A METHOD FOR SOLVING THE SCHRÖDINGER EQUATION FOR MANY-PARTICLE SYSTEMS

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A METHOD FOR SOLVING THE SCHRÖDINGER EQUATION FOR MANY-PARTICLE SYSTEMS

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§ 1. The three-particle Schrödinger equation.

The Schrödinger equation

$$\sum_{i=1}^{3}\left[-\frac{\hbar^2}{2m_i}\Delta_{r_i}+V_1(|\mathbf{r}_2-\mathbf{r}_1|)+V_2(|\mathbf{r}_3-\mathbf{r}_2|)+V_3(|\mathbf{r}_1-\mathbf{r}_3|)-E\right]\psi=0, \quad (1)$$

with respect to which, for simplicity, it is assumed that it does not depend on spin variables, takes a symmetric form in the relative coordinates

$$\vec{\eta}_1=\mathbf{r}_2-\mathbf{r}_1, \qquad \vec{\eta}_2=\mathbf{r}_3-\mathbf{r}_2, \qquad \vec{\eta}_3=\mathbf{r}_1-\mathbf{r}_3, \qquad \vec{\eta}_1+\vec{\eta}_2+\vec{\eta}_3\equiv 0. \quad (2)$$

To transform equation (1) to the coordinates (2), one may, by means of the relation

$$M\mathbf{R}=\sum_{i=1}^{3}m_i\mathbf{r}_i, \qquad M=\sum_{i=1}^{3}m_i, \quad (3)$$

and the equalities (2), relate the radius vectors of the particles $\mathbf{r}_i$ to the relative vectors $\vec{\eta}_i$, differentiate the resulting relations with respect to time, multiply by m_i, and obtain

$$\mathbf{p}_1=m_1\mathbf{P}/M-\mathbf{q}_1+\mathbf{q}_3, \qquad \mathbf{p}_2=m_2\mathbf{P}/M+\mathbf{q}_1-\mathbf{q}_2,$$

$$\mathbf{p}_3=m_3\mathbf{P}/M+\mathbf{q}_2-\mathbf{q}_3, \quad (4)$$

where $\mathbf{q}_i = \mu_i \dot{\vec{\eta}}_i$ are the relative momenta, and $\mu_1 = m_1 m_2/M$, $\mu_2 = m_2 m_3/M$, $\mu_3 = m_1 m_3/M$ are the effective masses. In addition, if identity (2) is differentiated with respect to time and multiplied by $m_1 m_2 m_3/M$, one obtains the condition

$$m_3 \mathbf{q}_1 + m_1 \mathbf{q}_2 + m_2 \mathbf{q}_3 \equiv 0, \tag{5}$$

which relates the relative momenta.

To determine the relative operators, it is evidently sufficient to obtain operator relations analogous to the classical relations (4) and (5). For this purpose one may differentiate the equalities (2) with respect to time and multiply by μ_i, which relates the relative momenta to the ordinary ones; then replace, in the relations obtained, the momenta $\mathbf{p}_i$ by the operators $-i\hbar\nabla_{r_i}$, and, with the aid of the relation

$$-i\hbar\nabla_R = \sum_{i=1}^{3} -i\hbar m_i \nabla_{r_i},$$

which follows from equality (3), find

$$\nabla_{r_1} = \frac{m_1}{M}\nabla_R - \nabla_{\vec{\eta}1} + \nabla_{\vec{\eta}3}, \qquad \nabla_{r_2} = \frac{m_2}{M}\nabla_R + \nabla_{\vec{\eta}1} - \nabla_{\vec{\eta}2},$$

$$\nabla_{r_3} = \frac{m_3}{M}\nabla_R + \nabla_{\vec{\eta}2} - \nabla_{\vec{\eta}3}, \tag{6}$$

$$[m_3 \nabla_{\vec{\eta}1} + m_1 \nabla_{\vec{\eta}2} + m_2 \nabla_{\vec{\eta}3}]\psi \equiv 0. \tag{7}$$

If equalities (6) are squared, and then the mixed products of the relative operators are eliminated from them with the aid of identity (7), then, substituting the resulting squares of the operators ∇_{r_i} into equation (1), one can bring it to the symmetric form

$$\left\{ -\frac{\hbar^2}{2M}\Delta_R + \sum_{i=1}^{3}\left[-\frac{\hbar^2}{2\mu_i}\Delta_{\vec{\eta}_i} + V_i(\eta_i)\right] - E \right\}\psi = 0, \tag{8}$$

where $-\dfrac{\hbar^2}{2M}\Delta_R$ is the kinetic-energy operator of the center of inertia.

To emphasize the correctness of the problem, it is necessary to note that equation (8) must be solved with the conditions

$$\left[m_3 \nabla_{\vec{\eta}_1} + m_1 \nabla_{\vec{\eta}_2} + m_2 \nabla_{\vec{\eta}_3} \right]\psi \equiv 0, \qquad \vec{\eta}_1 + \vec{\eta}_2 + \vec{\eta}_3 = 0, \tag{9}$$

since this equation is defined in a 12-dimensional space, whereas there exist only three independent vectors.

Before proceeding to the solution of the system (8) and (9), it is useful to give expressions for the angular-momentum vector of the system

$$\vec{\Lambda} = [\mathbf{R} \times \mathbf{P}] + \sum_{i=1}^{3} \vec{\Lambda}_i, \qquad \vec{\Lambda}_i = [\mathbf{r}_i \times \mathbf{q}_i], \tag{10}$$

and for the square of the angular-momentum vector of the dependent subsystem

$$\vec{\Lambda}_2^2 = \left(\frac{m_2}{m_1}\vec{\Lambda}_1\right)^2 + \left(\frac{m_2}{m_1}\vec{\Lambda}_3\right)^2 + 2\frac{m_2 m_3}{m_1^2}(\vec{\Lambda}_1\vec{\Lambda}_3) + \left(\frac{m_2}{m_1}\vec{\Lambda}_{31}\right)^2 + \left(\frac{m_3}{m_1}\vec{\Lambda}_{13}\right)^2 + \tag{11}$$

$$+2\left(\frac{m_3}{m_1}\vec{\Lambda}_1 + \frac{m_2}{m_1}\vec{\Lambda}_3\right)\left(\frac{m_3}{m_1}\vec{\Lambda}_{31} + \frac{m_2}{m_1}\vec{\Lambda}_{13}\right), \qquad \vec{\Lambda}_{13} = [\vec{\eta}_1 \times \mathbf{q}_3], \qquad \vec{\Lambda}_{31} = [\vec{\eta}_3 \times \mathbf{q}_1],$$

which is obtained by squaring the vector product from the equalities $\vec{\eta}_2 = -(\vec{\eta}_1 + \vec{\eta}_3)$, $\mathbf{q}_2 = -(m_3\mathbf{q}_1 + m_2\mathbf{q}_3)/m_1$.

§ 2. **Method for solving the many-particle Schrödinger equation.** For solving the system (8) and (9) it is convenient to use the method of one-particle Fock expansions ([1]). To this end, in equation (8) the operator $-\dfrac{\hbar^2}{2M}\Delta_R$ is omitted, since only the internal motion is of interest, and the remaining part is rewritten in relative spherical coordinate systems

$$\sum_{i=1}^{3} \frac{\hbar^2}{2\mu_i}\left[\frac{1}{\eta_i^2}\frac{\partial}{\partial \eta_i}\left(\eta_i^2\frac{\partial}{\partial \eta_i}\right) + \frac{\hat{\Lambda}_i}{\eta_i^2} - \frac{2\mu_i}{\hbar^2}(V_i - E)\right]\psi = 0, \tag{12}$$

where

$$\hat{\Lambda}_j^2 = \frac{1}{\hbar^2 \sin\vartheta_j}\left[\frac{\partial}{\partial\vartheta_j}\left(\sin\vartheta_j\frac{\partial}{\partial\vartheta_j}\right) + \frac{1}{\sin\vartheta_j}\frac{\partial^2}{\partial\varphi_j^2}\right], \qquad j = 1, 3,$$

and $\hat{\Lambda}_2^2$ is determined from relation (11), where by relative spherical coordinate systems one means coordinate systems whose origins are associated with the particles.

In order to simplify the solution of equation (12) with conditions (9), it must be noted that the internal motion in a three-particle system is completely described by the various orientations in space of a triangle whose sides are the independent variables $|\vec{\eta}_1|$, $|\vec{\eta}_3|$ and the dependent variable $|\vec{\eta}_2|$. The orientations in space of the triangle can, naturally, be specified by a set of spherical functions $Y_{l_1 m_1}(\vartheta_1, \varphi_1)$, $Y_{l_3 m_3}(\vartheta_3, \varphi_3)$, and therefore the wave function of the system, not depending on the variables ϑ_2, φ_2, must be constructed from the sequences

$$\psi_{l_1}(\eta_1) Y_{l_1 m_1}; \qquad \psi_{l_3}(\eta_3) Y_{l_3 m_3}; \qquad \psi_{l_1 l_3}(r_2). \tag{13}$$

Since among the arguments of the wave function there are not two angular variables ϑ_2, φ_2, in order to determine the radial parts in the sequences (13) one must solve equation (12) with one of the three operator conditions (9)

$$\left[m_3^2 \Delta_{\vec{\eta}1} + 2m_2 m_3 \nabla_{\vec{\eta}1} \nabla_{\vec{\eta}3} + m_2^2 \Delta_{\vec{\eta}3}\right] \psi = m_1^2 \Delta_{\vec{\eta}2} \psi \tag{14}$$

and, moreover, take into account in the integration the identity $\vec{\eta}_1 + \vec{\eta}_2 + \vec{\eta}_3$.

The wave function of the system, if one uses one-particle Fock expansions, is constructed from configurations

$$\psi_s(\vec{\eta}_1, \vec{\eta}_3, \vec{\eta}_2) = \psi_1 Y_{l_1 m_1} \psi_3 Y_{l_3 m_3} \psi_{1,3}, \qquad s = \{l_1, m_1; \, l_3, m_3\}, \tag{15}$$

whose radial functions can be determined in advance. For this purpose equation (12), if on its left-hand side one leaves the part of the kinetic operator

$$\begin{aligned} -\hat{T}_{13}\{\psi_s\} = -\Bigg\{ & Y_{l_1 m_1} \psi_3 Y_{l_3 m_3} \psi_{13} \frac{\hbar^2}{2\mu_1} \left[\Delta_{\eta_1} + \frac{l_1(l_1+1)}{\eta_1^2}\right] \psi_1 + \\ & + \psi_1 Y_{l_1 m_1} \psi_3 Y_{l_3 m_3} \frac{\hbar^2}{2\mu_2} \left[\Delta_{\eta_2} + \frac{l_1(l_1+1) + l_3(l_3+1)}{\eta_2^2}\right] \psi_{1,3} + \\ & + \psi_1 Y_{l_1 m_1} Y_{l_3 m_3} \psi_{13} \frac{\hbar^2}{2\mu_3} \left[\Delta_{\eta_3} + \frac{l_3(l_3+1)}{\eta_3^2}\right] \psi_3 \Bigg\}, \end{aligned} \tag{16}$$

where Δ_{η_i} are radial operators, is transformed into the form

$$\left[-\hat{T}_{13} + \sum_{i=1}^{3} V_i - E_s\right] \psi_s = -\left(\hat{T} + \hat{T}_{13}\right) \psi_s, \tag{17}$$

and the approximate radial functions are sought as eigenfunctions of the operators

$$\left\{-\frac{\hbar^2}{2\mu_i} \left[\Delta_{\eta_i} + \frac{l_i(l_i+1)}{\eta_i^2}\right] + V_i\right\} \psi_i = E_{is} \psi_i, \qquad E_s = \sum_{i=1}^{3} E_{is}, \tag{18}$$

in which $l_2(l_2+1) = l_1(l_1+1) + l_3(l_3+1)$.

Since the real motion of the subsystems takes place in effective potentials, by adding to and subtracting from the equations of the system (18) the expressions $\lambda_i u_i(\eta_i)\psi_i$, where λ_i are parameters, one can, by an identical transformation, improve the choice of the basis radial functions and make it possible to solve in analytic form the transformed equations (18) for practically interesting types of interactions

$$\left\{-\frac{\hbar^2}{2\mu_i}\left[\Delta_{\eta_i} + \frac{l_i(l_i+1)}{\eta_i^2} - \frac{2\mu_i}{\hbar^2}(\lambda_i u_i - E_{is})\right]\right\}\psi_i = [\lambda_i u_i - V_i]\,\psi_i, \qquad (19)$$

where, for atomic systems, u_i means Coulomb potentials, while for nuclear systems it is convenient to choose spherical wells for u_i and to solve equations (19) with the conditions $\psi_i|_{\eta_i=0} = 0$.

After determining the radial functions, one can antisymmetrize the configurations (15) and construct, from the antisymmetrized configurations $\psi_s(\vec{\eta}_1, \vec{\eta}_3, \eta_2)$, the wave function of the system

$$\psi(\vec{\eta}_1, \vec{\eta}_3, \eta_2) = \sum_s a_s \psi_s(\vec{\eta}_1, \vec{\eta}_3, \eta_2), \qquad (20)$$

whose unknown coefficients a_s are determined if, by the Bubnov-Galerkin method with the wave function (20), equation (17) is solved with condition (14). In the solution, the energy of the system E is obtained as a func-

of the parameters $E(\lambda_1, \lambda_2, \lambda_3)$, from which, upon minimization, these parameters are determined.

Thus, the paper describes a method for solving the many-particle Schrödinger equation in relative spherical coordinate systems; it should be noted that the method of reducing the Schrödinger equation to symmetric form does not depend on the number of particles in the system.

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CITED LITERATURE

1. V. A. Fock, *Zs. Phys.*, **61**, 126 (1930); **62**, 795 (1930).

Note: Figure translations are in progress. See original paper for figures.