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Do anticommutators give additional conditions on adiabatic time-dependent Hartree-Fock path?

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Abstract. Utilizing one-particle one-hole variations of ATDHF states by invoking commutators obtained from generators of complete set of coordinates and of momenta, the ATDHF equations were shown in an earlier work to yield the valley condition. In principle, variations of ATDHF states should also be exploited by using anticommutators involving the said generators. It is demonstrated here that owing to the canonicity condition relating the generators of coordinates and of momenta, use of anticommutators gives rise to exactly the same valley condition on the ATDHF path.

Keywords. ATDHF path; anticommutators; canonicity condition.

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The adiabatic time-dependent Hartree-Fock (ATDHF) theory for the microscopic description of large-amplitude collective motions of nuclei e.g. soft nuclear vibrations, fission, fusion etc. has been formulated by Villars (1977), Baranger and Vénéroni (1978) and Goeke and Reinhard (1978).

In Mukherjee and Pal (1982), the formal identity of the above approaches was established while arguing 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 (Villars) equations, has to be taken into account. Nonuniqueness [Mukherjee and Pal (1981, 1985)] of Villars equations was lifted by imposing the consistency condition derived from zeroth- and second-order equations via the elimination of the curvature term. Use of a formal but analytic operator algebra method then showed that the simultaneous fulfilment of Villars equations and the consistency condition results in a unique path following the bottom of the valley of the many-body potential energy surface for any adiabatic process. The canonicity condition completes (Mukherjee 1990) the above proof regarding the valley by determining the Lagrange multiplier.

The ATDHF variational equations are written in the form

$$\langle \delta\Phi | R | \Phi \rangle = \langle \Phi | R | \delta\Phi \rangle = 0. \tag{1}$$

Using complete set of particle-hole ($p-h$) operators Q_α, P_α, ($\alpha = 1, 2, \ldots, n$), eq. (1) can be written as

$$\langle \Phi | R Q_\alpha | \Phi \rangle = \langle \Phi | Q_\alpha R | \Phi \rangle = 0, \tag{2a}$$

$$\langle \Phi | R P_\alpha | \Phi \rangle = \langle \Phi | P_\alpha R | \Phi \rangle = 0. \tag{2b}$$

These can be expressed as two and only two pairs of necessary and sufficient conditions. One pair can be set up in the anticommutator form

$$\langle\Phi|[R, Q_\alpha]_+|\Phi\rangle = 0, \tag{3a}$$

$$\langle\Phi|[R, P_\alpha]_+|\Phi\rangle = 0, \tag{3b}$$

while the other the previous commutator form

$$\langle\Phi|[R, iQ_\alpha]|\Phi\rangle = 0 \tag{4a}$$

$$\langle\Phi|[R, -iP_\alpha]|\Phi\rangle = 0 \tag{4b}$$

where $[A, B] = AB - BA$ and $[A, B]_+ = AB + BA$. According as R is time-even or time-odd, eqs (3b) and (4a) or eqs (3a) and (4b) are identically satisfied and therefore the opposite pairs, namely, eqs (3a) and (4b) or eqs (3b) and (4a) are to be solved. The commutator-form eqs (4) have been used in Mukherjee and Pal (1982, 1985) (see also Fukui and Tsue 1991) to derive the valley condition on the ATDHF path. In this brief report we argue that in principle the anticommutator form, viz. eqs (3), should also be considered and examined whether these lead to any further conditions over and above those given by eqs (4).

The hermitian operators R for zeroth- and first-order Villars equations and the consistency condition, denoted by $R^{(0)}$, $R^{(1)}$ and $R^{(c)}$ respectively, are given by

$$R^{(0)} = H - \lambda Q, \tag{5}$$

$$R^{(1)} = [H, iQ] - P/m(q), \tag{6}$$

$$R^{(c)} = \tfrac{1}{2}\lambda^2[[H, iQ], iQ] + \frac{\lambda}{m}[H, -iP] - \lambda\omega_0(q)Q \tag{7}$$

where

$$\lambda = \frac{\mathrm{d}V}{\mathrm{d}q},$$

and

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

V and m being respectively the collective potential and collective mass. Here Q and P, the generators of momentum p and of coordinate q, are hermitian time-even and -odd $p-h$ operators respectively.

In eqs (2a) and (2b) we have used the fact that since time-even as well as -odd variations $|\delta\Phi\rangle$ of the time-even Slater determinantal state $|\Phi\rangle$ are, in general, $1p-1h$ excited states with respect to $|\Phi\rangle$ as vacuum, $|\delta\Phi\rangle$ can be expressed as

$$|\delta\Phi\rangle = Q_\alpha|\Phi\rangle \text{ or } P_\alpha|\Phi\rangle, (\alpha = 1, 2, \ldots, n).$$

Here P_α and Q_α are time-odd and -even $p-h$ operators obtained from the time-odd and -even linear combinations of the complete set of $p-h$ operators $C_p^+ C_h$ and $C_h^+ C_p$. The two complementary sets Q_α, P_α satisfy the orthogonality properties (Mukherjee and Pal 1982, 1985)

$$\langle\Phi|[Q_\alpha, Q_\beta]|\Phi\rangle = \langle\Phi|[P_\alpha, P_\beta]|\Phi\rangle = 0, \tag{8}$$

$$\langle\Phi|[Q_\alpha, -iP_\beta]|\Phi\rangle = \delta_{\alpha\beta}. \tag{9}$$

A representation for parameterizing the manifold of time-even Slater determinantal states was utilized. Such a state $|\Phi(x)\rangle$ in the neighbourhood of another determinantal state $|\Phi(0)\rangle$ was expressed through

$$|\Phi(x)\rangle = \exp(i\Sigma_\alpha x_\alpha P_\alpha)|\Phi(0)\rangle.$$

The set of real numbers $x=[x_\alpha]$, $(\alpha = 1,2,\ldots,n)$, parametrizes the state $|\Phi(x)\rangle$. Taking for time-even and -odd R eqs (5) and (6) respectively, the Villars equations as dictated by eqs (4) are reduced to differential conditions on the space $[x_\alpha]$ to be interpreted as lines of force orthogonal to equipotential surfaces. Then using eq. (7) for R it was shown that the restrictions imposed by the consistency condition single out the valley path as the consistent solution of the ATDHF theory from an infinite number of solutions of Villars equations. The canonicity relationship in turn identifies (Mukherjee 1990) $2\omega_0(q)$ as the Lagrange multiplier in the valley condition.

We shall now show that the conditions resulting from eqs (3) are same as those obtained from eqs (4). To this end we consider the case when R is *time*-even. The nontrivial conditions on the ATDHF path are in this situation [eqs (3a) and (4b)]. One can write

$$\begin{aligned}\langle\Phi|[R,-iP_\alpha]|\Phi\rangle = &-i\sum_\beta\{\langle\Phi|RQ_\beta|\Phi\rangle\langle\Phi|Q_\beta P_\alpha|\Phi\rangle \\ &+\langle\Phi|RP_\beta|\Phi\rangle\langle\Phi|P_\beta P_\alpha|\Phi\rangle\} \\ &+i\sum_\beta\{\langle\Phi|P_\alpha Q_\beta|\Phi\rangle\langle\Phi|Q_\beta R|\Phi\rangle \\ &+\langle\Phi|P_\alpha P_\beta|\Phi\rangle\langle\Phi|P_\beta R|\Phi\rangle\},\end{aligned} \tag{10}$$

where we have inserted complete set of $p-h$ states in between RP_α and $P_\alpha R$ and used the facts that P_α's are one-body $p-h$ operators and a complete set of $1p-1h$ states is generated by $P_\beta|\Phi\rangle$ and $Q_\beta|\Phi\rangle$, $(\beta = 1,2,\ldots,n)$.

Using the relation that follows from time-reversal

$$\langle\Phi|[P_\alpha,Q_\beta]_+|\Phi\rangle = 0,$$

in the first and third terms and (8) in the second and fourth terms of eq. (10), we find

$$\begin{aligned}\langle\Phi|[R,-iP_\alpha]|\Phi\rangle = &\sum_\beta\{\tfrac{1}{2}\langle\Phi|[R,Q_\beta]_+|\Phi\rangle\langle\Phi|[P_\alpha,iQ_\beta]|\Phi\rangle \\ &+\langle\Phi|[R,-iP_\beta]|\Phi\rangle\langle\Phi|P_\beta P_\alpha|\Phi\rangle\}.\end{aligned}$$

From the canonicity condition (9), one has

$$\langle\Phi|[R,-iP_\alpha]|\Phi\rangle = \tfrac{1}{2}\langle\Phi|[R,Q_\alpha]_+|\Phi\rangle + \sum_\beta\langle\Phi|[R,-iP_\beta]|\Phi\rangle\langle\Phi|P_\beta P_\alpha|\Phi\rangle. \tag{11}$$

If we require that (4b) is satisfied, the second term on the r.h.s. of (11) automatically vanishes and (3a) follows. We therefore conclude that (3a) gives the same condition on the ATDHF path as that originally given by (4b). Likewise in the case where R is time-odd, an identical conclusion ensues.

Thus, anticommutator-aided variations of ATDHF states do not lead to any additional condition on the ATDHF path because of the canonicity relation (9)—a manifestation that (x_α, π_α) are canonically conjugate variables satisfying Hamilton's equations. Therefore any one of the two conditions derived from either the commutator or the anticommutator may be used to delineate the collective valley path. Otherwise, new extraneous conditions emanating from the anticommutator could have generated unphysical restrictions on the valley path. Moreover, starting with a symplectic manifold (Rowe and Ryman 1982) ATDHF states can be shown to generate an underlying space which is in fact Riemanian (Klein *et al* 1991). Hence both anticommutators and commutators should give equivalent results and so previous findings by workers in this field are complete and fully consistent.

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