Excitations

RPA theory

Summary

- ❑ RPA theory (random-phase approximation)
    - ❑ Equations of motion for the harmonic oscillator
    - ❑ Theories of excitations in Fermion systems
    - ❑ RPA theory
    - ❑ Properties of the RPA solutions

- ❑ The schematic RPA model
    - ❑ Graphical solution
    - ❑ Fully degenerate case

❑ RPA theory

Random-phase approximation (historical name!)
Improves on TD theory
Sum rules
More sophisticated ground state

❑ 'Equations of motion' for the harmonic oscillator

Creation-annihilation operators for phonons: $O_\lambda^+ ,\ O_\lambda$

$$H = \sum_\lambda \hbar\omega_\lambda O_\lambda^+ O_\lambda$$

Bosonic commutator $[O_k, O_\lambda^+] = \delta_{k\lambda}, \qquad [O_k, O_\lambda] = 0, \qquad [O_k^+, O_\lambda^+] = 0$

Operator equation $\boxed{[H, O_\lambda^+] = \hbar\omega_\lambda O_\lambda^+}$ Determines the full spectrum!

Vacuum for phonons $|0\rangle$ $\qquad H|0\rangle = E_0|0\rangle$

λ phonon $O_\lambda^+|0\rangle$ $\qquad HO_\lambda^+|0\rangle = \left(O_\lambda^+ H + \hbar\omega_\lambda O_\lambda^+\right)|0\rangle = (E_0 + \hbar\omega_\lambda)O_\lambda^+|0\rangle$

condition of phonon vacuum $\qquad O_\lambda|0\rangle = 0, \quad \forall\lambda$

$$[H, O_\lambda^+] = \hbar\omega_\lambda O_\lambda^+ \quad \Rightarrow \quad [\underset{\substack{\uparrow \\ \text{variation}}}{\delta} O_\lambda, [H, O_\lambda^+]] = \hbar\omega_\lambda [\delta O_\lambda, O_\lambda^+]$$

Define the symmetrized double commutator

$$[\delta O_\lambda, H, O_\lambda^+] \equiv \frac{1}{2}\left\{ \left[[\delta O_\lambda, H], O_\lambda^+\right] + \left[\delta O_\lambda, [H, O_\lambda^+]\right] \right\}$$

Using results (exercise)

$$\left[[\delta O_\lambda, H], O_\lambda^+\right] = \left[\delta O_\lambda, [H, O_\lambda^+]\right] + \left[[\delta O_\lambda, O_\lambda^+], H\right]$$

$$\langle 0| \left[[\delta O_\lambda, H], O_\lambda^+\right] |0\rangle = \langle 0| \left[\delta O_\lambda, [H, O_\lambda^+]\right] |0\rangle + \underbrace{\langle 0| \left[[\delta O_\lambda, O_\lambda^+], H\right] |0\rangle}_{i\hbar \frac{\partial}{\partial t} \langle 0|[\delta O_\lambda, O_\lambda^+]|0\rangle = 0}$$

We get to

$$[\delta O_\lambda, [H, O_\lambda^+]] = \hbar\omega_\lambda [\delta O_\lambda, O_\lambda^+] \quad \Rightarrow \quad \boxed{\langle 0|[\delta O_\lambda, H, O_\lambda^+]|0\rangle = \hbar\omega_\lambda \langle 0|[\delta O_\lambda, O_\lambda^+]|0\rangle}$$

Equations of motion

❑ Theories of excitations for Fermion systems

Bosonic excitations
Based on the equations of motion of the harmonic oscillator

$$\langle\phi|[\delta O_\lambda, H, O_\lambda^+]|\phi\rangle = \hbar\omega_\lambda\langle\phi|[\delta O_\lambda, O_\lambda^+]|\phi\rangle$$

Approximation for the ground state of the Fermions,
Vacuum of boson-type excitations

Creation of boson-type excitation λ

variation

This scheme recovers TD for

$|\phi\rangle = |v\rangle$ of HF

$$O_\lambda^+ = \sum_{nj} Y_{nj}(\lambda) a_n^+ a_j$$

$$\delta O_\lambda = \{a_i^+ a_m,\ \forall mi\}$$

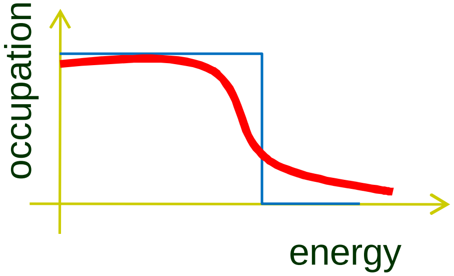
$$\sum_{nj}\langle v|[a_i^+ a_m, H, a_n^+ a_j]v\rangle Y_{nj}(\lambda) = \hbar\omega_\lambda \sum_{nj}\langle v|[a_i^+ a_m, a_n^+ a_j]|v\rangle Y_{nj}(\lambda)$$

$$\Downarrow$$

$$\sum_{nj}\left(\delta_{mn}\delta_{ij}\varepsilon_{mi} + \hat{v}_{mjin}\right)\ Y_{nj}(\omega) = \hbar\omega\ Y_{mi}(\omega)$$

❑ The RPA

Eq. of motion $\langle\phi|[\delta O_\lambda, H, O_\lambda^+]|\phi\rangle = \hbar\omega_\lambda\langle\phi|[\delta O_\lambda, O_\lambda^+]|\phi\rangle$



$$\left\{\begin{aligned}
&|\phi\rangle = |v\rangle \\
&O_\lambda^+ = \sum_{nj} Y_{nj}(\lambda)\; a_n^+ a_j - \underbrace{Z_{nj}(\lambda)\; a_j^+ a_n}_{} \\
&\delta O_\lambda = \{a_i^+ a_m \;\forall mi, \quad a_m^+ a_i \;\forall mi\}
\end{aligned}\right.$$

Annihilates over F and creates below F.
Correlations in reference state

$$\sum_{nj}\langle v|[a_i^+ a_m, H, a_n^+ a_j]|v\rangle Y_{nj} - \langle v|[a_i^+ a_m, H, a_j^+ a_n]|v\rangle Z_{nj} = \hbar\omega_\lambda \sum_{nj}\langle v|[a_i^+ a_m, a_n^+ a_j]|v\rangle Y_{nj} - \langle v|[a_i^+ a_m, a_j^+ a_n]|v\rangle Z_{nj}$$

$$\sum_{nj}\langle v|[a_m^+ a_i, H, a_n^+ a_j]|v\rangle Y_{nj} - \langle v|[a_m^+ a_i, H, a_j^+ a_n]|v\rangle Z_{nj} = \hbar\omega_\lambda \sum_{nj}\langle v|[a_m^+ a_i, a_n^+ a_j]|v\rangle Y_{nj} - \langle v|[a_m^+ a_i, a_j^+ a_n]|v\rangle Z_{nj}$$

We can rewrite

$$\boxed{\begin{aligned}\sum_{nj}\left(A_{mi,nj}Y_{nj}+B_{mi,nj}Z_{nj}\right) &= \hbar\omega_\lambda Y_{mi}\\ \sum_{nj}\left(B^*_{mi,nj}Y_{nj}+A^*_{mi,nj}Z_{nj}\right) &= -\hbar\omega_\lambda Z_{mi}\end{aligned}}$$

$$\begin{aligned}A_{mi,nj} &= \langle v|[a_i^+a_m, H, a_n^+a_j]|v\rangle &&= \delta_{mn}\delta_{ij}\varepsilon_{mi} + \overset{\overset{v_{mjin}-v_{mjni}}{\nearrow}}{\hat{v}_{mjin}}\\ B_{mi,nj} &= -\langle v|[a_i^+a_m, H, a_j^+a_n]|v\rangle &&= \underset{\underset{v_{mnij}-v_{mnji}}{\searrow}}{\hat{v}_{mnij}}\end{aligned}$$

Symmetries:

$$\begin{aligned}A_{mi,nj} &= A^*_{nj,mi} && \text{Hermitian}\\ B_{mi,nj} &= B_{nj,mi} && \text{symmetric}\end{aligned}$$

The RPA eigenvalue problem

$$\left(\begin{array}{cc} \left(\begin{array}{cc} A_{m_1i_1,m_1i_1} & \cdots \\ \cdots & \cdots \end{array}\right) & \left(\begin{array}{cc} B_{m_1i_1,m_1i_1} & \cdots \\ \cdots & \cdots \end{array}\right) \\ -\left(\begin{array}{cc} B^*_{m_1i_1,m_1i_1} & \cdots \\ \cdots & \cdots \end{array}\right) & -\left(\begin{array}{cc} A^*_{m_1i_1,m_1i_1} & \cdots \\ \cdots & \cdots \end{array}\right) \end{array}\right)\left(\begin{array}{c} Y_1(\lambda) \\ \cdots \\ Z_1(\lambda) \\ \cdots \end{array}\right) = \hbar\omega_\lambda \left(\begin{array}{c} Y_1(\lambda) \\ \cdots \\ Z_1(\lambda) \\ \cdots \end{array}\right)$$

$$\left(\begin{array}{cc} A & B \\ -B^* & -A^* \end{array}\right)\left(\begin{array}{c} Y(\lambda) \\ Z(\lambda) \end{array}\right) = \hbar\omega_\lambda \left(\begin{array}{c} Y(\lambda) \\ Z(\lambda) \end{array}\right)$$

non Hermitian matrix
Not guaranteed that eigenvalues are always real
Instability
For B=0 we recover Tamm-Dancoff

❑ Properties of RPA solutions

(i) Solutions come in pairs

$$\begin{pmatrix} Y \\ Z \end{pmatrix}, \ \hbar\omega \quad \Leftrightarrow \quad \begin{pmatrix} Z^* \\ Y^* \end{pmatrix}, \ -\hbar\omega$$

$$\begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix}\begin{pmatrix} Y \\ Z \end{pmatrix} = \hbar\omega\begin{pmatrix} Y \\ Z \end{pmatrix} \quad \Leftrightarrow \quad \begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix}\begin{pmatrix} Z^* \\ Y^* \end{pmatrix} = -\hbar\omega\begin{pmatrix} Z^* \\ Y^* \end{pmatrix}$$

'Mathematical' property
Physically meaningful only those solutions with $\hbar\omega \geq 0$

(ii) Orthogonality and normalization

$$\begin{pmatrix} Y(\lambda) \\ Z(\lambda) \end{pmatrix}, \ \hbar\omega_\lambda \qquad \begin{pmatrix} Y(k) \\ Z(k) \end{pmatrix}, \ \hbar\omega_k$$

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} Y(\lambda) \\ Z(\lambda) \end{pmatrix} = \hbar\omega_\lambda \begin{pmatrix} Y(\lambda) \\ -Z(\lambda) \end{pmatrix}$$

$$\begin{pmatrix} Y^*(k) & Z^*(k) \end{pmatrix} \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} = \hbar\omega_k \begin{pmatrix} Y^*(k) & -Z^*(k) \end{pmatrix}$$

Row vector

$$\Downarrow$$

$$0 = [\hbar\omega_k - \hbar\omega_\lambda] \begin{pmatrix} Y^*(k) & -Z^*(k) \end{pmatrix} \begin{pmatrix} Y(\lambda) \\ Z(\lambda) \end{pmatrix}$$

$$\sum_{mi} [\, Y^*_{mi}(k) Y_{mi}(\lambda) - Z^*_{mi}(k) Z_{mi}(\lambda) \,] = \delta_{k\lambda}$$

(iii) Quasi-boson behavior of excitations

$$O_\lambda^+ = \sum_{nj} Y_{nj}(\lambda)\; a_n^+ a_j - Z_{nj}(\lambda)\; a_j^+ a_n \qquad O_k^+ = \sum_{nj} Y_{nj}(k)\; a_n^+ a_j - Z_{nj}(k)\; a_j^+ a_n$$

$$\langle v|[O_k, O_\lambda^+]|v\rangle = \begin{pmatrix} Y^*(k) & -Z^*(k) \end{pmatrix} \begin{pmatrix} Y(\lambda) \\ Z(\lambda) \end{pmatrix} = \delta_{k\lambda}$$

$$\langle v|[O_k^+, O_\lambda^+]|v\rangle = \begin{pmatrix} -Y^*(-k) & Z^*(-k) \end{pmatrix} \begin{pmatrix} Y(\lambda) \\ Z(\lambda) \end{pmatrix} = 0$$

$$\langle v|[O_k, O_\lambda]|v\rangle = 0$$

The RPA ground state $|v_{\rm RPA}\rangle$

Excitations $|\lambda\rangle = O_\lambda^+|v_{\rm RPA}\rangle$

Vacuum condition $O_\lambda|v_{\rm RPA}\rangle = 0 \quad \forall\lambda$

Orthonormalization

$$\langle k|\lambda\rangle = \langle v_{\rm RPA}|O_k O_\lambda^+|v_{\rm RPA}\rangle = \langle v_{\rm RPA}|[O_k, O_\lambda^+]|v_{\rm RPA}\rangle \approx \langle v|[O_k, O_\lambda^+]]|v\rangle = \delta_{k\lambda}$$

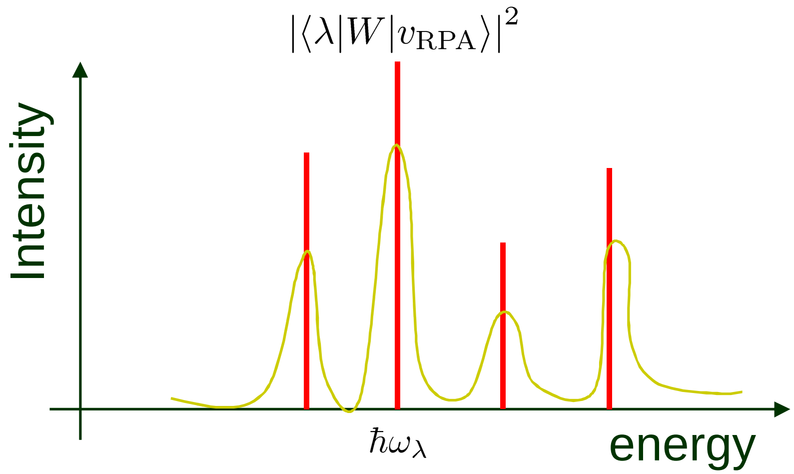
(iii) Transition matrix elements

1-body operator $W = \sum_{\alpha\beta} w_{\alpha\beta} a_\alpha^+ a_\beta$

$$\langle \lambda | W | v_{\rm RPA} \rangle = \langle v_{\rm RPA} | O_\lambda W | v_{\rm RPA} \rangle = \langle v_{\rm RPA} | [O_\lambda, W] | v_{\rm RPA} \rangle$$

$$\approx \langle v | [O_\lambda, W] | v \rangle = \sum_{mi} (Y_{mi}^* w_{mi} + Z_{mi}^* w_{im})$$

Spectra (absorption)



❑ Schematic RPA model

Separable interaction

1st quant. $$V = -\chi \sum_{i,j=1}^{N} Q(i)Q(j)$$

RPA Eq. $$\left\{ \begin{array}{rcl} AY + BZ & = & \hbar\omega Y \\ -B^*Y - A^*Z & = & \hbar\omega Z \end{array} \right.$$ with $$\left\{ \begin{array}{ll} A_{mi,nj} & = \delta_{mn}\delta_{ij}\varepsilon_{mi} + \hat{v}_{mjin} \\ B_{mi,nj} & = \hat{v}_{mnij} \end{array} \right.$$

Approximate $$\begin{array}{rcl} \hat{v}_{mjin} & \approx & v_{mjin} = -\chi\, Q_{mi}\, Q^*_{nj} \\ \hat{v}_{mnij} & \approx & v_{mnij} = -\chi\, Q_{mi}\, Q_{nj} \end{array}$$

➡ $$\left\{ \begin{array}{rcl} (\varepsilon_{mi} - \hbar\omega)Y_{mi} - \chi\, Q_{mi} \sum_{nj} \left(Q^*_{nj}Y_{nj} + Q_{nj}Z_{nj}\right) & = & 0 \\ (\varepsilon_{mi} + \hbar\omega)Z_{mi} - \chi\, Q^*_{mi} \sum_{nj} \left(Q^*_{nj}Y_{nj} + Q_{nj}Z_{nj}\right) & = & 0 \end{array} \right.$$

Define
$$\mathcal{N} = \chi \sum_{nj} \left(Q^*_{nj}\, Y_{nj} + Q_{nj}\, Z_{nj} \right)$$

$$\left\{ \begin{array}{rcl} (\varepsilon_{mi} - \hbar\omega) Y_{mi} - \chi\, Q_{mi} \sum_{nj} \left(Q^*_{nj} Y_{nj} + Q_{nj} Z_{nj} \right) & = & 0 \\ (\varepsilon_{mi} + \hbar\omega) Z_{mi} - \chi\, Q^*_{mi} \sum_{nj} \left(Q^*_{nj} Y_{nj} + Q_{nj} Z_{nj} \right) & = & 0 \end{array} \right. \Rightarrow \left\{ \begin{array}{rcl} Y_{mi} & = & \dfrac{\mathcal{N} Q_{mi}}{\varepsilon_{mi} - \hbar\omega} \\ Z_{mi} & = & \dfrac{\mathcal{N} Q^*_{mi}}{\varepsilon_{mi} + \hbar\omega} \end{array} \right.$$

Normalization
$$\sum_{mi} \left(|Y_{mi}|^2 - |Z_{mi}|^2 \right) = 1$$

Trascendent equation
$$\mathcal{N} = \chi \sum_{nj} \left(\frac{Q^*_{nj} \mathcal{N} Q_{nj}}{\varepsilon_{nj} - \hbar\omega} + \frac{Q^*_{nj} \mathcal{N} Q_{nj}}{\varepsilon_{nj} + \hbar\omega} \right)$$

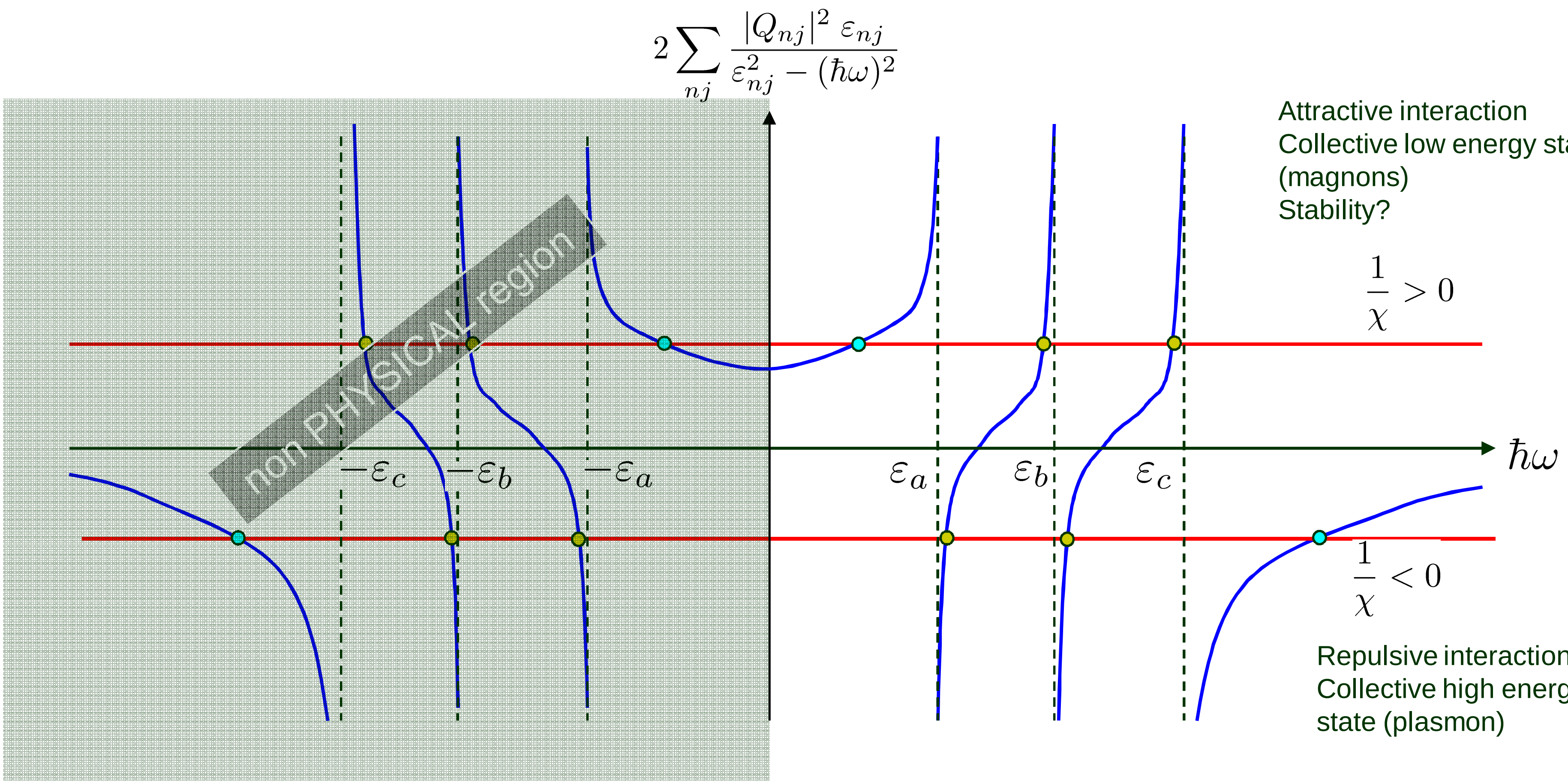
$$\boxed{2 \sum_{nj} \frac{|Q_{nj}|^2\, \varepsilon_{nj}}{\varepsilon^2_{nj} - (\hbar\omega)^2} = \frac{1}{\chi}}$$

Equation fixing the excitation energy $\hbar\omega$

The graphical resolution

Assume for simplicity there are only 3ph pairs $\{\varepsilon_{nj}\} = \{\varepsilon_a, \varepsilon_b, \varepsilon_c\}$

$$2\sum_{nj} \frac{|Q_{nj}|^2\ \varepsilon_{nj}}{\varepsilon_{nj}^2 - (\hbar\omega)^2} = \frac{1}{\chi}$$

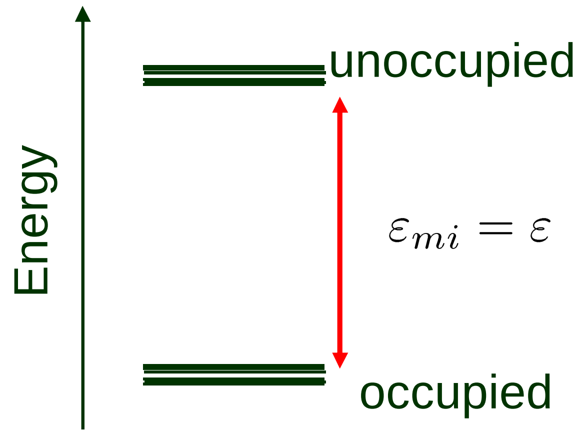


Attractive interaction
Collective low energy state
(magnons)
Stability?

Repulsive interaction
Collective high energy
state (plasmon)

Fully degenerate case

HF levels



$$\varepsilon_{mi} = \varepsilon \quad \forall mi$$

$$2\sum_{nj}\frac{|Q_{nj}|^2\,\varepsilon_{nj}}{\varepsilon_{nj}^2-(\hbar\omega)^2}=\frac{1}{\chi}$$ ⇒ $$(\hbar\omega)^2=\varepsilon^2-2\,\chi\,\varepsilon\sum_{nj}|Q_{nj}|^2$$

Attractive int.
$\chi > 0 \Rightarrow \hbar\omega < \varepsilon$

Repulsive int.
$\chi < 0 \Rightarrow \hbar\omega > \varepsilon$

(Tamm-Dancoff) ⇒ $$(\hbar\omega)^2=\varepsilon^2-2\,\chi\,\varepsilon\sum_{nj}|Q_{nj}|^2+\chi^2\left(\sum_{nj}|Q_{nj}|^2\right)^2$$

In the schematic model we find $\hbar\omega_{\mathrm{RPA}} < \hbar\omega_{\mathrm{TD}}$