Linear Response Theory

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1 Time Dependent Hartree-Fock Theory

1.1 The TDHF Equations

We start with an arbitrary wave packet $|\Psi(0)\rangle$. Its exact time evolution is given by

$$|\Psi(t)\rangle = \exp(-i\hat{H}t)|\Psi(0)\rangle \tag{1}$$

and its one-body density at time t is given by

$$\rho_{kl}(t) = \langle\Psi(t)|c_l^\dagger c_k|\Psi(t)\rangle. \tag{2}$$

To obtain an equation of motion, we calculate its time derivative:

$$i\dot{\rho}_{kl}(t) = \langle\Psi(t)|\left[c_l^\dagger c_k, \hat{H}\right]|\Psi(t)\rangle. \tag{3}$$

In the next step we assume, that $|\Psi(0)\rangle = |\Phi(0)\rangle$ is a Slater and that $|\Psi(t)\rangle = |\Phi(t)\rangle = |t\rangle$ stays at all times a Slater determinant. In this case we can apply the Wick theorem at each time. For a two-body Hamiltonian

$$\hat{H} = \hat{T} + \hat{V} = \sum_{pp'} t_{kk'} c_k^\dagger c_{k'} + \frac{1}{4}\sum_{pp'qq'} \bar{v}_{pp'qq'} c_p^\dagger c_{p'}^\dagger c_{q'} c_q \tag{4}$$

we find

$$\langle t|\left[c_l^\dagger c_k, \hat{T}\right]|t\rangle = (t\rho - \rho t)_{kl} = [t,\rho]_{kl}\,, \tag{5}$$

and in the same way we find

$$\langle t|\left[c_l^\dagger c_k, \hat{V}\right]|t\rangle = (\Gamma\rho - \rho\Gamma)_{kl} = [\Gamma,\rho]_{kl}\,, \tag{6}$$

where $\Gamma_{kl} = \sum \bar{v}_{kl'lk'}\rho_{k'l'}$. We find

$$i\dot{\rho} = [h,\rho]\,. \tag{7}$$

with $h = t + \Gamma$. It is a non-linear matrix equation for the one-body density matrix ρ and a first-order differential equation in time. Starting with an initial condition $\rho(0)$, it defines $\rho(t)$ for all times.

In the case of an external field $\hat{F}(t) = \sum_{kl} f_{kl}(t) c_k^\dagger c_l$, we find

$$i\dot{\rho} = [h + f(t), \rho]\,. \tag{8}$$

In *coordinate space* (it is obvious how to also include spin and isospin variables) with a spin independent tow-body potential $v(\mathbf{r}, \mathbf{r}')$ the TDHF equation (7) has the form

$$i\hbar\dot{\rho}(\mathbf{r}, \mathbf{r}', t) = -\frac{1}{2m}(\Delta_{\mathbf{r}} - \Delta_{\mathbf{r}'})\rho(\mathbf{r}, \mathbf{r}', t) + (\Gamma_H(\mathbf{r}, t) - \Gamma_H(\mathbf{r}', t))\rho(\mathbf{r}, \mathbf{r}', t) \tag{9}$$

$$+ \int d^3r'' \left(\Gamma_{Ex}(\mathbf{r}, \mathbf{r}'', t)\rho(\mathbf{r}'', \mathbf{r}', t) - \Gamma_{Ex}(\mathbf{r}'', \mathbf{r}, t)\rho(\mathbf{r}, \mathbf{r}'', t)\right)\,, \tag{10}$$

where Γ_H and Γ_{Ex} have the same form as in the static case, but now they depend on time-dependent densities. This is a relatively complicated equation. It is much easier to solve it by decomposing the density matrix into single particle wave functions. From the fact that the wave function $|\Phi(t)\rangle$ is a Slater determinant for all times, we have $\rho^2(t) = \rho(t)$ for all times and we can diagonalize $\rho(t)$ at each time

$$\rho(t) = \sum_{i=1}^{A} |\varphi_i\rangle\langle\varphi_i|. \tag{11}$$

Starting from the eigenfunctions of $\rho(0)$ we can solve A time dependent coupled equations

$$i|\dot{\varphi}_i\rangle = h(\rho)|\varphi_i\rangle \qquad \text{for } i = 1, \ldots A \tag{12}$$

and obtain

$$\rho(t) = \sum_{i=1}^{A} |\varphi_i(t)\rangle\langle\varphi_i(t)| \tag{13}$$

We find

$$i\dot{\rho} = i\sum_i |\dot{\varphi}_i\rangle\langle\varphi_i| + |\varphi_i\rangle\langle\dot{\varphi}_i| = \sum_i h|\varphi_i\rangle\langle\varphi_i| - |\varphi_i\rangle\langle\varphi_i|h = [h, \rho] \tag{14}$$

This form of the the solution of the TDHF equation is easier to handle for practical calculations, because it is simpler to solve A differential equations

depending on four coordinates ($\mathbf{r}$,t) than one differential equation depending on seven coordinates ($\mathbf{r}, \mathbf{r}', t$) as in Eq. (9).

Before we discuss the properties of the TDHF equations, we should mention that it can also be derived from a *time-dependent variational principle*. The Lagrangian is defined as

$$\mathcal{L} = \langle \Phi(t) | i\partial_t - \hat{H} | \Phi(t) \rangle. \tag{15}$$

Under the assumption that $|\Phi(t)\rangle$ is a Slater determinant of the single particle wave functions ($\varphi_1(\mathbf{r},t), \ldots, \varphi_A(\mathbf{r},t)$), $\mathcal{L}$ is a functional of the $2A$ independent variables $\varphi_1(\mathbf{r},t)$ and $\varphi_1^*(\mathbf{r},t)$. Using them as classical field variables, we can define an action

$$I_{12} = \int_{t_1}^{t_2} \mathcal{L}[\varphi, \varphi^*] dt \tag{16}$$

with fixed endpoints 1 and 2. The Hamiltonian variational principle

$$\delta I_{12} = 0 \tag{17}$$

with independent variation of φ_i and φ_i^* gives the equations of motion (12)

1.2 Conservation laws

1.2.1 Conservation of Product Character.

In the last section we assumed that the wave function $|\Phi(t)\rangle$ is a Slater determinant for all times and under this condition we derived the TDHF equation (7). Therefore, the first thing we have to show is that the theory is consistent, that is, if we start with a density of a Slater determinant ($\rho^2(0) = \rho(0)$) this property is conserved for all times:

$$i\hbar\partial_t(\rho^2 - \rho) = i\hbar(\dot{\rho}\rho + \rho\dot{\rho} - \dot{\rho}) = [h, \rho^2 - \rho] = 0. \tag{18}$$

This shows that, if $\rho(t)^2 - \rho(t) = 0$ at one time, it also vanishes for the next time step

$$\rho^2(t + dt) - \rho(t + dt) = \rho(t)^2 - \rho(t) + \partial_t(\rho^2 - \rho)dt. \tag{19}$$

The solution $|\Phi(t)\rangle$ of the TDHF equation therefore corresponds to a *trajectory* on the energy surface.

1.2.2 Conservation of Orthogonality

Closely connected to the property just discussed is the fact that single-particle wave functions $\varphi_i(\mathbf{r}, t)$ stay orthogonal for all times:

$$i\frac{d}{dt}\langle\varphi_i|\varphi_{i'}\rangle = \langle\varphi_i|h - h^\dagger|\varphi_{i'}\rangle = 0. \tag{20}$$

1.2.3 Conservation of Expectation Values of Symmetry Operators

For an arbitrary, time-independent, single particle operator $\hat{F} = \sum_{kl} f_{kl} c_k^\dagger c_l$, we obtain for the expectation values in the state $|\Phi(t)\rangle$

$$i\frac{d}{dt}\langle\hat{F}\rangle = i\hbar\mathrm{Tr}\left(f\dot{\rho}\right) = \mathrm{Tr}\left(f[h,\rho]\right)$$

or

$$i\frac{d}{dt}\langle\hat{F}\rangle = \langle[F,H]\rangle, \tag{21}$$

where the last expectation value was evaluated using Wick's theorem. There we find, that all symmetries of the Hamiltonian are conserved, at least on the average. Examples are

$$\text{(i) the particle number} \qquad (d/dt)\langle\hat{N}\rangle = \mathrm{Tr}(\dot{\rho}) = 0, \tag{22}$$

$$\text{(ii) the total linear momentum} \qquad (d/dt)\langle\hat{\mathbf{P}}\rangle = 0, \tag{23}$$

$$\text{(iii) the total angular momentum} \qquad (d/dt)\langle\hat{\mathbf{J}}\rangle = 0, \tag{24}$$

However, this does not mean that $|\Phi(t)\rangle$ has to be an eigenstate of these symmetry operators. Any localized density distribution $\rho(t)$, for instance, violates translational invariance.

Furthermore, for velocity independent forces we gt for the center of mass $\mathbf{R} = 1/A\sum \mathbf{r}_i$

$$\frac{d}{dt}\langle\hat{\mathbf{R}}\rangle = \frac{1}{Am}\langle\hat{\mathbf{P}}\rangle. \tag{25}$$

1.2.4 Conservation of Energy.

The derivative of the energy with respect to time can be expressed by the change of density $\dot{\rho}$

$$\frac{d}{dt}\langle\hat{H}\rangle = \frac{d}{dt}E = \sum_{kl}\frac{\partial E}{\partial\rho_{kl}}\dot{\rho}_{kl}.$$

Starting from the Hartree-Fock expression for the energy

$$E = \sum_{kl} t_{kl}\rho_{lk} + \frac{1}{2}\sum_{kl} \rho_{kl}\bar{v}_{lk'kl'}\rho_{l'k'}$$

we obtain

$$h_{kl} = \frac{\partial E}{\partial \rho_{lk}} = t_{kl} + \sum_{kl} \bar{v}_{kk'll'}\rho_{l'k'}$$

and find

$$\frac{d}{dt}\langle \hat{H}\rangle = \mathrm{Tr}(h\dot{\rho}) = -i\mathrm{Tr}(h[h,\rho]) = 0.$$

This means that the energy is conserved with time. The motion therefore has to take place on lines of constant energy in the multidimensional energy surface of Slater determinants. If, therefore, our initial conditions are inside a valley, such that the energy is smaller than the lowest saddle point, we can never leave that valley. The system runs on equipotential lines within the valley.

2 Linear Response Theory

The mean field approximation yields a single particle Hamiltonian and its excitations are multiparticle-multihole excitations. In experimental spectra, however, one has also observed, in particular at low energies, collective excitations, such as vibrations and rotations. In this section we consider vibrational excitations of small amplitude.

We investigate the influence of an external time-dependent field

$$\hat{F}(t) \;=\; \hat{F}e^{-i\omega t} + \hat{F}^{+}e^{i\omega t} \tag{26}$$

on the system.

We assume that $\hat{F}$ is a one-body operator

$$\hat{F}(t) \;=\; \sum_{kl} f_{kl}(t)a_k^{+}a_l, \tag{27}$$

and that the field F is weak, that is, it introduces only small changes of the nuclear density, which we can treat in linear order. We thus study the behavior of a system under the influence of a time-dependent Hamiltonian $\hat{H} + \hat{F}(t)$.

2.1 The Exact Response Function

We start with an exact static solution $|\Psi_0\rangle$ of the system

$$\hat{H}|\Psi_0\rangle \;=\; E|\Psi_0\rangle, \tag{28}$$

When we swich in the external field, the exact wave function changes under the influence of the time evolution operator

$$|\Psi(t)\rangle \;=\; \hat{U}(t)|\Psi_0\rangle, \tag{29}$$

which is determined by the Schrödinger equation

$$i\hbar\frac{d}{dt}\hat{U} \;=\; \left(\hat{H}+\hat{F}(t)\right)\hat{U} \tag{30}$$

For a weak external field $\hat{F}$ it is given in perturbation theory:

$$\hat{U}(t) \;=\; e^{-i\hat{H}t}\left(1-i\int\limits_{-\infty}^{t}dt'\hat{F}_H(t')\right) \tag{31}$$

where the Heisenberg representation $\hat{G}_H$ of any operator $\hat{G}$ is given by

$$\hat{G}_H = \; e^{i\hat{H}t}\hat{G}e^{-i\hat{H}t} \tag{32}$$

We find for the expectation value of an arbitrary operator at the time t

$$\langle\hat{G}\rangle(t) \;=\; \langle\hat{G}\rangle_0 \;-\; i\int\limits_{-\infty}^{t}dt'\left\langle\left[\hat{G}_H(t),\hat{F}_H(t')\right]\right\rangle \tag{33}$$

where $|\rangle$ is the static wave function and $G_0=\langle\hat{G}\rangle$ is the expectation value of $\hat{G}$ in the static case. In particular we have for the density $a_l^+a_k$

$$\rho(t) \;=\; \rho_0 \;+\; \delta\rho(t) \tag{34}$$

where ρ_0 is the static density.

For the transition density we obtain the equation of motion

$$\delta\rho_{kl}(t) \;=\; \sum_{kl}\int\limits_{-\infty}^{\infty}dt'R_{klk'l'}(t-t')f_{k'l'}(t') \tag{35}$$

Here the *response function* R is defined by

$$R_{klk'l'}(t) \;=\; -i\Theta(t)\langle 0|\left[a_l^+(t)a_k(t), a_{k'}^+a_{l'}\right]|0\rangle \tag{36}$$

the time-dependent creation and annihilation operators $a(t), a^+(t)$ are meant to be in the Heisenberg representation. Inserting a complete set of eigenstates of the Hamiltonian H we find after a Fourier transformation

$$R_{klk'l'}(\omega) = \sum_\nu \left\{ \frac{\langle 0|a_l^+a_k|\nu\rangle\langle\nu|a_{k'}^+a_{l'}|0\rangle}{\omega - E_\nu + E_0 + i\eta} - \frac{\langle 0|a_{k'}^+a_{l'}|\nu\rangle\langle\nu|a_l^+a_k|0\rangle}{\omega + E_\nu - E_0 + i\eta} \right\}. \tag{37}$$

So far we are still exact with respect to the many-body Hamiltonian H, we have applied perturbation theory only with respect to the external field. In that sense (37) is the exact *response function of the system.*If we expand the time-dependent wave function $|\Psi(t)\rangle$ in terms of the exact eigenstates $|\nu\rangle$ of the system

$$|\Psi(t)\rangle = |0\rangle + \sum_\nu c_v e^{-iE_vt}|\nu\rangle \tag{38}$$

we find the transition densities of the system

$$\delta\rho_{kl}(t) \;=\; \sum_\nu c_v\langle 0|a_l^+a_k|\nu\rangle e^{-iE_vt} \;+ c_v^*\langle\nu|a_l^+a_k|0\rangle e^{+iE_vt} \tag{39}$$

or introducing

$$\delta\rho_{kl}^{(\nu)} = \langle 0|a_l^+a_k|\nu\rangle \tag{40}$$

we have

$$\delta\rho_{kl}(t) \;=\; \sum_\nu c_v\delta\rho_{kl}^{(\nu)}e^{-iE_vt} \;+ c_v^*\delta\rho_{lk}^{(\nu)*}e^{+iE_vt} \tag{41}$$

and the response function

$$R_{klk'l'}(\omega) = \sum_\nu \left\{ \frac{\delta\rho_{kl}^{(\nu)}\delta\rho_{k'l'}^{(\nu)*}}{\omega - E_\nu + E_0 + i\eta} - \frac{\delta\rho_{l'k'}^{(\nu)}\delta\rho_{lk}^{(\nu)*}}{\omega + E_\nu - E_0 + i\eta} \right\}. \tag{42}$$

2.2 The Free Response

Without residual interaction, the excited states are given by the multi-particle multi-hole excitations and we obtain the free response function

$$R^0_{klk'l'}(\omega) = \sum_{mi} \left\{ \frac{\langle 0|a_l^+ a_k|mi\rangle\langle mi|a_{l'}^+ a_{k'}|0\rangle}{\omega - \epsilon_m + \epsilon_i + i\eta} - \frac{\langle 0|a_{l'}^+ a_{k'}|mi\rangle\langle mi|a_l^+ a_k|0\rangle}{\omega + \epsilon_m - \epsilon_i + i\eta} \right\}, \tag{43}$$

$$= \frac{n_l - n_k}{\omega - \epsilon_k + \epsilon_l + i\eta}\delta_{kk'}\delta_{ll'} \tag{44}$$

2.3 The Response in Mean Field Approximation

In the next step we we use the mean field approximation, i.e. we assume that the ground state of the system can be assumed to be at all times to be a Slater determinant. We therefore start with the TDHF equation in the external time-dependent field.

$$i\hbar\dot{\rho} \;=\; [h[\rho] + f(t), \rho]\,. \tag{45}$$

Since we assume that the external field $f(t)$ is weak and that it has a harmonic time dependence, it introduces only oscillations of *small amplitude* around the stationary density $\rho^{(0)}$, which is itself a solution of the stationary Hartree-Fock equation

$$\left[h^{(0)}, \rho^{(0)}\right] = 0 \tag{46}$$

Therefore, the density has the form

$$\rho(t) \;=\; \rho^{(0)} \;+\; \delta\rho(t) \tag{47}$$

where $\delta\rho$ is linear in the field f.

$$\delta\rho(t) \;=\; \delta\rho e^{-i\omega t} + \text{c.c} \tag{48}$$

We are now able to derive an equation for $\delta\rho$ by linearizing the equation of motion (E13), i.e. we consider only terms linear in f. This does not mean, however, that we assume the interaction to be small using perturbation theory in first order. In fact the resulting linear response and RPA equations go beyond any perturbation theory in finite order. They correspond to a partial summation of an infinite number of perturbative diagrams.

In the following we work in a basis, in which the static solution $\rho^{(0)}$ as well as the corresponding single particle field $h^{(0)}$ are diagonal.

$$\rho^{(0)}_{kl} \;=\; n_k \delta_{kl}, \qquad \text{where} \quad \begin{cases} n_i = 1 & \text{for hole states} \\ n_m = 0 & \text{for particle states} \end{cases} \tag{49}$$

and

$$h^{(0)}_{kl} \;=\; \left(h[\rho^{(0)}]\right)_{kl} \;=\; \epsilon_k \delta_{kl}. \tag{50}$$

In linear order in f and $\delta\rho$ we derive

$$i\hbar\delta\dot{\rho} \;=\; \left[h^{(0)}, \delta\rho\right] \;+\; \left[\frac{\partial h}{\partial \rho}\delta\rho, \rho^{(0)}\right] \;+\; \left[f, \rho^{(0)}\right], \tag{51}$$

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

$$\frac{\partial h}{\partial \rho}\delta\rho = \sum_{kk'} \left.\frac{\partial h}{\partial \rho_{kk'}}\right|_{\rho^{(0)}} \delta\rho_{kk'} \tag{52}$$

From $\rho^2 - \rho$ we find that $\delta\rho$ has only non-vanishing *ph*- and *hp*-matrix elements $\delta\rho_{mi}$ and $\delta\rho_{im}$.

Using the harmonic time dependence of $\delta\rho$ we obtain the *linear response equation*:

$$(\omega - \epsilon_m + \epsilon_i)\delta\rho_{mi} \;=\; f_{mi} + \sum_{m'i'} V_{mi'im'}\delta\rho_{m'i'} + V_{mm'ii'}\delta\rho_{im'} \tag{53}$$

$$(\omega - \epsilon_i + \epsilon_m)\delta\rho_{im} \;=\; f_{im} + \sum_{m'i'} V_{imi'm'}\delta\rho_{m'i'} + V_{im'mi'}\delta\rho_{im'} \tag{54}$$

with the effective interaction expressed as the second derivative of the energy as a function of the density:

$$V_{kl'lk'} \;=\; \sum_{kk'} \left.\frac{\partial h_{kl}}{\partial \rho_{k'l'}}\right|_{\rho^{(0)}} \;=\; \left.\frac{\partial^2 E}{\partial \rho_{lk}\partial \rho_{k'l'}}\right|_{\rho^{(0)}}. \tag{55}$$

For HF-theory without density dependent forces, these are the matrix elements of the interaction. For energy dependent forces we obtain in addition *rearrangement terms*.

Correspondingly to the RPA-matrices A and B are introduced:

$$\begin{aligned} A_{mim'i'} &= (\epsilon_m - \epsilon_i)\delta_{mm'}\delta_{ii'} + V_{mi'im'} \\ B_{mim'i'} &= V_{mm'ii'} \end{aligned} \tag{56}$$

We find the linear response equation in a more familiar form:

$$\left\{\omega \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} - \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix}\right\} \begin{pmatrix} \delta\rho_{mi} \\ \delta\rho_{im} \end{pmatrix} = \begin{pmatrix} f_{mi} \\ f_{im} \end{pmatrix} \tag{57}$$

This equation is an inhomogeneous equation and can be solved by inverting the matrix on the left-hand side. In short hand notation it can be written as

$$(\omega\mathcal{N} - \mathcal{S})\,\delta\rho = f \tag{58}$$

and

$$\delta\rho = Rf$$

with the response function

$$R^{-1} = \omega\mathcal{N} - \mathcal{S} = (R^0)^{-1} - V \tag{59}$$

or

$$R^{(0)}{=}R - R^{(0)}VR \tag{60}$$

and we find the linear response equation

$$R = R^0 + R^0VR \tag{61}$$

2.4 The Random Phase Approximation

2.4.1 Derivation of the RPA Equations from Linear Response

The response function R depends on the frequency of the external field. It has poles at the eigen-frequencies of the system, where already an infinitesimal field f is sufficient to excite the corresponding eigen-mode. To find these resonances ($\omega = \Omega_\nu$), we have to look for the solutions of the homogeneous equation (57) with vanishing external field

$$(\mathcal{S} - \Omega_\nu\mathcal{N})\,\delta\rho^\nu = 0 \tag{62}$$

Without external field the eigen-modes of the system by the solution of the RPA equations

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix}_\nu = \Omega^\nu \begin{pmatrix} X \\ -Y \end{pmatrix}_\nu \tag{63}$$

find non-vanishing transition the RPA equations for the eigensolutions of the system

and the RPA amplitudes X_{mi} and Y_{mi} are given by the transition densities

$$\begin{aligned} X^{\nu}_{mi} &= \delta\rho^{(\nu)}_{mi} \ = \langle 0|a^{+}_{i}a_{m}|\nu\rangle \\ Y^{\nu}_{mi} &= \delta\rho^{(\nu)}_{im} = \langle 0|a^{+}_{m}a_{i}|\nu\rangle \end{aligned} \tag{64}$$

The energy surface in the vicinity of the stationary point $\rho^{(0)}$ can be obtained by expanding the HF energy $E[\rho]$, up to second order in $\delta\rho$

$$E[\rho] = E_0 + \frac{\delta E}{\delta\rho}\delta\rho + \frac{1}{2}\delta\rho^{+}\frac{\delta^2 E}{\delta\rho\delta\rho}\delta\rho \tag{65}$$

where $E_0 = E[\rho^{(0)}]$ is the static energy. In term $(\delta E/\delta\rho)\delta\rho$ contains first order matrix elements $\delta\rho_{mi}$ and $\delta\rho_{mi}$. Their contribution vanishes because the ph-matrix elements of h vanish. However, going up to second order in the term $(\delta E/\delta\rho)\delta\rho$, we have to take into account also the pp- and hh-matrix elements of $\delta\rho$, which are (because of $\rho^2 = \rho$) of second order $\delta\rho_{mi}$. They lead to the ph-energies $\epsilon_m - \epsilon_i$ in the matrix A below. Finally we obtain

$$\begin{aligned} E[\rho] &= E_0 + \frac{1}{2}\begin{pmatrix} \delta\rho^{*}_{mi} & \delta\rho^{*}_{im} \end{pmatrix}\begin{pmatrix} A & B \\ B^{*} & A^{*} \end{pmatrix}\begin{pmatrix} \delta\rho_{mi} \\ \delta\rho_{im} \end{pmatrix} \\ &= E_0 + \frac{1}{2}\delta\rho^{+}\mathcal{S}\delta\rho. \end{aligned} \tag{66}$$

where the matrix

$$\mathcal{S} = \begin{pmatrix} A & B \\ B^{*} & A^{*} \end{pmatrix} \tag{67}$$

is the *stability matrix*

We eventually obtain *Goldstone modes* (in nuclear physics they are often called *spurious solutions*) at zero frequency in the case of a broken symmetry P (for instance momentum). We have only to use the fact that together with $\rho^{(0)}$ the shifted solution

$$\bar{\rho} = e^{i\alpha P}\rho^{(0)}e^{-i\alpha P}, \tag{68}$$

also fulfills the equation $[h(\bar{\rho}), \bar{\rho}] = 0$. Infinitesimal changes $\bar{\rho} = \rho^{(0)} + \delta\rho$, with $\delta\rho \propto [P, \rho^{(0)}]$, give

$$\left[h^{(0)}, \delta\rho\right] + \left[\frac{\partial h}{\partial\rho}\delta\rho, \rho^{(0)}\right] = 0, \tag{69}$$

which shows that $\delta\rho$, which is given by the matrix elements of P, correspond to a spurious solution at zero energy.

The RPA equation can also be written as

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} X & Y^* \\ Y & X^* \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} X & Y^* \\ Y & X^* \end{pmatrix} \begin{pmatrix} \Omega^\nu & 0 \\ 0 & -\Omega^\nu \end{pmatrix} \quad (70)$$

or with

$$\mathcal{X} = \begin{pmatrix} X & Y^* \\ Y & X^* \end{pmatrix} \quad (71)$$

one can derive orthogonality and completeness relations:

$$\mathcal{X}\mathcal{N}\mathcal{X}^\dagger = \mathcal{N} \ , \qquad \mathcal{X}^\dagger\mathcal{N}\mathcal{X} = \mathcal{N} \quad (72)$$

and

$$\mathcal{S}\mathcal{X} = \mathcal{N}\mathcal{X}\mathcal{N}\Omega \quad (73)$$

Knowing the eigen-modes of the system, that is the frequencies Ω_ν and the RPA amplitudes X^ν and Y^ν (the densities $\delta\rho^\nu$), makes it possible to solve to transform to normal coordinates and to express the solution of the linear response equation in these modes

$$\omega\mathcal{N} - \mathcal{S} = \mathcal{N}\mathcal{X}(\omega - \Omega)\mathcal{N}\mathcal{X}^+\mathcal{N} \quad (74)$$

and the response function

$$R = (\omega\mathcal{N} - \mathcal{S})^{-1} = \mathcal{X}(\omega - \mathcal{N}\Omega)^{-1}\mathcal{N}\mathcal{X}^\dagger \quad (75)$$

or

$$R_{klk'l'} \ = \ \sum_\nu \left(\frac{\delta\rho^\nu_{kl}\delta\rho^{\nu*}_{k'l'}}{\omega - \Omega_\nu + i\eta} - \frac{\delta\rho^\nu_{l'k'}\delta\rho^{\nu*}_{lk}}{\omega + \Omega_\nu + i\eta} \right) \quad (76)$$

The sum runs over all eigenstates of the RPA equation with positive eigenvalues.

2.4.2 Derivation from the Quasi-boson Approximation

The RPA theory can be derived also from the quasi-boson approximation. Here one assumes that the nuclear Hamiltonian for collective excitations can

be written a generalized one-boson operator, where the ph-operators $a_m^\dagger a_i \rightarrow B_{mi}^\dagger$ are mapped to boson operators with the commutation relations

$$[B_{mi}, B_{m'i'}] = \left[B_{mi}^\dagger, B_{m'i'}^\dagger\right] = 0, \qquad \left[B_{mi}, B_{m'i'}^\dagger\right] = \delta_{mm'}\delta_{ii'} \tag{77}$$

and the Hamiltonian in boson space has the form

$$H_B = E_{RPA} + \frac{1}{2}\begin{pmatrix} B^\dagger & B \end{pmatrix}\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix}\begin{pmatrix} B \\ B^\dagger \end{pmatrix} \tag{78}$$

The mapping is carried out in such a way that certain matrix elements in Fermion of the Hamiltonian are preserved by this mapping:

$$(0|\left[B_{mi}, \left[\hat{H}_B, B_{m'i'}^\dagger\right]\right]|0) = \langle \mathrm{HF}|\left[a_i^\dagger a_m, \left[\hat{H}, a_{m'}^\dagger a_{i'}\right]\right]|\mathrm{HF}\rangle = A_{mim'i'}, \tag{79}$$

$$(0|\left[B_{mi}, \left[\hat{H}_B, B_{m'i'}\right]\right]|0) = \langle \mathrm{HF}|\left[a_i^\dagger a_m, \left[\hat{H}, a_{i'}^\dagger a_{m'}\right]\right]|\mathrm{HF}\rangle = B_{mim'i'}, \tag{80}$$

where $|\mathrm{HF}\rangle$ is the static HF-state in Fermion space with and $|0)$ is the corresponding state in Boson space with $|0)$, i.e.

$$a_i^\dagger a_m|\mathrm{HF}\rangle = 0 \qquad \text{and} \qquad B_{mi}|0) = 0 \tag{81}$$

The Hamiltonian in Boson space has a similar form as the HFB-Hamiltonian in Fermion space. It can be diagonalized by forming new bosons (collective bosons)

$$O_\nu^\dagger = \sum_{mi} X_{mi}^\nu B_{mi}^\dagger - Y_{mi}^\nu B_{mi} \tag{82}$$

with boson commutation relations

$$[O_\nu, O_{\nu'}] = \left[O_\nu^\dagger, O_{\nu'}^\dagger\right] = 0, \qquad \left[O_\nu, O_{\nu'}^\dagger\right] = \delta_{\nu\nu'} \tag{83}$$

The RPA-ground state is a correlated state and defined as the vacuum of the bosons O_ν

$$O_\nu|\mathrm{RPA}) = 0 \text{ for all } \nu. \tag{84}$$

They lead to the orthogongonality and completeness relations for the coefficients X and Y with the norm operator $\mathcal{N}$. The diagonalization of the Boson Hamiltonian leads to

$$H_B = E_{RPA} + \frac{1}{2}\begin{pmatrix} O^\dagger & O \end{pmatrix}\mathcal{X}^\dagger\mathcal{S}\mathcal{X}\begin{pmatrix} O \\ O^\dagger \end{pmatrix} \tag{85}$$

$$= E_{RPA} + \sum_\nu \Omega_\nu O_\nu^\dagger O_\nu, \tag{86}$$

where

$$E_{RPA} = E_{HF} - \frac{1}{2}\mathrm{Tr}(A) + \frac{1}{2}\sum_{\nu>0}\Omega_\nu = E_{\mathrm{HF}} - \frac{1}{2}\sum_{\nu}\Omega_\nu \sum_{mi}|Y^\nu_{mi}|^2 \qquad (87)$$

This is a Hamiltonian of harmonic oscillatons. As compared to the RPA derived from linear response theory this theory allows (i) for a *correlated ground state* and (ii) *multi-boson excitations*, which are observed in nuclear spectra.

Introducing the generalized coordinates Q_ν and canonically conjugate momenta P_ν by

$$P_v = \frac{\hbar}{i}\sqrt{\frac{M_\nu\Omega_\nu}{\hbar}}\frac{1}{\sqrt{2}}(O_\nu - O^\dagger_\nu), \qquad (88)$$

$$Q_v = \sqrt{\frac{\hbar}{M_\nu\Omega_\nu}}\frac{1}{\sqrt{2}}(O_\nu + O^\dagger_\nu), \qquad (89)$$

we find for the Hamiltonian

$$\hat{H}_B = E_{HF} - \frac{1}{2}\mathrm{Tr}(A) + \sum_\nu\left(\frac{1}{2M_\nu}P^2_\nu + \frac{M_\nu}{2}\Omega^2_\nu Q^2_\nu\right) \qquad (90)$$

For a symmetry operator $\hat{P}$ belonging to a broken symmetry of the Hamiltonian in the HF-solution, we have

$$\left[\hat{H}, \hat{P}\right] = 0 \qquad (91)$$

and therefore

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix}\begin{pmatrix} P_{mi} \\ -P_{im} \end{pmatrix} = 0 \qquad (92)$$

This leads to a Goldstone mode (spurious solution) with vanishing energy and with the eigenvector $X_{mi} = P_{mi}$ and $Y_{mi} = -P_{im}$. For the Goldstone modes we have $|X_{mi}| = |Y_{mi}|$, i.e. the corresponding Bosons have infinite norm. Bosons cannot be defined. Th motion is no longer of small amplitude, because there is no restauring force. The Hamiltonian can only be expressed in terms of the momenta.

2.5 RPA in the continuum

In this case we have to solve the linear response equation in r-space. For a residual interaction of zero range ($V(\mathbf{r},\mathbf{r}') = V_0\delta(\mathbf{r}-\mathbf{r}')$) we find for the response function $R(\mathbf{r},\mathbf{r}') = R(\mathbf{r},\mathbf{r},\mathbf{r}',\mathbf{r}')$:

$$R(\mathbf{r},\mathbf{r}',\omega) = R^0(\mathbf{r},\mathbf{r}',\omega) + V_0 \int d^3r R^0(\mathbf{r},\mathbf{r}'',\omega)R(\mathbf{r}'',\mathbf{r}'). \tag{93}$$

When $R^0(\mathbf{r},\mathbf{r}',\omega)$ is know, this is easy to solve by discretization in r-space and matrix inversion. In this case it is the bigger problem to determine $R^0(\mathbf{r},\mathbf{r}',\omega)$:

We start from the full free response

$$R^0(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_1',\mathbf{r}_2',\omega) = \sum_{mi}\left\{\frac{\langle 0|a^\dagger(\mathbf{r}_2)a(\mathbf{r}_1)|mi\rangle\langle mi|a^\dagger(\mathbf{r}_1')a(\mathbf{r}_2')|0\rangle}{\omega-\epsilon_m+\epsilon_i+i\eta} - ...\right\} \tag{94}$$

$$= \sum_{mi}\left\{\frac{\varphi_m(\mathbf{r}_1)\varphi_i^*(\mathbf{r}_2)\varphi_m^*(\mathbf{r}_1')\varphi_i(\mathbf{r}_2')}{\omega-\epsilon_m+\epsilon_i+i\eta} - ...\right\}. \tag{95}$$

For simplicity the backward going parts are not given here. Since we need only the values for $\mathbf{r} = \mathbf{r}_1 = \mathbf{r}_2$, and $\mathbf{r} = \mathbf{r}_1' = \mathbf{r}_2'$ we find

$$R^0(\mathbf{r},\mathbf{r}',\omega) = \sum_{mi}\left\{\varphi_i^*(\mathbf{r})\langle\mathbf{r}|\frac{1}{\omega+\epsilon_i+i\eta-h^0}|\mathbf{r}'\rangle\varphi_i(\mathbf{r}') \right. \tag{96}$$

$$\left. + \,.\, \varphi_i^*(\mathbf{r}')\langle\mathbf{r}'|\frac{1}{-\omega+\epsilon_i+i\eta-h^0}|\mathbf{r}\rangle\varphi_i(\mathbf{r})\right\}. \tag{97}$$

Here we have inserted a unity $\sum_m |m\rangle\langle m| + \sum_i |i\rangle\langle i| = 1$ and used that for the sum over i the contributions from forward and backward-going parts cancel. We therefore need the single particle Greens's function

$$G(\mathbf{r},\mathbf{r}',\omega) = \langle\mathbf{r}|\frac{1}{\omega+i\eta-h^0}|\mathbf{r}'\rangle \tag{98}$$

For spherical nuclei the angular part can be carried anlytically and the radial part is given by

$$G(r,r',\omega) = 2m\frac{v(r_<)w(r_>)}{W(v,w)}. \tag{99}$$

Here $r_>$ and $r_<$ denote the greater and the lesser of r and r' and $v(r)$ and $w(r)$ are two linear independent solutions of $(h^0 - \omega)v = 0$ with the following boundary conditions

$$\begin{array}{lll} r = 0: & & v(r) \text{ regular, } w(r) \text{ irregular,} \\ r \to \infty: & \omega < 0: & v(r) \text{ increases and } w(r) \text{ decreases exponentially} \\ & \omega > 0: & v(r) \text{ standing wave and } w(r) \text{ outgoing wave.} \end{array}$$

Finally $W(v, w)$ is the Wronskian of the two functions.

If $\hat{F}$ is a local operator (for instance the dipole operator) the transition density is obtained as

$$\delta\rho(\mathbf{r}, \omega) = \int d^3r' R(\mathbf{r}, \mathbf{r}') F(\mathbf{r}') \tag{100}$$

and the strength function is found as

$$S(\omega) = -\frac{1}{\pi} \Im m \int d^3r d^3r' F^*(\mathbf{r}) R(\mathbf{r}, \mathbf{r}', \omega) F(\mathbf{r}') \tag{101}$$