APPROXIMATE METHODS IN NUCLEAR STRUCTURE CALCULATIONS

HARTREE-FOCK THEORY and RANDOM-PHASE-APPROXIMATION

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ABSTRACT — An attempt has been made to describe the correlation structure of the electron gas in terms of the collective modes only.

A very simple formalism is obtained which leads to very good agreement with the results of Nozières-Pines and Hubbard for low momentum transfer ($k/k_F < 1$), if one neglects the exchange terms.

1 — INTRODUCTION

1.1 — *Variational principles*

Let H be the hamiltonian of some quantum system. The Schrödinger equation

$$H\Psi_r = \mathcal{E}_r \Psi_r \tag{1.1}$$

gives us the eigenfunctions Ψ_r and the eigenvalues $\mathcal{E}_r$ of H. The stationary states of our system are described by the eigenfunctions Ψ_r and their energies are the eigenvalues $\mathcal{E}_r$. The time evolution of a general (possibly non-stationary) state described by a wave function Ψ is determined by the time-dependent Schrödinger equation

$$i\frac{\partial \Psi}{\partial t} = H\Psi \tag{1.2}$$

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(we will use units such that $\hbar = 1$). Now, eq. (1.1) is equivalent to the variational equation

$$\delta < \Psi \mid H \mid \Psi > = 0 \tag{1.3}$$

where the wave function Ψ is varied subject to the restriction

$$< \Psi \mid \Psi > = 1 . \tag{1.4}$$

Similarly, eq. (1.2) is equivalent to the variational equation

$$-i(< \delta \Psi \mid \dot{\Psi} > - < \dot{\Psi} \mid \delta \Psi >) + \delta < \Psi \mid H \mid \Psi > = 0 . \tag{1.5}$$

It is well known that eq. (1.3) is mainly useful for providing approximations to the ground state wave function and energy. This is so because the minimum value of $< \Psi \mid H \mid \Psi >$, assuming that Ψ is normalized to unity according to eq. (1.4), is the ground state energy $\mathcal{E}_o$, which is attained if Ψ is replaced by the ground state wave function Ψ_o. On the other hand, eq. (1.5) may be interpreted (1) as te condition for the error in $\dot{\Psi}$ to be minimum.

1.2 — *Main concepts in the Hartree-Fock method*

In order to introduce the main concepts and mathematical methods involved in the Hartree-Fock Theory, considering not only the time-independent version but also the time-dependent extension and the more recent developments such as a discussion of the stability conditions and of the Random-Phase-Approximation (RPA), we start by considering a simple exemple (2).

When we don't know how to solve the Schrödinger equation for a problem it may happen that we expect the ground state wave function $\Psi_o(x)$ to be well approximated by a member of some family of normalized functions $\Phi(x; \alpha_\mu)$, where x stands for the coordinates of the system under consideration and the α_μ are real parameters. Denoting by $\alpha_\mu = \alpha_\mu^{(o)}$ the solution set (we assume, for simplicity, that there is only one solution set) of the system of equations arising from the minimum condition

$$\frac{\partial}{\partial \alpha_\mu} (\Phi \mid H \mid \Phi) = 0 \tag{1.6}$$

the function which best describes the ground state is $\Phi(x; \alpha_\mu^{(o)})$. For later convenience we assume that the parametrization of the functions $\Phi(x; \alpha_\mu)$ has been made in such a way that $\alpha_\mu^{(o)} = 0$. In our approxi-

mation the ground state energy is the minimum value E_o of the expectation values of H with respect to the functions $\Phi(x; \alpha_\mu)$,

$$E_o = (\Phi \mid H \mid \Phi)_{\alpha_\rho = 0} . \tag{1.7}$$

1.3 — *Main concepts in the Tamm-Dancoff method*

We assume, for simplicity, that the functions $\Phi(x; \alpha_\mu)$ are real. Then, eq. (1.6) is equivalent to

$$\left(\frac{\partial}{\partial \alpha_\mu} \Phi \mid H \mid \Phi\right)_{\alpha_\rho = 0} = 0. \tag{1.8}$$

This equation means that at the minimum of $(\Phi \mid H \mid \Phi)$ the hamiltonian H has no matrix elements between Φ and $\partial \Phi / \partial \alpha_\mu$. Moreover, from the normalization condition

$$(\Phi \mid \Phi) = 1 \tag{1.9}$$

it follows that $\partial (\Phi \mid \Phi) / \partial \alpha_\mu = 0$, or, if Φ is real

$$\left(\frac{\partial}{\partial \alpha_\mu} \Phi \mid \Phi\right) = 0. \tag{1.10}$$

This means that $\partial \Phi / \partial \alpha_\mu$ is orthogonal to Φ. It is therefore tempting to try and obtain approximations to the excited states of H by diagonalizing the hamiltonian H in the subspace of the wave functions $\partial \Phi / \partial \alpha_\mu$. This leads to the eigenvalue problem

$$\sum_\nu \left[\left(\frac{\partial \Phi}{\partial \alpha_\mu} \mid H \mid \frac{\partial \Phi}{\partial \alpha_\nu}\right)_{\alpha_\rho = 0} - E_r \left(\frac{\partial \Phi}{\partial \alpha_\mu} \mid \frac{\partial \Phi}{\partial \alpha_\nu}\right)_{\alpha_\rho = 0}\right] C_\nu^{(r)} = 0 \tag{1.11}$$

(the matrix $(\partial \Phi / \partial \alpha_\mu \mid \partial \Phi / \partial \alpha_\nu)_{\alpha_\rho = 0}$ appears because the functions $\partial \Phi / \partial \alpha_\mu$ are in general not orthogonalized). This is the conceptual content of the so called method of Tamm-Dancoff. Since linear combinations of the functions $\partial \Phi / \partial \alpha_\mu$ do not belong in general to the family of the functions Φ there is no guarantee that the eigenvalues E_r of eq. (1.11) are larger than E_o. Some may be smaller and then we arrive at an inconsistency — excited states with an energy lower than the ground state. This type of inconsistency is avoided in the RPA as well shall see.

1.4 — *Main concepts in the RPA*

We look for a description of non stationary states of our system. Assume that the states in which the system finds itself in successive instants of time, for appropriate initial conditions, may be well represented by functions of the family $\{\Phi(x;\alpha_\mu)\}$. The function which best represents the state of the system at time t should be some function $\Phi(x;\alpha_\mu(t))$. The parameters α_μ become now time-dependent and eq. (1.5) should provide us with the law for their time evolution. However we must allow the parameters α_μ to become complex. We replace them by

$$\gamma_\mu = \alpha_\mu + i\beta_\mu \tag{1.12}$$

where α_μ and β_μ are real. The initial family $\{\Phi(x;\alpha_\mu)\}$ is therefore replaced by the family $\{\Phi(x;\gamma_\mu)\}$, where the functions $\Phi(x;\gamma_\mu)$ are defined by expanding $\Phi(x;\alpha_\mu)$ in a Taylor series in α_μ and replacing afterwards α_μ by γ_μ. (Notice that the functions $\Phi(x;\gamma_\mu)$ are no longer necessarily normalized). For small γ_μ we can write (1), up to second order in γ_μ,

$$\frac{(\Phi\,|\,H\,|\,\Phi)}{(\Phi\,|\,\Phi)} = E_o + \frac{1}{2}\sum_{\mu\nu}\left[(\gamma^*_\mu\gamma^*_\nu + \gamma_\mu\gamma_\nu)B_{\mu\nu} + 2\gamma^*_\mu\gamma_\nu A_{\mu\nu}\right] \tag{1.13}$$

where

$$\begin{aligned} B_{\mu\nu} &= \left[\left(\frac{\partial^2\Phi}{\partial\alpha_\mu\,\partial\alpha_\nu}\,|\,H\,|\,\Phi\right) - E_o\left(\frac{\partial^2\Phi}{\partial\alpha_\mu\,\partial\alpha_\nu}\,|\,\Phi\right)\right]_{\alpha_\rho=0} \\ A_{\mu\nu} &= \left[\left(\frac{\partial\Phi}{\partial\alpha_\mu}\,|\,H\,|\,\frac{\partial\Phi}{\partial\alpha_\nu}\right) - E_o\left(\frac{\partial\Phi}{\partial\alpha_\mu}\,\Big|\,\frac{\partial\Phi}{\partial\alpha_\nu}\right)\right]_{\alpha_\rho=0}. \end{aligned} \tag{1.14}$$

The stability of our wave function for the ground state requires that E_o is still the minimum value of $(\Phi\,|\,H\,|\,\Phi)/(\Phi\,|\,\Phi)$, even when the parameters α_μ are replaced by the γ_μ. Then it follows that the quadratic form in the right hand side of eq. (1.13) is necessarily positive definite. This has important consequences for the coefficients $B_{\mu\nu}$ and $A_{\mu\nu}$ which, however, we will not discuss. We also have

$$-i\left[(\delta\Phi\,|\,\dot\Phi) - (\dot\Phi\,|\,\delta\Phi)\right] = -i\sum_{\mu\nu}(\delta\gamma^*_\mu\dot\gamma_\nu - \dot\gamma^*_\mu\delta\gamma_\nu)N_{\mu\nu} \tag{1.15}$$

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(1) This expression depends on the assumption that $\Phi(x;\alpha_\mu)$ is real. The general result is not, however, essentially different.

where

$$N_{\mu\nu} = \left(\frac{\partial \Phi}{\partial \alpha_\mu} \middle| \frac{\partial \Phi}{\partial \alpha_\nu} \right). \tag{1.16}$$

Then eq. (1.5), with Ψ replaced by Φ, leads to the equations

$$\begin{cases} \sum_\nu (-i N_{\nu\mu} \dot{\gamma}_\nu + A_{\mu\nu} \gamma_\nu + B_{\mu\nu} \gamma_\nu^*) = 0 \\ \sum_\nu (i N_{\nu\mu} \dot{\gamma}_\nu^* + A_{\nu\mu} \gamma_\nu^* + B_{\nu\mu} \gamma_\nu) = 0 \end{cases} \tag{1.17}$$

which govern the time evolution of the parameters γ_μ. If we assume a time dependence of the form

$$\gamma_\mu(t) = \xi_\mu^{(r)} \exp(-i\omega_r t) + \eta_\mu^{(r)} \exp(i\omega_r t) \tag{1.18}$$

the following algebraic equations are obtained

$$\sum_\nu (-\omega_r N_{\mu\nu} \xi_\nu^{(r)} + A_{\mu\nu} \xi_\nu^{(r)} + B_{\mu\nu} \eta_\nu^{(r)}) = 0 \tag{1.19}$$

$$\sum_\nu (\omega_r N_{\nu\mu} \eta_\nu^{(r)} + A_{\nu\mu} \eta_\nu^{(r)} + B_{\nu\mu} \xi_\nu^{(r)}) = 0 \tag{1.20}$$

which are the analogue of the RPA equations for our model. Since the quantities $N_{\mu\nu}$, $A_{\mu\nu}$ and $B_{\mu\nu}$ are real (with our simplifying assumptions) and since E_o is the minimum of $(\Phi | H | \Phi)/(\Phi | \Phi)$ it follows that the eigenfrequencies ω_r are real and that the eigenvectors $(\xi_\nu^{(r)} \eta_\nu^{(r)})$ may be chosen real, as it has been done already. Since the matrices $N_{\mu\nu}$, $A_{\mu\nu}$ and $B_{\mu\nu}$ are symetric, it follows that the eigenfrequencies ω_r appearin pairs with opposit signs. (See section 3 below for detailed proofs of analogous statements). If $(\xi_\mu^{(r)} \eta_\mu^{(r)})$ is the eigenvector corresponding to the eigenvalue ω_r, the eigenvector $(\xi_\mu^{(\bar{r})} \eta_\mu^{(\bar{r})})$ corresponding to the eigenvalue $\omega_{\bar{r}} = -\omega_r$ is given by $\xi_\mu^{(\bar{r})} = \eta_\mu^{(r)}$ $\eta_\mu^{(\bar{r})} = \xi_\mu^{(r)}$.

1.5 — *Physical interpretation of the RPA*

Let us consider again eqs. (1.13) and (1.15) and eq. (1.5) with Ψ replaced by Φ. Since eq. (1.5) is valid for arbitrary $\delta\gamma_\mu$, as long

as $\gamma_\mu(t)$ satisfies eq. (1.17), it remains true if we replace $\delta\gamma_\mu$ by $\gamma_\mu(t)$. We may then write eq. (1.13) in the form

$$\frac{(\Phi \mid H \mid \Phi)}{(\Phi \mid \Phi)} = E_o + \frac{i}{2} \sum_{\mu\nu} (\gamma_\mu^* \dot{\gamma}_\nu - \dot{\gamma}_\mu^* \gamma_\nu) N_{\mu\nu}.$$

For a $\gamma_\mu(t)$ as given by eq. (1.18) we have

$$\frac{(\Phi \mid H \mid \Phi)}{(\Phi \mid \Phi)} - E_o = \omega_r \sum_{\mu\nu} (\xi_\mu^{(r)} \xi_\nu^{(r)} - \eta_\mu^{(r)} \eta_\nu^{(r)}) N_{\mu\nu}. \qquad (1.21)$$

Since the left-hand-side of this equation is positive the co-factor of ω_r has the same sign as ω_r. In order to interpret the right-hand-side of eq. (1.21) we consider the time-dependent wave function

$$\Psi(t) = \Psi_o \, e^{-i\mathcal{E}_o t} + C_r \Psi_r \, e^{-i\mathcal{E}_r t} \qquad (1.22)$$

where Ψ_o, $\mathcal{E}_o$ and Ψ_r, $\mathcal{E}_r$ are exact eigenfunctions and eigenvalues of H [eq. (1.1)] and C_r is small. Up to second order in C_r we have

$$\frac{<\Psi \mid H \mid \Psi>}{<\Psi \mid \Psi>} = \mathcal{E}_o + (\mathcal{E}_r - \mathcal{E}_o) C_r^* C_r. \qquad (1.23)$$

Comparing with eq. (1.21) it seems natural, for a positive ω_r, to identify ω_r with excitation energy $(\mathcal{E}_r - \mathcal{E}_o)$ and to identify

$$\sum_{\mu\nu} (\xi_\mu^{(r)} \xi_\nu^{(r)} - \eta_\mu^{(r)} \eta_\nu^{(r)}) N_{\mu\nu}$$

with the transition probability $C_r^* C_r$.

The interpretation given is confirmed if we consider the following expectation values of some arbitrary operator M, up to first order in the small quantities γ_μ and C_r,

$$\frac{(\Phi \mid M \mid \Phi)}{(\Phi \mid \Phi)} = (\Phi \mid M \mid \Phi)_{\alpha_\rho = 0} + \sum_\mu (\gamma_\mu^* + \gamma_\mu) \left(\frac{\partial \Phi}{\partial \alpha_\mu} \mid M \mid \Phi \right)_{\alpha_\rho = 0} \qquad (1.24)$$

$$= (\Phi \mid M \mid \Phi)_{\alpha_\rho = 0} + \sum_\mu (\xi_\mu^{(r)} + \eta_\mu^{(r)}) (e^{i\omega_r t} + e^{-i\omega_r t}) \left(\frac{\partial \Phi}{\partial \alpha_\mu} \mid M \mid \Phi \right)_{\alpha\rho = 0}$$

and

$$\frac{<\Psi|M|\Psi>}{<\Psi|\Psi>} = <\Psi_o|M|\Psi_o> \tag{1.25}$$

$$+ e^{i(\varepsilon_r - \varepsilon_o)t} C_r^* <\Psi_r|M|\Psi_o> + e^{-i(\varepsilon_r - \varepsilon_o)t} C_r <\Psi_o|M|\Psi_r>$$

Indeed, ω_r plays in eq. (1.24) the same role as $\mathcal{E}_r - \mathcal{E}_o$ in eq. (1.25). Moreover $C_r^* <\Psi_r|M|\Psi_o>$ corresponds to

$$\sum_\nu (\xi_\mu^{(r)} + \eta_\mu^{(r)}) \left(\frac{\partial \Phi}{\partial \alpha_\mu}|M|\Phi\right)_{\alpha_\rho = 0}$$

if ω_r is positive. Therefore, the matrix element $<\Psi_r|M|\Psi_o>$ should be identified with

$$\left[\sum_{\mu\nu} (\xi_\mu^{(r)} \xi_\nu^{(r)} - \eta_\mu^{(r)} \eta_\nu^{(r)}) N_{\mu\nu}\right]^{-\frac{1}{2}} \times \sum_\mu (\xi_\mu^{(r)} + \eta_\mu^{(r)}) \left(\frac{\partial \Phi}{\partial \alpha_\mu}|M|\Phi\right)_{\alpha_\rho = 0}.$$

The present method provides us, therefore, with a consistent procedure for calculating excitation energies and transition amplitudes and is free of the inconsistency of the method previously described, since it is the positive ω_r which play the role of excitation energies. We remark, however, that by neglecting the terms in $B_{\mu\nu}$ in eqs. (1.19) and (1.20) we recover eq. (1.11) and, therefore, the previous method.

1.6 — *Orthonormality relations of the RPA eigenvectors*

If we add the equations obtained by summing over μ te product of eq. (1.19) by $\xi_\mu^{(s)}$ and the product of eq. (1.20) by $\eta_\mu^{(s)}$, it may be shown that

$$(\omega_s - \omega_r) \sum_{\mu\nu} (\xi_\mu^{(s)} \xi_\nu^{(r)} - \eta_\mu^{(s)} \eta_\nu^{(r)}) N_{\mu\nu} = 0.$$

The orthogonality relations follow

$$\sum_{\mu\nu} (\xi_\mu^{(s)} \xi_\nu^{(r)} - \eta_\mu^{(s)} \eta_\nu^{(r)}) N_{\mu\nu} = 0, \quad (\text{if } \omega_r \neq \omega_s). \tag{1.26}$$

From eq. (1.21) it follows that it is possible to normalize the eigenvectors $(\xi_\mu^{(r)} \eta_\mu^{(r)})$ according to

$$\sum_{\mu\nu} (\xi_\mu^{(r)} \xi_\nu^{(r)} - \eta_\mu^{(r)} \eta_\nu^{(r)}) N_{\mu\nu} = \frac{\omega_r}{|\omega_r|}. \tag{1.27}$$

This normalization is useful and is frequently adopted. (Notice that the quantities $\xi_{\mu}^{(r)}$, $\eta_{\mu}^{(r)}$ we have used up to now were infinitesimals, therefore they were not normalized to unity). In general one may impose the orthonormality conditions

$$\sum_{\mu,\nu} (\xi_{\mu}^{(s)} \xi_{\nu}^{(r)} - \eta_{\mu}^{(s)} \eta_{\nu}^{(r)}) N_{\mu\nu} = \frac{\omega_r}{|\omega_r|} \delta_{rs} \tag{1.28}$$

which are obvious, from what has been said, if no two ω_r are equal.

2 — THE HARTREE-FOCK METHOD

2.1 — *Parametrization of a general Slater determinant*

We consider a system of N fermions. The hamiltonian may be written

$$H = T + V \tag{2.1}$$

where T is a one-body operator and V is a two-body operator. The operator T is, therefore, the kinetic energy plus the potential energy due to some external field $U(x)$

$$T = \sum_{i=1}^{N} \left(\frac{1}{2m} p_i^2 + U(x_i) \right) \tag{2.2}$$

while V is the potential energy of the two-body interactions

$$V = \sum_{i<j=1}^{N} v(x_i, x_j) . \tag{2.3}$$

The coordinate x_i stands for the space, spin and iso-spin coordinates of particle i

$$x_i = (r_i, \tau_i, \sigma_i) . \tag{2.4}$$

We denote by t_i the sum of the kinetic energy and of the external potential energy of particle i

$$t_i = \frac{1}{2m} p_i^2 + U(x_i) . \tag{2.5}$$

The potential energy of the pair i, j is

$$v_{ij} = v(x_i, x_j) . \tag{2.6}$$

If we consider N linearly independent single-particle wave functions $\psi_\alpha(x)$, the Slater determinant

$$\Psi(x_1, x_2, \ldots, x_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \psi_1(x_1) & \psi_1(x_2) & \ldots & \psi_1(x_N) \\ \psi_2(x_1) & \psi_2(x_2) & \ldots & \psi_2(x_N) \\ \ldots & \ldots & \ldots & \ldots \\ \psi_N(x_1) & \psi_N(x_2) & \ldots & \psi_N(x_N) \end{vmatrix} \tag{2.7}$$

is obviously antisymmetric with respect to the interchange of the coordinates of any pair of particles, so, in agreement with the Pauli principle, it represents a possible physical state of our system. We now assume that the behaviour of our system may be well described by Slater determinants. This assumption leads to the definition of the class of functions where we are going to look for a description of the ground state and of non stationary states (in general obtained by slightly deforming the ground state): we consider the class of Slater determinants of orthonormal single particle functions. It is always possible (even if the $\psi_\alpha(x)$ are not orthonormal) to construct orthonormal linear combinations $\xi_\alpha(x)$ of the functions $\psi_\alpha(x)$, $\xi_\alpha(x) = \sum_{\beta=1}^{N} C_{\alpha\beta}\psi_\beta(x)$. Now, the Slater determinant of the $\xi_\alpha(x)$ differs from the Slater determinant of the $\psi_\alpha(x)$ on a numerical factor, namely the determinant of the coefficients $C_{\alpha\beta}$. The two Slater determinants are, therefore, physically equivalent, so we would gain nothing by dropping the restriction of orthonormality on the functions $\psi_\alpha(x)$. The Slater determinant $\Psi(x_1, x_2, \ldots x_N)$ is normalized if the functions $\psi_\alpha(x)$ are orthonormal. Now let

$$\Phi(x_1, x_2, \ldots, x_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \varphi_1(x_1) & \varphi_1(x_2) & \ldots & \varphi_1(x_N) \\ \varphi_2(x_1) & \varphi_2(x_2) & \ldots & \varphi_2(x_N) \\ \ldots & \ldots & \ldots & \ldots \\ \varphi_N(x_1) & \varphi_N(x_2) & \ldots & \varphi_N(x_N) \end{vmatrix} \tag{2.8}$$

be the Slater determinant [of orthonormal single-particle functions $\varphi_\alpha(x)$] which minimizes the expectation value of the hamiltonian. In order to introduce a convenient parametrization of the general Slater determinant $\Psi(x_1, x_2, \ldots, x_N)$ we expand the set of the wave functions $\varphi_\alpha(x)$ ($\alpha = 1, 2, \ldots, N$) into a complet set of orthonormal functions $\varphi_i(x)$ ($i = 1, 2, \ldots, N, N+1, \ldots, \infty$). (This may be done in infinitely many ways). We also expand the set of the functions $\psi_\alpha(x)$ ($\alpha = 1, 2, \ldots, N$) into another orthonormal set $\psi_i(x)$ ($i = 1, 2, \ldots, \infty$). From now on we will denote by greek letters $\alpha, \beta, \gamma, \ldots$, the labels

of the single-particle states φ_i present in Φ (hole states) and by the letters $m, n, p, \ldots$ we will denote the labels of the single-particle states φ_i not present in Φ (particle states). The letters $i, j, \ldots$, may denote both types of labels.

The transformation of the orthonormal set of single-particle functions $\varphi_i(x)$ into the orthonormal set of the functions $\psi_i(x)$ defines a linear operator u such that

$$\psi_i = u\,\varphi_i\,. \tag{2.9}$$

Since both sets are orthonormal, the operator u is unitary

$$u\,u^+ = u^+\,u = I\,. \tag{2.10}$$

Therefore we may write

$$u = \mathrm{e}^{i\,s} \tag{2.11}$$

where s is an hermitian operator,

$$s = s^+\,. \tag{2.12}$$

The transformation of the functions $\varphi_i(x)$ into the functions $\psi_i(x)$ induces a transformation of the N-particle product wave functions

$$\varphi_{i_1}(x_1)\,\varphi_{i_2}(x_2)\ldots\varphi_{i_N}(x_N)$$

into the functions

$$\begin{aligned}\psi_{i_1}(x_1)\,\psi_{i_2}(x_2)\ldots\psi_{i_N}(x_N) &= u_1\,u_2\ldots u_N\,\varphi_{i_1}(x_1)\,\varphi_{i_2}(x_2)\ldots\varphi_{i_N}(x_N)\\ &= \mathrm{e}^{i\,(s_1+s_2+\ldots+s_N)}\,\varphi_{i_1}(x_1)\,\varphi_{i_2}(x_2)\ldots\varphi_{i_N}(x_N)\,.\end{aligned} \tag{2.13}$$

The label i in the operators u_i, s_i means that these operators act on functions of the coordinate x_i. The several u_i and the several s_i commute, therefore, between themselves. Let

$$\mathfrak{U} = \prod_{i=1}^{N} u_i \tag{2.14}$$

$$S = \sum_{i=1}^{N} s_i \tag{2.15}$$

From eq. (2.13) it follows that a general Slater determinant Ψ is related to a particular Slater determinant Φ through the equation

$$\Psi = \mathrm{e}^{i\,S}\,\Phi \tag{2.16}$$

The operator S replaces the variational parameters a_μ of the previous section. However, since there are several S connecting a given Ψ with a given Φ, a particular S contains in general much arbitrarines. In the next section we will show how to get rid of what is not essential.

2.2 — *The Hartree-Fock equations*

When S tends to zero Ψ approaches Φ. We are going to consider only functions Ψ near to the function Φ. Therefore we replace eq. (2.16) by

$$\Psi_\gamma = e^{i\gamma S}\,\Phi \tag{2.16'}$$

where γ is an infinitesimal real parameter introduced in order to enable one to keep easily track of orders of magnitude. We now define hermitian operators S' and S'' which are relate to the operator S,

$$\begin{aligned} S' &= \sum_{i=1}^{N} s_i' \\ S'' &= \sum_{i=1}^{N} s_i'' \end{aligned} \tag{2.17}$$

$$\begin{aligned} (\varphi_m \mid s' \mid \varphi_\alpha) &= (\varphi_\alpha \mid s' \mid \varphi_m)^* = (\varphi_m \mid s \mid \varphi_\alpha) \\ (\varphi_m \mid s' \mid \varphi_n) &= (\varphi_\alpha \mid s' \mid \varphi_\beta) = 0 \end{aligned} \tag{2.18}$$

$$\begin{aligned} (\varphi_m \mid s'' \mid \varphi_\alpha) &= (\varphi_\alpha \mid s'' \mid \varphi_m)^* = 0, \\ (\varphi_\alpha \mid s'' \mid \varphi_\beta) &= (\varphi_\alpha \mid s \mid \varphi_\beta), \\ (\varphi_m \mid s'' \mid \varphi_n) &= (\varphi_m \mid s \mid \varphi_n). \end{aligned} \tag{2.19}$$

Then we have

$$\begin{aligned} s &= s' + s'', \\ S &= S' + S''. \end{aligned} \tag{2.20}$$

It may now be verified that

$$e^{i\gamma S} = e^{i\left\{\gamma S' + i\,\frac{\gamma^2}{2!}[S', S''] + 0(\gamma^3)\right\}} e^{i\gamma S''}. \tag{2.21}$$

The operator $\exp(i\gamma S'')$ acting on Φ just produces a phase factor. This is so because the functions $\varphi'_\alpha(x) = \exp(i\gamma s'')\,\varphi_\alpha(x)$ are ortho-

normal linear combinations of the functions $\varphi_\alpha(x)$ (notice that $(\varphi_m \mid s'' \mid \varphi_\alpha) = (\varphi_\alpha \mid s'' \mid \varphi_m) = 0$). In order to obtain the Hartree-Fock equations we expand the expectation value

$$< \Psi_\gamma \mid H \mid \Psi_\gamma > = < \Phi \mid e^{-i\gamma S} H e^{i\gamma S} \mid \Phi >$$

up to second order in γ. Then we have

$$< \Psi_\gamma \mid H \mid \Psi_\gamma > = < \Phi \mid H \mid \Phi > - i\gamma < \Phi \mid [S, H] \mid \Phi > - \frac{1}{2!} \gamma^2 < \Phi \mid [S, [S, H]] \mid \Phi > + 0(\gamma^3). \tag{2.22}$$

In agreement with eq. (2.21) and with tha remarks following that equation, we may replace, in eq. (2.22), the operator S by $S' + i\frac{\gamma}{2}[S', S'']$.

Since $< \Psi_\gamma \mid H \mid \Psi_\gamma >$ must be stationary for $\Psi_\gamma = \Phi$, it follows that the terms linear in γ must be zero for arbitrary S,

$$< \Phi \mid [S, H] \mid \Phi > = < \Phi \mid [S', H] \mid \Phi > = 0 \tag{2.23}$$

showing that the component S'' of S is not relevant as far as the stationary condition is concerned. Now we have

$$[S', H] = \sum_{i=1}^{N} [s_i', t_i] + \sum_{i<j=1}^{N} [(s_i' + s_j'), v_{ij}] \tag{2.24}$$

Making use of the general expressions for the expectation values of one-and two-body operators with respect to a Slater determinant, we obtain

$$\begin{aligned} < \Phi \mid [S', H] \mid \Phi > &= \sum_\alpha (\varphi_\alpha \mid [s', t] \mid \varphi_\alpha) \\ &+ \sum_{\alpha<\beta} (\varphi_\alpha \varphi_\beta \mid [(s_1' + s_2'), v_{12}] \mid \varphi_\alpha \varphi_\beta) \\ &- \sum_{\alpha<\beta} (\varphi_\alpha \varphi_\beta \mid [(s_1' + s_2'), v_{12}] \mid \varphi_\beta \varphi_\alpha) = 0. \end{aligned} \tag{2.25}$$

If we consider the operator $\hat{v}$ such that

$$(\varphi_i \varphi_j \mid \hat{v} \mid \varphi_k \varphi_l) = (\varphi_i \varphi_j \mid v \mid \varphi_k \varphi_l) - (\varphi_i \varphi_j \mid v \mid \varphi_l \varphi_k) \tag{2.26}$$

we may replace eq. (2.25) by

$$\sum_{\alpha}(\varphi_\alpha|[s', t]|\varphi_\alpha) + \frac{1}{2}\sum_{\alpha\beta}(\varphi_\alpha\varphi_\beta|[(s_1' + s_2), \hat{v}_{12}]|\varphi_\alpha\varphi_\beta) = 0 \quad (2.27)$$

where the factor 1/2 comes from the equality $\sum_{\alpha<\beta} = \frac{1}{2}\sum_{\alpha\beta}$. With the help of standard techniques of matrix quantum mechanics (such as manipulating the completeness relation $\Sigma_i|\varphi_i)(\varphi_i| = I$) and considering eq. (2.18) we may replace eq. (2.27) by

$$\sum_{\alpha,m}[s_{\alpha,m}(t_{m,\alpha} + \sum_{\beta}\hat{v}_{m\beta,\alpha\beta}) - (t_{\alpha,m} + \sum_{\beta}\hat{v}_{\alpha\beta,m})s_{m,\alpha}] = 0 \quad (2.28)$$

where we have introduced the notation

$$t_{i,j} = (\varphi_i|t|\varphi_j),\ v_{ij,kl} = (\varphi_i\varphi_j|v|\varphi_k\varphi_l),\ \text{etc.} \quad (2.29)$$

Since the real and imaginary parts of $s_{\alpha,m}$ are arbitrary it follows that we may regard $s_{\alpha,m}$ and $s_{m,\alpha}$ as independent, although $s_{\alpha,m} = s^*_{m,\alpha}$. In order to see this it is enough to remark that if we replace $s_{\alpha,m}$ by $is_{\alpha,m}$, then $s_{m,\alpha}$ should be replaced by $-is_{m,\alpha}$. The co-factors of $s_{\alpha,m}$ and $s_{m,\alpha}$ in eq. (2.28) must, therefore, be both equal to zero,

$$t_{\alpha,m} + \sum_{\beta}\hat{v}_{\alpha\beta,m\beta} = 0\,. \quad (2.30)$$

Consider now the operator h such that

$$h_{i,j} = t_{i,j} + \sum_{\beta}\hat{v}_{i\beta,j\beta}\,. \quad (2.31)$$

The operator h is obviously hermitian. The matrices $h_{\alpha,\beta}$ and $h_{m,n}$ are diagonalised by a canonical transformation of the type of exp (is'') which does not mix hole states φ_α with particle states φ_m. Since such a canonical transformation leaves both eq. (2.30) and the Slater determinant Φ invariant, it follows that eq. (2.30) may be replaced, without loss of generality, by the following eigenvalue equations

$$t_{i,j} + \sum_{\beta}\hat{v}_{i\beta,j\beta} = \varepsilon_i\delta_{i,j}\,. \quad (2.32)$$

These are the Hartree-Fock equations, which determine the best single particle orbitals describing the structure of the ground state and, obviously, may also be written

$$h\,\varphi_i = \varepsilon_i\,\varphi_i\,. \tag{2.32'}$$

3 — SECOND ORDER VARIATION

3.1 — *The stability condition*

If eqs. (2.32) are satisfied we may be sure only that the expectation value $<\Psi\,|\,H\,|\,\Psi>$ is stationary when Ψ approaches Φ, but we do not know yet what tipe of stationary point we are dealing with. Since we are looking for a minimum, we ask under what conditions is the expectation value $<\Psi\,|\,H\,|\,\Psi>$ never smaller than $<\Phi\,|\,H\,|\,\Phi>$, at least for a Ψ close to Φ. In order to investigate this point we consider again eq. (2.22). Taking into account eq. (2.23) (the stationary condition) and eq. (2.21) we may write, up to second order in γ

$$\begin{aligned} <\Psi_\gamma\,|\,H\,|\,\Psi_\gamma> - <\Phi\,|\,H\,|\,\Phi> &= -\frac{\gamma^2}{2\,!}<\Phi\,|\,[S,[S,H]]\,|\,\Phi> \\ &= -\frac{\gamma^2}{2\,!}<\Phi\,|\,[S',[S',H]]\,|\,\Phi>\,. \end{aligned} \tag{3.1}$$

The right hand side of this equation must he a non-negative quantity (either positive or zero). If it were not we should look for a better solution of the Hartree-Fock equations. We may write

$$\begin{aligned} [S',[S',H]] = &-\sum_{i=1}^{N}[s_i',[s_i',t_i]] \\ &+\sum_{i<j=1}^{N}[(s_i'+s_j'),[(s_i'+s_j'),v_{ij}]]\,. \end{aligned} \tag{3.2}$$

Therefore we have

$$\begin{aligned} -\frac{1}{2}<\Phi\,|\,[S',[S',H]]\,|\,\Phi> = -\frac{1}{2}\{&\sum_{\alpha}(\varphi_\alpha\,|\,[s',[s',t]]\,|\,\varphi_\alpha) \\ &+\sum_{\alpha<\beta}(\varphi_\alpha\varphi_\beta\,|\,[(s_1'+s_2'),[(s_1'+s_2'),v_{12}]]\,|\,\varphi_\alpha\varphi_\alpha) \\ &-\sum_{\alpha<\beta}(\varphi_\alpha\varphi_\beta\,|\,[(s_1'+s_2'),[(s_1'+s_2'),v_{12}]]\,|\,\varphi_\beta\varphi_\alpha)\,\}\end{aligned} \tag{3.3}$$

$$= -\frac{1}{2}\{\sum_{\alpha}(\varphi_\alpha | [s', [s', t]] | \varphi_\alpha) + \frac{1}{2}\sum_{\alpha\beta}(\varphi_\alpha \varphi_\beta | [(s_1' + s_2'), [(s_1' + s_2'), \hat{v}_{12}]] | \varphi_\alpha \varphi_\beta)\} \tag{3.4}$$

$$= \sum_{\alpha m} s_{\alpha,m}\, s_{m,\alpha}(\varepsilon_m - \varepsilon_\alpha) + \sum_{\alpha\beta,mn}(s_{\alpha,m}\,\hat{v}_{m\beta,\alpha n}\, s_{n,\beta} - \frac{1}{2} s_{\alpha,m}\, s_{\beta,n}\,\hat{v}_{mn,\alpha\beta} - \frac{1}{2}\hat{v}_{\alpha\beta,mn}\, s_{m,\alpha}\, s_{n,\beta}) \tag{3.5}$$

where use has been made ef eq. (2.32). The right hand side of eq. (3.5) is a quadratic form in the quantities $s_{\alpha,m}$ and $s^*_{\alpha,m} = s_{m,\alpha}$. Since it must be non-negative, the sigenvalues λ of the following eigenvalue equation

$$\begin{aligned}(\varepsilon_m - \varepsilon_\alpha)\, s_{\alpha,m} + \sum_{\beta n}(s_{\beta,n}\,\hat{v}_{\alpha n,m\beta} - s_{n,\beta}\,\hat{v}_{\alpha\beta,mn}) &= \lambda\, s_{\alpha,m} \\ (\varepsilon_m - \varepsilon_\alpha)\, s_{m,\alpha} + \sum_{\beta n}(s_{n,\beta}\,\hat{v}_{m\beta,\alpha n} - s_{\beta,n}\,\hat{v}_{mn,\alpha\beta}) &= \lambda\, s_{m,\alpha}\end{aligned} \tag{3.6}$$

must also be non negative (3) — they are either positive or zero. Notice that eq. (3.6) insures that the quadratic form in eq. (3.5) is stationary with respect to variations of $s_{\alpha,m}$ subject to the restriction

$$\sum_{\alpha,m} s_{\alpha,m}\, s_{m,\alpha} = \sum_{\alpha,m} s_{\alpha,m}\, s^*_{\alpha,m} = 1.$$

If the $s_{\alpha,m}$ satisfy this normalization, the lowest eigenvalue λ is also the minimum value of the right hand side of eq. (3.5), which is attained if $s_{\alpha,m}$ is the eigensolution of eq. (3.6) corresponding to the lowest eigenvalue. There will be always zero eigenvalues if there are operators s such that Φ is not their eigenstate and which commute with the hamiltonian (4). Of course, Φ must not be an eigenstate of S because then we would have $\exp(is)\,\Phi = \exp(i\sigma)\,\Phi$, where σ is a real number, so the corresponding $s'_{\alpha,m}$ would be zero. Examples of operators S commuting with H which give rise to zero eigenvalues are the total momentum P and, for an asymmetric nucleus, the angular momentum J. It should be emphasized that the eigenvalues λ have no physical meaning although, if we neglect the matrix elements of the type of $\hat{v}_{\alpha\beta,mn}$, then eqs. (3.5) reduce to the so called Tamm-Dancoff equations

$$(\varepsilon_m - \varepsilon_\alpha)\, C_{\alpha m} + \sum_{\beta,m} C_{\beta n}\,\hat{v}_{\alpha n,m\beta} = E\, C_{\alpha m} \tag{3.7}$$

It is seen that the eigenvalues λ of eq. (3.6) are here replaced by the excitation energies E. There is however no guarantee that the eigenvalues E are positive (since the terms in $\hat{v}_{\alpha\beta,mn}$ are absent). This is a weakness of the Tamm-Dancoff method which is avoided by the RPA method.

3.2 — *The RPA equations*

We use now the variational principle expressed by eq. (1.5) to determine the best time evolution of Slater determinants Ψ_γ near the Slater determinant Φ, assuming we restrict ourselves to that class of functions. We allow, therefore, the operator S to become time-dependent. We may write, up to second order in γ

$$\begin{aligned} &-i\{<\delta\Psi_\gamma|\dot{\Psi}_\gamma> - <\dot{\Psi}_\gamma|\delta\Psi_\gamma>\} \\ &= -i\gamma^2 <\Phi|[\delta S, \dot{S}]|\Phi> = -i\gamma^2 <\Phi|[\delta\dot{S}', S']|\Phi> \end{aligned} \tag{3.8}$$

where use has been made again of eq. (2.21). Now we have

$$[\delta S', \dot{S}'] = \sum_{i=1}^{N} [\delta s_i', \dot{s}_i']$$

so that

$$-i<\Phi|[\delta S', \dot{S}']|\Phi> = -i\sum_\alpha (\varphi_\alpha|[\delta s', \dot{s}']|\varphi_\alpha)\,. \tag{3.9}$$

Finally the variational principle

$$-i(<\delta\Psi_\gamma|\dot{\Psi}_\gamma> - <\dot{\Psi}_\gamma|\delta\Psi_\gamma>) + \delta<\Psi_\gamma|H|\Psi_\gamma> = 0\,,$$

which now may be replaced by

$$-i<\Phi|[\delta S', \dot{S}']|\Phi> - \frac{1}{2}\delta<\Phi|[S', [S', H]]|\Phi> = 0\,. \tag{3.10}$$

leads, with the help of eqs. (3.4) and (3.9), to the following first order linear differential system

$$\begin{cases} i\dot{s}_{\alpha,m} + (\varepsilon_m - \varepsilon_\alpha)s_{\alpha,m} + \sum_{\beta n}(s_{\beta,n}\hat{v}_{\alpha n,m\beta} - s_{n,\beta}\hat{v}_{\alpha\beta,mn}) = 0\,, \\ -i\dot{s}_{m,\alpha} + (\varepsilon_m - \varepsilon_\alpha)s_{m,\alpha} + \sum_{\beta n}(s_{n,\beta}\hat{v}_{m\beta,\alpha n} - s_{\beta,n}\hat{v}_{mn,\alpha\beta}) = 0\,. \end{cases} \tag{3.11}$$

This may be written in a more compact form if we introduce a quantity $\theta(ij)$ defined by

$$\theta(\alpha m) = -\theta(m\alpha) = 1, \quad \theta(\alpha\beta) = \theta(mn) = 0. \tag{3.12}$$

We have then

$$i\dot{s}'_{ij} + (\varepsilon_j - \varepsilon_i)\, s'_{ij} + \sum_{kl} \hat{v}_{il,jk}\, \theta(kl)\, s'_{kl} = 0 \tag{3.13}$$

where s'_{ij} is given by eqs. (2.18). We look now for a solution of these equations in the form

$$s'_{ij}(t) = \theta(ij)\,(\psi^{(r)}_{ij}\, e^{i\omega_r t} - \psi^{(r)*}_{ji}\, e^{-i\omega^*_r t}) \tag{3.14}$$

where the quantities $\psi^{(r)}_{ij}$ are such that $\psi^{(r)}_{\alpha\beta} = \psi^{(r)}_{mn} = 0$ (remember that s'_{ij} must be hermitian). Then we arrive at the RPA equations in the form adopted by Fukuda *et al.* (5).

$$\omega_r\, \psi^{(r)}_{ij} = (\varepsilon_j - \varepsilon_i)\, \psi^{(r)}_{ij} + \theta(ij) \sum_{kl} \hat{v}_{il,jk}\, \psi^{(r)}_{kl}. \tag{3.15}$$

The quantities ω_r are the normal frequencies of our system and the amplitudes $\psi^{(r)}_{ij}$ describe the normal modes. A more physical interpretation of these equations will be given later.

3.3 — *Mathematical properties of RPA equations*

Let us consider again eq. (3.10). This equation is satisfied for arbitrary variations $\delta S'$ as long as S' is such that eq. (3.13) is verified. It follows that eq. (3.10) remains satisfied if we replace in it $\delta S'$ by S'. Therefore we may write, with the help of eq. (3.1),

$$\begin{aligned} \langle \Psi_\gamma | H | \Psi_\gamma \rangle - \langle \Phi | H | \Phi \rangle &= \frac{i\gamma^2}{2} \langle \Phi | [S', S'] | \Phi \rangle \\ &= \frac{i\gamma^2}{2} \sum_{\alpha m} (s_{\alpha,m}\, \dot{s}_{m,\alpha} - \dot{s}_{\alpha,m}\, s_{m,\alpha}). \end{aligned} \tag{3.16}$$

For a $s_{\alpha,m}$ as given by eq. (3.14) we obtain

$$\begin{aligned} &\langle \Psi_\gamma | H | \Psi_\gamma \rangle - \langle \Phi | H | \Phi \rangle \\ &= \frac{\gamma^2}{2} (\omega^*_r + \omega_r) \sum_{\alpha m} (\psi^{(r)*}_{\alpha m}\, \psi^{(r)}_{\alpha m} - \psi^{(r)*}_{m\alpha}\, \psi^{(r)}_{m\alpha}) \\ &= \frac{\gamma^2}{2} (\omega^*_r + \omega_r) \sum_{ij} \theta(ij)\, \psi^{(r)*}_{ij}\, \psi^{(r)}_{ij}. \end{aligned} \tag{3.17}$$

Let us now multiply eq. (3.15) by $\psi_{ij}^{(r)*}\,\theta(ij)$ and let us sum over i,j. We have

$$\omega_r \sum_{ij} \psi_{ij}^{(r)*}\,\theta(ij)\,\psi_{ij}^{(r)} = \sum_{ij} \psi_{ij}^{(r)*}\,\theta(ij)\,(\varepsilon_j - \varepsilon_i)\,\psi_{ij}^{(r)} + \sum_{ij,kl} \psi_{ij}^{(r)*}\,\hat{v}_{il,jk}\,\psi_{kl}^{(r)}. \tag{3.18}$$

It is a simple matter to verify that the right hand side of eq. (3.18) and the co-factor of ω_r are real quantities. Therefore ω_r is also real unless its co-factor is zero. But if the co-factor is zero, the right-hand-side of eq. (3.17) is also zero, so the minimum value of $<\Psi_\gamma \mid H \mid \Psi_\gamma>$ is attained for the $s'_{i,j}$ under consideration (eq. 3.14). The quantity $s'_{\alpha,m}$ is therefore a solution of eq. (3.6) corresponding to an eigenvalue λ equal to zero, but then it follows [taking again into account eq. (3.14)] that the eigenvalue ω_r in eq. (3.15) is zero. Summarizing, the eigenvalues ω^r of eq. (3.15) are always real. If the quantity

$$\sum_{ij} \theta(ij)\,\psi_{ij}^{(r)*}\,\psi_{ij}^{(r)}$$

is zero, then ω_r is also zero. Moreover, since the quantity

$$<\Psi_\gamma \mid H \mid \Psi_\gamma> - <\Phi \mid H \mid \Phi> = \gamma^2\,\omega_r \sum_{ij} \theta(ij)\,\psi_{ij}^{(r)*}\,\psi_{ij}^{(r)} \tag{3.19}$$

is non-negative, it is seen that ω_r has the same sign as $\sum_{ij} \theta(ij)\,\psi_{ij}^{(r)*}\,\psi_{ij}^{(r)}$.

We do not wish to discuss here the case of zero frequencies. For that the reader is referred to Thouless's paper (3). Since such frequencies are related to the degeneracies of the hamiltonian H, we may suppose that those degeneracies have been removed by adding to the hamiltonian a perturbation small enough to be otherwise negligible. Then the quantity $\sum_{ij} \theta(ij)\,\psi_{ij}^{(r)*}\,\psi_{ij}^{(r)}$ is different from zero and it may be conveniently normalized to ± 1,

$$\sum_{ij} \theta(ij)\,\psi_{ij}^{(r)*}\,\psi_{ij}^{(r)} = \frac{\omega_r}{|\omega_r|} \tag{3.20}$$

Consider now two different eigenfrequencies ω_r and ω_s and the corresponding eigenvalue equations. By the usual technique (complex conjugation of the equation for ω_s, multiplication of this equation

by $\psi_{ij}^{(r)}\,\theta(ij)$, multiplication of the other equation by $\psi_{ij}^{(s)\,*}\,\theta(ij)$ and subtraction of the equations so obtained) it may be shown that

$$(\omega_r - \omega_s)\sum_{ij}\psi_{ij}^{(s)\,*}\,\theta(ij)\,\psi_{ij}^{(r)} = 0 \tag{3.21}$$

It folows that, for $\omega_r \neq \omega_s$, the amplitudes $\psi_{ij}^{(r)}$ and $\psi_{ij}^{(s)}$ are orthogonal in the following sence $\sum_{ij}\psi_{ij}^{(s)}\,\theta(ij)\,\psi_{ij}^{(r)} = 0$.

If the $\psi_{ij}^{(r)}$ are properly normalized we have, therefore (we do not wish to discuss explicity the case of degenerate solutions, which involves no particular difficulty)

$$\sum_{ij}\psi_{ij}^{(s)\,*}\,\theta(ij)\,\psi_{ij}^{(r)} = \delta_{rs}\,\frac{\omega_r}{|\omega_r|}\,. \tag{3.22}$$

We will show now that, if $\psi_{ij}^{(r)}$ is an eigensolution of eq. (3.15) corresponding to te eigenvalue ω_r, then $\psi_{ij}^{(\bar{r})} = \psi_{ji}^{(r)\,*}$ is an eigensolution corresponding to the eigenvalue $\omega_{\bar{r}} = -\omega_r$. It is enough to consider the complex conjugate of eq. (3.15)

$$-\omega_r\,\psi_{ji}^{(r)\,*} = (\varepsilon_j - \varepsilon_i)\,\psi_{ji}^{(r)\,*} + \theta(ij)\sum_{kl}\hat{v}_{il,jk}\,\psi_{lk}^{(r)\,*}\,. \tag{3.15'}$$

It may be shown that the amplitudes $\psi_{ij}^{(r)}$ form a complet set, meaning that any collection of quantities $m_{\alpha,m}$, $m_{m,\alpha}$ may be expanded as

$$m_{i,j} = \theta(ij)\sum_{r\,(\omega_r > 0)}(n_r\,\psi_{ij}^{(r)} - m_r\,\psi_{,i}^{(r)\,*}) \tag{3.23}$$

where the summation extends only over positive frequencies. A discussion of this point may be fond elsewhere (6). Of course, from the orthonormality condition we have

$$\begin{aligned} n_r &= \sum_{ij} m_{i,j}\,\psi_{ij}^{(r)\,*}\,, \\ m_r &= \sum_{ij} m_{i,j}\,\psi_{ji}^{(r)}\,. \end{aligned} \tag{3.24}$$

Notice that if $m_{j,i} = m_{i,j}^{*}$ we have $n_r = m_r^{*}$.

3.4 — *Physical interpretation of the RPA solutions*

Let us consider again eq. (3.19), which involves an operator S as given by eq. (3.14) and let us assume that ω_r is positive and that $\psi_{ij}^{(r)}$ is normalized according to eq. (3.22). Then we may write

$$<\Psi_\gamma | H | \Psi_\gamma> = <\Phi | H | \Phi> + \omega_r \gamma^2 . \tag{3.25}$$

Consider now the non-stationary state Ψ_c obtained by admiting a small component of the exact excited state Ψ_r to the exact ground state Ψ_o. Its time evolution is rigorously given by

$$\Psi_c(t) = \Psi_o \, e^{-i\mathcal{E}_o t} + c\,\Psi_r \, e^{-i\mathcal{E}_r t} . \tag{3.26}$$

The expectation value of H with respect to $\Psi_c(t)$ is given by

$$\frac{<\Psi_c(t) | H | \Psi_c(t)>}{<\Psi_c(t \; | \Psi_c(t)>} = \mathcal{E}_o + c\,c^*(\mathcal{E}_r - \mathcal{E}_o) . \tag{3.27}$$

This expression is correct up to second order in c. The comparison of this result, which is exact, with the approximate result expressed by eq. (3.25) suggests the interpretation of a (positive) ω_r as an excitation energy $\mathcal{E}_r - \mathcal{E}_o$. The correctness of this interpretation is confirmed if we consider also the expectation value of an arbitrary one-body operator

$$M = \sum_{i=1}^{N} m_i . \tag{3.28}$$

We have, indeed, up to first order in γ and for an operator S as given by eq. (3.14)

$$\begin{aligned} <\Psi_\gamma | M | \Psi_\gamma> &= <\Phi | M | \Phi> - i\gamma <\Phi | [S, M] | \Phi> \\ &= <\Phi | M | \Phi> - i\gamma \sum_{\alpha\, m} (s_{\alpha,m} m_{m,\alpha} - m_{\alpha,m} s_{m,\alpha}) \\ &= <\Phi | M | \Phi> + (i\gamma)^* e^{i\omega_r t} \sum_{ij} \psi_{ij}^{(r)} m_{j,i} + (i\gamma) e^{-i\omega_r t} \sum_{ij} \psi_{ij}^{(r)*} m_{i,j} \end{aligned} \tag{3.29}$$

On the other hand we may write, up to first order in c

$$\begin{aligned} &\frac{<\Psi_c(t) | M | \Psi_c(t)>}{<\Psi_c(t) | \Psi_c(t)>} = <\Psi_o | M | \Psi_o> \\ &+ c^* e^{i(\mathcal{E}_r - \mathcal{E}_o)t} <\Psi_r | M | \Psi_o> + c \;\; e^{-i(\mathcal{E}_r - \mathcal{E}_o)t} <\Psi_o | M | \Psi_r> \end{aligned} \tag{3.30}$$

Comparing the rigorous eq. (3.30) with the approximate eq. (3.39), we not only find that ω_r plays the role of an excitation energy,

$$\omega_r \Longrightarrow \mathcal{E}_r - \mathcal{E}_o, \tag{3.31}$$

but we also discover the significance of the amplitudes $\psi_{ij}^{(r)}$ which is provided by the following correspondence

$$<\Psi_r | M | \Psi_o> \Longrightarrow m_r = \sum_{ij} \psi_{ij}^{(r)} m_{j,i} \tag{3.32}$$

[Notice that an abstract quantity m_r had been previously introduced in connection with eq. (3.24)]. This interpretation is confirmed if we compare the exact treatment of the polarization of a quantal system by an external time dependent perturbation with the approximate treatment based on the Hartree-Fock method.

Let us consider again a hermitian transition operator M as given by eq. (3.28). There is an important sum-rule refering to the transition amplitudes $<\Psi_r | M | \Psi_o>$: it is the so called Thomas-Reiche-Kuhn sum-rule

$$\begin{aligned} \sum_r (\mathcal{E}_r - \mathcal{E}_o) <\Psi_o | M | \Psi_r> <\Psi_r | M | \Psi_o> \\ = \frac{1}{2} <\Psi_o | [M, [H, M]] | \Psi_o> \end{aligned} \tag{3.33}$$

A remarkable property of the time-dependent Hartree-Fock method or RPA is that it preserves this sum-rule (6). In order to prove this we define a time dependent operator $M(t)$ by

$$\begin{aligned} M(t) &= \sum_{i=1}^{N} m_i(t) \\ m_{i,j}(t) &= \theta(ij) \sum_{r\,(\omega_r > 0)} (m_r^* \psi_{ij}^{(r)} e^{i\omega_r t} - m_r \psi_{ji}^{(r)*} e^{-i\omega_r t}) \end{aligned} \tag{3.34}$$

The last equation does not refer to the matrix elements $m_{\alpha,\beta}(t)$, $m_{m,n}(t)$ which are not required in the proof. Taking into account eq. (3.23), with $n_r = m_r^*$, it follows that $M(0) = M$, if m_r is given by eq. (3.24). This is the reason why we have used the same letter to represent both operators M and $M(t)$. Mereover $m_{i,j}(t)$ satisfies eq. (3.13), (since it is a linear combination of solutions of the type of eq. (3.14)) so eq. (3.16) is applicable. Considering also eq. (3.1) we

may write (for an M' related to M in the same way as S' is related to S)

$$\frac{1}{2}<\Phi|[M,[H,M]]|\Phi>=\frac{i}{2}<\Phi|[M',\dot{M}']|\Phi>$$

$$=\frac{i}{2}\sum_{ij} m_{i,j}\dot{m}_{j,i}\theta(ij)$$

$$=\frac{1}{2}\sum_{ij}\theta(i)\sum_{r}(m_r^*\psi_{ij}^{(r)}e^{i\omega_r t}-m_r\psi_{ji}^{(r)*}e^{-i\omega_r t}) \tag{3.35}$$

$$\times\sum_{s}\omega_s(m_s\psi_{ij}^{(s)*}e^{-i\omega_s t}-m_s^*\psi_{ji}^{(s)}e^{i\omega_s t})$$

$$=\sum_{r(\omega_r>0)}\omega_r m_r^* m_r .$$

Considering eqs. (3.31) and (3.32), the proof is completed. An important consequence of this result is that if $[M,H]=0$ then we either have $m_r=0$ or $\omega_r=0$. This demonstrates again that the so called spurious states, generated by an operator M which commutes H, have zero energy.

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