Technique for evaluating the optimal path in adiabatic time-dependent Hartree-Fock theory

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A method of achieving the consistent solution of the adiabatic time-dependent Hartree-Fock theory as the optimal path is discussed. The method is applied to evaluate the valley path in the soluble three-level model.

The adiabatic time-dependent Hartree-Fock (ATDHF) theory for the microscopic description of the large-amplitude collective motions of nuclei, e.g., soft nuclear vibrations, fission, fusion, etc., has been formulated by Villars,[1] by Baranger and Véneroni,[2] and by Goeke and Reinhard.[3]

The formal identity of the above approaches has been established in Ref. 4 and it has been argued there[4] that for consistent exploitation of the TDHF variation principle in the adiabatic limit, the second-order ATDHF equation in conjunction with the zeroth- and first-order equations, the latter two being usually called the Villars equations, has to be taken into account. With the use of a formal but analytic method involving operator algebra it has been shown[4] that for any adiabatic process the simultaneous fulfillment of the Villars equations and the consistency condition, the latter being derived[4] from the second-order ATDHF equation, lifts the non-uniqueness[5,6] inherent in the Villars equations and results in a unique path following the bottom of the valley of the many-body potential-energy surface. The canonicity condition has been shown[7] to be a normalization requirement which, when taken into account, completes the above proof that the solution of the ATDHF theory follows the valley.

The ATDHF equations in the one-body form have been cast[8,9] in a representation in which the one-body time-even density matrix is diagonal. The Villars equations are combined to yield[8,9] a TDHF-like evolution equation for the occupied (hole) single-particle states $|\phi_h(q)\rangle$,

$$\frac{\partial}{\partial q}|\phi_h(q)\rangle = -i\hat{p}(q)|\phi_h(q)\rangle \ . \tag{1}$$

Here,

$$-i\hat{p}(q)=c(q)(1-\rho_0)\hat{e}(q) \ , \tag{2a}$$

$$c(q)=m(q)/\lambda(q) \ , \tag{2b}$$

$$\lambda(q)=\frac{dV}{dq} \ , \tag{2c}$$

$$\hat{e}(q)=h_0(1-2\rho_0)h_0+\bar{h}_1 \ , \tag{3a}$$

$$\rho_0(q)=\sum_h |\phi_h(q)\rangle\langle\phi_h(q)| \ , \tag{3b}$$

where $V(q)$ and $m(q)$ are the usual collective potential and collective mass.

The consistency condition is reduced[8,9] to the form

$$(1-\rho_0)R|\phi_h(q)\rangle=0 \ , \tag{4}$$

where the consistency operator R is given by

$$R=[h_0,\hat{e}]+\bar{h}_c-\omega_0(q)h_0 \ . \tag{5}$$

Here,

$$\bar{h}_c=\bar{h}_q-\tfrac{1}{2}\bar{h}_2 \ , \tag{6a}$$

$$\bar{h}_q=\mathrm{Tr}\bar{v}[\hat{e},\rho_0] \ , \tag{6b}$$

$$\omega_0(q)=\frac{1}{2\lambda}\frac{d}{dq}(\lambda^2/m) \ . \tag{2d}$$

The TDHF Hamiltonian in different orders of the adiabaticity parameter p is given by

$$h_0=t+\mathrm{Tr}\bar{v}\rho_0 \ , \tag{6c}$$

$$\bar{h}_1=\mathrm{Tr}\bar{v}[h_0,\rho_0] \ , \tag{6d}$$

$$\bar{h}_2=\mathrm{Tr}\bar{v}[(1-\rho_0)h_0\rho_0+\rho_0h_0(1-\rho_0),[h_0,\rho_0]] \ . \tag{6e}$$

Here t and v are, respectively, the kinetic energy and the two-body interaction potential. We thus have a representation of the ATDHF equations in which the occupied single-particle states evolve in accordance with a TDHF-like evolution equation (1) while in order to choose the optimal valley solution from the infinite number of solutions of the Villars equations (1) we are required to fulfill a one-body consistency condition (4).

Though given a nonsingular initial condition, the TDHF-like evolution Eq. (1) appearing here in ATDHF theory can be solved in a manner similar to those followed in TDHF calculations; the method of fulfillment of the consistency condition (4) is not yet clear. In what follows we describe a method to achieve the optimal path with the use of the consistency check (4) along with the evolution Eq. (1), the knowledge of the Hartree-Fock (HF) ground state, and the lowest-energy random-phase-approximation (RPA) mode there. With the HF configuration as the state to start with, the following procedure is suggested.

(i) Displace the HF state at $H(q=q_0)$ to a point at $P_I(q=q_I)$ by the generator of the lowest-frequency RPA mode (P_{RPA}).

(ii) In general, the point $q=q_I$ does not satisfy the consistency condition (4). However, it is a nonsingular

point of the differential equation (1). With $q=q_I$ as the initial condition the evolution equation (1) is solved in the forward (up-the-hill) direction along which $V(q)$ increases [$\lambda(q)>0$] to roll the system to a point $P_1(q=q_1)$ away from the valley.

(iii) At the point $q=q_1$ a kick[10] is given to the system to reach a point $P_e(q=q_e)$ with the generator $\hat{p}(q_1)$ at the state $q=q_1$ in the backward (down-the-hill) direction. Along the kick q_1q_e the satisfaction of the consistency condition(4) is checked at regular intervals at the points $P_1(q=q_1)$, $P_2(q=q_2)$, $P_3(q=q_3)$, etc.

(iv) If in the interval q_1q_e [Eq. (4)] is satisfied to a desired accuracy, say, at a point $P_v(q=q_v)$ then the evolution Eq. (1) can be solved with $q=q_v$ as the initial condition down the hill along which the ATDHF solutions are stable and thus obtain the segment of the valley q_vq_0. If Eq. (4) is not satisfied to a desired accuracy, whence we guess that the kick given in (iii) does not intersect the valley as may be the case in three- and higher-dimensional problems, then the measure of satisfaction of Eq. (4) can be minimized at a certain point $q=q_1$ which is nearest to the valley in the kick q_1q_3. With $q=q_1$ as the initial condition in place of $q=q_1$ for the kick of step (iii) the processes (iii) and (iv) are repeated. We expect that after a plausible number of such processes Eq. (4) will be satisfied to a desired accuracy and we have a point $q=q_v$ on the optimal path.

(v) With $q=q_v$ as the initial condition we solve the evolution equation (1) up the hill to reach a point $P_1'(q=q_1')$. In general, $q=q_1'$ will not be on the valley path. However, with $q=q_1'$ as the initial condition for kick in step (iii) we repeat steps (iii) and (iv) to obtain further segment of the valley P_vP_v'; in this way we can trace the entire valley path and obtain the collective mass and collective potential on it.

Goeke *et al.*[11–13] have also used a trial and error method for achieving the optimal path. However, they have not used the consistency check which is required to assure that the solution chosen is really the optimal valley solution. Further, the trial and error method used by Goeke *et al.* is effective only when one has an idea of the saddle configuration and uses a configuration near it as the initial condition.

We shall now use the aforementioned method of exploring the optimal path for evaluating the valley path in the three-level model. We shall only use the knowledge of the Hartree-Fock minimum and the lowest-energy RPA mode in the model as input and the solution of Eq. (1) which represents the lines of force orthogonal to the equipotential surfaces as the guide in exploring the valley path designated by Eq. (4).

Since the description of the three-level Lipkin model is discussed extensively in the literature[14] and the ATDHF formulation in the framework of the model has also been discussed in Refs. 5, 6, 14, and 15, we shall omit the necessary steps for arriving at the equation of the path and shall cite these references at appropriate places.

In the three-level model there are three N-fold degenerate states having N particles distributed between them in accordance with the interaction among N-particles, which is assumed to be only of monopole-monopole nature.

The solution of the zeroth- and first-order Villars equations or equivalently Eq. (1) can be written[16] in the model as a system of partial differential equations,

$$c^{-1}(q)\frac{\partial\theta_i}{\partial q}=\sum_{j=1}^{2}M_{ij}^{-1}\frac{\partial V}{\partial\theta_j}\ . \tag{7}$$

Here θ_i ($i=1,2$) are a set of real numbers required to parametrize the time-even Slater determinants in the three-level Lipkin model. q is the collective coordinate designating the collective path. $M_{ij}^{-1}(\theta_1,\theta_2)$ ($i,j=1,2$) and $V(\theta_1,\theta_2)$ are, respectively, the mass matrix and the many-body potential function. $c(q)$ is given in Eq. (2b).

It can be shown easily following the steps used in Ref. 4 that the simultaneous fulfillment of the second-order ATDHF equation leads, in the model, to the condition

$$\left[\frac{\partial U}{\partial\theta_i}\right]-\omega_0(q)\left[\frac{\partial V}{\partial\theta_i}\right]=0,\quad i=1,2\ . \tag{8}$$

Here U is the first-order gradient function defined as

$$U=|\mathrm{grad}V|^2=\sum_{i,j=1}^{2}\left[\frac{\partial V}{\partial\theta_i}\right]M_{ij}^{-1}\left[\frac{\partial V}{\partial\theta_j}\right]\ , \tag{9}$$

and $\omega_0(q)$ is an arbitrary Lagrange multiplier given in Eq. (2d). Equations (8) are essentially the same as Eq. (4). Equations (8) express the fact that the first-order gradient function is minimal for excursions along the equipotentials and thus Eqs. (8) are the conditions for valley path.

$V(\theta_1,\theta_2)$ and $M_{ij}^{-1}(\theta_1,\theta_2)$ for the three-level model can be explicitly calculated[15,16] as functions of (θ_1,θ_2) and are given in Refs. 15 and 16 and we would not repeat it here.

Equation (7), representing the solution of Villars equations, can be written[5,6,15,15] as a first-order ordinary differential equation,

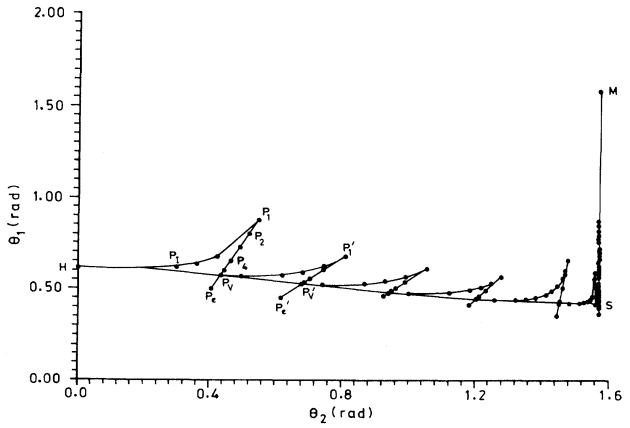

FIG. 1. The entire topography in the three-level model ($\kappa=3.0$, $n=1$) of the roll and kick method of exploring the optimal path described in the text. H, M, and S are, respectively, the minimum, maximum, and saddle point of $V(\theta_1,\theta_2)$. HP_I is the lowest-frequency RPA mode. $HP_vP_v'\cdots$ is the optimal valley path.

TABLE I. The numerical results of the application to the three-level model of the roll and kick method of exploring the optimal path described in the text. The nomenclature of different points used is the same as those used in the text.

Reference point in Fig. 1	θ_1 (rad)	θ_2 (rad)	$F(\theta_1,\theta_2)$	Obtained from the earlier point with the use of	Remarks
H	0.615	0.0	×	Initial point	Static Hartree-Fock pt.
P_I	0.615	0.3	55.23	Lowest-frequency RPA displ. at H	Away from the valley
P_1	0.873	0.55	178.69	Forward roll with P_I as the initial condition	Further away from the valley
P_2	0.798	0.521	134.05	Backward kick at P_1 with $P_{\mathrm{ATDHF}}(q_1)$	Nearer to the valley
P_3	0.723	0.492	107.62	Backward kick at P_1 with $P_{\mathrm{ATDHF}}(q_1)$	Nearer to the valley
P_4	0.648	0.463	49.93	Backward kick at P_1 with $P_{\mathrm{ATDHF}}(q_1)$	Nearer to the valley
P_5	0.573	0.434	1.9	Backward kick at P_1 with $P_{\mathrm{ATDHF}}(q_1)$	Nearer to the valley
P_e	0.498	0.406	−20.48	Backward kick at P_1 with $P_{\mathrm{ATDHF}}(q_{1)}$	Opposite side of the valley
P_v	0.569	0.433	0.0002	Backward kick at P_1 with $P_{\mathrm{ATDHF}}(q_1)$	Converges on the valley
P_1'	0.673	0.808	147.83	Forward roll with P_v as the initial condition	Away from the valley
P_e'	0.448	0.614	−21.73	Backward kick at P_1' with $P_{\mathrm{ATDHF}}(q_1')$	Opposite side of the valley
P_v'	0.521	0.677	0.0009	Backward kick at P_1' with $P_{\mathrm{ATDHF}}(q_1')$	Converges on the valley

$$\frac{d\theta_1}{d\theta_2}=\frac{X_1(\theta_1,\theta_2)}{X_2(\theta_1,\theta_2)}\ , \tag{10}$$

where the functions $X_i(\theta_1,\theta_2)$ $(i=1,2)$ are given by

$$X_i(\theta_1,\theta_2)=\sum_{j=1}^{2} M_{ij}^{-1}\frac{\partial V}{\partial\theta_j},\quad i=1,2\ . \tag{11}$$

The lines of force are therefore the solution to the first-order differential equation (10).

Eliminating the Lagrange multiplier $\omega_0(q)$ between the two Eqs. (8) the valley condition reduces to

$$F(\theta_1,\theta_2)=0\ , \tag{12}$$

where the function $F(\theta_1,\theta_2)$ is given by

$$F(\theta_1,\theta_2)=\frac{\partial(U,V)}{\partial(\theta_1,\theta_2)}\ . \tag{13}$$

Here the Jacobian is given by

$$\frac{\partial(u,v)}{\partial(x,y)}=\frac{\partial u}{\partial x}\frac{\partial v}{\partial y}-\frac{\partial u}{\partial y}\frac{\partial v}{\partial x}\ . \tag{14}$$

We are required to solve the differential Eq. (10) satisfying the consistency check (12). To achieve this we apply the method of exploring the optimal path described earlier in this paper. The numerical results are given in Table I and Fig. 1, in which the minimum value of $F(\theta_1,\theta_2)$, for which we conclude that the point (θ_1,θ_2) is on the valley, is chosen to be 10^{-3}. Even though the solution of Eq. (12) can be obtained in a straightforward manner without using the said method, we observe from Fig. 1 and Table I how for nontrivial problems the above method converges on the valley path.

We conclude the present paper with the notion that an efficacious method for exploring the optimal path has been successfully applied for evaluating the valley path in the soluble three-level model.

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