \left| \sum_i F_{\mu}^{ipm}(\mathbf{r}_i, \mathbf{p}_i) \right| gs \right\rangle \\ &- \sum_{\nu} \int_{-\infty}^{\infty} dt' \tilde{\chi}_{\mu\nu}^{ipm}(t - t') [Q_{\nu}(t') - Q_{\nu}^0 + Q_{\nu}^{ext}(t')] \end{aligned} \quad (25)$$

Harmonic Vibrations in the Random Phase Approximation

RPA Response to an External Field

- We can now use equation 8.1.11 to calculate the rate of change of the energy due to this external field.

$$\begin{aligned}\frac{dE}{dt} &= \sum_{\mu} \frac{dQ_{\mu}^{ext}}{dt} \left\langle \psi(t) \left| \sum_i F_{\mu}^{ipm}(\mathbf{r}_i, \mathbf{p}_i) \right| \psi(t) \right\rangle \\ &\equiv \frac{d}{dt} \langle \psi(t) | H(t) | \psi(t) \rangle\end{aligned}\quad (26)$$

- Using Ehrenfest's theorem again we can write

$$\begin{aligned}\frac{d}{dt} \langle \psi(t) | H(t) | \psi(t) \rangle &= \left\langle \psi(t) \left| \frac{\partial H}{\partial t} \right| \psi(t) \right\rangle \\ &= \sum_{\mu} \frac{dQ_{\mu}^{ext}}{dt} \left\langle \psi(t) \left| \sum_i F_{\mu}^{ipm}(\mathbf{r}_i, \mathbf{p}_i) \right| \psi(t) \right\rangle \\ &\quad + \sum_{\mu} \frac{dQ_{\mu}}{dt} \left\langle \psi(t) \left| \frac{\partial H_{sp}}{\partial Q_{\mu}} \right| \psi(t) \right\rangle\end{aligned}\quad (27)$$

Harmonic Vibrations in the Random Phase Approximation

RPA Response to an External Field

- Putting these two equations together we see that equation 9 (8.4.9) is still true even with the external field.
- After some computation it can be shown that

$$\left\langle \psi(t) \left| \sum_i F_{\mu}^{ipm}(\mathbf{r}_i, \mathbf{p}_i) \right| \psi(t) \right\rangle = \left\langle gs \left| \sum_i F_{\mu}^{ipm}(\mathbf{r}_i, \mathbf{p}_i) \right| gs \right\rangle - \sum_{\nu} \int_{-\infty}^{\infty} dt' \tilde{\chi}_{\mu\nu}^{RPA}(t-t') (Q_{\nu}^{ext}(t') + \sum_{\sigma} (\kappa^{-1})_{\nu\sigma} \langle gs | F_{\sigma} | gs \rangle), \quad (28)$$

which shows the RPA response tensor to be

$$\tilde{\chi}_{\mu\nu}^{RPA}(t) = \frac{1}{2\omega} \int d\omega e^{-i\omega t} \chi_{\mu\nu}^{RPA}(\omega) \quad (29)$$

$$\tilde{\chi}_{\mu\nu}^{RPA}(\omega) = \sum_{\rho\lambda} \kappa_{\mu\lambda} [\kappa + \chi^{ipm}(\omega)]_{\lambda\rho}^{-1} \chi_{\rho\nu}^{ipm}(\omega). \quad (30)$$

Harmonic Vibrations in the Random Phase Approximation

RPA Response to an External Field

- This RPA response tensor describes the total force on the external field due to the nucleons' rearrangement.
- Analogous to dielectric theory in E&M
 - $Q^{ext} \rightarrow D$
 - $Q - Q^0 \rightarrow P$
 - $Q + Q^{ext} \rightarrow E$
- So the polarization (response) tensor, which is proportional to the matrix in equation 17 whose determinant is zero, which implies that $\chi_{\mu\nu}^{RPA}$ has poles at ω_n .

$$\chi_{\mu\nu}^{RPA}(\omega) = \sum_n \left[\frac{P}{\omega_n - \omega} - i\pi\delta(\omega_n - \omega) \right] \quad (31)$$

$$D_{\mu\nu}^n = -\lim_{\epsilon \rightarrow 0} \epsilon \sum_{\rho\lambda} [\kappa + \chi^{ipm}(\omega_n + \epsilon)]_{\lambda\rho}^{-1} \chi_{\rho\nu}^{ipm}(\omega_n) \quad (32)$$

Harmonic Vibrations in the Random Phase Approximation

RPA Response to an External Field

- Simplifying to one variable to analyze the nature of the singularities, we get

$$D^n = \frac{\kappa^2}{\partial \chi^{ipm'}/\partial \omega} \Big|_{\omega_n}, \quad (33)$$

where D^n tells how easy it is to excite the nucleus with an external field of ω_n .

- He says that, from figure 8.4, these are the eigenfrequencies that lie farthest from the ipm excited energies. The states are the states when the external field acts on all particles equally, and are called “collective” states.

Harmonic Vibrations in the Random Phase Approximation

Vibrational Parameters: the Coupling Constant and the Sum Rule

- An important step in calculating the collective vibrational motion of nuclei is to determine the Q 's and the associated form factors,

$$F_{\mu}^{sp} = \left. \frac{\partial H^{sp}}{\partial Q_{\mu}} \right|_{Q_{\alpha}=Q_{\alpha}^0} \quad (34)$$

- To do this we need to know the Hamiltonian and associated states and energies, $H_0^{sp} |k\rangle = \hat{\varepsilon}_k |k\rangle$.
- One way to do this is to calculate κ using the definition.

$$\kappa_{\mu\nu} \equiv - \left\langle gs \left| \left. \frac{\partial^2 H_{sp}}{\partial Q_{\mu} \partial Q_{\nu}} \right|_{Q_{\alpha}=Q_{\alpha}^0} \right| gs \right\rangle \quad (35)$$

Harmonic Vibrations in the Random Phase Approximation

Vibrational Parameters: the Coupling Constant and the Sum Rule

- Now, like Bohr and Mottelson, let's use the ipm potential (8.3.1), and look at vibrations about a spherical equilibrium to obtain an estimate of the coupling constant in 8.4.20.

$$\kappa_l = -R(A)^2 \int_0^{\infty} dr r^2 \hat{n}(r) \left(\frac{\partial^2 \hat{U}}{\partial r^2} + \frac{2}{R(A)} \frac{\partial \hat{U}}{\partial r} \right) \quad (36)$$

$$\approx -R(A)^2 \int_0^{\infty} dr r^2 \hat{n}(r) \left(\frac{\partial^2 \hat{U}}{\partial r^2} + \frac{2}{r} \frac{\partial \hat{U}}{\partial r} \right) \quad (37)$$

$$= \frac{R(A)^2}{4\pi} \int d^3 \mathbf{r} \nabla \hat{n}(\mathbf{r}) \cdot \nabla \hat{U}(\mathbf{r}) \quad (38)$$

- It turns out that κ is very sensitive to the choice of $H^{sp}(Q)$, and requires a second order approximation, whereas F_{μ}^{sp} only requires a first order approximation.

Harmonic Vibrations in the Random Phase Approximation

Vibrational Parameters: the Coupling Constant and the Sum Rule

- 8.4.20 was a second order approximation. There is another way to calculate $\kappa_{\mu\nu}$ that only requires first order variables.
- This method involves determining the shape of the potential from the density, as we did before.
- First, given a density distribution due to vibrational motion, we calculate the mean value of F_μ^{sp} and the parameters $Q_\mu - Q_\mu^0$. We can then use equation 8.4.12 to first order to get

$$\kappa_{\mu\nu} = \frac{\partial}{\partial Q_\nu} \langle \{Q_\alpha\} | \sum_i F_\mu^{sp} | \{Q_\alpha\} \rangle |_{Q_\alpha^0} \quad (39)$$

Harmonic Vibrations in the Random Phase Approximation

Vibrational Parameters: the Coupling Constant and the Sum Rule

- Let's apply this to a deformed Woods-Saxon potential. Use equations 5.3.1 to describe the deformation in both $\hat{U}(\mathbf{r})$ and the density $\hat{n}(\mathbf{r})$.
- Assuming that $F_{\mu\nu}$ is real tells us that $m = 0$. Also note that F_{l0}^{ipm} is proportional to $Y_l^0(\theta, \phi)$ (8.4.38), so the only part of the density that contributes to the expectation value is the part with the same angular dependence,

$$\delta n_{l0}(\mathbf{r}) = -\alpha_{l0} Y_l^0(\theta, \phi) R(A) \frac{\partial}{\partial r} \hat{n}(\mathbf{r}) \quad (40)$$

- Now using equations 8.3.2 and 8.4.39 we get

$$\kappa_l = \frac{\partial}{\partial \alpha_{l0}} \int_0^\infty f^2 dr \frac{\partial \hat{U}}{\partial r} \frac{\partial \hat{n}}{\partial r} \cdot \int d\Omega Y_l^0(\theta, \phi)^2 \alpha_{l0} R(A)^2, \quad (41)$$

which is the same as equation 8.4.37 (which was second order).

Harmonic Vibrations in the Random Phase Approximation

Vibrational Parameters: the Coupling Constant and the Sum Rule

- Now we define a quantity called the energy-weighted sum rule,

$$S_{\mu\nu} = \frac{1}{2} \left\langle gs \left| \left[\sum_i F_{\mu}^{sp}, \left[H_{sp}(\{Q_{\alpha}^0\}), \sum_i F_{\nu}^{sp} \right] \right] \right| gs \right\rangle \quad (42)$$

$$= \sum_n (E_n - E_0) \left\langle gs \left| \sum_i F_{\mu}^{sp} \right| n \right\rangle \left\langle n \left| \sum_i F_{\nu}^{sp} \right| gs \right\rangle. \quad (43)$$

- Comparing this with equation 8.1.24 we can write this as

$$S_{\mu\nu} = \frac{\hbar^2}{2\pi} \int_{-\infty}^{\infty} d\omega \chi_{\mu\nu}^{ipm''}(\omega) \cdot \omega. \quad (44)$$

Harmonic Vibrations in the Random Phase Approximation

Vibrational Parameters: the Coupling Constant and the Sum Rule

- From the hamiltonian from the RPA (8.4.11)

$$H_{sp}^{RPA} \approx \sum_i H_0^{sp}(\mathbf{r}_i, \mathbf{p}_i) + \sum_\mu (Q_\mu - Q_\mu^0) \sum_i F_\mu^{sp}(\mathbf{r}_i, \mathbf{p}_i, \{Q_\alpha^0\}) \\ - \frac{1}{2} \sum_{\mu\nu} \kappa_{\mu\nu} (Q_\mu - Q_\mu^0)(Q_\nu - Q_\nu^0) \quad (45)$$

we see that the commutator in $S_{\mu\nu}$ would be the same wether we use $H_{sp}(\{Q_\alpha\})$ or $H_{sp}(\{Q_\alpha^0\})$, and thus we can write

$$S_{\mu\nu} = \frac{\hbar^2}{2\pi} \int_{-\infty}^{\infty} d\omega \chi_{\mu\nu}^{RPA''}(\omega) \cdot \omega \quad (46)$$

$$= \hbar^2 \sum_{\omega_n > 0} D_{\mu\nu}^n \cdot \omega_n \quad (47)$$

Harmonic Vibrations in the Random Phase Approximation

Vibrational Parameters: the Coupling Constant and the Sum Rule

- S is interesting because it only depends on the nuclear ground state, F_{μ}^{sp} and H_{sp} , and the right-hand side depends on the individual RPA vibrational solutions. Thus when you only know some of these, you can use it to deduce if the rest are “collective” (contribute) or not.
- From the inverse FT we can write

$$S_{\mu\nu} = \hbar^2 \frac{d}{dt} \tilde{\chi}_{\mu\nu}^{RPA}(t) \Big|_{t=0} = \hbar^2 \frac{d}{dt} \tilde{\chi}_{\mu\nu}^{ipm}(t) \Big|_{t=0}. \quad (48)$$

- From this we can see that $S_{\mu\nu}$ represents the short-time behavior of the response function $\tilde{\chi}_{\mu\nu}$ and that it's the same for ipm and RPA.
- Meaning that the interactions of the field only affect the long-time behavior of the response.