

Is the solution to the ATDHF equation unique?

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The adiabatic time-dependent Hartree-Fock (ATDHF) theory is a microscopic theory for describing large-amplitude collective motion in atomic nuclei. Although several versions of the ATDHF theory have been proposed since the 1970's, they encounter difficulties such as non-uniqueness of solutions. To overcome these problems, Matsuo *et al.* proposed 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 Schrödinger equation

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

where q and p represent the collective coordinate and its conjugate momentum, respectively. 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 , and the expansion only up to the first order is considered in the conventional ATDHF and ASCC theories. The author proposed the ASCC theory including the second-order collective operator, wherein $\hat{G}(q,p)$ 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 is highlighted.²⁾ The ASCC equations of motion with $\hat{Q}^{(2)}$ are given by

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

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

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

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

Equations (2) and (3) are derived from the $O(1)$ and $O(p)$ expansions, respectively. $\hat{Q}^{(2)}$ contributes to the equation of $O(p)$; however, it is neglected in the conventional ATDHF theory. Without $\hat{Q}^{(2)}$, Eqs. (2) and (3) coincide with the ATDHF equations reported by Villars.^{3,4)} Thus, we focus on the Villars ATDHF theory in this report. In Villars ATDHF theory, 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 $|\phi(q)\rangle$. In the ASCC theory, \hat{P} is treated as an unknown operator, which can be determined by solving the equations of motion. In the ASCC theory with $\hat{Q}^{(2)}$, the above four equations are

simultaneously solved. Equations (4) and (5) involve $\partial_q \hat{Q}^{(1)}$, and therefore, one has to solve a differential equation for $\hat{Q}^{(1)}$. This is the essential difference from the conventional ASCC theory without $\hat{Q}^{(2)}$. The conventional ASCC 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 reduced to an eigenvalue problem with eigenvalues $\omega^2(q)$ in Eq. (4). In the ASCC theory with $\hat{Q}^{(2)}$, the differential equation for $\hat{Q}^{(1)}$ is solved, and thus, one idea emerges as a new approach to solve the ATDHF equation, *i.e.*, to adopt Eqs. (3) and (4) by omitting $\hat{Q}^{(2)}$ and solve the differential equations for $\hat{Q}^{(1)}$. In fact, Eqs. (3) and (4) without $\hat{Q}^{(2)}$ are reduced to one ordinary differential equation in the matrix form given below.

$$\partial_q V \frac{d}{dq} \mathbf{Q}_\lambda^{(1)} = [(\mathbf{A} + \mathbf{B})(\mathbf{A} - \mathbf{B}) + \mathbf{D}' - \omega_\lambda^2] \mathbf{Q}_\lambda^{(1)}, \quad (6)$$

where λ denotes the mode index, and $\mathbf{D}' = \partial_q V \mathbf{D}$ is a contribution from $\partial_q \hat{Q}^{(1)}$. At an equilibrium point $q = q_0$ where $\partial_q V(q_0) = 0$, Eq. (6) reduces to the RPA equation. Without loss of generality, one can set $q_0 = 0$. By dividing the both sides by $\partial_q V \neq 0$ and taking the limit $q \rightarrow 0$, we get a singular point of this differential equation. To analyze its behavior around the equilibrium, we consider the deviation from the RPA solution $\mathbf{Q}_\lambda^{(1)}(0)$ by putting $\mathbf{Q}_\lambda^{(1)}(q) = \mathbf{Q}_\lambda^{(1)}(0) + \delta\mathbf{Q}_\lambda^{(1)}(q)$ and linearizing Eq. (6). By expanding $\delta\mathbf{Q}_\lambda^{(1)}$ as $\delta\mathbf{Q}_\lambda^{(1)}(q) = \sum_i z_{\lambda i}(q) \mathbf{Q}_i^{(1)}(0)$, we obtain the solution $z_{\lambda i} = \beta_{\lambda i} / (1 - \eta_{\lambda i} q + \sum_i c_{\lambda i} q^{\eta_{\lambda i}})$, where $\eta_{\lambda i} = [(\omega_i^2 - \omega_\lambda^2) / \omega_0^2]_{q=0}$ with the RPA eigenfrequencies $\omega_\alpha^2(0)$. From the initial condition, $z_{\lambda i}(q)$ should vanish at $q = 0$. Around the potential minimum, where $\omega_0^2 > 0$ and $\eta_{\lambda i} \leq 0$ for $\lambda \geq i$, $c_{\lambda i} = 0$ follows from the initial condition. However, for $\lambda < i$, the initial condition is met for arbitrary $c_{\lambda i}$, which leads to the non-uniqueness of the solution that can be interpreted as one of the reasons for the numerical instability observed in the ATDHF studies. In other words, an additional condition is necessary for determining the solution uniquely. More detailed analysis on this equation will be reported in a future publication.

References

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