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A NEW THREE-BODY EQUATION

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To describe the internal motion of the system of three nonrelativistic particles with masses M_1, M_2 and M_3, we choose the vector $\vec{R}$ connecting M_1 and M_2 and the vector $\vec{r}$ connecting the midpoint of $\vec{R}$ and particle M_3. Then we introduce spherical coordinates R, Θ and Φ for $\vec{R}$ and prolate spheroidal coordinates (ξ, η, φ) for r

$$
\begin{aligned}
x &= \frac{R}{2} S \cos\varphi, \quad y = \frac{R}{2} S \sin\varphi, \\
z &= \frac{R}{2} \xi\eta; \quad S = \sqrt{(\xi^2-1)(1-\eta^2)}, \\
1 &\leq \xi < \infty, \quad -1 \leq \eta \leq 1.
\end{aligned}
\tag{1}
$$

The alternative expressions for ξ and η are

$$
\xi = \frac{r_1 + r_2}{R}, \quad \eta = \frac{r_1 - r_2}{R}. \tag{2}
$$

Here $r_1 = r_{13}$ and $r_2 = r_{23}$ are the distances between the particles.

Hence, any function of interparticle distances including the potential energy will have a simple form in the above coordinates.

The kinetic energy operator of this system is

$$
\begin{aligned}
T = &- \frac{1}{2m} \Delta_{\vec{r}} - \frac{1}{2M}\left(\frac{1}{R} + \frac{\partial}{\partial R}\right)^2 + \frac{1}{MR} \hat{q} \left(\frac{1}{R} + \frac{\partial}{\partial R}\right) \\
&+ \frac{1}{2MR^2}\left(\vec{K}^2 - B - 2\ell_z^2\right) - \frac{1}{8M}\left(\xi^2 + \eta^2 - 1 + 2\varkappa\xi\eta + \varkappa^2\right)\Delta_{\vec{r}}.
\end{aligned}
\tag{3}
$$

In formula (3) we use the following notation for the particle mass functions:

$$
\frac{1}{m} = \frac{1}{M_3} + \frac{1}{M_1 + M_3}, \quad \frac{1}{M} = \frac{1}{M_1} + \frac{1}{M_2}
\tag{4}
$$

$$
\varkappa = \frac{M_2 - M_1}{M_2 + M_1}
$$

and for the operators:

$$\Delta_{\vec z}=\frac{4}{R^2(\xi^2-\eta^2)}\Big[\frac{\partial}{\partial\xi}(\xi^2-1)\frac{\partial}{\partial\xi}+\frac{\partial}{\partial\eta}(1-\eta^2)\frac{\partial}{\partial\eta}+\frac{\xi^2-\eta^2}{(\xi^2-1)(1-\eta^2)}\frac{\partial^2}{\partial\varphi^2}\Big],$$

$$\hat q=\frac{1}{\xi^2-\eta^2}\Big[(\xi+\varkappa\eta)(\xi^2-1)\frac{\partial}{\partial\xi}+(\eta+\varkappa\xi)(1-\eta^2)\frac{\partial}{\partial\eta}\Big],$$

$$\vec K^2=-\Big(ctg\Theta+\frac{\partial}{\partial\Theta}\Big)\frac{\partial}{\partial\Theta}-\frac{1}{\sin^2\Theta}\Big(\frac{\partial}{\partial\Phi}-i\ell_z\cos\Theta\Big)^2+\ell_z^2,$$

$$B=2i\Big(\ell_x-\frac{\varkappa R}{2}p_y\Big)\Big(\frac{1}{\sin\Theta}\frac{\partial}{\partial\Phi}-\ell_z\,ctg\,\Theta\Big)-2i\Big(\ell_y+\frac{\varkappa R}{2}p_x\Big)\frac{\partial}{\partial\Theta}. \qquad (5)$$

In its turn formula (5) involves the projections of the orbital momentum $\vec\ell$ and linear momentum $\vec p$, which also should be given by the coordinates (ξ,η,φ)

$$\pm ip_x-p_y=exp(\pm i\varphi)\frac{2}{R}\Big[\pm\frac{S}{\xi^2-\eta^2}\Big(\xi\frac{\partial}{\partial\xi}-\eta\frac{\partial}{\partial\eta}\Big)+\frac{i}{S}\frac{\partial}{\partial\varphi}\Big]$$

$$\ell_x\pm i\ell_y=exp(\pm i\varphi)\Big[\pm\frac{S}{\xi^2-\eta^2}\Big(\eta\frac{\partial}{\partial\xi}-\xi\frac{\partial}{\partial\eta}\Big)+\frac{\xi\eta}{S}i\frac{\partial}{\partial\varphi}\Big]. \qquad (6)$$

$$\ell_z=-i\frac{\partial}{\partial\varphi}$$

To complete the notation, we write down the formula for

$$p_z=-\frac{2i}{R(\xi^2-\eta^2)}\Big[\eta(\xi^2-1)\frac{\partial}{\partial\xi}+\xi(1-\eta^2)\frac{\partial}{\partial\eta}\Big]. \qquad (6a)$$

The Hamiltonian is in the usual form

$$H=T+V. \qquad (7)$$

where $V=V_1(r_1)+V_2(r_2)+V_3(R)$, and the volume element

$$d\tau=\frac{R^5}{8}(\xi^2-\eta^2)d\xi\,d\eta\,d\varphi\,dR\,d(\cos\Theta)\,d\Phi.$$

Thus, the initial representation is defined completely [1].

The cross derivatives in the operator (3) hinder its use in the asymptotic region, when the physical system disintegrates into subsystems, the kinetic energy operator should split into the sum of two Laplace operators with the relevant reduced masses, and the total wave function factorizes into subsystem wave functions.

Unifying the first and last terms in formula (3) for the kinetic energy of the three-particle system, we get an interesting candidate for the role of the kinetic energy operator of the subsystem [2]

$$t_\rho=-\frac{1}{2\frac{m}{\rho}}\Delta_{\vec z},\quad \rho=1+\frac{m}{4M}(\xi^2+\eta^2-1+2\varkappa\xi\eta+\varkappa^2) \qquad (8)$$

and the corresponding Hamiltonian

$$h_\rho=t_\rho+V_1+V_2+V_3. \qquad (9)$$

For definiteness we assume that the terms V_1 and V_2 correspond to attraction and the term V_3 to repulsion. A classical example of such a problem is the molecular hydrogen ion H_2^+.

Now we use the asymptotic properties of the coordinates ξ and η as $R\to\infty$. In this case [3]

$$\xi\longrightarrow 1+\frac{\lambda_1}{R}\approx 1+\frac{\lambda_2}{R},$$

$$\eta\longrightarrow -1+\frac{\mu_1}{R}\approx 1-\frac{\mu_2}{R}, \qquad (10)$$

where

$$\lambda_1=r_1(1-\cos\Theta_1),\quad \lambda_2=r_2(1+\cos\Theta_2),$$

$$\mu_1=r_1(1+\cos\Theta_1),\quad \mu_2=r_2(1-\cos\Theta_2) \qquad (11)$$

are two sets of parabolic coordinates (λ,μ), and formula (11) expresses them through the polar coordinates at each center.

Substituting expressions (10) into the formula (8) for ρ and using the leading term only, we come to the conclusion that

$$\rho\xrightarrow[R\to\infty]{}\begin{cases}\rho_+=1+\frac{m}{M}\left(\frac{1+\varkappa}{2}\right)^2\\ \rho_-=1+\frac{m}{M}\left(\frac{1-\varkappa}{2}\right)^2\end{cases} \qquad (12)$$

and then using formulae (4), we get

$$\frac{\rho_+}{m}=\frac{1}{M_3}+\frac{1}{M_1},$$

$$\frac{\rho_-}{m}=\frac{1}{M_3}+\frac{1}{M_2}. \qquad (13)$$

The physical meaning of formulae (7), (10) and (13) is the following. The Schrödinger equation with the Hamiltonian (9)

$$h_\rho\varphi_\rho=\mathcal{E}\varphi_\rho \qquad (14)$$

which may be called a generalized two-center problem /3/, has two types of solutions. At finite R (this distance enters into the problem (14) as a parameter) the wave functions of eq. (14) are formed due to the total particle interaction. However, as $R\to\infty$ the solutions of the first type group at the point $\eta=-1$ and due to the interaction V_1 form a subsystem (1+3) with the precise reduced mass from the upper formula (13). As $R\to\infty$ the solutions of the second type describe a subsystem (2+3), they group at the point $\eta=1$. Moreover, eq. (14) has a continuous spectrum, the wave functions of which resemble the delta function $\delta(\eta)$ as $R\to\infty$ /4/.

Thus, the solutions of problem (14) in the asymptotic region (i.e. as $R\to\infty$) gather in different configuration regions. If a pair of particles is coupled, the Hamiltonian h_ρ turns into the corresponding precise two-particle Hamiltonian. All these solutions are mutually orthogonal.

Now we introduce the operator

$$\Lambda = f(\rho)R\left(\frac{1}{R}+\frac{\partial}{\partial R}\right). \tag{15}$$

where $f(\rho)$ is an unknown function of the argument which is determined by formula (8) and enters into the Hamiltonian h_ρ (9). Then we introduce a unitary transformation of the total Hamiltonian

$$H=-\frac{1}{2\frac{m}{\rho}}\Delta_{\vec z}+V-\frac{1}{2M}\left(\frac{1}{R}+\frac{\partial}{\partial R}\right)^2+\frac{\hat q}{MR}\left(\frac{1}{R}+\frac{\partial}{\partial R}\right)-\frac{\vec K^2-B-2\ell_z^2}{2MR^2} \tag{16}$$

in the form of

$$H_\Lambda=e^{-\Lambda}He^{\Lambda}=H-[\Lambda,H]+\frac{1}{2!}[\Lambda,[\Lambda,H]]+\ldots \tag{17}$$

According to formula (17) each term of the operator (16) transforms into an infinite series

$$\begin{aligned}e^{-\Lambda}\left(-\frac{1}{2\frac{m}{\rho}}\Delta_{\vec z}\right)e^{\Lambda}=&-(1+2f+\ldots)\frac{1}{2\frac{m}{\rho}}\Delta_{\vec z}\\&-\frac{2\rho}{M}f'\frac{\hat q}{R}\left(\frac{1}{R}+\frac{\partial}{\partial R}\right)\\&-\frac{\rho}{2MR}\left[6f'+4f''(\rho-1)\right]\left(\frac{1}{R}+\frac{\partial}{\partial R}\right)+\ldots\end{aligned} \tag{18}$$

$$e^{-\Lambda}\left[-\frac{1}{2M}\left(\frac{1}{R}+\frac{\partial}{\partial R}\right)^2\right]e^{\Lambda}=(1+2f+\ldots)\left[-\frac{1}{2M}\left(\frac{1}{R}+\frac{\partial}{\partial R}\right)^2\right] \tag{19}$$

$$\begin{aligned}e^{-\Lambda}\left[\frac{\hat q}{MR}\left(\frac{1}{R}+\frac{\partial}{\partial R}\right)\right]e^{\Lambda}=&(1+2f+\ldots)\frac{\hat q}{MR}\left(\frac{1}{R}+\frac{\partial}{\partial R}\right)+\\&+\frac{2(\rho-1)}{M}f'\left[\left(\frac{1}{R}+\frac{\partial}{\partial R}\right)^2+\frac{1}{R}\left(\frac{1}{R}+\frac{\partial}{\partial R}\right)\right]+\ldots\end{aligned} \tag{20}$$

$$e^{-\Lambda}\left[\frac{\vec K^2-B-2\ell_z^2}{R^2}\right]e^{\Lambda}=(1+2f+\ldots)\frac{\vec K^2-B-2\ell_z^2}{R^2}. \tag{21}$$

Formulae (18)-(21) contain two terms each from the corresponding infinite series, thus giving an idea about their structure.

Collecting similar terms and summing up the corresponding series, we find

$$\begin{aligned}H_\Lambda=e^{2f}\Big\{&-\frac{1}{2\frac{m}{\rho}}\Delta_{\vec z}+(1-2\rho f')\frac{\hat q}{MR}\left(\frac{1}{R}+\frac{\partial}{\partial R}\right)\\&-\frac{1}{2M}\left[1-4(\rho-1)f'+4\rho(\rho-1)(f')^2\right]\left(\frac{1}{R}+\frac{\partial}{\partial R}\right)^2+\frac{\vec K^2-B-2\ell_z^2}{R^2}\\&+\frac{1}{MR}\left[2f'(\rho-1)-3f'\rho-2f''\rho(\rho-1)-2\rho(\rho-1)(f')^2\right]\left(\frac{1}{R}+\frac{\partial}{\partial R}\right)\Big\}+e^{-\Lambda}Ve^{\Lambda}.\end{aligned} \tag{22}$$

Killing the term $\frac{\hat q}{MR}\left(\frac{1}{R}+\frac{\partial}{\partial R}\right)$ with the cross derivatives $\frac{\partial^2}{\partial R\partial\xi}$ and $\frac{\partial^2}{\partial R\partial\eta}$, we get an equation for f

$$f'=\frac{1}{2\rho}$$

with the solution

$$f=\ln\sqrt{\rho}+\text{const}.$$

Assuming an arbitrary constant to be zero, we substitute $f=\ln\sqrt{\rho}$ into expression (22). After some simple transformations, we arrive at the final expression for H_Λ

$$\begin{aligned}H_\Lambda=\rho\Big[&-\frac{1}{2\frac{m}{\rho}}\Delta_{\vec z}-\frac{1}{2M\rho}\left(\frac{\partial^2}{\partial R^2}+\frac{5}{R}\frac{\partial}{\partial R}\right)-\frac{3}{2}\frac{1}{M\rho R^2}\\&+\frac{1}{2MR^2}\left(\vec K^2-B-2\ell_z^2\right)\Big]+V_\Lambda.\end{aligned} \tag{23}$$

Finally, instead of the reduced mass M there arises the combination $M\rho$, so that

$$\frac{1}{M\rho} \xrightarrow[R\to\infty]{} \begin{cases} (\rho_+ M)^{-1} = \frac{1}{M_2} + \frac{1}{M_1+M_3} \\ (\rho_- M)^{-1} = \frac{1}{M_1} + \frac{1}{M_2+M_3} \end{cases} . \tag{24}$$

This means that in the asymptotic region, i.e. as $R\to\infty$, the combination $M\rho$ turns into precise reduced mass either for the case (1+3)+2 or for the case (2+3)+1. The important point is that this happens at the same time when the proper reduced mass arises in the h_ρ subsystem Hamiltonian, as it has been shown above, formula (13).

The summing up: We started with the three-body molecular Hamiltonian. After a simple regrouping of its terms, we succeeded in extracting the subsystem Hamiltonian h_ρ with a good asymptotic behaviour. Then we introduced a unitary transformation of the total Hamiltonian, which simplifies it drastically and simultaneously improves its asymptotic properties. The action of this operator is equivalent to a certain extension with respect to the R coordinate with the coefficient depending on the (ξ, η) coordinates.

The potential energy operator "dresses" and becomes

$$\frac{1}{\rho} e^{-\Lambda} V e^{\Lambda}$$

being easily calculated for any analytical form.

There appears an addition to the potential energy in the form

$$-\frac{3}{2}\,\frac{1}{R^2 M\rho}$$

which may be regarded as the three-particle interaction. It is of the kinematic origin.

The Schrödinger equation acquires naturally the mass operators which are the coordinate functions. This phenomenon is thought as the emergence of quasiparticles.

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Матвеенко А.В. E4-83-50

Новое уравнение для задачи трех тел

Исходным берется уравнение Шредингера для задачи трех тел в молекулярном представлении. Строится представление, при помощи которого в новом уравнении Шредингера "убиваются" перекрестные производные. Это уравнение имеет простой вид и "хорошие" асимптотические свойства. Его можно интерпретировать как уравнение для квазичастиц, массы которых зависят от координат. Кроме того, в новом уравнении возникает добавка к потенциальной энергии, которая имеет вид трехчастичного взаимодействия. Эта добавка имеет кинематическое происхождение.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

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Matveenko A.V. E4-83-50

A New Three-Body Equation

We start with the Schrödinger equation for the three-body problem in the molecular state approach. A new representation is built, which "kills" cross derivatives in the Schrödinger equation. This new equation has a simple form and "good" asymptotic properties. It may be interpreted as an equation for quasiparticles with masses depending on coordinates. Moreover, a potential energy term is modified and acquires the form of the three-particle interaction. This modification is of the kinematic nature.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

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