DETERMINATION OF THE COLLECTIVE PATH IN THE ADIABATIC TIME DEPENDENT HARTREE-FOCK THEORY

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Many large amplitude collective processes like low energy heavy ion reactions, fission, vibrations of soft nuclei etc. have the property that there exist certain classical parameters $q_1(t)$, $q_2(t)$, ... whose evolution in time is intimately connected with the time evolution of the total many body wave function. This suggests to extract from the total Hamiltonian a collective Hamiltonian H_c in the form of a Schrödinger equation in terms of the $q_1, q_2, \ldots$ and characterized by a collective mass tensor $M_{ik}(q_1, q_2, \ldots)$ and a collective potential $V(q_1, q_2, \ldots)$. The M and the V can be obtained from the corresponding classical quantities $\mathcal{M}_{ik}(q_1, q_2, \ldots)$ and $\mathcal{V}(q_1, q_2, \ldots)$ by quantizing the classical collective Hamiltonian $\mathcal{H}_c = \frac{1}{2}\sum_{ik} \mathcal{M}_{ik}\, \dot{q}_i\, \dot{q}_k + \mathcal{V}(q_i)$. This quantization can be performed uniquely without the well known ambiguities (see P.-G. Reinhard and K. Goeke, subm. to Annals of Physics, and these proceedings) yielding eventually expressions similar to the GCM. The purpose of formulating a new version of an adiabatic time dependent Hartree--Fock theory (ATDHF) is to derive consistently a set of equations, which determines simultaneously the classical mass $\mathcal{M}$, the classical potential $\mathcal{V}$ and the collective path, i.e. the parameter dependent set of Slater determinants $|q_1, q_2, \ldots\rangle$ along which $\mathcal{M}$ and $\mathcal{V}$ are to be calculated. Not all trajectories of TDHF are appropriate to derive a collective Schrödinger equation from, but only those, along which the system may travel regardless of its velocity $\dot{q}_1, \dot{q}_2, \ldots$ since otherwise the resulting $\mathcal{H}_c$ and H_c were energy dependent which contradicts the concept of a

collective Schrödinger equation. It is the aim of the present formalism to determine just those trajectories on the basis of an ATDHF theory. (This is the point from which on the present approach deviates from the one of Brink et al., Nucl. Phys. A258 (1976) 237 hence allowing to give a prescription for the path explicitely).

In terms of the single particle density matrix ρ the TDHF equations are $i\dot{\rho} = [W, \rho]$. We assume $\rho(t) = \rho_0(t) + \rho_1(t) + \rho_2(t) + \ldots$ with $\rho_0(t) = \rho_0(q)$ characterizing the collective path and $\rho_1(t) = \dot{q}\,\bar{\rho}_1(q)$, where we restrict to one parameter $q = q(t)$ for sake of simplicity. The TDHF Hamiltonian $W = T + \mathrm{Tr}\, v\rho$ is split into $W = H_0 + W_1 + W_2 + F + \ldots$ with $W_0 = T + \mathrm{Tr}\, v\rho_0 = H_0 + F$, $W_1 = \mathrm{Tr}\, v\rho_1$, ... The H_0 has been constructed in such a way that it has ρ_0 as solution. Then one obtains a set of equations:

$$\text{(I)} \quad [H_0 , \rho_0] = 0$$

$$\text{(II)} \quad [H_0 , \rho_1] + [W_1 , \rho_0] = i\dot{\rho}_0$$

$$\text{(III)} \quad [H_0 , \rho_2] + [W_2 , \rho_0] + [W_1 , \rho_1] + [F , \rho_0] = i\dot{\rho}_1$$

Since $\dot{q}$ is a small but free parameter eq. (III) can be split into a part which determines the path

$$\text{(IIIa)} \quad [F , \rho_0] = -\frac{i}{\mathcal{M}} \frac{\partial \mathcal{V}}{\partial q} \bar{\rho}_1$$

and an equation for the p-h elements of ρ_2, which can be used to check the assumption of adiabacity

$$\text{(IIIb)} \quad [H_0 , \bar{\rho}_2] + [\bar{W}_2 , \rho_0] + [\bar{W}_1 , \bar{\rho}_1] = i\sqrt{\mathcal{M}}\, \partial/\partial_q (\bar{\rho}_1/\mathcal{M}) .$$

The mass $\mathcal{M}(q)$ and the potential $\mathcal{V}(q)$ can be obtained by applying the same perturbation expansion to the TDHF energy $E = \mathrm{Tr}\, T\rho + \frac{1}{2}\mathrm{Tr}\,\mathrm{Tr}\,\rho v \rho$ giving $\mathcal{M}(q) = i\,\mathrm{Tr}\{[\rho_0 , \bar{\rho}_1] \frac{\partial \rho_0}{\partial q}\}$ and $\mathcal{V}(q) = \mathrm{Tr}\, T\rho_0 + \frac{1}{2}\mathrm{Tr}\,\mathrm{Tr}\,\rho_0 v \rho_0$. It can be shown that the above equations are consistent with those obtained from the normalizations $\rho^2 = \rho$ and $\rho_0^2 = \rho_0$. Eqs. (I - IIIa) can be rewritten to

$$\text{(I')} \quad \left[W_0 - \frac{\partial \mathcal{V}}{\partial q} \bar{Q} , \rho_0\right] = 0$$

$$\text{II')} \quad \left[W_0 \, , \, \bar{\rho}_1 \right] + \left[\bar{W}_1 \, , \, \rho_0 \right] = i \, \frac{\partial \rho_0}{\partial q}$$

$$\text{III')} \quad \bar{Q} = \frac{i}{\mathcal{M}} \left[\rho_0 \, , \, \bar{\rho}_1 \right]$$

which determine simultaneously the collective path $\rho_0(q)$ and the first order correction $\bar{\rho}_1(q)$ needed for the mass $\mathcal{M}$. The equations can be solved e.g. iteratively by starting with an initial guess $\tilde{\rho}_0(q)$, then II') provides $\bar{\rho}_1$ and then III') a new $\hat{Q}$ which can be used in the CHF eq. I') to give an improved $\rho_0(q)$, etc

In the adiabatic limit the present theory for the collective path is more general than the local harmonic approach (LHA) of Holzwarth and Jukawa (Nucl. Phys. A219 (1974) 125) and of Rowe and Bassermann (Can. Journ. Phys. 54 (1976) 1941) since it takes into account the term $\partial\hat{Q}/\partial q$ which has been neglected by these authors and which is not necessary small. Both collective paths, however, have the desirable feature, that they can easily be transformed to a collective path consisting out of correlated wave functions, such that GCM and the uniquely quantized ATDHF, both used along this correlated path, are equivalent. With the operator $\hat{P}$ given by $\left[P \, , \, \rho_0 \right] = i \, \partial\rho_0 / \partial q$ and having the property $\mathrm{Tr} \{ \left[\hat{Q} \, , \, \hat{P} \right] \rho_0 \} = i$ one can define a local collective boson

$$b_0 = \sqrt{\frac{\mathcal{G}}{2}} \left(\hat{Q} + \frac{i}{\mathcal{G}} \hat{P} \right)$$

such that the correlated state $| \tilde{q} >$ is defined as the vacuum of b_0:

$$| \tilde{q} > = \Sigma \, \frac{(-)^n}{n!} \, (b_0^+)^n \, b_0^n \, (q)$$

where $| q >$ is the Slater determinant corresponding to $\rho_0(q)$. Along $| \tilde{q} >$ the two parameters GCM with two conjugate parameters $\tilde{p}$, $\tilde{q}$ reduces to a one parameter one which has then the same collective mass as ATDHF, hence giving the same quantized collective Schrödinger equation, H_c.