ATDHF THEORY WITH A CONSISTENCY CONDITION

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The adiabatic time-dependent Hartree-Fock theory for the microscopic description of large amplitude collective motion was formulated in two seemingly different ways by (i) Villars[1] and by (ii) Baranger and Vēnēroni[2]. The formal identity of these approaches has been demonstrated in ref. 3) and it has been shown that the solution of the zeroth and first order equations satisfying a consistency condition derived from the second-order equation follows the bottom of the potential energy valley.

In this paper we have shown the identity of the two approaches in a different way and in the process the ATDHF equations have been reduced to computationally tractable form. We have then discussed how the solution of the ATDHF equations along with the consistency requirement can be achieved in practice.

The decomposition of the single-particle density operator $\rho(t)$ in the forms

$$\rho(t) = e^{-i\chi(t)} \rho_0(t)\, e^{i\chi(t)} \tag{1}$$

where $\rho_0(t)$ and $\chi(t)$ are time-even hermitian operators, enables one to write the TDHF equation

$$i\dot{\rho} = [h, \rho] \tag{2}$$

as two coupled equations for the time-even and time-odd components ρ_+ and ρ_- of ρ. In the adiabatic approximation $\chi(t)$ is "small" and a series expansion in powers of χ enables one to pick up terms up to any desired order. Retaining terms up to the second order, the two coupled equations reduce to

time-even: $$i\dot{\rho}_1 = [h_0, \rho_0] + [h_0, \rho_2] + [h_1, \rho_1] + [h_2, \rho_0] \tag{3}$$

time-odd: $$i\dot{\rho}_0 = [h_0, \rho_1] + [h_1, \rho_0] \tag{4}$$

where

$$\rho_1 = [\chi, \rho_0] \tag{5}$$

$$\rho_2 = -\tfrac{1}{2}\,[\chi, [\chi, \rho_0]] \tag{6}$$

$$h_0 = t + Tr\,\tilde{v}\,\rho_0 \tag{7}$$

$$h_1 = Tr\,\tilde{v}\,\rho_1 \;;\; h_2 = Tr\,\tilde{v}\,\rho_2 \tag{8}$$

As in ref. 3) substituting $\rho_0(t) = \rho_0(q)$ and $\chi = \hat{pq}$, where p is the small adiabaticity parameter and q the collective coordinate eq. (3) reduces to:

$$p\left[\left\{[h_0, \hat{q}] + \bar{h}_1 + i\frac{\hat{p}}{m}\right\}, \rho_0\right] = 0 \tag{9}$$

Here $\hat{q}$ and $\hat{p}$ are p-h type operators and the latter, in particular, is defined through

$$\frac{\partial \rho_0}{\partial q} = -i\left[\hat{P}, \rho_0\right] \tag{10}$$

The quantity $\bar{h}_1$ is given by

$$\bar{h}_1 = \frac{1}{p} h_1 = Tr\,\tilde{v}\,[\hat{q}, \rho_0] \tag{11}$$

Similarly eq. (2) reduces to

$$[h_0 - \lambda\hat{q}, \rho_0] + p^2\left[\left\{-\tfrac{1}{2}\left([[h_0, \hat{q}], \hat{q}] + 2[\bar{h}_1, \hat{q}] + \right.\right.\right.$$
$$\left.\left.\left. + \bar{h}_2\right) + m^{-1}(q)\frac{\partial \hat{q}}{\partial q} - \tfrac{1}{2}\frac{\partial m^{-1}}{\partial q}\hat{q}\right\}, \rho_0\right] = 0 \tag{12}$$

where

$$\bar{h}_2 = -\frac{1}{2p^2} h_2 = [\hat{q}, [\hat{q}, \rho_0]] \tag{13}$$

In deriving eqs. (9) and (12) we have made use of the Hamilton equations

$$\dot{q} = \frac{\partial \mathcal{H}}{\partial p} = \frac{p}{m} \;;\; \dot{p} = -\frac{\partial \mathcal{H}}{\partial q} = -\frac{\partial V}{\partial q} - \frac{p^2}{2}\frac{\partial m^{-1}}{\partial q}$$

corresponding to the collective Hamiltonian

$$\mathcal{H}(p, q) = \frac{p^2}{2m(q)} + V(q) \tag{14}$$

where

$$m^{-1}(q) = Tr\,h_0\,[[\hat{q}, \rho_0], \hat{q}] + Tr\,Tr\,[\hat{q}, \rho_0]\tilde{v}\,[\hat{q}, \rho_0] \tag{15}$$

$$V(q) = Tr\,t\,\rho_0 + \frac{1}{2} Tr\,Tr\,\rho_0\,\tilde{v}\,\rho_0 \tag{16}$$

We thus conclude as in ref. 3) that while the time-odd eq. (9) of Baranger-Vénéroni (BV) is of first order in the adiabaticity parameter p, the time-even eq. (12) mixes the zeroth- and second-order terms in p. In the spirit of the perturbation approach we write them as separate equations

$$p^0 \rightarrow \qquad [h_0 - \lambda \hat{q}\,,\, \rho_0] = 0 \tag{DI}$$

$$p^1 \rightarrow \qquad \left[\left\{ [h_0, \hat{q}] + \bar{h}_1 + i\frac{\hat{p}}{m} \right\},\, \rho_0\right] = 0 \tag{DII}$$

$$p^2 \rightarrow \qquad \left[\left\{ -\tfrac{1}{2}([[h_0,\hat{q}],\hat{q}] + 2[\bar{h}_1,\hat{q}] + \bar{h}_2) + m^{-1}(q)\frac{\partial \hat{q}}{\partial q} - \tfrac{1}{2}\frac{\partial m^{-1}}{\partial q}\hat{q} \right\},\, \rho_0\right] = 0 \tag{DIII}$$

Notice that in the basis of the eigenstates of ρ_0 only the particle-hole (p-h) matrix elements of the eqs. (DI), (DII) and (DIII) are relevant, since the p-p and h-h matrix elements of an operator of the form $[A,\rho_0]$ identically vanish.

In order to derive the consistency requirement we differentiate eq. (DI) with respect to q,

$$\left[\frac{\partial h_0}{\partial q} - \frac{\partial \lambda}{\partial q}\hat{q} - \lambda\frac{\partial \hat{q}}{\partial q}\,,\, \rho_0\right] + \left[h_0 - \lambda\hat{q}\,,\, \frac{\partial \rho_0}{\partial q}\right] = 0$$

which after some algebraic manipulations gives

$$\left[m^{-1}(q)\frac{\partial \hat{q}}{\partial q}\,,\, \rho_0\right] = \frac{1}{\lambda m}\left[\left\{ \mathrm{Tr}\,\tilde{v}\,[-i\hat{p},\rho_0] + [h_0, -i\hat{p}] - \frac{\partial \lambda}{\partial q}\hat{q} \right\},\, \rho_0\right] - m^{-1}\left[[\hat{q}, -i\hat{p}], \rho_0\right] \tag{17}$$

Substituting eq. (17) in eq. (DIII) we have

$$\left[\left\{ -\frac{\lambda^2}{2}([[h_0,\hat{q}],\hat{q}] + 2[\bar{h}_1,\hat{q}] + \bar{h}_2) + \frac{\lambda}{m}([h_0, -i\hat{p}] + \mathrm{Tr}\,\tilde{v}\,[-i\hat{p},\rho_0]) - \lambda G_0(q)\hat{q} \right\},\, \rho_0\right] = 0 \tag{DIII'}$$

where

$$G_0(q) = \frac{1}{2\lambda}\frac{d}{dq}(\lambda^2/m) \tag{18}$$

In ref. 3) we had the ATDHF equations of Villars

$$\langle \delta\Phi(q) \mid H - \lambda Q \mid \Phi(q)\rangle = 0 \tag{SI}$$

$$\langle \delta\Psi(q) | [H, iQ] - P/m(q) | \Psi(q) \rangle = 0 \qquad \text{(SII)}$$

along with the consistency requirement

$$\langle \delta\Psi(q) | \tfrac{1}{2}\lambda^2 [[H, iQ], iQ] + \frac{\lambda}{m}[H, -iP] - \lambda \omega_0(q) Q | \Psi(q) \rangle = 0 \qquad \text{(SIII')}$$

The similarity of the eqs. (DI), (DII) and (DIII') with eqs. (SI), (SII) and (SIII'), where $|\delta\Phi(q)\rangle$ are in general 1p-1h type states with respect to $|\Phi(q)\rangle$ as vacuum, can be easily seen from the following relations

$$\langle \Psi_{ph} | H | \Psi \rangle = \langle p | h_0 | h \rangle$$

$$\langle \Psi_{ph} | [H, Q] | \Psi \rangle = \langle \Psi_{ph} | [\sum_i t_i, \sum_j \hat{q}_j] + [\sum_{i<j} v_{ij}, \sum_k \hat{q}_k] | \Psi \rangle$$

$$= \langle \Psi_{ph} | \sum_i [t_i, \hat{q}_i] + \sum_{i<j} [v_{ij}, \hat{q}_i + \hat{q}_j] | \Psi \rangle$$

since the operators corresponding to different particles commute. Therefore,

$$\langle \Psi_{ph} | [H, Q] | \Psi \rangle$$

$$= \langle p | [t, \hat{q}] | h \rangle + \sum_{h'} [\langle ph' | [v_{12}, \hat{q}_1 + \hat{q}_2] | hh' \rangle - \langle ph' | [v_{12}, \hat{q}_1 + \hat{q}_2] | h'h \rangle]$$

where, since $\sum_i [t_i, \hat{q}_i]$ and $\sum_{i<j} [v_{ij}, \hat{q}_i + \hat{q}_j]$ are respectively one-body and two-body type symmetric operators, we have used the results

$$\langle \Psi_{ph} | \sum_i O_i | \Psi \rangle = \langle p | O | h \rangle$$

$$\langle \Psi_{ph} | \sum_{i<j} O_{ij} | \Psi \rangle = \sum_{h'} (ph' | O_{12} | hh')$$

Therefore

$$\langle \Psi_{ph} | [H, Q] | \Psi \rangle = \sum_{\alpha\beta} [(p\alpha | [v_{12}, q_1] | h\beta) \times$$

$$\times \langle \beta | \rho | \alpha \rangle + (p\alpha | [v_{12}, q_2] | h\beta) \langle \beta | \rho | \alpha \rangle] + \langle p | [t, q] | h \rangle$$

$$= \langle p | [t, \hat{q}] + Tr_2 [\tilde{v}_{12}, q_1] \rho_2 + Tr_2 [\tilde{v}_{12}, q_2] \rho_2 | h \rangle$$

$$= \langle p | [h, \hat{q}] + \bar{h}_1 | h \rangle$$

where we have used the definition of the trace

$$\langle a|\, Tr_2 \tilde{V}_{12} O_2 \,|b\rangle = \sum_{\alpha\beta} (a\alpha|V|b\beta)\langle\beta|O|\alpha\rangle$$

and the cyclic property of trace, which leads to

$$Tr\,[A,B]C = Tr\,(ABC - BAC) = Tr\,(BCA - CBA)$$
$$= Tr\,[B,C]A$$

The round-bracket matrix element of V here stands for the usual "direct" minus "exchange" matrix elements.

In a similar manner it can be easily seen that

$$\langle \Phi_{ph}|\,[H,-i\hat{P}]\,|\Phi\rangle = \langle h|\,[h_0,-i\hat{p}] + Tr\,\hat{v}\,[-i\hat{p},\rho_0]\,|h\rangle$$

$$\langle \Phi_{ph}|\,[[H,i\hat{Q}],i\hat{Q}]\,|\Phi\rangle = -\langle h|\,[[h_0,\hat{q}],\hat{q}] + 2[\bar{h}_1,\hat{q}] + \bar{h}_2\,|h\rangle$$

Since the eqs. (DI), (DII) and (DIII) are one-body equations they can be easily reduced to equations for the single particle states $|\phi_\alpha(q)\rangle$. Since $\hat{q}$ and $\hat{p}$ are p-h type operators eq. (DI) gives

$$\lambda\hat{q} = (1-\rho_0)h_0\rho_0 + \rho_0 h_0 (1-\rho_0) \tag{19}$$

and eq. (DII) gives

$$-i\hat{p} = c(q)\{(1-\rho_0)h_0(1-2\rho_0)h_0\rho_0 - \rho_0 h_0(1-2\rho_0)h_0(1-\rho_0) + (1-\rho_0)\bar{h}_1'\rho_0 + \rho_0\bar{h}_1'(1-\rho_0)\} \tag{20}$$

where $c(q) = m/\lambda$ and we have substituted $\hat{q}$ from eq. (19). Recognizing that $-i\hat{p}|\phi_\alpha(q)\rangle = \frac{\partial}{\partial q}|\phi_\alpha(q)\rangle$, we have from eq. (20)

$$\frac{\partial}{\partial q}|\phi_\lambda(q)\rangle = c(q)\{(1-\rho_0)h_0(1-2\rho_0)h_0 + (1-\rho_0)\bar{h}_1'\}|\phi_\lambda(q)\rangle \tag{21a}$$

$$\frac{\partial}{\partial q}|\phi_\nu(q)\rangle = c(q)\{-\rho_0 h_0(1-2\rho_0)h_0 + \rho_0\bar{h}_1'\}|\phi_\nu(q)\rangle \tag{21b}$$

where $\bar{h}_1' = \frac{1}{\lambda}\bar{h}_1 = Tr\tilde{V}[h_0,\rho_0]$. In eq. (21a) since no particle states appear, in order to obtain the occupied states which are sufficient to evaluate the relevant quantities of the ATDHF theory, one needs not consider infinite number of particle states.

In ref. 3) it has been shown that solutions of eqs. (21) represent lines of force normal to the equipotential surfaces revealing the non-uniqueness of their solutions. It has been shown in ref. 3) that the particular solution of eq. (21) that satisfies the consistency condition (DIII') follows the bottom of the potential energy valley.

Substituting $\hat{q}$ and $\hat{p}$ from eqs. (19) and (20), eq. (DIII') reduces to

$$(1-\rho_0)\{h_0(1-\rho_0)h_0(1-2\rho_0)h_0 - h_0(1-2\rho_0)h_0\rho_0 h_0 + h_0\bar{h}_1' - \bar{h}_1' h_0 - \omega_0(q)h_0 + T^r\tilde{v}\hat{r}\}|\phi_\lambda(q)\rangle = 0 \tag{22a}$$

$$\rho_0\{h_0(1-2\rho_0)h_0(1-\rho_0)h_0 - h_0\rho_0 h_0(1-2\rho_0)h_0 + h_0\bar{h}_1' - \bar{h}_1' h_0 - \omega_0(q)h_0 + T^r\tilde{v}\hat{r}\}|\phi_\mu(q)\rangle = 0 \tag{22b}$$

where the one-body operator $\hat{r}$ is given by

$$\hat{r} = (1-\rho_0)h_0(1-2\rho_0)h_0\rho_0 + \rho_0 h_0(1-2\rho_0)h_0(1-\rho_0) - \rho_0 h_0(1-\rho_0)h_0\rho_0 + (1-\rho_0)h_0\rho_0 h_0(1-\rho_0) + (1-\rho_0)\bar{h}_1'\rho_0 - \rho_0\bar{h}_1'(1-\rho_0) \tag{23}$$

In order to solve the eqs. (21) the prescription

$$|\phi_\alpha(q+\delta q)\rangle = (1 - i\delta q\,\hat{P}(q))|\phi_\alpha(q)\rangle \tag{24}$$

does not preserve the scalar product of the states. One has to use some unitary evolution operator

$$|\phi_\alpha(q+\delta q)\rangle = e^{-i\delta q\,\hat{P}(q)}|\phi_\alpha(q)\rangle \tag{25}$$

or some approximation[6] to it. Given an initial set of states corresponding to an initial deformation

$$q_0 = \langle\Phi(q_0)|\hat{D}|\Phi(q_0)\rangle$$

one first calculates λ/m from the normalization condition

$$\frac{\partial q}{\partial q} = 1 = \langle\Phi(q)|[\hat{D}, -iP]|\Phi(q)\rangle$$

$$\text{or, } c^{-1}(q) = \frac{\lambda}{m} = \langle\Phi(q)|[\hat{D}, -ic^{-1}(q)P]|\Phi(q)\rangle$$

and then using eq. (25) the set of states corresponding to deformation $q_0+\delta q$ can be calculated and so on. There is another normalization condition

$$\langle \Phi(q) | [Q, -iP] | \Phi(q) \rangle = 1$$

which gives λ^2/m and thus at each step we obtain λ and m separately.

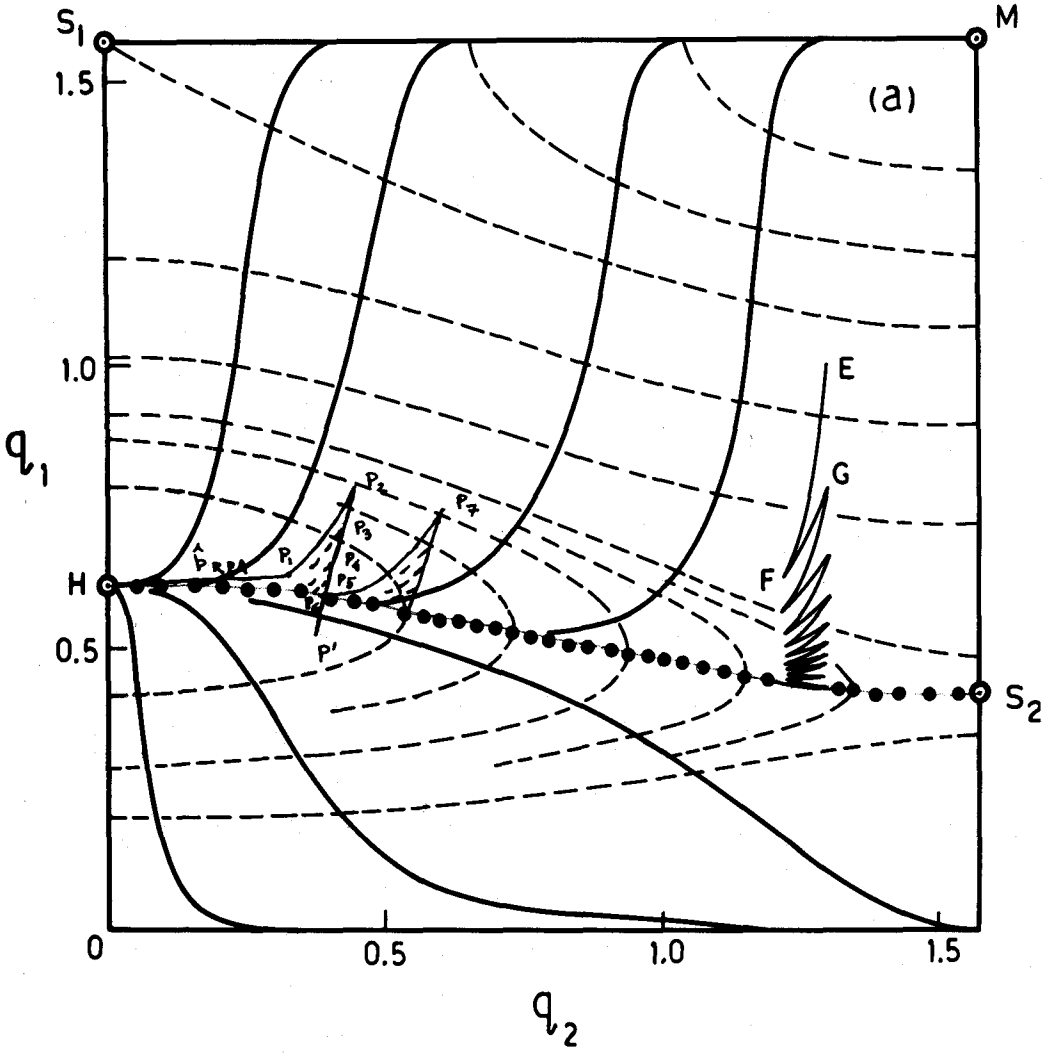

Figure: Schematic plot of ATDHF trajectory of the two-dimensional Lipkin model. Crossed line represents the valley path. The procedure to trace out the valley path is also shown (see the text). H is the static HF minimum and S_1 and S_2 are the saddle points of the potential.

Along with eq. (25) one has to satisfy the consistency conditions (22). The following procedure schematically explained in the figure can be adopted to achieve the consistency. With the displacement operator $\hat{p}_{RPA}$ of the lowest frequency RPA mode at the HF minimum we displace the static HF state by an amount δq and reach a point P_1 which is not a singular point of the eqs. (21). With P_1 as the initial condition we solve the eqs. (21) along which V(q) increases and after a few steps reach the point P_2 which in general does not satisfy eqs. (22). At P_2 we give a kick to the system with the momentum operator $\hat{p}$ corresponding to the point P_2 and at each step of this kick we solve the ATDHF equations for two or three steps and check the consistency conditions (22). Thus along the kick P_2P' we will reach a point P_6 on the valley path where the consistency condition is satisfied. With P_6 as the initial condition we solve eqs. (21) in a direction along which V(q) diminishes and trace out a portion of the valley path. Repeat the process with the point P_6 playing the role of P_1 one obtains the collective path along with the classical Hamiltonian defined in eq. (14).

The coordinate representation of the ATDHF equations with a generalized Skyrme force is in progress. However in order to apply ATDHF theory to nuclear fission some relevant features have to be incorporated. The collective coordinate q represents the fission degree of freedom. Though the vibration of the nucleus along the fission path is trivially included in the theory the rotational motion of the nucleus along its fission path has to be incorporated. This can be done by using cranked TDHF equation to derive the ATDHF equations and including a centrifugal term in the classical Hamiltonian (14).

Discussions with D.M. Brink, K. Goeke and a correspondence with P.-G. Reinhard are gratefully acknowledged.

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