Spin-orbit force in time-dependent Hartree-Fock calculations of heavy-ion collisions

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We discuss the time-dependent Hartree-Fock equations which maintain independent nucleon spin degrees of freedom, and which include spin-orbit interactions. The complex numerical task of including the spin-orbit force in reaction studies is described in detail.

I. INTRODUCTION

It is generally accepted that the time-dependent Hartree-Fock (TDHF) theory provides a microscopic basis for building a many-body theory of low-energy heavy-ion reactions. The TDHF theory has been widely used in the study of fusion excitation functions, fission, deep-inelastic scattering of heavy-mass systems, and nuclear molecular resonances,[1-3] while providing a natural foundation for many other studies. A complete account of the previous TDHF applications can be found in Refs. 1 and 2.

The TDHF studies of heavy-ion reactions show an unusual degree of transparency for central low-energy collisions. This lack of dissipation is due partially to the symmetries assumed to simplify the numerical computations and partially to the absence of higher-order correlations in the mean-field approximation. The latter requires us to go beyond the mean-field approximation, and various attempts to include collision terms into TDHF have been reported in the literature.[4,5] The understanding of the dissipative mechanisms in the TDHF theory is vital for establishing the region of validity of the mean-field approximation and providing estimates for the importance of the mean-field effects at higher energies. The most critical approximations are the assumption of spin-degeneracy and spin-saturated states, and the restriction of calculations to an axially symmetric geometry. A limited number of comparisons of axially symmetric TDHF calculations with the corresponding three-dimensional calculations is available.[6-8] The three-dimensional calculations show more dissipation. However, none of these calculations includes the spin-orbit part of the effective interaction. In TDHF the dissipation of the translational kinetic energy of the two ions is due to the collisions of single-particle states with the walls of the Hartree-Fock potential. This leads to the randomization of the motion characterized by the distribution of energy among all possible degrees of freedom of the system. The complete equilibration of the translational kinetic energy among all possible degrees of freedom is commonly accepted as being the definition of fusion, whereas the incomplete equilibration results in inelastic collisions. From this point of view, it is clear that an increase in the number of degrees of freedom will result in an enhanced dissipation. Thus one expects that removing the spin degeneracy will enhance the dissipation.

We have recently reported TDHF calculations which also include a spin-orbit part for the effective nucleon-nucleon interaction.[9-11] These calculations, indeed, have shown a substantial enhancement of dissipation in comparison to the earlier TDHF calculations. The numerical realizations of these calculations are quite complex and have only been briefly reported. It is the aim of this paper to give a detailed description of the numerical realization of TDHF calculations with the spin-orbit force.

In Sec. II, we give a detailed description of the numerical procedures used in adding the spin-orbit force to the TDHF calculations. This section can be viewed as an extension of the previously published[12] procedures which did not include the spin-orbit interaction. In Sec. III a summary and outlook are provided.

II. THEORY AND CALCULATIONAL DETAILS

In Ref. 12 the theory and the numerical methods for axially symmetric Skyrme-Hartree-Fock calculations were presented. Finite difference techniques on a coordinate space grid have been used to discretize the action integral. The dynamical equations on the grid are obtained

from variation of the discretized action. In this section we generalize the methods of Ref. 12 to include a spin-orbit potential. We have attempted to parallel the discussions and derivations of Ref. 12 as closely as possible. Many of the functions defined here will be the same as or analogous to those of Ref. 12; thus we will not extensively define all quantities again since the interested reader can find the exact definitions in that paper. Note that our discretization method is similar to that used in Ref. 13 but our notation and equations have been somewhat changed.

A. The energy functional

We begin with the Skyrme energy functional which includes a spin-orbit force and a finite-range Yukawa interaction[12–22]

$$\mathcal{H}=\mathcal{H}_n+\mathcal{H}_y+\mathcal{H}_{1s}+\mathcal{H}_C+\mathcal{H}_R \ , \tag{1}$$

where

$$\mathcal{H}_n=\int d^3r\left\{\frac{\hbar^2}{2m}\tau+\frac{t_0}{2}\left[1+\frac{x_0}{2}\right]\rho^2-\frac{t_0}{2}\left(\tfrac{1}{2}+x_0\right)\sum_q\rho_q^2+\frac{t_3}{12}\left[1+\frac{x_3}{2}\right]\rho^{\alpha+2}-\frac{t_3}{12}\left(\tfrac{1}{2}+x_3\right)\rho^\alpha\sum_q\rho_q^2\right.$$
$$\left.+\tfrac{1}{4}(t_1+t_2)(\rho\tau-j^2)-\tfrac{1}{8}(t_1-t_2)\sum_q(\rho_q\tau_q-j_q^2)\right\} , \tag{2}$$

$$\mathcal{H}_y=\int d^3r\,d^3r'\frac{\exp(-|\mathbf{r}-\mathbf{r}'|/a)}{4\pi a^2|\mathbf{r}-\mathbf{r}'|}\left[\frac{t_y}{2}\left[1+\frac{x_y}{2}\right]\rho(\mathbf{r})\rho(\mathbf{r}')-\frac{t_y}{2}\left(\tfrac{1}{2}+x_y\right)\sum_q\rho_q(\mathbf{r})\rho_q(\mathbf{r}')\right] , \tag{3}$$

$$\mathcal{H}_{1s}=-\frac{t_4}{2}\int d^3r\left[\rho\nabla\cdot\mathcal{J}+\sum_q\rho_q(\nabla\cdot\mathcal{J}_q)\right] , \tag{4}$$

$$\mathcal{H}_C=\frac{1}{2}e^2\int d^3r\,d^3r'\rho_p(\mathbf{r})\frac{1}{|\mathbf{r}-\mathbf{r}'|}\rho_p(\mathbf{r}')-\frac{3}{4}\left[\frac{3}{\pi}\right]^{1/3}e^2\int d^3r[\rho_p(\mathbf{r})]^{4/3} . \tag{5}$$

The energy functional $\mathcal{H}_R$ describes the classical rotational energies for the rotating frame approximation; its definition is found in Ref. 12. The particle, kinetic energy, current, and spin-current densities are, respectively, given by

$$\begin{aligned}
\rho_q(\mathbf{r})&=\sum_{\substack{\alpha\in q\\ \mu}}n_\alpha|\psi_\alpha(\mathbf{r}\mu)|^2 ,\\
\tau_q(\mathbf{r})&=\sum_{\substack{\alpha\in q\\ \mu}}n_\alpha|\nabla\psi_\alpha(\mathbf{r}\mu)|^2 ,\\
\mathbf{j}_q(\mathbf{r})&=\sum_{\substack{\alpha\in q\\ \mu}}n_\alpha\mathrm{Im}[\psi_\alpha^*(\mathbf{r}\mu)\nabla\psi_\alpha(\mathbf{r}\mu)] ,\\
\mathcal{J}_q(\mathbf{r})&=-i\sum_{\substack{\alpha\in q\\ \mu\mu'}}n_\alpha\psi_\alpha^*(\mathbf{r}\mu)\nabla\times\sigma\psi_\alpha(\mathbf{r}\mu') ,
\end{aligned} \tag{6}$$

where μ and μ' are z components of spin, σ is the Pauli spin matrix, the sums are over all single-particle states having isospin q. The n_α is the occupation probability for the state α. For filled shells one has $n_\alpha=1$. Fractional occupancies may occur in the filling approximation or if pairing is included. A quantity without an isospin label refers to a sum over both isospins, e.g.,

$$\mathcal{J}=\mathcal{J}_n+\mathcal{J}_p \ . \tag{7}$$

We also note that $\nabla\cdot\mathcal{J}_q$ in Eq. (4) may be expressed as

$$\nabla\cdot\mathcal{J}_q(\mathbf{r})=-i\sum_{\substack{\alpha\in q\\ \mu\mu'}}\nabla\psi_\alpha^*(\mathbf{r}\mu)\cdot(\nabla\times\sigma)\psi_\alpha(\mathbf{r}\mu') . \tag{8}$$

The possible time dependence of the wave functions and densities is suppressed.

We want to point out that the energy functional (1)–(5) does not only include the spin-orbit term (4) but also a generalized three-body term, i.e., the terms which depend on the parameter t_3. It allows arbitrary powers α in the density dependence and it has a parameter x_3 for the exchange force. For $x_3=1$ and $\alpha=1$ the form of Ref. 12 is recovered. The generalized three-body term gives a better fit to the data,[19,20] particularly for the compressibility of nuclear matter and for the surface thickness.[19,23,11]

Furthermore, we have rescaled the parameters in the Yukawa term $\mathcal{H}_y$. Rather than using the V_u and V_l as in Ref. 12, we introduce t_y and x_y by

$$\begin{aligned}
4\pi a^3V_u&=t_y\left[1+\frac{x_y}{2}\right] ,\\
4\pi a^3V_l&=t_y\left[\frac{1}{2}-\frac{x_y}{2}\right] .
\end{aligned} \tag{9}$$

The advantage of the t_y and x_y is that they are directly comparable to t_0,x_0, and t_3,x_3. For example, in nuclear matter they contribute in a similar way.

All previous fits with the Skyrme potential were obtained using a fully zero-range form of the energy density. In this form the Yukawa terms are replaced by surface terms proportional to $\rho\nabla^2\rho$. In Refs. 12 and 13 a prescription was given to deduce approximate values for the parameters V_u and V_l. As reported in Ref. 13, this

procedure has an intrinsic error due to the higher-order terms neglected in the Taylor expansion of the Yukawa term, and leads to an error of about 0.5 MeV/nucleon in the binding energy of the ^{16}O nucleus. We have recently determined, by least-squares fits, parameters for the new energy functional (2); see Ref. 11. In Table I we compile the parameters for the three forces Skyrme II, Skyrme M^*,[19] and the newly fitted force $FY1$.

The functional, Eq. (4), is not the most general spin interaction. Reference 17 gives a more complete Skyrme energy functional which includes a spin density, a spin kinetic-energy density, and the full spin-current tensor. In the present stage we have chosen to consider only the spin-orbit force because we expect it to be the most important of the spin interactions. There is, furthermore, the problem that the microscopic spin-orbit interaction still contains some ambiguities.[24–26] For symmetric collisions, such as the ^{16}O+^{16}O system, the TDHF equations are exactly Galilean invariant. This is due to the fact that the two ions are boosted with velocities that are equal in magnitude but opposite in direction. This leads to a cancellation among the velocity-dependent terms arising from the Galilean transformation. The change in the spin-orbit splitting as a function of time in the entrance channel is conserved to an accuracy commensurate with the error in the total energy conservation. Furthermore, in all of our calculations, quantities such as particle number, energy, etc., were numerically conserved at the usual levels of accuracy. It is the main purpose of the present work to demonstrate that the spin-orbit force is manageable in TDHF calculations and that it has significant effects on heavy-ion collisions.

TABLE I. Parameters as defined in the Skyrme energy functional for the three parametrizations, Skyrme II, Skyrme M^* (finite-range Yukawa versions), and FY1, a newly fitted set. Note that V_u and V_l depend on t_y and x_y; they are tabulated for completeness.

	Skyrme II	Skyrme M^*	FY1
t_0	−104.49	−1784.69	0.0
x_0	4.01	0.19302	0.0
t_1	585.6	410.0	510.971
t_2	−27.10	−135.0	−97.749
t_3	9331.1	15595.0	11282.1
x_3	1.0	0.0	−0.665746
t_4	120.0	130.0	120.0
t_y	−1065.5	−860.364	−2131.29
x_y	−0.02	−0.1237	−0.234242
a	0.4598	0.4598	0.319073
α	1.0	1/6	0.2
V_u	−863.53	−660.747	−4609.61
V_l	−444.85	−395.722	−3222.05

B. Specialization to axial symmetry

We let the z direction define an axis of symmetry for the system, so that all equations are expressed in cylindrical coordinates, $\mathbf{r}=(r,z,\phi)$. Each single-particle wave function is given by

$$\psi_\alpha(\mathbf{r})=\Phi_\alpha^{(+)}(r,z)e^{i\Lambda_\alpha^{(-)}\phi}\begin{bmatrix}1\\0\end{bmatrix}+\Phi_\alpha^{(-)}(r,z)e^{i\Lambda^{(+)}\phi}\begin{bmatrix}0\\1\end{bmatrix}, \tag{10}$$

where

$$\Lambda_\alpha^{(\pm)}=K_\alpha\pm\tfrac{1}{2}, \tag{11}$$

and K_α is the z component of the total angular momentum. Comparing with Eqs. (6), we see that

$$\begin{aligned}\psi_\alpha(\mathbf{r},\tfrac{1}{2})&=\Phi_\alpha^{(+)}(r,z)e^{i\Lambda_\alpha^{(-)}\phi},\\ \psi_\alpha(\mathbf{r},-\tfrac{1}{2})&=\Phi_\alpha^{(-)}(r,z)e^{i\Lambda_\alpha^{(+)}\phi}.\end{aligned} \tag{12}$$

Also, each α pertains to a given spin K_α, and by convention $-\alpha$ corresponds to $-K_\alpha$. We will impose the condition that the state for $-K_\alpha$ is degenerate to that of $+K_\alpha$ by which we mean

$$\Phi_{-\alpha}^{(\pm)}(r,z)=\mp\Phi_\alpha^{(\mp)}(r,z). \tag{13}$$

If we further assume that both $\pm K$ have equal occupancies, then it can be shown that densities and currents in Eqs. (6) only depend on r and z and there are no azimuthal currents, i.e., $j_\Phi=0$ and $\mathcal{J}_\Phi=0$.

Thus, the energy functionals (2) and (4) are completely symmetric under the interchange of K_α and $-K_\alpha$, as we see from the explicit expressions

$$\begin{aligned}\mathcal{H}_n=\int d^3r\Bigg\{&\frac{\hbar^2}{2m}(\tau_z+\tau_r+s)+\frac{t_0}{2}\left[\left(1+\frac{x_0}{2}\right)\rho^2-(\tfrac{1}{2}+x_0)\sum_q\rho_q^2\right]+\frac{t_3}{12}\left[1+\frac{x_3}{2}\right]\rho^{\alpha+2}\\&-\frac{t_3}{12}(\tfrac{1}{2}+x_3)\rho^\alpha\sum_q\rho_q^2+\tfrac{1}{4}(t_1+t_2)[\rho(\tau_z+\tau_r+s)-j_z^2+j_r^2]-\tfrac{1}{8}(t_1-t_2)\sum_q[\rho_q(\tau_{zq}+\tau_{rq}+s_q)-j_{zq}^2-j_{rq}^2]\Bigg\},\end{aligned} \tag{14}$$

and

$$\mathcal{H}_{1s}=-\frac{t_4}{2}\int d^3r\sum_{qq'}(1+\delta_{qq'})\rho_q[\mathcal{J}_{rzq'}+\mathcal{J}_{rq'}+\mathcal{J}_{zq'}], \tag{15}$$

where the r or z index denotes the parts with the r or z derivative,

$$\tau_{zq}=\sum_{\alpha\in q}\left[\left|\frac{\partial\Phi_\alpha^{(+)}}{\partial z}\right|^2+\left|\frac{\partial\Phi_\alpha^{(-)}}{\partial z}\right|^2\right], \tag{16}$$

$$\tau_{rq}=\sum_{\alpha\in q}\left[\left|\frac{\partial\Phi_\alpha^{(+)}}{\partial r}\right|^2+\left|\frac{\partial\Phi_\alpha^{(-)}}{\partial r}\right|^2\right], \tag{17}$$

$$s_q=\sum_{\alpha\in q}\frac{1}{r^2}(|\Lambda_\alpha^{(-)}\Phi_\alpha^{(+)}|^2+|\Lambda_\alpha^{(+)}\Phi_\alpha^{(-)}|^2), \tag{18}$$

$$j_{zq}=\sum_{\alpha\in q}\mathrm{Im}\left[\Phi_\alpha^{(+)*}\frac{\partial\Phi_\alpha^{(+)}}{\partial z}+\Phi_\alpha^{(-)*}\frac{\partial\Phi_\alpha^{(-)}}{\partial z}\right], \tag{19}$$

$$j_{rq}=\sum_{\alpha\in q}\mathrm{Im}\left[\Phi_\alpha^{(+)*}\frac{\partial\Phi_\alpha^{(+)}}{\partial r}+\Phi_\alpha^{(-)*}\frac{\partial\Phi_\alpha^{(-)}}{\partial r}\right], \tag{20}$$

$$\mathcal{J}_{rzq}=2\sum_{\alpha\in q}\mathrm{Re}\left[\frac{\partial\Phi_\alpha^{(+)*}}{\partial r}\frac{\partial\Phi_\alpha^{(-)}}{\partial z}-\frac{\partial\Phi_\alpha^{(+)*}}{\partial z}\frac{\partial\Phi_\alpha^{(-)}}{\partial r}\right], \tag{21}$$

$$\mathcal{J}_{rq}=\frac{2}{r}\sum_{\alpha\in q}\mathrm{Re}\left[\Lambda_\alpha^{(-)}\Phi_\alpha^{(+)*}\frac{\partial\Phi_\alpha^{(+)}}{\partial r}-\Lambda_\alpha^{(+)}\Phi_\alpha^{(-)*}\frac{\partial\Phi_\alpha^{(-)}}{\partial r}\right], \tag{22}$$

$$\mathcal{J}_{zq}=-\frac{2}{r}\sum_{\alpha\in q}\mathrm{Re}\left[\Lambda_\alpha^{(-)}\Phi_\alpha^{(+)*}\frac{\partial\Phi_\alpha^{(-)}}{\partial z}+\Lambda_\alpha^{(+)}\Phi_\alpha^{(-)*}\frac{\partial\Phi_\alpha^{(+)}}{\partial z}\right]. \tag{23}$$

Eqs. (16)–(20) are the analog to the functions defined in Eqs. (2.14) of Ref. 12 if, in the latter, we make the identifications $\psi_\alpha\rightarrow\Phi_\alpha^{(\pm)}$ and $\mu_\alpha\rightarrow\Lambda_\alpha^{(\pm)}$, and also note that the sum over α implicitly includes the $\pm$ (degenerate) spin states.

C. Spatial discretization of the energy functional

The discretization in cylindrical coordinates proceeds just as in Ref. 12 (see also Refs. 13, 14, and 27). We define the discretized mesh points r_i and z_j

$$\begin{aligned} r_i&=(i-\tfrac{1}{2})\Delta r;\quad 1\le i\le N_R\ ;\\ z_j&=(j-1)\Delta z;\quad -N_Z\le j\le N_Z\ ; \end{aligned} \tag{24}$$

the volume element

$$\Delta V_i=2\pi(i-\tfrac{1}{2})(\Delta r)^2\Delta z\ ; \tag{25}$$

and the discretized wave functions

$$g_\alpha^{(\pm)}(i,j)=(i-\tfrac{1}{2})^{1/2}\Phi_\alpha^{(\pm)}(r_i,z_j)\ . \tag{26}$$

The wave functions vanish on the mesh boundaries

$$g_\alpha^{(\pm)}(N_R,j)=0=g_\alpha^{(\pm)}(i,\pm N_Z) \tag{27}$$

and satisfy the orthonormality relations

$$2\pi(\Delta r)^2\Delta z\sum_{ij}\{[g_\alpha^{(+)}(i,j)]^*g_\beta^{(+)}(i,j)+[g_\alpha^{(-)}(i,j)]^*g_\beta^{(-)}(i,j)\}=\delta_{\alpha\beta}\ . \tag{28}$$

The energy functional (1–5) is discretized before variation. For the parts $\mathcal{H}_y$, $\mathcal{H}_C$, and $\mathcal{H}_R$ the results are the same as in Ref. 12. The discretized $\mathcal{H}_n$ is almost the same as in Ref. 12 except for an obvious generalization for the terms proportional to t_3. The important new piece is the spin-orbit functional (4). This becomes

$$H_{1s}=-\frac{t_4}{2}\sum_{i,j}\Delta V_i\sum_{qq'}(1+\delta_{qq'})[\rho_q(i+\tfrac{1}{2},j+\tfrac{1}{2})\mathcal{J}_{rzq'}(i+\tfrac{1}{2},j+\tfrac{1}{2})+\rho_q(i+\tfrac{1}{2},j)\mathcal{J}_{rq'}(i+\tfrac{1}{2},j)+\rho_q(i,j+\tfrac{1}{2})\mathcal{J}_{zq'}(i,j+\tfrac{1}{2})]\ , \tag{29}$$

where $\rho_q(i+\frac{1}{2},j)$ and $\rho_q(i,j+\frac{1}{2})$ are defined in Ref. 12 and

$$\rho_q(i+\tfrac{1}{2},j+\tfrac{1}{2})=\tfrac{1}{4}[\rho_q(i,j)+\rho_q(i+1,j)+\rho_q(i,j+1)+\rho_q(i+1,j+1)]\ , \tag{30}$$

$$\mathcal{J}_{rzq}(i+\tfrac{1}{2},j+\tfrac{1}{2})=\frac{i}{2(i-\frac{1}{2})\Delta z\Delta r}\sum_{\substack{\alpha\in q\\ s}}s\left\{\left[\frac{g_\alpha^{(s)}(i+1,j)}{x_{i+1}}-\frac{g_\alpha^{(s)}(i,j+1)}{x_i}\right]^*\left[\frac{g_\alpha^{(-s)}(i+1,j+1)}{x_{i+1}}-\frac{g_\alpha^{(-s)}(i,j)}{x_i}\right]\right.$$
$$\left.-\left[\frac{g_\alpha^{(s)}(i+1,j+1)}{x_{i+1}}-\frac{g_\alpha^{(s)}(i,j)}{x_i}\right]^*\left[\frac{g_\alpha^{(-s)}(i+1,j)}{x_{i+1}}-\frac{g_\alpha^{(-s)}(i,j+1)}{x_i}\right]\right\}, \tag{31}$$

$$\mathcal{J}_{rq}(i+\tfrac{1}{2},j)=\frac{1}{(i-\frac{1}{2})(\Delta r)^2}\sum_{\substack{\alpha\in q\\ s}}s\left[K_\alpha-\frac{s}{2}\right]\left[\left|\frac{g_\alpha^{(s)}(i+1,j)}{x_{i+1}}\right|^2-\left|\frac{g_\alpha^{(s)}(i,j)}{x_i}\right|^2\right], \tag{32}$$

$$\mathcal{J}_{zq}(i,j+\tfrac{1}{2})=\frac{-1}{(i-\frac{1}{2})^2\Delta r\Delta z}\sum_{\substack{\alpha\in q\\ s}}\left\{K_\alpha[g_\alpha^{(s)*}(i,j+1)g_\alpha^{(-s)}(i,j+1)-g_\alpha^{(s)*}(i,j)g_\alpha^{(-s)}(i,j)]\right.$$
$$\left.+\frac{s}{2}[g_\alpha^{(s)*}(i,j+1)g_\alpha^{(-s)}(i,j)-g_\alpha^{(s)*}(i,j)g_\alpha^{(-s)}(i,j+1)]\right\}, \tag{33}$$

with $s=\pm 1$ in the summations and $x_i=\sqrt{i-(1/2)}$.

D. Derivation of the spatially discretized TDHF equations

The discretized TDHF equations are determined by variation of the action integral[28]

$$\mathcal{S}=\int dt\left[\sum_{i,j}\Delta V_i\sum_{\alpha,s}\Phi_\alpha^{(s)*}(r_i,z_j)i\hbar\frac{\partial\Phi_\alpha^{(s)}}{\partial t}(r_i,z_j)-\mathcal{H}\right], \tag{34}$$

with respect to the wave functions $g_\alpha^{(s)*}$ where $\mathcal{H}$ is the functional of Eq. (1), discretized as described in the previous section. After straightforward but lengthy algebra it can be shown that

$$i\hbar\frac{\partial g_\alpha^{(s)}(i,j)}{\partial t}=(Hg_\alpha^{(s)})(i,j)+(Vg_\alpha^{(s)})(i,j)+W_0^{(K_\alpha q)}(i,j)g_\alpha^{(s)}(i,j)+(W_Hg_\alpha^{(s)})(i,j)+(W_Vg_\alpha^{(s)})(i,j)\ ;\quad \alpha=1,2,\ldots,A\ , \tag{35}$$

where H and V refer to the *horizontal* (z-direction) and *vertical* (r-direction) parts of the single-particle Hamiltonian. The W matrices are spin-orbit matrices which "flip" the spin of the single-particle wave functions. The various terms in Eq. (35) are in detail

$$(Hg_\alpha^{(s)})(i,j)=B_q^{(+)}(i,j)g_\alpha^{(s)}(i,j+1)+B_q^{(+)*}(i,j-1)g_\alpha^{(s)}(i,j-1)+[B_q^{(0)}(i,j)+\tfrac{1}{2}h_{0q}(i,j)]g_\alpha^{(s)}(i,j)\ , \tag{36}$$

$$(Vg_\alpha^{(s)})(i,j)=A_q^{(+)}(i,j)g_\alpha^{(s)}(i+1,j)+A_q^{(+)*}(i-1,j)g_\alpha^{(s)}(i-1,j)+\left[A^{(0)}_{\Lambda_\alpha^{(s)}q}(i,j)+\frac{1}{2}h_{0q}(i,j)\right]g_\alpha^{(s)}(i,j)\ , \tag{37}$$

$$W_0^{(K_\alpha q)}(i,j)=K_\alpha F_q^{(0)}(i,j)\ , \tag{38}$$

$$(W_Hg_\alpha^{(s)})(i,j)=sF_q^{(+)}(i,j)g_\alpha^{(-s)}(i,j+1)-sF_q^{(+)}(i,j-1)g_\alpha^{(-s)}(i,j-1)\ , \tag{39}$$

$$(W_Vg_\alpha^{(s)})(i,j)=sE_q^{(+)}(i,j)g_\alpha^{(-s)}(i+1,j)-sE_q^{(+)}(i-1,j)g_\alpha^{(-s)}(i-1,j)\ , \tag{40}$$

and the constituents of these expressions are

$$h_{0q}(i,j)=t_0\left[\left(1+\frac{x_0}{2}\right)\rho(i,j)-(\tfrac{1}{2}+x_0)\rho_q(i,j)\right]+\frac{t_3}{12}\left[\left(1+\frac{x_3}{2}\right)(2+\alpha)[\rho(i,j)]^{\alpha+1}-(\tfrac{1}{2}+x_3)\left\{\alpha[\rho(i,j)]^{\alpha-1}\sum_q[\rho_q(i,j)]^2+2[\rho(i,j)]^\alpha\rho_q(i,j)\right\}\right]$$
$$+\frac{t_y}{4\pi a^3}\left[\left(1+\frac{x_y}{2}\right)U_y(i,j)-(\tfrac{1}{2}+x_y)U_{yq}(i,j)\right]+\delta_{q,p}\left\{U_C(i,j)-\left[\frac{3}{\pi}\right]^{1/3}e^2[\rho_p(i,j)]^{1/3}\right\}$$
$$-\frac{t_4}{8}\left\{\frac{(i-3/2)}{(i-1/2)}[\hat{\mathcal{J}}_{rzq}(i-\tfrac{1}{2},j-\tfrac{1}{2})+\hat{\mathcal{J}}_{rzq}(i-\tfrac{1}{2},j+\tfrac{1}{2})]+\hat{\mathcal{J}}_{rzq}(i+\tfrac{1}{2},j-\tfrac{1}{2})+\hat{\mathcal{J}}_{rzq}(i+\tfrac{1}{2},j+\tfrac{1}{2})\right\}, \tag{41}$$

where $U_{yq}(i,j)$ and $U_C(i,j)$ are the discretized approximations to the Yukawa and direct Coulomb potentials, respectively.[12] Furthermore,

$$B_q^{(0)}(i,j)=\frac{\hbar^2}{m(\Delta z)^2}+\frac{t_1+t_2}{4}\left\{\frac{\rho(i,j+\frac{1}{2})+\rho(i,j-\frac{1}{2})}{(\Delta z)^2}+\frac{1}{2}[\tau_z(i,j+\frac{1}{2})+\tau_z(i,j-\frac{1}{2})]\right\}$$
$$+\frac{t_2-t_1}{8}\left\{\frac{\rho_q(i,j+\frac{1}{2})+\rho_q(i,j-\frac{1}{2})}{(\Delta z)^2}+\frac{1}{2}[\tau_{zq}(i,j+\frac{1}{2})+\tau_{zq}(i,j-\frac{1}{2})]\right\}-\frac{t_4}{4}[\hat{\mathscr{J}}_{zq}(i,j-\tfrac{1}{2})+\hat{\mathscr{J}}_{zq}(i,j+\tfrac{1}{2})]\ , \tag{42}$$

$$B_q^{(+)}(i,j)=-\frac{\hbar^2}{2m(\Delta z)^2}-\frac{t_1+t_2}{4(\Delta z)^2}\left[\rho(i,j+\tfrac{1}{2})+\frac{\Delta z}{\sqrt{-1}}j_z(i,j+\tfrac{1}{2})\right]-\frac{t_2-t_1}{8(\Delta z)^2}\left[\rho_q(i,j+\tfrac{1}{2})+\frac{\Delta z}{\sqrt{-1}}j_{zq}(i,j+\tfrac{1}{2})\right]\ . \tag{43}$$

The $A^{(0)}$ is split further

$$A_{\mu q}^{(0)}(i,j)=C_{\mu q}(i,j)+D_q(i,j) \tag{44}$$

with

$$C_{\mu q}(i,j)=\frac{\mu^2}{r_i^2}\left[\frac{\hbar^2}{2m}+\frac{t_1+t_2}{4}\rho(i,j)+\frac{t_2-t_1}{8}\rho_q(i,j)\right] \tag{45}$$

$$D_q(i,j)=\frac{\hbar^2}{m(\Delta r)^2}+\frac{t_1+t_2}{4}s(i,j)+\frac{t_2-t_1}{8}s_q(i,j)$$
$$+\frac{t_1+t_2}{4}\left\{\frac{i\rho(i+\frac{1}{2},j)+(i-1)\rho(i-\frac{1}{2},j)}{(i-\frac{1}{2})(\Delta r)^2}+\frac{1}{2}\left[\tau_r(i+\tfrac{1}{2},j)+\frac{i-\frac{3}{2}}{i-\frac{1}{2}}\tau_r(i-\tfrac{1}{2},j)\right]\right\}$$
$$+\frac{t_2-t_1}{8}\left\{\frac{i\rho_q(i+\frac{1}{2},j)+(i-1)\rho_q(i-\frac{1}{2},j)}{(i-\frac{1}{2})(\Delta r)^2}+\frac{1}{2}\left[\tau_{rq}(i+\tfrac{1}{2},j)+\frac{i-\frac{3}{2}}{i-\frac{1}{2}}\tau_{rq}(i-\tfrac{1}{2},j)\right]\right\}$$
$$-\frac{t_4}{4}\left[\frac{i-\frac{3}{2}}{i-\frac{1}{2}}\hat{\mathscr{J}}_{rq}(i-\tfrac{1}{2},j)+\hat{\mathscr{J}}_{rq}(i+\tfrac{1}{2},j)\right]-\frac{t_4}{2}\frac{s(\Lambda_\alpha^{(s)}-s)}{(i-\frac{1}{2})(\Delta r)^2}[\rho_q(i-\tfrac{1}{2},j)+\rho(i+\tfrac{1}{2},j)]\ . \tag{46}$$

Furthermore,

$$A_q^{(+)}(i,j)=\frac{i}{(i^2-\frac{1}{4})^{1/2}(\Delta r)^2}\left[-\frac{\hbar^2}{2m}-\frac{t_1+t_2}{4}\rho(i+\tfrac{1}{2},j)-\frac{t_2-t_1}{8}\rho_q(i+\tfrac{1}{2},j)\right]$$
$$-\frac{1}{\sqrt{-1}\Delta r}\left[\frac{i}{i-\frac{1}{2}}\right]^{1/2}\left[\frac{t_1+t_2}{4}j_r(i+\tfrac{1}{2},j)+\frac{t_2-t_1}{8}j_{rq}(i+\tfrac{1}{2},j)\right]\ . \tag{47}$$

Finally the terms for the spin-flip parts become

$$F_q^{(0)}(i,j)=\frac{t_4}{2\Delta r\Delta z(i-\frac{1}{2})}[\hat{\rho}_q(i,j-\tfrac{1}{2})-\hat{\rho}_q(i,j+\tfrac{1}{2})]\ , \tag{48}$$

$$F_q^{(+)}(i,j)=-\frac{t_4}{4\Delta r\Delta z(i-\frac{1}{2})}[\hat{\rho}_q(i,j+\tfrac{1}{2})+(i-1)\hat{\rho}(i-\tfrac{1}{2},j+\tfrac{1}{2})-i\hat{\rho}_q(i+\tfrac{1}{2},j+\tfrac{1}{2})]\ , \tag{49}$$

$$E_q^{(+)}(i,j)=-\frac{t_4}{4}\frac{i}{\Delta r\Delta z(i^2-\frac{1}{4})^{1/2}}[\hat{\rho}_q(i+\tfrac{1}{2},j+\tfrac{1}{2})-\hat{\rho}_q(i+\tfrac{1}{2},j-\tfrac{1}{2})]\ , \tag{50}$$

where

$$\hat{\rho}_q(i,j)\equiv\rho(i,j)+\rho_q(i,j)\ , \tag{51}$$

$$\hat{\mathscr{J}}_{rzq}(i,j)\equiv\mathscr{J}_{rz}(i,j)+\mathscr{J}_{rzq}(i,j)\ , \tag{52}$$

$$\hat{\mathscr{J}}_{rq}(i,j)\equiv\mathscr{J}_r(i,j)+\mathscr{J}_{rq}(i,j)\ , \tag{53}$$

$$\hat{\mathscr{J}}_{zq}(i,j)\equiv\mathscr{J}_z(i,j)+\mathscr{J}_{zq}(i,j)\ . \tag{54}$$

(On the right-hand sides of Eqs. (51)–(54), remember that a function without an isospin label is the sum of the separate neutron and proton parts.)

Equation (35) may be written in a compact manner as

$$i\hbar\frac{\partial g_\alpha}{\partial t}=h(t)g_\alpha(t) \tag{55}$$

where

$$h = H + V + W_0 + W_H + W_V \tag{56}$$

with the terms on the right-hand side given by Eqs. (36)–(40), and the g_α represents the Pauli spinor on the grid, $g_\alpha^{(s)}(i,j)$. The h and the five terms in Eq. (56) are matrix operators in (i,j,s) space. They are split such that each term has "minimum off-diagonality." The notation uses the mnemonics H = *horizontal* = "along the z axis" and V = *vertical* = "along the r axis." The separable structure displayed in Eq. (56) will play a role in the following considerations of the time step.

E. Time discretization and evolution

The formal solution of the TDHF equation (55) is

$$g_\alpha(t) = U(t,t_0) g_\alpha(t_0) ,$$
$$U(t,t_0) = \mathcal{T} \exp\left[-\frac{i}{\hbar} \int_{t_0}^{t} dt' h(t') \right] , \tag{57}$$

where we have now reintroduced explicitly the time argument in g_α. The $\mathcal{T}$ denotes time ordering, and $U(t,t_0)$ is the time-evolution operator for the TDHF wave functions. We employ discrete time according to the relation

$$t_n = n\Delta t, \quad n = 0,1,2,\ldots , \tag{58}$$

express the time-evolution operator in successive pieces

$$U(t,t_0) = U(t,t_{n-1}) \times U(t_{n-1},t_{n-2}) \cdots U(t_1,t_0) , \tag{59}$$

and approximate the exponential in Eq. (57) by the unitary Padé approximant

$$U(t_n,t_{n-1}) \approx \left[1 + i\frac{\Delta t}{2\hbar} h(t_n - \tfrac{1}{2}\Delta t) \right]^{-1} \times \left[1 - i\frac{\Delta t}{2\hbar} h(t_n - \tfrac{1}{2}\Delta t) \right] . \tag{60}$$

Note that the Hamiltonian h is evaluated at the half-time point using the Crank-Nicholson step. The full inversion involved is extremely expensive on a large two-dimensional grid. We take advantage of the separable form (56) for the Hamiltonian and write the step (60) as successive products

$$U \approx U_{PR} \tag{61}$$

$$U_{PR} = \left[1 + i\frac{\Delta t}{2\hbar} V \right]^{-1} \left[1 + i\frac{\Delta t}{2\hbar} H \right]^{-1} \left[1 + i\frac{\Delta t}{2\hbar} W_V \right]^{-1} \left[1 + i\frac{\Delta t}{2\hbar} W_H \right]^{-1} \times \left[1 + i\frac{\Delta t}{2\hbar} W_0 \right]^{-1} \left[1 - i\frac{\Delta t}{2\hbar} W_0 \right] \left[1 - i\frac{\Delta t}{2\hbar} W_H \right] \left[1 - i\frac{\Delta t}{2\hbar} W_V \right] \left[1 - i\frac{\Delta t}{2\hbar} H \right] \left[1 - i\frac{\Delta t}{2\hbar} V \right] , \tag{62}$$

and V, H, W_V, W_H, and W_0 are defined in Eqs. (36)–(40). This is a generalization of the Peaceman-Rachford method.[12,14,29] It approximates the exponential time operator in Eq. (58) through terms in $(\Delta t)^2$ even if the various operators do not commute. This is an important property for time evolution with Hamiltonians containing two or more noncommuting operators.

We see from Eqs. (35)–(40) that the V, H, and W matrices are tridiagonal. Thus in Eq. (61) the matrix inversions involving V and H may be performed with a Gaussian elimination[30] method. Although $[1 + i(\Delta t/2\hbar) W_x]$ is a sparse matrix, it connects different spin blocks. Using an implicit matrix notation,

$$\left[1 + i\frac{\Delta t}{2\hbar} W_x \right]^{-1} = \begin{bmatrix} \left[1 - \left[\frac{\Delta t}{2\hbar} \right]^2 W_x^2 \right]^{-1} & 0 \\ 0 & \left[1 - \left[\frac{\Delta t}{2\hbar} \right]^2 W_x^2 \right]^{-1} \end{bmatrix} \left[1 - \frac{\Delta t}{2\hbar} W_x \right] , \tag{63}$$

with $x = 0, V, H$. This representation is sparse, with off-diagonal elements in i or j differing at most by ± 2 units. From Eqs. (35), (36)–(40), and (38), we find explicitly that

$$(W_0^2 g_\alpha^{(s)})(i,j) = K_\alpha^2 [F_q^{(0)}(i,j)]^2 g_\alpha^{(s)}(i,j) , \tag{64}$$

$$(W_V^2 g_\alpha^{(s)})(i,j) = -E_q^{(+)}(i,j) E_q^{(+)}(i+1,j) g_\alpha^{(s)}(i+2,j) - E_q^{(+)}(i-1,j) E_q^{(+)}(i-2,j) g_\alpha^{(s)}(i-2,j) + \{ [E_q^{(+)}(i,j)]^2 + [E_q^{(+)}(i-1,j)]^2 \} g_\alpha^{(s)}(i,j) , \tag{65}$$

$$(W_H^2 g_\alpha^{(s)})(i,j) = -F_q^{(+)}(i,j) F_q^{(+)}(i,j+1) g_\alpha^{(s)}(i,j+2) - F_q^{(+)}(i,j-1) F_q^{(+)}(i,j-2) g_\alpha^{(s)}(i,j-2) + \{ [F_q^{(+)}(i,j)]^2 + [F_q^{(+)}(i,j-1)]^2 \} g_\alpha^{(s)}(i,j) . \tag{66}$$

Thus in Eq. (63), for $x=0$ the first matrix is diagonal, which is trivial to invert, while for $x=V$ and H the matrix is tridiagonal with two off-diagonal units and can be inverted using a special form of a sparse Gaussian elimination[31] scheme. The time evolution with the spin-orbit force included is a straightforward generalization of the case without spin orbit.[12] But it is considerably slower because of the more complicated Peaceman-Rachford steps needed in Eq. (61).

F. Calculation of final-state quantities

The final state of the system is analyzed by computing various observables. For example, the asymptotic center-of-mass scattering and the total fragment kinetic energies are obtained by matching to a pure Coulomb trajectory, for details see Ref. 12. The charges and masses of the final fragments are obtained by computing the density distributions to the *left* and *right* of a dividing plane (between the two separating fragments) where the density is negligible. The total kinetic energies of the left- and right-hand fragments are given by

$$T_L=\frac{\pi\hbar^2}{m}\int_{-\infty}^{z_{\min}}dz\int_0^{\infty}dr\,r[\tau_z(r,z)+\tau_r(r,z)+s(r,z)]\ , \tag{67}$$

and

$$T_R=\frac{\pi\hbar^2}{m}\int_{z_{\min}}^{\infty}dz\int_0^{\infty}dr\,r[\tau_z(r,z)+\tau_r(r,z)+s(r,z)]\ , \tag{68}$$

where τ_z, τ_r, and s are defined in Eqs. (16)–(18). Each of these kinetic energies include both the energy of motion in the center of mass and the internal kinetic energy of the fragment.

Another quantity of interest is the dispersion of the number distribution for a given isospin. The left-hand fragment dispersion is,[12]

$$\sigma_q^2=\mathrm{Tr}[\rho_q^{(L)}-(\rho_q^{(L)})^2]\ , \tag{69}$$

where

$$\rho_q^{(L)}(\mathbf{r}\mu,\mathbf{r}'\mu')=\theta(z_{\min}-z)\times\sum_{\alpha\in q}n_\alpha\psi_\alpha(\mathbf{r}\mu)\psi_\alpha^*(\mathbf{r}'\mu')\theta(z_{\min}-z')\ . \tag{70}$$

The location of the dividing plane is at $z=z_{\min}$ and n_α is the occupation probability for the state α. From Eqs. (10), (69), and (70) we obtain

$$\sigma_q^2=\sum_{\alpha\in q}n_\alpha\omega_{\alpha\alpha}-\sum_{\alpha,\beta\in q}n_\alpha n_\beta|\omega_{\alpha\beta}|^2\ , \tag{71}$$

with

$$\omega_{\alpha\beta}=2\pi\delta_{K_\alpha K_\beta}\int_{-\infty}^{z_{\min}}dz\int_0^{\infty}dr\,r[\Phi_\alpha^{(+)*}(r,z)\Phi_\beta^{(+)}(r,z)+\Phi_\alpha^{(-)*}(r,z)\Phi_\beta^{(-)}(r,z)]\ . \tag{72}$$

Notice that $\omega_{\alpha\beta}$ depends implicitly on the angular momentum since the only contributions to the integral occur for α and β having the same K value. For a further detailed discussion of the full width at half maximum and corrections due to the use of the filling approximation (fractional values for n_α's in unfilled shells), see Ref. 12.

III. CONCLUSION

The evolution of the TDHF studies of heavy-ion reactions is marked by increasingly sophisticated calculations trying to eliminate as many of the assumed symmetries as possible.[2] This progress has closely paralleled the advances in computer technology. Thus it became possible to remove the spin degeneracy and to include the full spin-orbit force in axially symmetric TDHF calculations. In this work we have provided the details of such calculations with the spin-orbit term. The wave function and potentials are represented on an axial coordinate space grid using finite differences to compute derivatives. It was possible to generalize the Peaceman-Rachford method for the time step using a separable form for the time-evolution matrix. The method works well, although the expense is higher than in calculations without the spin-orbit force.

Application of the methods we have outlined to light and heavy systems[9–11] show a significant increase in the dissipation of the translational kinetic energy of the two ions. Since in TDHF the total energy of the system is conserved, the dissipation of the translational kinetic energy implies the excitation of internal degrees of freedom of the system. This means that the breakdown of mean-field approximation does not show up as soon as suspected before, and one might get out even more dissipative effects in the future if one includes the other spin-dependent forces hitherto neglected. It seems as if the mean-field approach has not yet been fully exhausted, and improved TDHF calculations may display more realistic features for heavy-ion collisions at low and medium energies.

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