A new approach to the ATDHF equation

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To describe large-amplitude collective motion in atomic nuclei, several versions of the adiabatic time-dependent Hartree-Fock (ATDHF) theory have been proposed since the 1970's, but they encounter difficulties such as non-uniqueness of solutions. To overcome these problems, Matsuo *et al.* proposed an advanced version of the ATDHF theory, the adiabatic self-consistent collective coordinate (ASCC) method.[1)] Both the ATDHF and ASCC equations are given by the adiabatic expansion of the invariance principle of the Schödinger equation,

$$\delta\langle\phi(q,p)|i\partial_t - \hat{H}|\phi(q,p)\rangle = 0. \tag{1}$$

Here, q is the collective coordinate and p is its conjugate momentum. In this report, we focus on the ATDHF equation by Villars.[2,3)] According to the generalized Thouless theorem, the state vector in the ATDHF/ASCC theory can be written in the form of $|\phi(q,p)\rangle = e^{i\hat{G}(q,p)}|\phi(q)\rangle$. In the adiabatic expansion, $\hat{G}$ is expanded in powers of p. In the conventional ATDHF and ASCC theories, the expansion up to only the first order is considered. Recently, the ASCC theory including the second-order collective operator has been proposed.[4)] There, $\hat{G}(q,p)$ is expanded as $\hat{G}(q,p) = p\hat{Q}^{(1)}(q) + \frac{1}{2}p^2\hat{Q}^{(2)}(q)$, and the possible contribution of $\hat{Q}^{(2)}$ to the collective dynamics has been highlighted. In the ASCC theory including $\hat{Q}^{(2)}$, the equations of motion comprise the four equations below.

$$\delta\langle\phi(q)|\hat{H} - \partial_q V\hat{Q}^{(1)}|\phi(q)\rangle = 0, \tag{2}$$

$$\delta\langle\phi(q)|[\hat{H},\hat{Q}^{(1)}] - \frac{1}{i}\hat{P} - \frac{1}{i}\partial_q V\hat{Q}^{(2)}|\phi(q)\rangle = 0, \tag{3}$$

$$\delta\langle\phi(q)|[\hat{H},\frac{1}{i}\hat{P}] - \omega^2(q)\hat{Q}^{(1)} - \partial_q V\partial_q\hat{Q}^{(1)}|\phi(q)\rangle = 0, \tag{4}$$

$$\delta\langle\phi(q)|[\hat{H},\frac{1}{i}\hat{Q}^{(2)}] + [[\hat{H},\hat{Q}^{(1)}],\hat{Q}^{(1)}] - 2\partial_q\hat{Q}^{(1)}|\phi(q)\rangle = 0. \tag{5}$$

We have adopted the coordinate system in which the inverse inertial mass $B(q)$ is unity. In the conventional ATDHF/ASCC theory, $\hat{Q}^{(2)}$ is omitted. In the ATDHF theory,[2,3)] Eqs. (2) and (3) are employed as the equations of motion, and the collective momentum operator $\hat{P}$ is treated as the differential operator $i\partial_q$, which leads to the differential equation for the state vector $|\phi(q)\rangle$. By contrast, in the conventional ASCC theory, the equations of motion comprise three equations, two of which are Eqs. (2) and (3). The last one is derived by considering a linear combination of Eqs. (4) and (5) and eliminating $\partial_q\hat{Q}^{(1)}$. The equations derived from Eqs. (3)–(5) are called the moving-frame RPA equations. It is the extension of the RPA equations for large-amplitude collective motion and is an eigenvalue problem with eigenvalues given by $\omega^2(q)$ in Eq. (4).

As in the general RPA equations, the moving-frame Eqs. (3)–(5) can be rewritten in the matrix form.

$$(\boldsymbol{A} - \boldsymbol{B})\boldsymbol{Q}^{(1)} - \boldsymbol{P} - \partial_q V\boldsymbol{Q}^{(2)} = 0, \tag{6}$$

$$(\partial_q V\boldsymbol{D} - \omega^2)\boldsymbol{Q}^{(1)} + (\boldsymbol{A} + \boldsymbol{B})\boldsymbol{P} = \partial_q V\partial_q\boldsymbol{Q}^{(1)}, \tag{7}$$

$$(2\boldsymbol{D} + \boldsymbol{C})\boldsymbol{Q}^{(1)} + (\boldsymbol{A} + \boldsymbol{B})\boldsymbol{Q}^{(2)} = 2\partial_q\boldsymbol{Q}^{(1)}. \tag{8}$$

Here, $\boldsymbol{C}$ and $\boldsymbol{D}$ are contributions from $[[\hat{H},\hat{Q}^{(1)}],\hat{Q}^{(1)}]$ and $\partial_q\hat{Q}^{(1)}$, respectively. In this approach, Eqs. (6)–(8) are simultaneously solved, and $\boldsymbol{Q}^{(1)}$ is obtained as a solution to these differential equations, rather than a eigenvector of the moving-frame RPA equations as in the conventional ASCC theory. This is the essential difference between the two ASCC approaches. Here, one idea may arise, that is, to adopt Eqs. (3) and (4) omitting $\hat{Q}^{(2)}$, and solve the differential equations for $\hat{Q}^{(1)}$. This serves as a new approach to solve the ATDHF equation. Here, the differential equation for $\hat{Q}^{(1)}$ is solved rather than the state vector. In fact, one can easily see that Eqs. (6) and (7) reduce to one ordinary differential equation as below.

$$\partial_q V\frac{d}{dq}\boldsymbol{Q}^{(1)} = \left[(\boldsymbol{A}+\boldsymbol{B})(\boldsymbol{A}-\boldsymbol{B}) + \boldsymbol{D}' - \omega^2\right]\boldsymbol{Q}^{(1)},$$

with $\boldsymbol{D}' = \partial_q V\boldsymbol{D}$. At an equilibrium point $q = q_0$ where $\partial_q V(q_0) = 0$, it reduces to the RPA equation. By dividing the both sides by $\partial_q V \neq 0$ and taking the limit $q \to q_0$, one can see that it is a singular point of this differential equation. Actually, this singularity leads to non-uniqueness of the solution that may be interpreted as one of the reasons for the numerical instability observed in the ATDHF studies. Detailed analysis on this equation will be reported in a future publication.

References

1) M. Matsuo, T. Nakatsukasa, and K. Matsuyanagi, Prog. Theor. Phys. **103**, 959 (2000).
2) F. Villars, Nucl. Phys. A **285**, 269 (1977).
3) K. Goeke, P.-G. Reinhard, and D. J. Rowe, Nucl. Phys. **A359**, 408 (1981), and references therein.
4) K. Sato, Prog. Theor. Exp. Phys. **2018**, 103D01 (2018).

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