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Time-Dependent Hartree-Fock Theory in a Two-Dimensional Rotating Frame

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PHYSICS DIVISION

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TWO-DIMENSIONAL ROTATING FRAME

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CONTENTS

	<u>Page</u>
I. VARIATIONAL PRINCIPLE	1
II. ROTATING FRAME	2
A. Action $\mathcal{A}$ Written in the Rotating Frame	3
B. Time-Dependent Hartree-Fock Equations in the Rotating Frame	3
C. Restriction on Two Dimensions: Axially Symmetry . .	4
C.1. Variation of the phases χ_λ	5
C.2. Solutions and boundary conditions for eqs. (20) and (21)	7
C.3. Variations of the single-particle wavefunctions $\tilde{\psi}_\lambda$	9
D. Expectation Values for Rotational Energy, Angular Momentum, Moment of Inertia, and Angular Velocity . .	10
E. Two Special Cases	11
III. DISCUSSION	13

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ABSTRACT

From a variational principle, which is equivalent to Schrödinger's equation, equations are derived which allow one to describe a system of axial symmetry rotating around an axis perpendicular to the symmetry-axis. Expressions are given for the moment of inertia, the angular velocity, and the contribution of the rotational energy to the total kinetic energy.

TIME-DEPENDENT HARTREE-FOCK THEORY IN A
TWO-DIMENSIONAL ROTATING FRAME

H. T. Feldmeier

I. VARIATIONAL PRINCIPLE

The time-dependent Hartree-Fock (TDHF) equations may be derived from the following variational principle. An action $\mathcal{A}$ for a given wavefunction and time interval is defined as

$$\mathcal{A}(\Psi) = \int_{t_1}^{t_2} \langle \Psi | i\hbar \frac{\partial}{\partial t} - H | \Psi \rangle dt \quad (1.1)$$

and is required to be extreme under variations of the wavefunction Ψ .

$$\lim_{\lambda \rightarrow 0} \frac{1}{\lambda} \{ \mathcal{A}(\Psi + \lambda \delta\Psi) - \mathcal{A}(\Psi) \} = 0. \quad (1.2)$$

The variation $\delta\Psi$ vanishes for t_1 and t_2 . In the Hartree-Fock case the allowed set of wavefunctions to be varied is restricted on Slater determinants of orthonormalized single-particle wavefunctions ψ_λ .

$$\Psi = \sqrt{A!} \mathcal{A}(\psi_{\alpha_1} \psi_{\alpha_2} \dots \psi_{\alpha_A}) \quad (2)$$

where $\mathcal{A}$ is a projection operator which antisymmetrizes.

Remark: In the following capital letters are used for many particle wavefunctions (Greek) and for operators in the many-particle Hilbert space (Latin). Small letters are used for single-particle quantities.

The Hamiltonian H in (1.1) consists of

$$H = \sum_{\lambda} \frac{1}{2m} \vec{p}^2 + \sum_{\lambda < \kappa} V_{\lambda\kappa}. \quad (3)$$

The two-particle potential $V_{\lambda\kappa}$ is assumed to be translational, galilean

and rotational invariant:

$$[\vec{r}_1 + \vec{r}_2, v_{12}] = 0; [\vec{p}_1 + \vec{p}_2, v_{12}] = 0; [\vec{\ell}_1 + \vec{\ell}_2, v_{12}] = 0. \quad (4)$$

II. ROTATING FRAME

New coordinates $\{x, y, z\}$ are introduced which belong to a frame rotated around the y' axis by an angle η against the inertial system $\{x', y', z'\}$.

The transformation between the two is given by:

$$\begin{aligned} x &= x' \cos \eta - z' \sin \eta & x' &= x \cos \eta + z \sin \eta \\ y &= y' & y' &= y & \text{or: } d_{\eta}(\vec{r}) &= \vec{r}' & (5) \\ z &= x' \sin \eta + z' \cos \eta & z' &= -x \sin \eta + z \cos \eta \end{aligned}$$

The wavefunction Ψ' in the inertial system transforms into the rotated system by:

$$\begin{aligned} D_{\eta} \Psi'(\vec{r}') &= \Psi(d_{\eta}^{-1}(\vec{r}')) = \Psi(\vec{r}) \\ D_{\eta} &= e^{\frac{i}{\hbar} \eta L_y}; D_{\eta}^{\dagger} = D_{\eta}^{-1} = D_{-\eta}; L_y = \sum_{\lambda=1}^A \ell_{y\lambda} \end{aligned} \quad (6)$$

A. The Action $\mathcal{A}$ Written in the Rotating Frame

The action $\mathcal{A}(\Psi')$ in the inertial system (primed) expressed in the rotating frame:

$$\mathcal{A} = \int_{t_1}^{t_2} \langle \Psi' | i\hbar \frac{\partial}{\partial t} - H | \Psi' \rangle dt = \int_{t_1}^{t_2} \langle \Psi | D_\eta \{ i\hbar \frac{\partial}{\partial t} - H \} D_\eta^{-1} | \Psi \rangle dt$$

The kinetic energy operator $\sum_\lambda \frac{\vec{p}_\lambda^2}{2m}$ commutes with L_y as well as the two-particle potential $\sum_{\lambda < \kappa} V_{\lambda\kappa}$ (rotational invariance). Therefore:

$$\mathcal{A} = \int_{t_1}^{t_2} \langle \Psi | D_\eta i\hbar \frac{\partial}{\partial t} D_\eta^{-1} - H | \Psi \rangle dt$$

$$\mathcal{A}(\Psi) = \int_{t_1}^{t_2} \langle \Psi | i\hbar \frac{\partial}{\partial t} + \omega L_y - H | \Psi \rangle dt; \quad \omega = \frac{\partial \eta}{\partial t}. \quad (7)$$

B. Time-Dependent Hartree-Fock Equations in the Rotating Frame

The TDHF equations in the rotating frame are given by varying the action $\mathcal{A}$ of eq. (7). The usual procedure of varying the real and imaginary part of each single-particle wavefunction provides us with the following single-particle equations:

$$i\hbar \frac{\partial}{\partial t} \psi_\lambda = \left[\frac{\vec{p}^2}{2m} - \omega \ell_y + v_{\text{HF}} \right] \psi_\lambda; \quad \lambda = 1, 2, \dots, A \quad (8)$$

$$v_{\text{HF}} \psi_\lambda = \sum_{\kappa} \left\{ \int \psi_\kappa^*(\vec{r}_2) V(\vec{r}, \vec{r}_2) \psi_\kappa(\vec{r}_2) d^3 \vec{r}_2 \cdot \psi_\lambda(\vec{r}) - \int \psi_\kappa^*(\vec{r}_2) V(\vec{r}, \vec{r}_2) \psi_\lambda(\vec{r}_2) d^3 \vec{r}_2 \cdot \psi_\kappa(\vec{r}) \right\}.$$

C. Restriction on Two Dimensions: Axially Symmetry

In the two-dimensional case we restrict the many-body wavefunction Ψ not only to a Slater determinant, but we require furthermore that each single-particle density is axially symmetric around the z-axis. Introducing the new coordinates r, z, ϕ in the rotating frame

$$\begin{aligned} r &= \sqrt{x^2 + y^2} \\ z &= z \\ \phi &= \arctan \frac{y}{x} \end{aligned} \tag{9}$$

$$\begin{aligned} \frac{\partial}{\partial x} &= \cos\phi \frac{\partial}{\partial r} - \frac{1}{r} \sin\phi \frac{\partial}{\partial \phi} \\ \frac{\partial}{\partial y} &= \frac{\hbar}{i} \left[z \cos\phi \frac{\partial}{\partial r} - \frac{z}{r} \sin\phi \frac{\partial}{\partial \phi} - r \cos\phi \frac{\partial}{\partial z} \right] \end{aligned}$$

the single-particle wavefunctions can be written as:

$$\psi_\lambda(r, z, \phi) = \hat{\psi}_\lambda(r, z) e^{i\chi_\lambda \phi} e^{i\chi_\lambda(r, z, \phi)} \tag{10}$$

$\hat{\psi}_\lambda(r, z)$ depends on r and z only and is complex. $\chi_\lambda(r, z, \phi)$ depends on ϕ as well as on r and z and is real. The wavefunction has to be continuous at $\phi = 2\pi$ and $\phi = 0$. Therefore the only possible form of $\chi_\lambda(r, z, \phi)$ can be expressed as:

$$\chi_\lambda(r, z, \phi) = \sum_{\kappa=1}^{\infty} g_{\kappa}^{(\lambda)}(r, z) \cos \kappa \phi + f_{\kappa}^{(\lambda)}(r, z) \sin \kappa \phi. \tag{11}$$

There is no $g_0^{(\lambda)}(r, z)$ term, because it is already included in $\hat{\psi}_\lambda(r, z)$.

By varying each χ_λ and $\hat{\psi}_\lambda$ separately in the expression for the action $\mathcal{A}$ (eq. (7)), we shall get the single-particle TDHF equations for $\hat{\psi}_\lambda$ associated with the χ_λ and equations for the χ_λ .

C.1. Variation of the phases χ_λ

$$\mathcal{A} = \int_{t_1}^{t_2} \langle \Psi | i\hbar \frac{\partial}{\partial t} + \frac{\hbar^2}{2m} \sum_{\lambda} \vec{\nabla}_{\lambda}^2 + \frac{\hbar}{i} \sum_{\lambda} \vec{\omega}(\vec{r}_{\lambda}) \times \vec{\nabla}_{\lambda} - \sum_{\lambda < \kappa} V_{\lambda\kappa} | \Psi \rangle dt. \quad (12)$$

Let us define $\tilde{\Psi} = \sqrt{A!} \mathcal{A}(\tilde{\psi}_{\alpha_1} \dots \tilde{\psi}_{\alpha_A})$

and $\tilde{\psi}_{\alpha}(r, z, \phi) = \hat{\psi}_{\alpha}(r, z) e^{i n_{\alpha} \phi}$

and assume

$$\langle \psi_{\alpha} \psi_{\beta} | V_{12} | \psi_{\alpha} \psi_{\beta} - \psi_{\beta} \psi_{\alpha} \rangle = \langle \tilde{\psi}_{\alpha} \tilde{\psi}_{\beta} | V_{12} | \tilde{\psi}_{\alpha} \tilde{\psi}_{\beta} - \tilde{\psi}_{\beta} \tilde{\psi}_{\alpha} \rangle. \quad (14)$$

At this point assumption (14) is a very helpful simplification. It is verified for the case where the same phase χ is used for all wavefunctions and V_{12} is local and not velocity dependent. It is even true for the Skyrme interaction and an overall phase χ not depending on the particular single-particle quantum numbers. An overall phase also guarantees the $\tilde{\psi}_{\alpha}$ to be orthonormalized if the ψ_{α} are.

$$\langle \psi_{\alpha} | \psi_{\beta} \rangle = \int \tilde{\psi}_{\alpha}^* e^{-i\chi} \psi_{\beta} e^{i\chi} d^3 \vec{r} = \langle \tilde{\psi}_{\alpha} | \tilde{\psi}_{\beta} \rangle = \delta_{\alpha\beta}.$$

Using assumption (14), the action $\mathcal{A}$ can be written as:

$$\begin{aligned} \mathcal{A} = & \int_{t_1}^{t_2} \langle \tilde{\Psi} | i\hbar \frac{\partial}{\partial t} + \frac{\hbar^2}{2m} \sum_{\lambda} \vec{\nabla}_{\lambda}^2 - \sum_{\lambda < \kappa} V_{\lambda\kappa} | \tilde{\Psi} \rangle \\ & + \int_{t_1}^{t_2} \sum_{\lambda} \langle \tilde{\psi}_{\lambda} | -\hbar \frac{\partial \chi_{\lambda}}{\partial t} + \frac{\hbar^2}{2m} \{ 2i \vec{\nabla} \chi_{\lambda} \cdot \vec{\nabla} + i \vec{\nabla}^2 \chi_{\lambda} - (\vec{\nabla} \chi_{\lambda})^2 \} + \hbar \vec{\omega}(\vec{r}) \times \vec{\nabla} \chi_{\lambda} | \tilde{\psi}_{\lambda} \rangle dt. \end{aligned} \quad (15)$$

In deriving eq. (15), the special choice of $\vec{\omega} = \omega \vec{e}_y$ should be considered; furthermore, in our coordinate system, ℓ_y (eq. 9) gives no contribution to the $\tilde{\Psi}$ part

$$\langle \tilde{\Psi} | \sum_{\lambda} \ell_{y_{\lambda}} | \tilde{\Psi} \rangle = 0.$$

For the case where the phases χ_{λ} are not the same for all single-particle states λ additional terms arise from the potential part. Besides that, the fact that the $\tilde{\psi}_{\lambda}$ are not orthonormal requires further attention.

In the following, we shall restrict ourselves to assumption (14) to avoid discussing the special structure of the potential. Nevertheless, for the kinetic energy and angular momentum parts, the most general expressions will be used. Those can be reduced easily to the overall phase case.

Let us now consider a special variation of Ψ :

$$\Psi + \delta\Psi = \sqrt{A!} \mathcal{Q}(\psi_{\alpha_1} \dots \tilde{\psi}_{\alpha_s} e^{i(\chi_{\alpha_s} + \delta\chi_{\alpha_s})} \dots \psi_{\alpha_A}) \quad (16)$$

where $\delta\chi_{\alpha_s}$ really means that we vary the functions $g_{\kappa}^{(\alpha_s)}(r,z)$ or $f_{\kappa}^{(\alpha_s)}(r,z)$ which depend only on r and z (eq. 11). Then the variational principle (1) provides us the following equation:

$$\int_{t_1}^{t_2} \langle \tilde{\psi}_s | -\hbar \frac{\partial}{\partial t} (\delta\chi_s) + \frac{\hbar^2}{2m} \{ 2i\vec{\nabla}(\delta\chi_s)\vec{\nabla} + i\vec{\nabla}^2 (\delta\chi_s) - 2\vec{\nabla}\chi_s\vec{\nabla}(\delta\chi_s) \} + \hbar\vec{\omega}(\vec{r} \times \vec{\nabla} \delta\chi_s) | \tilde{\psi}_s \rangle dt = 0. \quad (17)$$

We define $\rho_s = \psi_s^* \psi_s = \tilde{\psi}_s^* \tilde{\psi}_s = \hat{\psi}_s^* \hat{\psi}_s$ and use the relations

$$\langle \tilde{\psi}_s | \frac{\partial}{\partial t} (\delta\chi_s) | \tilde{\psi}_s \rangle = \langle \tilde{\psi}_s | \vec{\nabla}(\delta\chi_s) \vec{\nabla} | \tilde{\psi}_s \rangle = \langle \tilde{\psi}_s | \vec{\nabla}^2 (\delta\chi_s) | \tilde{\psi}_s \rangle = 0. \quad (18)$$

These matrix elements are equal to zero because $\delta\chi_s$ contains functions $\cos\kappa\phi$ and $\sin\kappa\phi$ for $\kappa \neq 0$. Partial integration gives us

$$\int_{t_1}^{t_2} dt \int d^3\vec{r} (\delta\chi_s) \left[\frac{\hbar^2}{m} \vec{\nabla} (\rho_s \vec{\nabla} \chi_s) - \hbar\omega(\vec{r} \times \vec{\nabla} \rho_s) \right] = 0. \quad (19)$$

At this point let us remember the special structure of χ

$$\chi_s(r, z, \phi) = \sum_{\kappa=1}^{\infty} g_{\kappa}^{(s)}(r, z) \cos\kappa\phi + f_{\kappa}^{(s)}(r, z) \sin\kappa\phi \quad (11)$$

and vary each $g_{\kappa}^{(s)}$ and $f_{\kappa}^{(s)}$ separately. Herewith we get differential equations for these functions

$$\begin{aligned} \frac{\partial \rho_s}{\partial r} \frac{\partial g_{\kappa}^{(s)}}{\partial r} + \frac{\partial \rho_s}{\partial z} \frac{\partial g_{\kappa}^{(s)}}{\partial z} + \rho_s \left\{ \frac{\partial^2 g_{\kappa}^{(s)}}{\partial r^2} + \frac{1}{r} \frac{\partial g_{\kappa}^{(s)}}{\partial r} + \frac{\partial^2 g_{\kappa}^{(s)}}{\partial z^2} - \frac{\kappa^2}{r^2} g_{\kappa}^{(s)} \right\} \\ - \frac{m\omega}{\hbar} \left\{ z \frac{\partial \rho_s}{\partial r} - r \frac{\partial \rho_s}{\partial z} \right\} \delta_{\kappa,1} \end{aligned} \quad (20)$$

$$\frac{\partial \rho_s}{\partial r} \frac{\partial f_{\kappa}^{(s)}}{\partial r} + \frac{\partial \rho_s}{\partial z} \frac{\partial f_{\kappa}^{(s)}}{\partial z} + \rho_s \left\{ \frac{\partial^2 f_{\kappa}^{(s)}}{\partial r^2} + \frac{1}{r} \frac{\partial f_{\kappa}^{(s)}}{\partial r} + \frac{\partial^2 f_{\kappa}^{(s)}}{\partial z^2} - \frac{\kappa^2}{r^2} f_{\kappa}^{(s)} \right\} = 0. \quad (21)$$

For an overall phase, the subscript s should be omitted.

C.2. Solutions and boundary conditions for eqs. (20) and (21)

The wavefunctions might be enclosed in a cylindrical box large enough not to influence the physical events inside. At the boundaries $(r \lesssim r_B, z \lesssim z_B)$ the density might be written as

$$\rho(r \lesssim r_B, z) = C_1(z)(r-r_B)^2 \quad ; \quad \rho(r, z \lesssim z_B) = C_2(r)(z-z_B)^2.$$

Herewith eq. (20) becomes for $k = 1$ near the boundaries, neglecting terms

proportional to $(r-r_B)^2$

$$\lim_{r \rightarrow r_B} \frac{\partial g_1}{\partial r} (r, z) = \frac{m\omega}{\hbar} z$$

and analogue

$$\lim_{z \rightarrow z_B} \frac{\partial g_1}{\partial z} (r, z) = - \frac{m\omega}{\hbar} r.$$

(22)

Since $g_1(r, z)$ exactly at the boundaries is arbitrary, we assume

$g_1(r_B, z) = \lim_{r \rightarrow r_B} g_1(r, z)$; analogue for $g_1(r, z_B)$. With boundary conditions (22), the differential eq. (20) can be solved for $g_1(r, z)$.

For $k = 2, 3, \dots$ eq. (20) is the same differential equation as (21).

These equations have in principle besides the zero solution also non-trivial solutions. But in going back to our variational principle (1), we see that non-zero solutions for f_k , $k = 1, 2, \dots$ and g_k , $k = 2, 3, \dots$ always increase the kinetic energy since these functions appear quadratic:

$$\begin{aligned} \langle \Psi | \sum_{\lambda} \frac{\vec{p}^2}{2m} | \Psi \rangle &= \sum_{\lambda} \langle \tilde{\psi}_{\lambda} | \frac{\hbar^2}{2m} \vec{\nabla}^2 | \tilde{\psi}_{\lambda} \rangle + \\ &\sum_{\lambda} \frac{\hbar^2}{2m} \langle \tilde{\psi}_{\lambda} | \frac{1}{2} \sum_{\kappa=1}^{\infty} \left(\frac{\partial g_{\kappa}^{(\lambda)}}{\partial r} \right)^2 + \left(\frac{\partial g_{\kappa}^{(\lambda)}}{\partial z} \right)^2 + \left(\frac{g_{\kappa}^{(\lambda)}}{r} \right)^2 | \tilde{\psi}_{\lambda} \rangle + \\ &\sum_{\lambda} \frac{\hbar^2}{2m} \langle \tilde{\psi}_{\lambda} | \frac{1}{2} \sum_{\kappa=1}^{\infty} \left(\frac{\partial f_{\kappa}^{(\lambda)}}{\partial r} \right)^2 + \left(\frac{\partial f_{\kappa}^{(\lambda)}}{\partial z} \right)^2 + \left(\frac{f_{\kappa}^{(\lambda)}}{r} \right)^2 | \tilde{\psi}_{\lambda} \rangle. \end{aligned} \quad (23)$$

On the other hand, these functions give no contribution to

$$\langle \Psi | i\hbar \frac{\partial}{\partial t} | \Psi \rangle = \sum_{\lambda} i\hbar \langle \tilde{\psi}_{\lambda} | \frac{\partial}{\partial t} \tilde{\psi}_{\lambda} \rangle. \quad (\text{see Eq. 18})$$

Therefore, $\mathcal{A}(\Psi)$ is always decreased for changing $g_k(r, z) = 0$; $k = 2, 3, \dots$ to any function $g_k(r, z) \neq 0$. The same holds for $f_k(r, z)$; $k = 1, 2, \dots$.

$\mathcal{A}(\Psi)$ is extreme only for

$$\begin{aligned} g_k(r, z) &= 0 \quad ; \quad k = 2, 3, \dots \\ f_k(r, z) &= 0 \quad ; \quad k = 1, 2, \dots \end{aligned} \quad (24)$$

For this reason we omit in the following these functions and use only $g(r, z) \equiv g_1(r, z)$ and $\chi(r, z, \phi) = g(r, z) \cos \phi$. Note that $\tilde{g} = \frac{1}{\omega} g$ is a solution of Eq. (20) for $\omega = 1$ if g is a solution.

C.3. Variations of the single-particle wavefunctions $\tilde{\psi}_\lambda$

Let us now consider the following special variation of Ψ :

$$\Psi + \delta\Psi = \sqrt{A!} \mathcal{Q}(\psi_{\alpha_1} \dots (\tilde{\psi}_{\alpha_s} + \delta\tilde{\psi}_{\alpha_s}) e^{i\chi_{\alpha_s}} \dots \psi_{\alpha_A}) \quad (25)$$

where $\langle \tilde{\psi}_\lambda | \tilde{\psi}_s + \delta\tilde{\psi}_s \rangle = \delta_{\lambda s}$ and therefore $\langle \tilde{\psi}_s | \delta\tilde{\psi}_s \rangle = 0$ without confining the variation.

Using Eq. (15) for the action, we get

$$\begin{aligned} \int_{t_1}^{t_2} \left[\langle \delta\tilde{\psi}_s | i\hbar \frac{\partial}{\partial t} + \frac{\hbar^2}{2m} \vec{\nabla}^2 - \hbar \frac{\partial \chi_s}{\partial t} + \frac{\hbar^2}{2m} \{ 2i\vec{\nabla}\chi_s \vec{\nabla} + i\vec{\nabla}^2 \chi_s - (\vec{\nabla}\chi_s)^2 \} \right. \\ \left. + \hbar\omega(\vec{r} \times \vec{\nabla}) \chi_s - v_{\text{HF}} |\tilde{\psi}_s\rangle + \text{c.c.} \right] dt = 0. \end{aligned} \quad (26)$$

Again the two-particle potential which contributes to v_{HF} is assumed to fulfill condition (14). Considering now the special structure of $\tilde{\psi} = \hat{\psi} e^{i\ln\phi}$ and $\chi = g(r, z)\cos\phi$ and the fact that the real and the imaginary part of $\delta\psi_s$ may be varied separately, we get the

Single-Particle TDHF Equations:

$$i\hbar \frac{\partial}{\partial t} \hat{\psi}_s = - \frac{\hbar^2}{2m} \left\{ \frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} + \frac{\partial^2}{\partial z^2} - \frac{n_s^2}{r^2} \right\} \hat{\psi}_s + v_{HF} \hat{\psi}_s \quad (27.1)$$

$$+ \frac{\hbar^2}{2m} \frac{1}{2} \left\{ \left(\frac{\partial g(s)}{\partial r} \right)^2 + \left(\frac{\partial g(s)}{\partial z} \right)^2 + \left(\frac{g(s)}{r} \right)^2 \right\} \hat{\psi}_s \quad (27.2)$$

$$- \hbar\omega \frac{1}{2} \left\{ z \left(\frac{\partial g(s)}{\partial r} + \frac{g(s)}{r} \right) - r \frac{\partial g(s)}{\partial z} \right\} \hat{\psi}_s \quad (27.3)$$

D. Expectation Values for Rotational Energy, Angular Momentum, Moment of Inertia, and Angular Velocity

The total angular momentum L with respect to the y -axis is given by

$$L = \sum_{\lambda} \langle \psi_{\lambda} | \ell_y | \psi_{\lambda} \rangle = \hbar \sum_{\lambda} \langle \hat{\psi}_{\lambda} | (\vec{r} \times \vec{\nabla} \chi_{\lambda}) | \hat{\psi}_{\lambda} \rangle. \quad (28.1)$$

For the case of an overall phase, this is equal to

$$L = \hbar\omega \int \rho \left\{ z \left(\frac{\partial \tilde{g}}{\partial r} + \frac{\tilde{g}}{r} \right) - r \frac{\partial \tilde{g}}{\partial z} \right\} \pi r dr dz \quad (28.2)$$

where $\tilde{g} = \frac{1}{\omega} g$.

Herewith a natural definition of the moment of inertia I with respect to the y -axis is given by

$$I = \frac{1}{\omega} L = \hbar \sum_{\lambda} \langle \hat{\psi}_{\lambda} | (\vec{r} \times \vec{\nabla} \chi_{\lambda}) | \hat{\psi}_{\lambda} \rangle \quad (29.1)$$

where $\tilde{\chi} = \frac{1}{\omega} \chi$. For an overall phase

$$I = \hbar \int \rho \left\{ z \left(\frac{\partial \tilde{g}}{\partial t} + \frac{\tilde{g}}{r} \right) - r \frac{\partial \tilde{g}}{\partial z} \right\} \pi r dr dz. \quad (29.2)$$

The moment of inertia can be calculated without knowing ω only by using the density ρ and the solution $\tilde{g}$ of Eq. (20). The angular velocity ω is

then given by

$$\omega = \frac{L}{I}. \quad (30)$$

The rotational energy E_{rot} which is the part of the total kinetic energy contributed by the phase χ of the wavefunctions is given by

$$E_{\text{rot}} = \sum_{\lambda} \langle \hat{\psi}_{\lambda} | \frac{\hbar^2}{2m} (\vec{\nabla} \chi_{\lambda})^2 | \hat{\psi}_{\lambda} \rangle. \quad (31.1)$$

For an overall phase:

$$E_{\text{rot}} = \frac{\hbar^2}{2m} \int \rho \left\{ \left(\frac{\partial g}{\partial r} \right)^2 + \left(\frac{g}{r} \right)^2 + \left(\frac{\partial g}{\partial z} \right)^2 \right\} \pi r dr dz. \quad (31.2)$$

The usual relation $E_{\text{rot}} = \frac{L^2}{2I}$ can be proved by using the relations

$$\frac{L^2}{2I} = \frac{1}{2} \vec{\omega} \vec{L} = \frac{1}{2} \hbar \vec{\omega} \int \rho (\vec{r} \times \vec{\nabla} \chi) d^3 r = - \frac{1}{2} \hbar \vec{\omega} \int \chi (\vec{r} \times \vec{\nabla} \rho) d^3 r.$$

From Eq. 19 we know that

$$\hbar \vec{\omega} (\vec{r} \times \vec{\nabla} \rho) = \frac{\hbar^2}{m} \vec{\nabla} (\rho \vec{\nabla} \chi).$$

Therefore

$$\begin{aligned} \frac{L^2}{2I} &= - \frac{\hbar^2}{2m} \int \chi \vec{\nabla} (\rho \vec{\nabla} \chi) d^3 r = \frac{\hbar^2}{2m} \int \rho (\vec{\nabla} \chi)^2 d^3 r = E_{\text{rot}} \\ E_{\text{rot}} &= \frac{L^2}{2I}. \end{aligned} \quad (31.3)$$

E. Two Special Cases

The case of a head-on collision of two systems with axial symmetry and with a common symmetry axis is obviously a problem with cylindrical symmetry and therefore exactly solvable in our framework.

Another case which, despite its three-dimensional structure, can be reduced to two dimensions is the so-called "passing by case". Two

spherical density distributions pass each other with an impact parameter large enough to avoid any interaction worth mentioning. In the following, we show that the "passing by case" is a solution of Eq. (20).

For spherical densities, we get the following relations for a density ρ_s centered at z_s

$$\rho_s(r, z) = \tilde{\rho}_s(r^2 + (z - z_s)^2)$$

$$\frac{\partial \rho_s}{\partial r} = 2r \tilde{\rho}'_s ; \quad \frac{\partial \rho_s}{\partial z} = z(z - z_s) \tilde{\rho}'_s ; \quad \tilde{\rho}'_s = \frac{\partial}{\partial \xi} \tilde{\rho}_s(\xi).$$

For uniformly moving systems with momentum $\hbar \vec{k}$ and $-\hbar \vec{k}$ and mass $A_R m$ and $A_L m$ for the right- and left-hand side, respectively, the phases assume the form

$$g(r, z > 0) = \frac{K \sin \eta}{A_R} r \quad \text{in the region of the right-hand system}$$

$$g(r, z < 0) = - \frac{K \sin \eta}{A_L} r \quad \text{in the region of the left-hand system.}$$

Equation (20) becomes for a wavefunction ψ_s belonging to the right-hand side

$$\frac{K \sin \eta}{A_R} \tilde{\rho}'_s 2r + \tilde{\rho}_s \left\{ \frac{K \sin \eta}{A_R} \frac{1}{r} - \frac{K \sin \eta}{A_R} \frac{1}{r} \right\} = \frac{m\omega}{\hbar} \left\{ z \tilde{\rho}'_s 2r - r \tilde{\rho}'_s 2(z - z_R) \right\}$$

or

$$\frac{K \sin \eta}{A_R} = \frac{m\omega}{\hbar} z_R \rightarrow \hbar K \sin \eta = m A_R z_R \omega$$

which gives the correct relation between the angular velocity ω , the center of mass z_R and the momentum perpendicular to the z -axis $\hbar K \sin \eta$.

The same holds for the left-hand side

$$\hbar K \sin \eta = - m A_L z_L \omega = m A_R z_R \omega \quad \text{since } A_L z_L + A_R z_R = 0.$$

III. DISCUSSION

The method presented here reduces the usual TDHF equation for three dimensions to the same type of equations and an additional differential equation both depending on two variables only. The TDHF equations are modified by an additional rotational potential whose shape and strength is determined self-consistently. Both centrifugal and Coriolis effects are included. In cases where the axial symmetry is applicable, the computational effort solving the TDHF equations is considerably reduced.

Besides this more practical advantage, a separation between the collective rotation of the system and other degrees of freedom is possible. Terms like moment of inertia and angular velocity are well defined.

The validity of this approximation has to be proved by comparison with three-dimensional calculations. Averaged quantities might be described well over a wide range of impact parameters, whereas the detailed structure of single-particle wavefunctions might deviate more under the additional constraints.

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