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Adiabatic time-dependent Hartree-Fock theory with the consistency condition

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Abstract. Adiabatic time-dependent Hartree-Fock (ATDHF) theory, including the authors' work in this field, has been summarised. In response to the criticism of Yamamura *et al* the role of curvature in preventing the choice of *pure* RPA mode as the solution near the static Hartree-Fock minimum has been discussed.

Keywords. ATDHF; nuclear fission; Lipkin model; pure RPA mode.

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1. Introduction

In recent years there has been an increasing interest among nuclear theorists in developing a microscopic theory for the description of nuclear dynamics. The success of the mean-field approximation in describing the static properties of nuclei as well as the incredible ease of the Hartree-Fock (HF) calculation (Vautherin and Brink 1973) attained with the use of the density-dependent effective two-body interaction suggests that the mean-field approximation could also be used to describe nuclear dynamics. The old formulation on the time-dependent Hartree-Fock (TDHF) theory due to Dirac (1930) has been revived (Bonche *et al* 1976) designing it for the description of the time-dependent nuclear processes, especially for the large amplitude collective motions of nuclei. Sufficient progress has been made (Negele 1982) in the last decade in applying the TDHF theory for the description of heavy-ion collision and encouraging results for the deep-inelastic scattering, fusion events etc have been obtained. However, the limitations of TDHF in describing such many-body processes like nuclear fission, for which a description in terms of barrier penetration is traditionally employed, have become clear (Reinhardt 1981), the TDHF solution gets trapped inside the barrier and can never lead to fission into separated fragments.

An independent formalism, namely, the adiabatic time-dependent Hartree-Fock (ATDHF) theory has been formulated (Baranger and Veneroni 1978; Brink *et al* 1976; Villars 1977; Moya De Guerra and Villars 1977; Goeke and Reinhard 1978) in the last few years especially designed for those processes whose dynamical evolution is governed by one or a few collective variables and in which the collective motion is slow compared to the single particle oscillations. Typical examples of such process are the nuclear fission and the inverse process, the sub-barrier fusion of two heavy ions.

Investigations have been carried out by several groups of workers (Reinhard and Goeke 1978; Goeke *et al* 1981; Rowe 1982; Rowe and Ryman 1982; Moya De Guerra and Villars 1978; Mukherjee and Pal 1981, 1982a, b) on whether the conditions derived from the mean-field theory of the adiabatic many-body process provide a unique

specification of the collective subspace. It has turned out in these investigations (Mukherjee and Pal 1982a, b; Pal 1984) that the zeroth- and first-order ATDHF equations, called the Villars equations, supplemented with a consistency condition derived from the second-order ATDHF equation specify the collective path uniquely. Further, it is a satisfying result, as has been proved analytically by Mukherjee and Pal (1982a) that the path followed by the many-body system during its adiabatic motion is indeed the 'fission path' which follows the bottom of the valley. In §2 a short review of the ATDHF theory has been included.

However there has been a certain criticism due to Yamamura *et al* (1984) on the results obtained by Mukherjee and Pal (1981) regarding the non-uniqueness of the solution of Villars equations. In the context of the three-level Lipkin model it has been argued by Yamamura *et al* (1984) that in the neighbourhood of a critical point of the collective potential the canonicity condition along with the RPA boundary condition restricts the solutions of the Villars equations to be unique and is given by the lowest-frequency principal line. In §3 emphasizing the role of curvature of the collective path, the ambiguity of the prescription used by Yamamura *et al* (1984) in order to choose the unique path has been clarified. Concluding remakrs are presented in §4.

2. The ATDHF theory

The ATDHF theory has been developed primarily by Baranger and Veneroni (BV) (1978), Brink *et al* (1976), Villars (1977), Moya De Guerra and Villars (1977).

Baranger and Veneroni (1978) used the language of density matrix and the theory was cast in a form independent of any initial parametrisation. Using the TDHF equation the equations of motion as a function of time for the evolution of the time-even single-particle density matrix and the corresponding momentum matrix have been obtained; adiabaticity in this work implies that the momentum matrix is 'small' in some sense. Given the initial values of the time-even density and the momentum matrix the equations of motion can be integrated taking small time steps. Using the density and the momentum matrix the existence of a collective Hamiltonian has been established and the Schrödinger equation corresponding to the classical Hamiltonian can be solved to compute any observables pertaining to the collective motion.

In the formulation of Villars and coworkers (Villars 1977; Moya De Guerra and Villars 1977) the theory is cast in terms of the state vectors that are parametrised right from the beginning in terms of two parameters—one to play the role of collective co-ordinate q and the other that of the collective momentum p. Assuming that the momentum p is small which assures the adiabaticity the TDHF equation has been used (Villars 1977) perturbatively in powers of the adiabaticity parameter p and the hierarchy of ATDHF equations has been obtained (Villars 1977). The zeroth- and first-order ATDHF equations, usually called the Villars equations, are given by

$$\langle \delta\Phi(q) \left| H - \frac{\mathrm{d}V}{\mathrm{d}q} Q \right| \Phi(q) \rangle = 0, \tag{I}$$

$$\langle \delta\Phi(q) | [H, iQ] - P/m(q) | \Phi(q) \rangle = 0. \tag{II}$$

Here P and Q are one-body particle-hole (p-h) type operators and the former is the generator of displacement in the time-even Slater determinantal space $|\Phi(q)\rangle$. The

collective potential $V(q)$ and the collective mass $m(q)$ are given by,

$$V(q) = \langle \Phi(q)|H|\Phi(q)\rangle, \tag{1a}$$

$$m^{-1}(q) = \langle \Phi(q)|[[H, iQ], iQ]|\Phi(q)\rangle. \tag{1b}$$

At any point in the Slater determinantal space defined by $|\Phi(q)\rangle$ and its 1p-1h excited states $|\Phi_{ph}(q)\rangle$, (I) is an equation for the determination of the ph-components of Q in terms of those of the given Hamiltonian, while (II) determines the ph-components of the operator P which is the generator of displacement. In obtaining the time-even state $|\Phi(q+\delta q)\rangle$ at the neighbouring point with the help of the generator P a normalisation factor (λ/m) is required which is obtained by choosing the collective submanifold (in this case a single collective co-ordinate q) in terms of a measuring operator D,

$$q = \langle \Phi(q)|D|\Phi(q)\rangle, \tag{2a}$$

or

$$\langle \Phi(q)|[D, -iP]|\Phi(q)\rangle = 1. \tag{2b}$$

It is to be emphasized here that the direction in the ph-space defined by the operator P is independent of the choice of this normalisation.

In this manner starting from *any* point (not a critical point) in the Slater determinantal space a unique path can always be obtained. By varying the starting point one can thus generate an infinite number of non-intersecting paths which are solutions of the Villars equations and converge at the nodal point of the potential function. It should be noted here that at the critical points where $dV/dq = 0$ (I) does not determine Q and hence the procedure for generating a solution of the Villars equations (I) and (II), as described above, does not go through if a critical point is chosen in practice to start the solution.

In order to explore the feasibility of obtaining the ATDHF path, the theory has been applied (Moya De Guerra and Villars 1978; Mukherjee and Pal 1981) to describe a solvable model, namely, the three-level Lipkin model. In the context of the three-level model the Villars equations reduce (Moya De Guerra and Villars 1978; Mukherjee and Pal 1981) to a non-linear first-order ordinary differential equation of which the critical points of the collective potential *i.e.* the minimum, maximum, the saddle point etc are the singular points. All the solutions of the differential equation passes through the HF minimum which is then called the nodal point. With the use of a property regarding the behaviour of the solutions of the differential equation near the nodal point it has been shown (Mukherjee and Pal 1981) analytically that at the HF minimum the slopes of all the solutions including the valley path but excluding the higher-frequency principal line are the same as that of the lowest frequency RPA mode and thus the non-uniqueness of the solution of the Villars equations has been established.

The solutions of Villars equations are shown (Mukherjee and Pal 1982a) to represent the lines of force orthogonal to the equipotential surface on the curved space of the time-even Slater determinants and thus the non-uniqueness of the solution has been established in general, irrespective of the model. Through any point in the space of time-even Slater determinants there exists a line of force representing the solution of the Villars equations at that point. All these infinite numbers of non-intersecting solutions converge at the HF minimum and therefore the Villars equations with the boundary condition that the solution should behave like the lowest-frequency RPA mode near the HF minimum does not in general yield a unique ATDHF path. In particular in the case of a finite dimensional model like the Lipkin model where there are only two RPA modes, it is

obvious that an infinite number of lines of force representing the solution of the Villars equations ought to behave at the nodal point as either of the RPA modes.

It is to be noted here that in the ATDHF theory one is specifically interested in extracting a collective submanifold (in this case a one-dimensional path) on which the dynamics of the many-body system is governed by the Hamilton's equations of motion corresponding to a classical collective Hamiltonian defined on the collective submanifold. It is, however, intuitive on physical grounds as has been recognized frequently in the past in the macroscopic description of nuclear fission (Hill and Wheeler 1953) that physical systems describing adiabatic motion should follow the path along which the energy is minimised *i.e.* the path following the bottom of the valley. The valley of a potential function V is defined variationally as,

$$\delta\{|\text{grad } V|^2\} - \Lambda\,\delta V = 0, \tag{3}$$

i.e. the magnitude of the potential gradient is stationary for excursions along the equipotential surfaces. Here Λ plays the role of a Lagrange multiplier taking care of the constraint.

In view of the above non-uniqueness of the solution of Villars equations and the desire to explore the valley path as the optimal ATDHF solution Goeke and coworkers (Goeke and Reinhard 1978; Reinhard and Goeke 1978; Goeke *et al* 1980, 1981, 1983a, b) proposed a validity criteria for exploring the ATDHF path. It has been argued that to make the adiabatic assumption valid, a second-order quantity obtained from the second-order ATDHF equation should be *small* compared to the first-order contribution. In practice, however, they find (Goeke *et al* 1980, 1983a, b) that the ratio of the two contribution be *minimum* along the optimal path. Indeed the validity of the adiabatic assumption requires that the second-order quantity should be *small* compared to the first-order contribution; it is however not clear from theoretical grounds why their ratio should be *minimum* for the optimal solution of the ATDHF theory. Nevertheless in numerical calculations (Goeke *et al* 1980, 1983a, b) they have used 'trial and error' method for exploring the optimal ATDHF path.

However, to describe nuclear fission, the theory should provide in a consistent manner the optimal path as the lowest valley of the many-body potential energy surface. It has been established by Mukherjee and Pal (1982a) that simultaneous solution of the zeroth-, first- and second-order ATDHF equations indeed delineates the lowest valley as the optimal solution of the ATDHF theory.

The formal identity of the ATDHF approaches of Villars and of Baranger and Veneroni (BV) has been established (Mukherjee and Pal 1982a; Pal 1984). It has been demonstrated that while the BV approach mixes the zeroth- and second-order quantities, Villars neglects the second-order quantity altogether. In the spirit of the perturbation approach the second-order equation,

$$\langle \delta\Phi(q)|\tfrac{1}{2}[[H, iQ], iQ] - \tfrac{1}{2}\frac{dm^{-1}}{dq}Q + m^{-1}\frac{dQ}{dq}|\Phi(q)\rangle = 0, \tag{III}$$

should be considered as a separate equation. It has been shown by Mukherjee and Pal (1982a) that for consistent exploitation of the time-dependent equation in the adiabatic limit the second-order equation (III) should be considered as a separate equation along with the zeroth- and first-order Villars equations (I) and (II).

Since, as has been noted earlier, the zeroth- and first-order equations can be solved,

given a time-even determinantal state as the initial condition, the simultaneous fulfilment of the second-order equation calls for a consistency condition,

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

derived from the zeroth- and second-order equations to be satisfied. Here,

$$\omega_0(q) = \frac{1}{\lambda}\frac{\mathrm{d}}{\mathrm{d}q}(\lambda^2/m). \qquad (4)$$

It is a satisfying result as has been proved by Mukherjee and Pal (1982a) by an analytic method (without invoking any model) that the consistent solution of Villars equations (I) and (II) satisfying the consistency condition (III') yields a unique path. In the space of the time-even Slater determinant for which the mass matrix plays the role of the metric tensor characterising the space, the solution represents the valley of the collective potential satisfying the variational equation (3) with $\omega_0(q)$ playing the role of the Lagrange multiplier Λ.

It should be noted here that having obtained the optimal collective path, the classical Hamiltonian defined on the optimal path can be established and with the use of the Schrödinger equation corresponding to the classical Hamiltonian the observables pertaining to fission may be computed.

However it is to be noted that the ATDHF theory indeed yields the Hamilton's equation of motion corresponding to the classical Hamiltonian,

$$\mathscr{H}(p, q) = \frac{p^2}{2m(q)} + V(q) \qquad (5)$$

provided the canonicity condition,

$$\langle \Phi(q) | [Q, -iP] | \Phi(q)\rangle = 1 \qquad (6)$$

is satisfied.

The canonicity condition (6) is interpreted (Villars 1977; Goeke and Reinhard 1978; Reinhard and Goeke 1978; Mukherjee and Pal 1982a, b; Goeke *et al* 1980, 1983a, b) as a normalisation condition of the operators Q and P. Along with the equation (2b) that specifies the collective co-ordinates in terms of the measuring operator D, the canonicity condition (6) has been shown (Mukherjee and Pal 1982b; Goeke *et al* 1980, 1983a, b) to yield an equation for determining the collective mass $m(q)$ consistent with the definition (1b).

3. Non-uniqueness in the Lipkin model

In the context of the three-level Lipkin model Yamamura *et al* (1984) obtained the solution of the linearised Villars equations (I) and (II) in the neighbourhood of a critical point which are in essence the same as those obtained by Mukherjee and Pal (1981). Yamamura *et al* (1984) concluded that the slopes of all these solutions at the critical point are the same as that of the lowest frequency RPA mode. The above conclusion is true only when the critical point is a nodal point characterised by the fact that the square of the RPA eigenvalues are of the same sign. If the RPA eigenvalues (squared) are of

opposite sign characterising the saddle point the principal lines which designate the RPA mode is the only solution (Mukherjee and Pal 1981).

The requirement of the RPA boundary condition demands that,

$$(\partial^2 V/\partial q^2)_{q=q_{HF}} = \lambda_1, \tag{7}$$

where λ_1 is the lowest eigenvalue of the RPA matrix.

The canonicity condition of (6) linearised about the critical point along with the substitution of (7) and the afore-mentioned solution of the linearised Villars equations, can be written, following Yamamura *et al* (1984) as

$$(A^2-1)\lambda_1^2\xi^2 + B^2\lambda_2^2\xi^{2\mu} = 0. \tag{8}$$

Here A and B are constants of integration, λ_1, λ_2 are the RPA eigenvalues (squared) with $\mu = \lambda_2/\lambda_1$. In order to avoid confusion with the operator Q a new notation $\xi = q - q_{HF}$ has been used in place of the notation Q of Yamamura *et al* (1984).

It is to be noted here that in deriving (8) the orthonormality of the RPA eigenvectors with respect to the metric $\mathbf{M}^{-1}$ (Mukherjee and Pal 1981) has been used.

It has been argued by Yamamura *et al* (1984) that (8) is satisfied if and only if,

$$A^2 \approx 1, \tag{9a}$$

$$B = 0. \tag{9b}$$

Condition (9) is a particular solution of the linearised Villars equations namely the principal line designating the lowest-frequency RPA mode. Yamamura *et al* (1984) concluded that the solution of the Villars equations (I) and (II) satisfying the canonicity condition (Baranger and Veneroni 1978) yields a unique path which is given by the solution of the ATDHF equations (I) and (II) satisfying the boundary condition that the solution in the neighbourhood of the critical point is given by the lowest-frequency principal line characterised by (9). The lacuna in this argument of Yamamura *et al* (1984) will now be clarified.

Let us discuss the linearisation of the Villars equations (I) and (II) about the static Hartree-Fock (HF) state. Since (I) is satisfied for all values of q its derivative with respect to q should also be satisfied,

$$\langle \delta\Phi(q)|[H, -iP] - C(q)Q - \lambda(q)\frac{dQ}{dq}|\Phi(q)\rangle = 0. \tag{10}$$

Here $\lambda(q) = dV/dq$ and $C(q) = d\lambda/dq$. At the critical point of the potential where $\lambda(q) = 0$ (I) does not determine, as noted earlier after (2b), the p-h components of Q; instead at that point it represents the static HF condition. In the *neighbourhood* of the HF point if the curvature of the path is neglected then $dQ/dq = 0$ and (10) can be written as,

$$\langle \delta\Phi(q)|[H, -iP] - C(q)Q|\Phi(q)\rangle = 0. \tag{11}$$

Note that exactly at the HF point, $\lambda(q) = 0$, the third term in (10) drops out and (11) is exact.

Equation (11) along with (II) can easily be reduced to the RPA eigenvalue equation,

$$\mathbf{R}|X_{hp}\rangle = \omega(q)|X_{hp}\rangle, \tag{12}$$

where $\omega(q) = C(q)/m(q)$ and $\mathbf{R}$ is the RPA matrix. We thus conclude that at the HF point the solutions are the RPA modes and the lowest energy solution is the lowest RPA mode.

However, due to the curvature effect, this does not preclude the possibility of many solutions in the neighbourhood of the HF point terminating at that point with the slope of the pure lowest RPA mode.

The curvature term (dQ/dq) in (10) cannot be neglected in the neighbourhood of the HF point as can be seen from the second-order equation (III), which gives (Mukherjee and Pal 1982a)

$$\langle \delta\Phi(q)|\frac{dQ}{dq}|\Phi(q)\rangle = \frac{m}{2}\langle \delta\Phi(q)|[[H, iQ], iQ] - \frac{dm^{-1}}{dq} Q|\Phi(q)\rangle. \tag{13}$$

It therefore follows that although the solution of the ATDHF equations in the limit $(q \to q_{HF})$ behaves like the decoupled RPA solution, in the neighbourhood of the HF minimum, the solution cannot be given by a *pure* RPA mode but is a superposition of the RPA modes which is dictated by the non-vanishing curvature.

The above assertion has been demonstrated in the context of the three-level Lipkin model by Mukherjee and Pal (1981) and in order to clarify further we reproduce here (figure 1) one of the figures of Mukherjee and Pal (1981) where the lowest-frequency RPA mode is shown as the line HR which excepting at the HF point is not an ATDHF solution. In the ATDHF numerical calculations (Goeke *et al* 1980, 1983a, b) of the fusion of $O^{16} + O^{16}$ this ambiguity of starting the solution at the HF state of the compound system has been clearly felt and the optimal path is obtained by trial and error method starting from a point far off from the HF state.

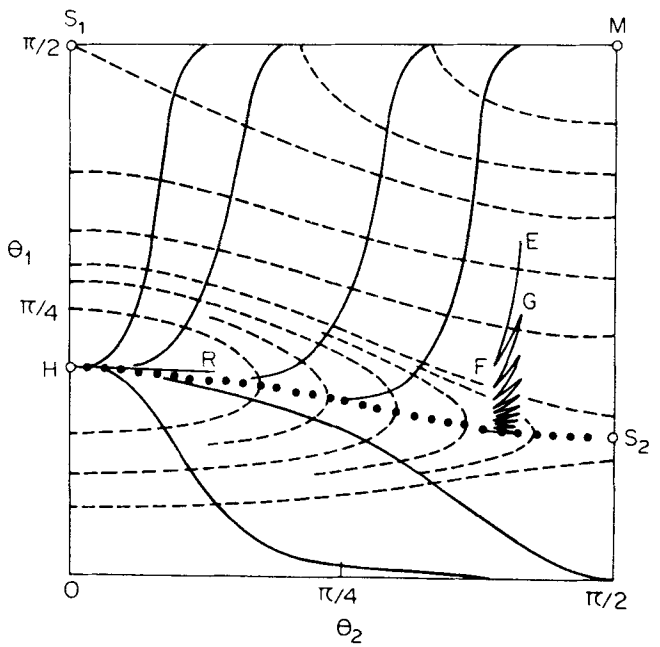

Figure 1. The entire topography of ATDHF paths (continuous lines) along with the contour plot (dashed lines) of $V(\theta_1, \theta_2)$ for the case $x > (n+1)$ $(x = 3, n = 1)$ with the maximum M, minimum H and the two saddle points S_1 and S_2 of $V(\theta_1, \theta_2)$ are shown. The optimal path following the bottom of the valley is shown by heavy dots. The line HR (parallel to the θ_2-axis) represents the lowest-frequency RPA mode.

In the adiabatic motion the nuclear system will in general start oscillations in a superposed mode and is expected to choose an optimal path along which the energy is minimised. This is the path which satisfies the consistency condition (III'). We therefore conclude that instead of constraining the system to choose a *pure* RPA mode, the system should be given the freedom to choose its lowest energy path which is obtained numerically by satisfying the canonicity condition. Constraining the solution deliberately as is done in Yamamura *et al* (1984) may be at best a good mathematical exercise with no utility for the physics of the large-amplitude nuclear collective motion for which delineating the valley path is to be set as a physically more desirable goal. Even within the three-level model the solution generated with the mathematical constraint of Yamamura *et al* (1984) departs considerably from the valley path as seen from the figure.

In the context of the three-level Lipkin model it thus follows from the above discussions that even in the neighbourhood of the HF point, the principal lines are not a solution to the ATDHF equations (I) and (II) which in the Lipkin model reduce to a non-linear first-order ordinary differential equation and thus the prescription of solving (I) and (II) or equivalently the non-linear differential equation with a boundary condition of particular solution (in the neighbourhood of the HF point) which itself is not a solution to the ATDHF equations is not clear to the present authors.

In our view (8) does not always imply that the condition (9) should be satisfied because of the following reason. The solutions of Villars equations (I) and (II) are obtained by linearising (I) about the critical point and therefore in essence is equivalent to (11) in which the curvature has been neglected. Further the canonicity condition is also linearised about the critical point. In such a linearised ATDHF theory we can only demand that (8) should be satisfied only in the limit ($\xi \to 0$). If the limit ($\xi \to 0$) of (8) is utilised two situations arise:

(i) If $\mu > 0$ characterising the nodal point then in the limit ($\xi \to 0$) (8) is satisfied for *all values* of A and B including those of (9) and thus the principal line is not the only solution that satisfies the canonicity condition (8) but a whole host of solutions of Villars equations along with the principal line satisfies the canonicity condition and behave like the lowest-frequency RPA mode near the HF minimum.

(ii) If $\mu < 0$ characterising the saddle point then in the limit ($\xi \to 0$) (8) implies that (9) must be satisfied and thus the principal line is the only solution.

Thus the assertion of Yamamura *et al* (1984) that in the neighbourhood of a *critical point* the only solution of Villars equations that satisfies the canonicity condition (6) and *behave* like the lowest frequency RPA mode is the lowest-frequency principal line is true only when the *critical point* is a *saddle point* but *not* a *nodal point* and therefore the results established in our work (Mukherjee and Pal 1981, 1982a, b) contrary to the criticism of Yamamura *et al* (1984) are correct and valid.

4. Conclusions

In this paper the non-uniqueness of the solution of Villars equations satisfying the canonicity equation and the RPA boundary condition, in contrast to the criticism due to Yamamura *et al* (1984) has been established. The adiabatic time-dependent Hartree-Fock theory with the consistency condition which delineates in a consistent manner the 'fission path' desired by workers in this field has been summarised.

Until now the application of the ATDHF theory to realistic calculations has been limited to the fusion of two heavy-ions; the work has been carried out by Goeke *et al* (1980, 1983a, b). However the ATDHF theory is most suitable for describing nuclear fission as is clear from the text. So far it has not been applied to nuclear fission. Though theoretical investigations are required to incorporate some of the relevant features of fission, the numerical application of the theory to nuclear fission is the challenging problem to nuclear theorists in recent times.

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