LETTERS TO THE EDITOR

THE TIME-DEPENDENT PARTICLES + CORE MODEL

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The time-dependent particles + core (TDPC) model is formulated as a reduction of the general time-dependent Hartree-Fock-Bogolyubov (TDHFB) approach. Particles of the core are described by the Slater determinant which depends only on few collective parameters. The external particles are treated explicitely in the frame of the TDHFB theory. Equations which describe the evolution of both coupled parts of the system are derived. Finally, the relevance of this model for the description of heavy ion reactions is shortly discussed.

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The time-dependent Hartree-Fock (TDHF) theory [1] provides a microscopic description of the fission process as well as the heavy ion fusion reaction. In heavy nuclei the computational effort in the calculation of the evolution of all single particle (s.p.) orbitals is enormous. It is even impossible to perforum such calculations for the realistic, momentum-dependent nucleon-nucleon interaction and (or) for the s.p. density which has several broken symmetries. Therefore, it is necessary to look for the simplified solutions of the nuclear dynamics.

In the peripheral collision of ions the detailed information about the evolution of deep lying s.p. orbitals is less important. In this process valence nucleons are mainly responsible for the dissipation of the kinetic energy and the angular momentum of the relative motion. It is then obvious to divide all nucleons in the nucleus into the external, active particles and the particles which form the inert core described by a few collective parameters. The residual interaction among valence particles determines largely the fusion cross section, the further evolution of the binary system and the mass spectrum of fragments in the final state.

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In this letter we formulate the time-dependent particles + core (TDPC) model. In the absence of the pairing force between valence nucleons this model was recently discussed by Jensen and Koonin [2]. In the derivation we use the canonical Hamiltonian formulation for the time-dependent variational principle (TDVP) [3]

$$\delta \int_{t_1'}^{t_2'} \langle \Psi(t)| \left(\hat{H} - i\hbar \frac{\partial}{\partial t} \right) |\Psi(t)\rangle dt = 0,$$

$$\langle \delta\Psi(t_1')| = \langle \delta\Psi(t_2')| = |\delta\Psi(t_1')\rangle = |\delta\Psi(t_2')\rangle = 0, \tag{1}$$

which implies the Schrödinger equation. For the wave function Ψ, decribed by a set of variational parameters $\{u_i\}$, the TDVP (1) leads to the dynamical equations [3]

$$\{u_i, u_j\}\dot{u}_j = \frac{\partial}{\partial u_i}(\langle \Psi|\hat{H}|\Psi\rangle),$$

$$\{u_i, u_j\} \equiv i\hbar \left(\left\langle \frac{\partial \Psi}{\partial u_i} \middle| \frac{\partial \Psi}{\partial u_j} \right\rangle - \left\langle \frac{\partial \Psi}{\partial u_j} \middle| \frac{\partial \Psi}{\partial u_i} \right\rangle \right), \tag{2}$$

for the parameters $\{u_i\}$. The basic assumption of the model is that the core levels can be described by the Slater determinant $\Phi_C = \prod_a c_a^\dagger |0\rangle$ parametrized by a few collective parameters $\{\beta_i\}$. The interaction between valence particles has both the particle-hole and the particle-particle components. Therefore, we perform the Bogolyubov transformation for the particle operators $c_a^\dagger(c_a)$ and form the quasi-particle (q.p.) operators $\alpha_\nu^\dagger(\alpha_\nu)$

$$\alpha_\nu^\dagger = A_{\nu k} c_k^\dagger + B_{\nu k} c_k,$$

$$\alpha_\nu = A_{\nu k}^* c_k + B_{\nu k}^* c_k^\dagger, \tag{3}$$

which define the vacuum

$$|\Phi_V\rangle = \exp\{-\tfrac{1}{2} M_{k_1 k_2} c_{k_1}^\dagger c_{k_2}^\dagger\} |0\rangle, \tag{4}$$

$$M_{k_1 k_2} \equiv B_{\nu k_2}^* A_{\nu k_1}^{*-1}. \tag{5}$$

The summation in Eq. (5) runs over q.p. states in the valence shell and indices k_i denote all basis states. The TDVP with the wave function $\Psi = \Phi_C \otimes \Phi_V$ leads to the equations for coupled parameters $\{\beta_i\}$, $\{A_{\lambda m}\}$, $\{A_{\lambda m}^*\}$, $\{B_{\lambda m}\}$, $\{B_{\lambda m}^*\}$. The corresponding Lagrange brackets can be easily evaluated using Eqs. (2)–(5)

$$\{B_{\lambda m}, B_{\alpha k}^*\} = i(\delta_{mk}\delta_{\lambda\alpha} - \delta_{\lambda\alpha} B_{\gamma k} B_{\gamma m}^* + B_{\alpha k} B_{\lambda m}^* - A_{\alpha m} A_{\lambda k}^*),$$

$$\{B_{\lambda m}, A_{\alpha k}^*\} = i(B_{\gamma k}^* A_{\gamma m} \delta_{\lambda\alpha} - B_{\lambda k}^* A_{\alpha m} + B_{\gamma k}^* A_{\gamma i}^{*-1} B_{\lambda m}^* B_{\alpha i}),$$

$$\{A_{\lambda m}, A_{\alpha k}^*\} = i(B_{\gamma k}^* B_{\gamma m} \delta_{\lambda\alpha} - B_{\lambda k}^* B_{\alpha m} + B_{\gamma i} A_{\gamma m}^{-1} B_{\delta j}^* A_{\delta k}^{*-1} B_{\lambda i}^* B_{\alpha j}),$$

$$\{B_{\lambda m}, \beta_n\} = i(d^n_{mi}B^*_{\lambda i} + d^n_{k_2k_1}B^*_{\nu k_1}B_{\nu k_2}B^*_{\lambda m} - d^n_{ij}B^*_{\lambda j}B_{\gamma i}B^*_{\gamma m} - d^n_{ij}B^*_{\gamma j}A_{\gamma m}A^*_{\lambda i}),$$

$$\{A_{\lambda m}, \beta_n\} = i(d^n_{ij}B_{\gamma m}B^*_{\lambda j}A^*_{\gamma i} - d^n_{ij}B_{\gamma m}B^*_{\gamma j}A^*_{\lambda i} - d^n_{k_2k_1}B_{\gamma i}A^{-1}_{\gamma m}B^*_{\nu k_1}B_{\nu k_2}B^*_{\lambda i}),$$

$$\{\beta_n, \beta_m\} = i(d^m_{k_4k_3}d^n_{k_2k_1} - d^n_{k_4k_3}d^m_{k_2k_1})(B_{\mu k_4}B^*_{\mu k_1}\delta_{k_3k_2} - B_{\mu k_4}A^*_{\mu k_2}B^*_{\nu k_1}A_{\nu k_3}),$$

$$\{A_{\lambda m}, A_{\alpha k}\} = \{B_{\lambda m}, B_{\alpha k}\} = \{A^*_{\lambda m}, A^*_{\alpha k}\} = \{B^*_{\lambda m}, B^*_{\alpha k}\} = 0,$$

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$$\{B^*_{\lambda m}, B_{\alpha k}\} = \{B_{\lambda m}, B^*_{\alpha k}\}^*,$$

$$\{B^*_{\lambda m}, \beta_n\} = \{B_{\lambda m}, \beta_n\}^*. \tag{6}$$

The anti-hermitian matrices in Eqs. (6) are defined as

$$d^m_{k_ik_j} \equiv \left\langle \varphi_{k_i} \left| \frac{\partial}{\partial \beta_m} \right| \varphi_{k_j} \right\rangle \tag{7}$$

and φ_{k_i} is the s.p. wave function corresponding to the basis state k_i. The derivatives of the Hamilton function

$$H = \operatorname{tr}(\varrho\varepsilon + \tfrac{1}{2}\varrho\Gamma - \tfrac{1}{2}\kappa^*\Delta),$$

$$\Gamma_{lm} = V_{lrms}\varrho_{sr},$$

$$\Delta_{lm} = \tfrac{1}{2}V_{lmrs}\kappa_{rs},$$

$$\varrho_{sr} = B_{\mu r}B^*_{\mu s},$$

$$\kappa_{rs} = A_{\mu s}B^*_{\mu r} \tag{8}$$

are given by

$$\frac{\partial H}{\partial B^*_{\lambda m}} = h^*_{ml}B_{\lambda l} + \Delta^*_{ml}A_{\lambda l},$$

$$\frac{\partial H}{\partial A^*_{\lambda m}} = -h_{ml}A_{\lambda l} - \Delta_{ml}B_{\lambda l},$$

$$\frac{\partial H}{\partial \beta_n} = B_{\mu k_1}B^*_{\mu k_2}(h_{k_1k_3}d^n_{k_3k_2} - d^n_{k_1k_3}h_{k_3k_2}) + 2\operatorname{Re}(A^*_{\mu k_1}B_{\mu k_2}d^n_{k_1k_3}\Delta_{k_3k_2}), \tag{9}$$

where, $\alpha, \gamma, \delta, \lambda(\mu, \nu)$ denote q.p. states in $\Phi_V(\Phi_C \times \Phi_V)$,

$$h_{ml} = \varepsilon_{ml} - \lambda\delta_{ml} + \Gamma_{ml} \tag{10}$$

and the Lagrange multipliers are introduced to conserve number of particles in the average. Inserting Eqs. (9) and (6) one obtains the final equations

$$i\hbar\begin{bmatrix}\dot{A}\\ \dot{B}\end{bmatrix}=\begin{bmatrix}(h-i\hbar\dot{\beta}_n d^n) & \Delta\\ -\Delta^* & -(h-i\hbar\dot{\beta}_n d^n)^*\end{bmatrix}\begin{bmatrix}A\\ B\end{bmatrix},$$

$$\hbar\dot{\beta}_m \operatorname{Im}(d^m_{k_3k_2}d^n_{k_2k_1}B_{\mu k_3}B^*_{\mu k_1}-d^m_{lk}d^n_{ki}B^*_{\alpha i}B_{\alpha l}-d^m_{kl}d^n_{ij}B_{\gamma k}B^*_{\gamma j}A^*_{\alpha i}A_{\alpha l})$$

$$=-\operatorname{Re}(h_{k_3k_2}d^n_{k_2k_1}B_{\mu k_3}B_{\mu k_1}-h_{lk}d^n_{ki}B^*_{\alpha i}B_{\alpha l}-h_{kl}d^n_{ij}B_{\gamma k}B^*_{\gamma j}A^*_{\alpha i}A_{\alpha l})$$

$$+\operatorname{Re}[d^n_{k_2k_1}\Delta_{kl}(M_{kl}B^*_{\nu k_1}B_{\nu k_2}+B_{\gamma l}\dot{A}^*_{\gamma k_2}\delta_{k_1k})]. \tag{11}$$

The lowest equation in (11) describes the complicated coupling between parameters of the valence particles and the collective parameters of the core. The first two equations in (11) remind the "free" TDHFB equations for states evolving in the HF-field h modified by the presence of the core field $-i\hbar\dot{\beta}_m d^m$. Eqs. (11) allow for the strong reduction of the TDHFB dynamic equations and the TDPC model can be a useful tool for the investigation of the dynamics of complicated nuclear systems.

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