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A Self-Consistent Description of Particle Scattering on a Bound System That Conserves Unitarity

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Abstract—A new way of solving the problem of scattering while conserving unitarity for real and complex interaction potentials is proposed: Finding a self-consistent solution to the many-particle Schrödinger equation.

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INTRODUCTION

A stationary Schrödinger equation is often used to solve a two-particle scattering problem in quantum mechanics. A solution with the real potential of interacting particles is usually sought by expanding the wave function over partial waves. The normalization of the wave function that is the solution of this equation is thus conserved and the S-matrix is unitary. It should be noted that an analytical solution can be found only for a small number of potentials and mainly for small values of the partial moments.

There are several approaches to this problem in theoretical studies of the scattering of systems with many-particle structure.

This many-particle problem is often considered within a two-particle problem by solving the Schrödinger equation with complex potentials [1, 2]. As a rule, such potentials are introduced phenomenologically. The solution obtained via partial wave decomposition does not conserve normalization in this case, leading to uncertainty in estimates of processes' probabilities. The method of a mathematical eikonal was first proposed in [3, 4], allowing us to obtain for a T-matrix an analytical expression in the form of a functional satisfying the optical theorem and valid for a wide range of potentials under the condition that the profile function small. This method successfully described the experimental differential cross-sections for elastic proton-proton scattering in a wide range of energies, from moderate to ultra-high [5, 6].

In [7], integral equations were obtained for the three-particle scattering problem using the Lippmann–Schwinger equation. The unitarity condition was fulfilled or purely real potentials describing two-particle interaction, but this was not obvious for complex ones. In the diagram approach [8, 9], the question of the fulfilling the unitarity condition remains open as well.

This work summarizes a self-consistent method for solving the Schrödinger equation for three particles. The asymptotic solution obtained by this method conserves the normalization [10, 11] and allows us to restore the potentials in a three-particle system.

SCHRÖDINGER EQUATION FOR THE PROBLEM OF PARTICLE SCATTERING ON A BOUND SYSTEM CONSISTING OF TWO PARTICLES

Let us consider the scattering of particle 1 with mass m_1 and impulse k_1 on a bound system of particles 2 and 3 with masses m_2, m_3 and impulses k_2, k_3, respectively. To select the degrees of freedom associated with the relative movement of particles (2, 3) and the relative movement of their center of mass and particle 1, we introduce the Jacobi coordinates

$$\vec{r} = \{x, y, z\} = \vec{r}_2 - \vec{r}_3 \text{ и } \vec{R} = \{X, Y, Z\} = \vec{r}_1 - \vec{R}_{23},$$

where $\vec{R}_{23} = \dfrac{m_2\vec{r}_2 + m_3\vec{r}_3}{m_2 + m_3}$ is coordinate of the center of mass of particles (2, 3), while $\vec{r}_1$, $\vec{r}_2$, and $\vec{r}_3$ are Cartesian coordinates of particles 1, 2, and 3, respectively.

The Schrödinger equation for the scattering of a particle on a two-particle bound system

$$\left[-\sum_{i=1}^{3}\frac{\hbar}{2m_i}\Delta_i + \sum_{i>j=1}^{3} V_{ij}\right]\Psi(\vec{r}_1,\vec{r}_2,\vec{r}_3) = E\Psi(\vec{r}_1,\vec{r}_2,\vec{r}_3) \quad (1)$$

in Jacobi coordinates in the system of the mass center at $Q = 0$ is written as

$$\left[-\frac{\hbar}{2M}\Delta_{\vec{R}} - \frac{\hbar}{2m}\Delta_{\vec{r}} + V_{12}(\vec{R},\vec{r}) + V_{13}(\vec{R},\vec{r}) + V_{23}(\vec{r})\right] \times \Psi(\vec{R},\vec{r}) = E\Psi(\vec{R},\vec{r}). \quad (2)$$

In Eqs. (1, 2), V_{ij} are the pair potentials of particles interaction. V_{23} are purely real, while V_{12} and V_{13} can in principle be complex. In Eq. (2), we introduce

reduced mass $m = \dfrac{m_2 m_3}{m_2 + m_3}$ for particles 2 and 3 and reduced mass $M = \dfrac{m_1(m_2 + m_3)}{m_1 + m_2 + m_3}$ for all three particles.

We select function $\Psi(\vec{R},\vec{r})$ in the optical limit [1]

$$\Psi(\vec{R},\vec{r}) = (2\pi\hbar)^{-3/2} e^{if(\vec{R},\vec{r})}\Phi_{i,s}(\vec{r}). \quad (3)$$

We assume that function $f(\vec{R},\vec{r})$ is valid [10, 11] and that function (3) retains its normalization.

In Eq. (2), Jacobi coordinates $\vec{R}$ and $\vec{r}$ are used as variables. Division of these variables in it is impossible, since potentials V_{12} and V_{13} depend on both Jacobi coordinates. We assume that at infinitely great distance ($|\vec{R}| \to \infty$), the state of system (2, 3) after scattering is described by the equation

$$\left[-\frac{\hbar}{2m}\Delta_{\vec{r}} + V_{23}(\vec{r})\right]\Phi_s(\vec{r}) = E_s\Phi_s(\vec{r}), \quad (4)$$

where $\Phi_s(\vec{r})$ is the normalized eigenfunction of the state of system (2, 3), and E_s is the energy of this system's state. Prior to interaction, function (3) is determined by a plane wave and normalized function of the initial state $\Phi_i(\vec{r})$, which is the solution to Eq. (4) for energy E_i.

Applying the operation of differentiation by argument $\vec{r}$ to the multiplication of functions $e^{if(\vec{R},\vec{r})}\Phi_s(\vec{r})$ in (2) and using (4), we obtain

$$\left\{-\frac{\hbar}{2M}\Delta_{\vec{R}} - i\frac{\hbar}{2m}\Delta_{\vec{r}} f(\vec{R},\vec{r}) - i\frac{\hbar}{m}\vec{\nabla}_{\vec{r}} f(\vec{R},\vec{r})\cdot\vec{\nabla}_{\vec{r}}\ln\Phi_s(\vec{r}) + V_{12}(\vec{R},\vec{r}) + V_{13}(R,\vec{r}) + \frac{\hbar}{2m}[\vec{\nabla}_{\vec{r}} f(\vec{R},\vec{r})]^2\right\}\Psi(\vec{R},\vec{r}) = (E - E_s)\Psi(\vec{R},\vec{r}), \quad (5)$$

in which $\vec{\nabla}_{\vec{r}} = \dfrac{\partial}{\partial x}\vec{i} + \dfrac{\partial}{\partial y}\vec{j} + \dfrac{\partial}{\partial z}\vec{k}$ is the gradient of function $\Phi_s(\vec{r})$ in the direction of vector $\vec{r}$.

If we introduce complex potential

$$V(\vec{R},\vec{r}) = v(\vec{R},\vec{r}) + iu(\vec{R},\vec{r}), \quad (6)$$

the real part of which is given by

$$v(\vec{R},\vec{r}) = \mathrm{Re}V_{12}(\vec{R},\vec{r}) + \mathrm{Re}V_{13}(\vec{R},\vec{r}) + \frac{\hbar}{2m}[\vec{\nabla}_{\vec{r}} f(\vec{R},\vec{r})]^2, \quad (7)$$

and the imaginary part has the form

$$u(\vec{R},\vec{r}) = -\frac{\hbar}{m}\vec{\nabla}_{\vec{r}} f(\vec{R},\vec{r})\cdot\vec{\nabla}_{\vec{r}}\ln\Phi_s(\vec{r}) - \frac{\hbar}{2m}\Delta_{\vec{r}} f(\vec{R},\vec{r}) + \mathrm{Im}V_{12}(\vec{R},\vec{r}) + \mathrm{Im}V_{13}(\vec{R},\vec{r}), \quad (8)$$

Eq. (2) can be written as

$$\left[-\frac{\hbar}{2M}\Delta_{\vec{R}} + V(\vec{R},\vec{r})\right]\Psi(\vec{R},\vec{r}) = (E - E_s)\Psi(\vec{R},\vec{r}). \quad (9)$$

In principle, complex potential (6–8) contains information on both the states of the bound two-particle system and the states of the entire three-particle system.

FINDING FUNCTION $f(\vec{R},\vec{r})$ AND RESTORING THE FORM OF THE OPTICAL POTENTIAL

Let us consider the asymptotic case $|\vec{R}| \gg |\vec{r}|$.

We expand function $f(\vec{R},\vec{r})$ in a Maclaurin series up to third derivatives inclusive, taking into account the considerations of symmetry

$$f(\vec{R},\vec{r}) \approx f(\vec{R}) + C(\vec{R})(x + y + z) + \frac{1}{2!}\Big[B(\vec{R})(x^2 + y^2 + z^2) + 2\tilde{B}(\vec{R})(xz + xy + yz)\Big] + \frac{1}{3!}\Big[D(\vec{R})(x^3 + y^3 + z^3) + 3\tilde{D}(\vec{R})(x^2z + x^2y + y^2z + z^2y + z^2x + y^2x) + 2\tilde{\tilde{D}}(\vec{R})xyz)\Big]. \quad (10)$$

In expansion (10), we introduce the notation $f(\vec{R},\vec{r})\big|_{|\vec{r}|=0} = f(\vec{R})$, and $C(\vec{R})$, $B(\vec{R})$, $\tilde{B}(\vec{R})$, $D(\vec{R})$, $\tilde{D}(\vec{R})$, $\tilde{\tilde{D}}(\vec{R})$ are partial derivatives of the first, second, and third order, respectively, when $\vec{r} = 0$.

We also expand potentials $V_{ij}(R,r)$ to a Maclaurin series by the powers of components of vector $\vec{r}$ and consider in the expansion the first-order terms relative to x, y, z:

$$\mathrm{Re}\Big[V_{12}(\vec{R},\vec{r}) + V_{13}(\vec{R},\vec{r})\Big] = V_0(\vec{R}) + V_1(\vec{R})(x + y + z), \quad (11)$$

$$\mathrm{Im}\Big[V_{12}(\vec{R},\vec{r}) + V_{13}(\vec{R},\vec{r})\Big] = U_0(\vec{R}) + U_1(\vec{R})(x + y + z), \quad (12)$$

where $V_0(\vec{R})$ and $U_0(\vec{R})$ are values of the real and imaginary parts of the potentials, and $V_1(\vec{R})$ and $U_1(\vec{R})$ are their partial derivatives when $\vec{r} = 0$.

Inserting expansion (10) into Eq. (9) and equating imaginary and real parts of the expressions on the right and left sides, we obtain a system of two differential equations with respect to $f(\vec{R})$, $C(\vec{R})$, $B(\vec{R})$, $\tilde{B}(\vec{R})$, $D(\vec{R})$, and $\tilde{D}(\vec{R})$:

$$\frac{\hbar}{2M}\left[\Delta_{\vec{R}}\left(f(\vec{R})+C(\vec{R})(x+y+z)\right)\right]+\frac{\hbar}{2m}\left[3B(\vec{R})+D(\vec{R})(x+y+z)\right.$$
$$\left.+\tilde{D}(\vec{R})(x+y+z)\right]+\frac{\hbar}{2m}\left[C(\vec{R})\left(\frac{\partial \ln\Phi_s}{\partial x}+\frac{\partial \ln\Phi_s}{\partial y}+\frac{\partial \ln\Phi_s}{\partial z}\right)\right] \quad (13)$$
$$=-U_0(\vec{R})-U_1(\vec{R})(x+y+z),$$

$$\frac{\hbar}{2M}\left[\left(\vec{\nabla}_{\vec{R}}f(\vec{R})\right)^2+2\vec{\nabla}_{\vec{R}}C(\vec{R})\vec{\nabla}_{\vec{R}}f(\vec{R})(x+y+z)\right]+\frac{\hbar}{2m}\left\{3C^2(\vec{R})\right. \quad (14)$$
$$\left.+\left[B(\vec{R})C(\vec{R})+2\tilde{B}(\vec{R})C(\vec{R})\right](x+z+y)\right\}=-V_0-V_1(x+y+z)+(E-E_s).$$

Since asymptotic wave function (3) included plane wave $e^{i\vec{k}\vec{R}}$ before interaction, it is natural to assume that

$$f(\vec{R}) = \vec{k}\vec{R}. \quad (15)$$

It then follows from Eq. (14) that

$$\frac{\hbar}{2M}\left|\vec{k}\right|^2 = (E-E_s). \quad (16)$$

To determine the partial derivatives $C(\vec{R})$, $B(\vec{R})$, $\tilde{B}(\vec{R})$, $D(\vec{R})$, and $\tilde{D}(\vec{R})$, we equate the zero-degree terms with Jacobi coordinates in (14). As a result, we obtain relation

$$C^2(\vec{R}) = -\frac{2m}{3\hbar}V_0(\vec{R}), \quad (17)$$

which determines $C(\vec{R})$, from which it follows that $V_0(\vec{R})$ must be negative in order for $C(\vec{R})$ to be a real function.

Coefficient $B(\vec{R})$ is found from (13)

$$B(\vec{R}) = -\frac{2m}{3\hbar}U_0(\vec{R}). \quad (18)$$

Given the condition of normalization, we may assume that

$$\tilde{B}(\vec{R}) = -\frac{1}{2}B(\vec{R}). \quad (19)$$

From Eq. (14), we then obtain

$$\frac{\hbar}{2M}[2\vec{k}\vec{\nabla}_{\vec{R}}C(\vec{R})] = -V_1(\vec{R}). \quad (20)$$

As derivatives of higher order, $D(\vec{R})$ and $\tilde{D}(\vec{R})$ can be found by setting a specific form of function $\Phi_s(\vec{r})$ that is a solution to Eq. (4) and considering the higher degree coordinates of vector $\vec{r}$ in expansion (10).

CONCLUSIONS

It was shown that function $f(\vec{R},\vec{r})$ contained in the exponent of wave function (3), which is the solution to Eq. (9), can be obtained with the required number of members in Maclaurin expansion (10). The convergence of this expansion for each $\vec{R}$ will suffice when $\left|\vec{r}\right|/\left|\vec{R}\right| \ll 1$, since each successive term contains a coefficient at the $\left(\left|\vec{r}\right|/\left|\vec{R}\right|\right)^n$ degree of the order of first degrees of two-particle potentials V_0 and $U_0(\vec{R})$ rather than their positive powers, as in perturbation theory. In addition, nuclear physics uses potentials that are decreasing exponents. To determine the coefficients in expansion (10) along with overridden two-particle potentials (11, 12), we used information on two-particle interaction potentials $V_0(\vec{R})$ and $U_0(\vec{R})$, and about the function of the two-particle system on which scattering occurs.

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