FORMULATION OF THE TDHF THEORY IN THE BASIS EVOLVING WITH THE TIME

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(Received September 17, 1980)

The general time-dependent Hartree-Fock (TDHF) equations are derived in the restricted basis which is variationally adjusted during the evolution of the system. The canonical Hamiltonian formulation for the time-dependent variational principle (TDVP) associated with the Schrödinger equation is used here to determine the time dependence of both the nuclear wave function and the basis parameters. This approach provides a method to calculate the evolution of the complicated many-body system in the numerically convenient way.

PACS numbers: 21.60.Jz, 24.10.Dp

Calculation of the dynamics of complicated nuclear systems have to deal with the truncation of the basis in the expansion of the nuclear wave function. This is a severe problem in the scattering of two ions described in the basis with fixed parameters. The separation distance of ions changes with time, but the distance between two centers of the basis remains fixed. Consequently, in realistic calculations one has to use a large number of basis states even for light nuclei and the accurate treatment of the nuclear dynamics is often imposible. In the following we derive the TDHF equations in the basis which is variationally adjusted during the evolution of the system. In this derivation we use the formulation of the TDVP for the Schrödinger equation as given by Kerman and Koonin [1].

Let us take the first N vectors $\hat{\phi}_\lambda$ of the complete basis $\{\hat{\phi}_\lambda\}$ which depends on parameters $\{\beta_n(t)\}$. These parameters change with the time and characterize the basis $\{\hat{\phi}_\lambda\}$ itself. The nuclear wave function is further approximated by the Slater determinant

$$\Psi(\{\alpha_{i\mu}\}, \{\beta_n\}) = (A!)^{-1/2} \det [\psi_1 \ldots \psi_A], \tag{1}$$

where A is the number of particles and the single particle (s.p.) wave function ψ_i is given by

$$\psi_i = \alpha_{i\mu}\phi_\mu, \quad \mu = 1, \ldots, N. \tag{2}$$

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In general, parameters $\alpha_{i\mu}$ are complex and therefore Ψ is parametrized by $\{\beta_n\}$ and $\{\alpha_{i\mu}\}$ as well as by $\{\alpha^*_{i\mu}\}$. The time evolution of the many-body wave function Ψ given in Eq. (1) is governed by the variational principle

$$\delta\langle\Psi|i\hbar\frac{\partial}{\partial t}-\hat{H}|\Psi\rangle=0, \tag{3}$$

where $\hat{H}$ is the Hamiltonian of the system. $\hat{H}$ is a sum of the one-body kinetic energy operator and the two-body interaction. Equation (3) with the wave function in Eq. (1) can be written as follows:

$$\begin{aligned}
\{\alpha^*_{i\mu},\alpha_{j\nu}\}\dot{\alpha}_{j\nu}+\{\alpha^*_{i\mu},\alpha^*_{j\nu}\}\dot{\alpha}^*_{j\nu}+\{\alpha^*_{i\mu},\beta_m\}\dot{\beta}_m&=\frac{\partial H}{\partial\alpha^*_{i\mu}},\\
\{\alpha_{i\mu},\alpha_{j\nu}\}\dot{\alpha}_{j\nu}+\{\alpha_{i\mu},\alpha^*_{j\nu}\}\dot{\alpha}^*_{j\nu}+\{\alpha_{i\mu},\beta_m\}\dot{\beta}_m&=\frac{\partial H}{\partial\alpha_{i\mu}},\\
\{\beta_n,\alpha_{j\nu}\}\dot{\alpha}_{j\nu}+\{\beta_n,\alpha^*_{j\nu}\}\dot{\alpha}^*_{j\nu}+\{\beta_n,\beta_m\}\dot{\beta}_m&=\frac{\partial H}{\partial\beta_n},
\end{aligned} \tag{4}$$

where $\{u_i,u_j\}$ denotes the real Lagrange bracket

$$\{u_i,u_j\}=i\hbar\left(\left\langle\frac{\partial\Psi}{\partial u_i}\middle|\frac{\partial\Psi}{\partial u_j}\right\rangle-\left\langle\frac{\partial\Psi}{\partial u_j}\middle|\frac{\partial\Psi}{\partial u_i}\right\rangle\right) \tag{5}$$

and H:

$$H(\{u_i\})=\langle\Psi(\{u_i\})|\hat{H}|\Psi(\{u_i\})\rangle \tag{6}$$

is the expectation value of $\hat{H}$. The orthogonality and the normalization of s.p. states ψ_i (Eq. (2)) during the evolution of the system is assured by adding the Lagrange multiplier $-\varepsilon_{ji}\alpha^*_{i\lambda}\alpha_{j\lambda}$ to the expectation value of $\hat{H}$. With those contributions the derivatives of the Hamilton functions are

$$\begin{aligned}
\frac{\partial H}{\partial\alpha^*_{i\mu}}&=\langle\mu|h|i\rangle-\varepsilon_{ki}\alpha_{k\mu},\\
\frac{\partial H}{\partial\alpha_{i\mu}}&=\langle i|h|\mu\rangle-\varepsilon_{ik}\alpha^*_{k\mu},\\
\frac{\partial H}{\partial\beta_n}&=\langle k|h\frac{\partial}{\partial\beta_n}|k\rangle+\langle k|\frac{\overleftarrow{\partial}}{\partial\beta_n}h|k\rangle,
\end{aligned} \tag{7}$$

where h denotes the HF Hamiltonian. The Lagrange brackets in Eq. (5) can be easily calculated and are given by

$$\{\alpha_{i\mu}, \alpha_{jv}\} = \{\alpha^*_{i\mu}, \alpha^*_{jv}\} = 0,$$

$$\{\alpha^*_{i\mu}, \alpha_{jv}\} = ih(\delta_{ij}\delta_{\mu v} - \delta_{ij}\alpha_{k\mu}\alpha^*_{kv} + \alpha_{i\mu}\alpha^*_{jv}),$$

$$\{\alpha^*_{i\mu}, \beta_m\} = ih\left(\langle\mu|\frac{\partial}{\partial\beta_m}|i\rangle + \alpha_{i\mu}\langle k|\frac{\partial}{\partial\beta_m}|k\rangle - \alpha_{j\mu}\langle j|\frac{\partial}{\partial\beta_m}|i\rangle\right),$$

$$\{\alpha_{i\mu}, \beta_m\} = \{\alpha^*_{i\mu}, \beta_m\}^*,$$

$$\{\beta_n, \beta_m\} = ih\left(\langle k|\frac{\overleftarrow{\partial}}{\partial\beta_n}\frac{\partial}{\partial\beta_m}|k\rangle - \langle k|\frac{\overleftarrow{\partial}}{\partial\beta_m}\frac{\partial}{\partial\beta_n}|k\rangle\right). \tag{8}$$

Inserting above expressions to Eq. (4) and choosing appropriately the Lagrange multipliers ε_{ji}

$$\varepsilon_{ji} = \langle j|h|i\rangle - \delta_{ji}\langle k|h|k\rangle \tag{9}$$

one obtains final equations for the dependence of basis parameters $\{\beta_n\}$ and expansion coefficients $\{\alpha_{i\mu}\}$

$$i\hbar\dot{\alpha}_{i\mu} = \left(\langle\mu|h|v\rangle - i\hbar\langle\mu|\frac{\partial}{\partial\beta_m}|v\rangle\dot{\beta}_m\right)\alpha_{iv}$$

$$-\hbar\,\mathrm{Im}\left(\langle k|\frac{\overleftarrow{\partial}}{\partial\beta_n}\frac{\partial}{\partial\beta_m}|k\rangle + \langle k|\frac{\partial}{\partial\beta_n}|v\rangle\langle v|\frac{\partial}{\partial\beta_m}|k\rangle\dot{\beta}_m\right.$$

$$= \mathrm{Re}\left(\langle k|\frac{\overleftarrow{\partial}}{\partial\beta_n}h|k\rangle + \langle k|\frac{\partial}{\partial\beta_n}|v\rangle\langle v|h|k\rangle\right). \tag{10}$$

The above equations reduce to the well known TDHF equations [2]

$$i\hbar\dot{\alpha}_{i\mu} = \langle\mu|h|v\rangle\alpha_{iv}, \tag{11}$$

in the case where a complete set of basis states $\{\hat{\phi}_\lambda\}$ is used. The adventage in using Eqs. (10) rather than Eq. (11) is that the truncation error and its changes are minimized during the evolution of the system. Numerical solution of Eqs. (10) is rather straightforward and involves the calculation of matrix elements between states $(\partial/\partial\beta_n)|v\rangle$ in addition to those matrix elements which appear in Eq. (11). Moreover, number of basis vectors can be strongly reduced leading to the reduction of the computation time in the realistic calculations. This allows for the extensive application of those equations for the description of the evolution of complicated nuclear systems.

REFERENCES

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