QUANTIZED ATDHF

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Abstract

A new quantization procedure of ATDHF in the small amplitude limit is presented. Results concerning ground state energy and density are compared with those obtained in the G.C.M. and by time averaging of the time-dependent Hartree-Fock density. This quantization procedure is applied to the small amplitude oscillations perpendicular to the "fission path" in order to see to what extent coupling between large and small amplitude modes may result in damping-like terms.

I. Selfconsistent Microscopic Description of Zero Point Motion Effects

It should be by now well understood that the ATDHF approach is not merely intended to provide an approximate solution of time-dependent Hartree-Fock theory, but rather, to provide a self-consistent microscopic description of quantum collective nuclear modes. In dealing with collective nuclear phenomena one is generally interested in reducing the many-body Schrödinger equation to a few-body one, by deriving a collective Hamiltonian which depends on a few collective coordinates and is quadratic in the momenta. ATDHF approaches this problem in two steps.

In a first stage the TDHF equation is used to derive a classical Hamiltonian, $\mathcal{H}(p_i, q_i)$, by parametrizing the time-dependence of the Slater determinants $\phi(t)$ in terms of the collective coordinates, $q_i(t)$, which are supposed to be relevant to the problem at hand, and their canonical conjugate momenta, $p_i(t)$. Since the classical Hamiltonian is expected to be quadratic in the velocities, an expansion of the TDHF equation to first order in the velocities is sufficient to derive a set of self-consistency conditions for the static determinants $\phi(q_i)$ and constraining operators Q_i at every point $\{q_i\}$; and hence the potential energy and inertial tensor governing the classical dynamics. To summarize, these conditions are [1]

$$\text{I} \quad \langle \delta\phi(q_i) | H - \sum_i \left(\frac{\partial V}{\partial q_i} Q_i\right) | \phi(q_i) \rangle = 0$$

$$\text{II} \quad \langle \delta\phi(q_i) | \{H, iQ_i\}_- - \sum_j \left(\frac{P_j}{M_{ij}}\right) | \phi(q_i) \rangle = 0$$

$$\text{III} \quad \langle \phi(q_i) | \{Q_i, -iP_j\}_- | \phi(q_i) \rangle = \delta_{ij}$$

with V, M_{ij} and Q_i, P_i as defined in ref.[1].

In a second stage one must proceed to a quantal interpretation of this dynamics. While the first part of this program is now rather well established[1-3], the second one remains open, and as a whole the theory has not been used in its full power. In these lectures I will focus on the problem of quantization. I shall first restrict the discussion to the case of small amplitude oscillations around the equilibrium shape in rigid nuclei. This, apart from being an interesting problem in itself, has the advantage that it allows us to compare easily with other theories, and in particular, with the generator coordinate method (GCM) which is in principle more reliable. Then I shall apply the method developed here to the problem of fission.

As can be easily shown[1] at the stable equilibrium point, $\{q_i = q_i^M\}$, condition I is just the static H-F equation for the unconstrained H-F ground state $\phi_o = \phi(q_i = q_i^M)$. In addition, its first derivative together with conditions II, III give the RPA equations for the normal modes of the system

$$\begin{aligned} &\langle \delta\phi_o | \{H, A_i^+\}_- - \omega_i A_i^+ | \phi_o \rangle = 0 \\ &\langle \delta\phi_o | \{H, A_i\}_- + \omega_i A_i | \phi_o \rangle = 0 \\ &\langle \phi_o | \{A_i, A_j^+\}_- | \phi_o \rangle = \delta_{ij} \,, \end{aligned} \tag{1}$$

with

$$A_i^+ = \left(\frac{M_i K_i}{4}\right)^{1/4} Q_i - i \left(\frac{1}{4 M_i K_i}\right)^{1/4} P_i, \quad A_i = (A_i^+)^+ \tag{2}$$

$$\omega_i = \sqrt{\frac{K_i}{M_i}}, \quad M_i^{-1} = \langle \phi_o | \{\{H, iQ_i\}_-, iQ_i\}_- | \phi_o \rangle$$
$$K_i = \langle \phi_o | \{\{H, -iP_i\}_-, -iP_i\}_- | \phi_o \rangle . \tag{3}$$

The energy of the system to second order in the coordinates and momenta is given by

$$\mathcal{H}(p_i, q_i) = \langle \phi(t) | H | \phi(t) \rangle = \langle \phi_o | H | \phi_o \rangle + \sum_i \left(\frac{p_i^2}{2M_i} + \frac{1}{2} q_i^2 K_i\right) \tag{4}$$

corresponding to the time-dependent Slater determinants

$$\phi(t) = \exp i \sum_i (p_i Q_i - q_i P_i) |\phi_o\rangle = (1 + i \sum_i (p_i Q_i - q_i P_i) + \ldots) |\phi_o\rangle \tag{5}$$

where the one-body operators Q_i, P_i are given by the transformation (2) in terms of the solutions of the RPA equations:

$$A_i^+ = \sum_{ph} (X_{ph}^i a_p^+ a_h - Y_{ph}^i a_h^+ a_p). \tag{6}$$

To simplify the notation the assumption is made that $q_i^M = 0$ for all i, otherwise q_i in eqs. (4), (5) should be replaced by $q_i - q_i^M$. Henceforth we can proceed in two ways: 1) by considering the time evolution of the classical variables q_i, p_i governed by Hamilton's equations. This is the semiclassical approximation in which the collective variables are supposed to evolve in time according to classical mechanics, with inertial and restoring force parameters determined microscopically in a self-consistent way. 2) By quantizing the collective variables.

1) Semiclassical approximation

Let us consider the time dependent one-body density associated to the Slater determinant in eq.(5). It can be obtained as the expectation value of the one-body density operator in $\phi(t)$ (eq.(5)), where $q_i(t)$, $p_i(t)$ are the classical solutions of the equations of motion $\dot{q}_i = \frac{\partial \mathcal{H}}{\partial p_i}$, $\dot{p}_i = -\frac{\partial \mathcal{H}}{\partial q_i}$, i.e.,

$$q_i(t) = q_i^o \cos(\omega_i t), \quad p_i(t) = -M_i \omega_i q_i^o \operatorname{sen}(\omega_i t) \tag{7}$$

In particular for q_i^o corresponding to the zero-point amplitudes, $\overline{q_i^2} = \frac{1}{2} q_i^{o2} = \frac{\omega_i}{2K_i}$, for all i. The (local) time-dependent Hartree-Fock density is given in coordinate space by

$$\rho(\vec{r},t) = \langle\phi(t)|\hat{\rho}(\vec{r})|\phi(t)\rangle = \rho(\vec{r}) + \rho^1(\vec{r},t) \tag{8}$$

$\rho^1(\vec{r},t)$ in eq. (8) is the oscillating part,

$$\rho^1(\vec{r},t) = \frac{1}{\sqrt{2}} \sum_i \{e^{-i\omega_i t} \sum_{ph} (X_{ph}^i \varphi_h^*(\vec{r}) \varphi_p(\vec{r}) + Y_{ph}^i \varphi_p^* \varphi_h) + c.c.\} \tag{9}$$

and states simply[14] that the density oscillates with the normal frequencies ω_i of the system. The static density $\rho(\vec{r})$ around which those oscillations take place is the time average of $\rho(\vec{r},t)$ in eq. (8) and to lowest order it is just the static H-F density ($\rho_{H-F}(\vec{r})$). However, keeping to quadratic terms in q_i^o, as in the classical Hamiltonian, one instead obtains

$$\rho(\vec{r}) = \rho_{H\text{-}F}(\vec{r}) + \frac{1}{2} \sum_i \sum_{\substack{ph \\ p'h'}} \rho^{ph}_{p'h'}(\vec{r}) \; (X^{i*}_{ph} X^{i}_{p'h'} + Y^{i}_{ph} Y^{i*}_{p'h'}) \tag{10}$$

with

$$\rho^{ph}_{p'h'}(\vec{r}) = \delta_{hh'} \; \varphi^*_p(\vec{r}) \; \varphi_{p'}(\vec{r}) - \delta_{p'p} \; \varphi^*_{h'}(\vec{r}) \; \varphi_h(\vec{r}) \tag{11}$$

This corresponds to an energy

$$\mathcal{H}(p_i, q_i) = E_o + \frac{1}{2} \sum_i \omega_i \tag{12}$$

greater than the H-F energy, $E_o = \langle \phi_o | H | \phi_o \rangle$, which suggests that $\rho(\vec{r})$ in eq. (10) does not correspond to the ground state density but rather to an average over real excitations.

2) Quantization

The problem of quantization has already been discussed by Goeke and Reinhard [3]. Here we shall address this problem from a different point of view. Let us discuss first for simplicity the case of just one collective coordinate (q); suppose we have solved the set of self-consistency conditions I-III and therefore we know the optimal structure of the determinantal wave functions $\phi(p,q)$ and classical collective Hamiltonian $\mathcal{H}(p,q)$. The quantization of $\mathcal{H}(p,q)$ would provide us with a collective basis $f_n(q)$ with corresponding eigenvalues E_n. Then the eigenstates ψ_n of the nuclear Hamiltonian H, for that particular mode, could be constructed in a generator coordinate method fashion from $f_n(q)$ and $\phi(p,q)$ [5]. However, one is not really interested in what the exact form of these eigenstates is, but rather in observable quantities as the matrix elements of given operators θ between those states. Such matrix elements would be given by [1,5]

$$\langle \psi_n | \theta | \psi_m \rangle = \int dq \; f^*_n(q) \; \Theta(p,q) \; f_m(q) \tag{13}$$

with $\Theta(p,q) \equiv \Theta(-i \frac{\partial}{\partial q}, q)$ being the effective collective operator equivalent to θ. Then the whole problem of quantization is actually reduced to finding those effective collective operators from $\phi(p,q)$ as

$$\Theta(p,q) = \langle \phi(p,q) | \boldsymbol{\theta} | \phi(p,q) \rangle \tag{14}$$

The handling of eq. (14) requires some care for $\Theta(p,q)$ must represent an operator in collective space, not a function of time!

Concentrating now on the case of small amplitude oscillations it is clear what we should do: change the classical variables $p_i(t)$, $q_i(t)$ in eq. (5) into the operators

$$q_i = \sqrt{\frac{1}{2M_i\omega_i}}\,(c_i+c_i^+)\ , \qquad p_i = \sqrt{\frac{M_i\omega_i}{2}}\,i\,(c_i^+-c_i) \tag{15}$$

where $c_i^+(c_i)$ are creation (annihilation) operators of one quantum of the mode i (satisfying boson conmutation relations $\{c_i,c_j^+\}_- = \delta_{ij}$) and act only on the collective basis:

$$|\{n_i\}> = \prod_i \frac{(c_i^+)^{n_i}}{\sqrt{n_i!}}\,|0> \tag{16}$$

Then the effective collective operators $\theta(p_i,q_i) \equiv \hat{\theta}(c_i^+,c_i)$ are given by

$$\hat{\theta}(c_i^+,c_i) = <\phi_0|\theta + \{\theta,iT\}_- + \tfrac{1}{2}\{\{\theta,iT\}_-,iT\}_-|\phi_0> \tag{17a}$$

where the two-fold operator $T = \sum_i (p_iQ_i - q_iP_i)$ can be written using the transformations (2) and (15) as

$$T = -i \sum_i (A_i^+c_i - A_ic_i^+) \tag{17b}$$

with the operators A_i^+, A_i defined on the s.p. H-F basis as in eq. (6). The matrix elements of the operator θ between "eigenstates" $\psi_{\{n_i\}}\psi_{\{m_i\}}$ can then be calculated as (see eq. (13))

$$<\psi_{\{n_i\}}|\theta|\psi_{\{m_i\}}> = <\{n_i\}|\hat{\theta}(c_i^+,c_i)|\{m_i\}> \tag{18}$$

from the explicit expression of $\hat{\theta}(c_i^+,c_i)$ that can be found in ref.[6]. As is shown in that reference the matrix elements in eq. (18) are identical to those obtained with the generator coordinate method. It has been pointed out[5] that after quantization ATDHF provides a description of excited states and energy levels analogous to that provided by the GCM, but that the latter method, being fully quantum mechanical, should be used to identify the zero point energy correction not included in the former. In what follows we shall show that with the quantization procedure presented here the effective collective operators in eq. (17) already contain the zero point corrections prescribed by the generator coordinate method. Let us first recall what the GCM results are for the correlated ground state energy ($E_{g.s.}$) and density ($\rho_{g.s.}$). To second order in the small amplitudes one gets in the usual quasi-boson approximation[7]

$$E_{g.s.} = E_0 - \sum_i \omega_i \left(\sum_{ph} |Y^i_{ph}|^2\right) \tag{19}$$

$$\rho_{g.s.}(\vec{r}) = \rho_{HF}(\vec{r}) + \sum_i \sum_{\substack{ph \\ p'h'}} Y^i_{ph}\, Y^{i*}_{p'h'}\, \rho^{ph}_{p'h'}(\vec{r}) \tag{20}$$

with $\rho^{ph}_{p'h'}(\vec{r})$ as defined in eq. (11). This correction to the H-F density due to RPA correlations, is equivalent to the sum of the graphs

for each vibrational mode in Nuclear Field Theory[8]. It is easily seen that these results are identical to the ones that follow from ATDHF using our quantization procedure. Using equations (17), together with the self-consistent conditions, the effective collective Hamiltonian and density operator in collective space are found to be:

$$\hat{\mathcal{H}}(c_i^+, c_i) = \left[E_0 - \sum_i \omega_i \left(\sum_{ph} |Y^i_{ph}|^2\right)\right] + \sum_i \omega_i \, c_i^+ c_i \tag{21}$$

$$\hat{\rho}(\vec{r})(c_i^+, c_i) = \left[\rho_{HF}(\vec{r}) + \sum_i \sum_{\substack{ph \\ p'h'}} Y^i_{ph} \, Y^{i*}_{p'h'} \, \rho^{ph}_{p'h'}(\vec{r})\right]$$

$$+ \sum_i \left\{\sum_{ph} \left(X^i_{ph} \, \varphi^*_h(\vec{r}) \, \varphi_p(\vec{r}) + Y^i_{ph} \, \varphi^*_p(\vec{r}) \, \varphi_h(\vec{r})\right) c_i + \text{h.c.}\right\}$$

$$+ \sum_{ij} \left\{\sum_{\substack{ph \\ p'h'}} \left(X^{i*}_{ph} \, X^j_{p'h'} + Y^{i*}_{p'h'} \, Y^j_{ph}\right) \rho^{ph}_{p'h'}(\vec{r}) \, c_i^+ c_j\right\} + \ldots \tag{22}$$

The expectation values of these operators in the ground state $\psi_0 = \psi_{\{n_i=0\}}$ are then the terms within square brackets in eqs. (21) and (22), and are identical to eqs. (19) and (20), respectively.

It is now clear what the limitations of the semiclassical approximation discussed before are. Comparing eqs. (10) and (20) one sees that the semiclassical approximation is only valid (as it should be) for highly collective modes for which ω_i is much smaller than the average one particle - hole excitation energies, for only then $|X^i_{ph}| \simeq |Y^i_{ph}|$.

To summarize, we have shown that after a proper quantization ATDHF provides a description of vibrational modes that goes beyond the semiclassical description furnished by TDHF. This description is analogous in all respects to that provided by the GCM, with the advantage that it is simpler to handle and that having a parallel semiclassical interpretation is more appealing to intuition. This aspect may be very valuable in addressing more complex collective nuclear phenomena.

II. The Fission Path

The adiabatic limit of time-dependent Hartree-Fock has been mainly used to provide a basis for the description of large amplitude slow collective modes, under the assumption that they may be treated as completely decoupled (see refs.|1a| - |3|). In order to be able to describe phenomena such as friction or damping, the coupling between large amplitude modes and intrinsic excitations must be taken into account. In ref. |1b| a set of selfconsistency conditions was derived from conditions I-III in part I to determine as well the coupling between the "fission" mode and the intrinsic excitations (see eqs. IA - VIA in ref.|1b|). The simplifying assumption was made that a single collective coordinate is sufficient to describe the deformation of the nucleus in the fission (or fusion) mode, and the intrinsic excitations were described in the form of RPA modes at any given deformation. Calling q_1 the fission mode coordinate (defined as the line of minimal potential energy), q_K (with $K \geq 2$) the vibrational coordinates, and p_1, p_K their canonical conjugate momenta, the classical Hamiltonian was found to be|1b|:

$$\mathcal{H}(p_i,q_i) = \mathcal{H}_a(p_1,q_1) + \frac{1}{2} \sum_K \left(\frac{p_K^2}{M_K^o} + K_K\, q_K^2\right) + \frac{1}{2}\, p_1^2 \sum_K \frac{q_K}{M_{11}^{(K)}} +$$

$$+ p_1 \sum_{K,K'} \frac{q_K p_{K'}}{M_{K'1}^{(K)}} \qquad (1)$$

where $\mathcal{H}_a(p_1,q_1) = \dfrac{p_1^2}{2M_1^o(q_1)} + V(q_1)$ represents the pure adiabatic motion in the fission direction and is identical to that in ref.|1a|. All the mass and restoring force parameters in eq. (1) are functions of q_1 and are to be determined together with the Slater determinants $\phi(q_1)$ and the 1 p-h operators Q_i^o , P_i^o in a selfconsistent way as prescribed in ref. |1b|. It is seen from eq. (1) that to lowest order in the small amplitudes and velocities the motion in the fission direction and the bound motion in the perpendicular surfaces, q_1 = cte, are decoupled except for the dependence of the vibrational frequencies

$\omega_K = \sqrt{\dfrac{K_K}{M_K^o}}$, on q_1. The explicit coupling comes from the dependence of the kinetic energy on the vibrational amplitudes. The Hamiltonian (1) corresponds to the time-dependent Slater determinant|1b|

$$\phi(t) = \left(1 - i \sum_{K\geq 2} q_K\, P_K^o + i \sum_{i\geq 1} p_i\, \tilde{Q}_i + \ldots\right) |\phi(q_i)\rangle \qquad (2)$$

with $\tilde{Q}_i = Q_i^o + Q_1^o \sum_{K\geq 2} q_K \gamma_K^i$, where the q_1-dependent quantities γ_K^i are given by $\gamma_K^i = \langle \{Q_i^o, i \frac{\partial p_K^o}{\partial q_1}\} \rangle$ and are crucial in defining the explicit coupling (the notation $\langle A \rangle$ is used for $\langle \phi(q_1)|A|\phi(q_1)\rangle$).

The quantization procedure discussed above can now be applied to find the effective Hamiltonian at every point p_1, q_1 in the collective path ($\hat{\mathcal{H}}(c_K^+, c_K; p_1 q_1)$ by quantizing the variables of the bound motion in eq. (2). Using the tranformation (15) in part I for the normal modes $K(K\geq 2)$, we find

$$\hat{\mathcal{H}}(c_K^+, c_K; p_1, q_1) = \mathcal{H}'(p_1, q_1) + \sum_K \omega_K c_K^+ c_K + \frac{1}{2} \sum_K F_K (p_1, q_1)(c_K^+ + c_K) +$$

$$+ \frac{1}{2} \sum_{K,K'} G_{K,K'}(p_1, q_1)\, i(c_K^+ c_{K'}^+ - c_K c_{K'} + c_K^+ c_{K'} - c_{K'}^+ c_K) \qquad (3)$$

where $\mathcal{H}'(p_1, q_1)$ can be interpreted as the classical Hamiltonian for the "frozen" motion in the fission direction, i.e., for the path along which the vibrational modes remain in their ground state. It is given by:

$$\mathcal{H}'(p_1, q_1) = V(q_1) + \frac{1}{2} \sum_K \left(\omega_K - \frac{\langle (P_K^o)^2 \rangle}{M_K^o} - K_K \langle (Q_K^o)^2 \rangle - K_{1K} \langle Q_K^o Q_1^o \rangle\right) +$$

$$+ \frac{p_1^2}{2M_1^o} - \frac{p_1}{M_1^o} \left(\sum_K \left\langle \frac{\partial p_K^o}{\partial q_1} Q_K^o \right\rangle\right) \qquad (4)$$

and only differs from $\mathcal{H}_a(p_1, q_1)$ in the last term (which is linear in the collective velocity) and in the renormalization of the potential energy due to the zero point motion of the vibrational modes. Note that since $\langle \frac{\partial p_K^o}{\partial q_1} Q_K^o \rangle$ must be imaginary, $\mathcal{H}'(p_1, q_1)$ is time-reversal invariant and therefore, although the equation of motion $\dot{p}_1 = -\frac{\partial \mathcal{H}'}{\partial q_1}$ contains a term linear in p_1, this term is imaginary and has, in principle, nothing to do with the usual viscosity term introduced by means of the Rayleigh dissipation function[9]. Analogous remarks stand for the whole effective Hamiltonian in eq. (3), where the coefficients in the coupling terms are given by:

$$F_K(p_1, q_1) = \frac{1}{\sqrt{2M_K^o \omega_K}} \left(\frac{p_1^2}{M_{11}^{(K)}} - \sum_{\ell\geq 2} \gamma_K^\ell \left\langle \frac{P_1^o P_\ell^o}{M_1^o} + K_\ell Q_\ell^o Q_1^o + K_{1\ell} (Q_1^o)^2 \right\rangle\right) \qquad (5)$$

$$G_{K,K'}(p_1,q_1) = \frac{p_1}{M^{(K)}_{K'1}} \sqrt{\frac{M^o_{K'}\,\omega_{K'}}{M^o_K\,\omega_K}} \qquad (6)$$

showing its manifest time-reversal invariance. A complete quantum mechanical description of the collective (large amplitude) motion coupled to the intrinsic excitations can be finally obtained by quantizing the fission mode variables. However this is only necessary to describe purely quantum mechanical phenomena such as tunneling[10] and one would like to attach to a semiclassical description of the large amplitude mode in the classically accesible regions. For $M^{(K)}_{K'1} = 0$ the Hamiltonian (3) has the usual form[11] of that for a system consisting of a subsystem coupled to a thermal reservoir and the method of ensemble averages can be used to derive time-irreversible equations from the time-reversal ones. This Hamiltonian could then be taken as the starting point for models of damped collective motion based on linear response theory[12]. The fact that in our approach the inertia of the fission mode and the frequencies of the bound motion (as well as the coupling) are determined in a selfconsistent way at every point in the path would also allow to elucidate the regions at which the intrinsic excitations can be treated globally as a heat bath, as well as the modes that must be excluded from that treatment (and considered as collective) in a given region[13]. Another model with which one could establish connection is that of Broglia, Dasso and Winther for heavy ion collisions[14], where the relative motion is described in terms of classical equations and the nuclear degrees of freedom are described in terms of low-lying surface vibrations and damped giant resonances.

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