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Integral equations for the wave function of particle systems

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Abstract. Constructions of integral equations to the wave function of particle systems in bound state have been proposed in this work. We obtain the kernel of the Fredholm type integral equation for an odd number of particles in explicit form. Besides, an integral equation that can be attributed to the class of Volterra integral equations was built. Their equivalence to known equations in limiting cases has been shown.

Keywords: integral equation, particle system, wave function.

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1. Introduction

Investigation of the state of a many-particle system, in most cases, is carried out by numerical simulation by using multidimensional differential equations. Besides, the equally popular method is one-particle approximation. However, in fundamental and applied researches of processes occurring in physical systems, integral equations corresponding to the wave function of a particle system are a powerful, effective means to obtain results. Therefore, in recent years, interest to the integral form of the equations of quantum mechanics has increased [1-7].

The form of the Helmholtz equation can be given to the stationary Schrodinger equation for a single particle in the case of negative energy as follows:

$$\left(\Delta-k_1^2\right)\varphi_1(\vec{r}_1)=u_1\varphi_1(\vec{r}_1), \tag{1.1}$$

where $u_1=\dfrac{2\mu_1 W_{P1}}{\hbar^2}$, $k_1=\dfrac{\sqrt{2\mu_1(-E_1)}}{\hbar}$; μ_1 – particle mass, E_1, W_{P1} – energy and potential energy of the particle, respectively.

The integral equation of the Fredholm [8, 9] type corresponds to Eq. (1.1):

$$\varphi_1(\vec{r}_1)=\int_{-\infty}^{+\infty}G_1(\vec{r}-\vec{\xi})u_1(\vec{\xi})\varphi_1(\vec{\xi})d\vec{\xi}\ , \tag{1.2}$$

where

$$G_1(\vec{r}-\vec{\xi})=-\frac{\exp\left\{-k_1\left|\vec{r}_1-\vec{\xi}_1\right|\right\}}{4\pi\left|\vec{r}_1-\vec{\xi}_1\right|}. \tag{1.3}$$

The integral equation of the Volterra [10] type corresponds to the one-dimensional case of the equation (1.1), when $\Delta=\dfrac{\partial^2}{\partial x_1^2}$:

$$\varphi_1=\varphi_{01}-\frac{1}{k_1}\int_{x_1}^{+\infty}\operatorname{sh}\{k_1(x_1-\xi_1)\}u_1\varphi_1(\xi_1)d\xi_1\ , \tag{1.4}$$

where φ_{01} is the solution of the homogeneous one-dimensional equation (1.1).

The aim of this work is to generalize the integral equation (1.3) for one particle in the case of a particle system, and to build an equation that can be attributed to the class of equations of the Volterra type for the wave function of the stationary bound states of the particle system.

2. Setting the task

In this work, we used the method of inverse differential operator. We can construct the equation as an illustration of this method (1.4).

For the operator inverse to the operator $\frac{\partial}{\partial x_1}$, we would choose the following two possible representations:

$$\hat{t}_{1+} = -\int_{x_1}^{+\infty} d\xi_1 , \quad (2.1)$$

$$\hat{t}_{1-} = \int_{+\infty}^{x_1} d\xi_1 . \quad (2.2)$$

The action of operators (2.1) and (2.2) to the power m on some function $f(x_1)$, according to the formula for multiple integration, will be:

$$\left(\hat{t}_{1+}\right)^m f(x_1) = -\int_{x_1}^{+\infty} \frac{(x_1-\xi_1)^{m-1}}{(m-1)!} f(\xi_1) d\xi_1 , \quad (2.3)$$

$$\left(\hat{t}_{1-}\right)^m f(x_1) = \int_{+\infty}^{x_1} \frac{(x_1-\xi_1)^{m}}{(m-1)!} f(\xi_1) d\xi_1 . \quad (2.4)$$

From one-dimensional equation (1.1), it follows that

$$\varphi_1 = \varphi_{01} + \left(\frac{\partial^2}{\partial x_1^2} - k_1^2\right)^{-1} u_1 \varphi_1 . \quad (2.5)$$

Let us expand the inverse operator in the right side of expression (2.5) into a power series by the operators (2.1):

$$\left(\frac{\partial^2}{\partial x_1^2} - k_1^2\right)^{-1} = \left(\hat{t}_{1+}\right)^2 \sum_{n_1=0}^{\infty} k_1^{2n_1} \left(\hat{t}_{1+}\right)^{2n_1} . \quad (2.6)$$

Substituting the inverse operator (2.6) into the equality (2.5), one can find:

$$\varphi_1 = \varphi_{01} - \sum_{n_1=0}^{\infty} \int_{x_1}^{+\infty} \frac{k_1^{2n_1} (x_1-\xi_1)^{2n_1+1}}{(2n_1+1)!} u_1 \varphi_1(\xi_1) d\xi_1 =$$
$$= \varphi_{01} - \frac{1}{k_1} \int_{x_1}^{+\infty} \mathrm{sh}\{k_1(x_1-\xi_1)\} u_1 \varphi_1(\xi_1) d\xi_1 . \quad (2.7)$$

The resulting equality (2.7) coincides with the equation (1.4).

Let's denote by N the number of particles in the system, by x_j – coordinates of the particles, where $j = 1, 2, \ldots, 3N$, by μ_j – masses of the particles (with taking into account the equality of particle masses for the indexes of its three coordinates).

We introduce the weighted coordinates of the particles z_j according to the rule:

$$z_j = x_j \sqrt{\mu_j} . \quad (2.8)$$

If in the stationary Schrödinger equation for a system of particles in the bound state to go from the ordinary coordinates to the weighted ones, then it can be represented as a multidimensional Helmholtz equation:

$$\left(\Delta_{3N} - k^2\right)\varphi_N(\vec{z}) = u(\vec{z})\varphi_N(\vec{z}) , \quad (2.9)$$

where $u = \frac{2W_P}{\hbar^2}$, $k = \frac{\sqrt{2(-E)}}{\hbar}$; E, W_P – energy and potential energy of the system of particles, respectively.

$\Delta_{3N} = \sum_{j=1}^{3N} \frac{\partial^2}{\partial z_j^2}$.

$3N$-dimensional integral equation of the Fredholm type must match to Eq. (2.9) as follows:

$$\varphi_N(\vec{z}) = \int_{-\infty}^{+\infty} G_N\left(\vec{z}-\vec{\xi}\right) u \varphi\left(\vec{\xi}\right) d\left(\vec{\xi}\right) . \quad (2.10)$$

The task of the work is as follows: using the direct and inverse Fourier transforms to find the kernel of the integral equation (2.10) and using the method of inversion of differential operators to build the integral equation from the class of Volterra type equations corresponding to Eq. (2.9).

3. Construction of integral equations

The function $G_N = \left(\vec{z}-\vec{\xi}\right)$ must satisfy the differential equation:

$$\left(\Delta_{3N} - k^2\right) G_N\left(\vec{z}-\vec{\xi}\right) = \delta\left(\vec{z}-\vec{\xi}\right) , \quad (3.1)$$

where $\delta\left(\vec{z}-\vec{\xi}\right)$ is the Dirac delta-function.

Using the direct and inverse Fourier transforms of the Dirac delta-function, the function $G_N = \left(\vec{z}-\vec{\xi}\right)$ can be represented as an integral:

$$G_N = -\frac{1}{(2\pi)^{3N}} \int_{(-\infty)}^{(+\infty)} \frac{\exp\left\{-i\vec{q}\left(\vec{z}-\vec{\xi}\right)\right\}}{q^2+k^2} d\vec{q} . \quad (3.2)$$

With direct substitution, one can be assured that the function (3.2) is the solution of Eq. (3.1).

When introducing auxiliary integration by the parameter λ, the right part of Eq. (3.2) can be represented in the form of an integral from the product of independent integrals that are taken explicitly:

$$G_N = -\frac{1}{(2\pi)^{3N}} \int_0^{\lambda} \prod_{j=1}^{3N} \{I_j\} d\lambda \ , \tag{3.3}$$

where

$$I_j = \int_{-\infty}^{+\infty} \exp\left\{-\lambda q_j^2 - i q_j (z_j - \xi_j)\right\} dq_j \ . \tag{3.4}$$

Taking the integrals (3.4) and substituting them into Eq. (3.3) and integrating by parameter λ, one can find the function G_N.

If the number of particles in the system is odd, that is $N = 2m + 1$; $m = 0, 1, 2, ...$, then

$$G_N = \frac{(-1)^{m+1} \exp\{-kR\}}{4\pi^{3m+1} R^{6m+1}} P_{3m}(R), \tag{3.5}$$

where

$$R = \left|\vec{z} - \vec{\xi}\right|, \tag{3.6}$$

$$P_{3m} = \exp\left\{kR\sqrt{\beta}\right\} \left(\frac{\partial}{\partial \beta}\right)^{3m} \left(\frac{\exp\left\{-kR\sqrt{\beta}\right\}}{\sqrt{\beta}}\right)\Bigg|_{\beta=1} . \tag{3.7}$$

When $m = 0$, in the case of one-particle system the function (3.5) coincides with the well-known function (1.3).

If the number of particles in the system is even, as: $N = 2(m + 1)$, then

$$G_N = \frac{(-1)^m f_{3m+1}(R)}{16\pi^{3m+3} R^{6m+2}}, \tag{3.8}$$

$$f_{3m+1} = \left(\frac{\partial}{\partial \beta}\right)^{3m+1} \left(\int_0^{+\infty} \exp\left\{-\frac{k}{\lambda} - \frac{\lambda}{4} R\beta\right\} d\lambda \right)\Bigg|_{\beta=1} . \tag{3.9}$$

From Eq. (2.9) it follows:

$$\varphi_N(\vec{z}) = \varphi_{0N} + \left(\Delta_{3N} - k^2\right)^{-1} u(\vec{z}) \varphi_N(\vec{z}) \ . \tag{3.10}$$

Expanding the inverse operator in Eq. (3.10) into a series in the Laplacian powers, and introducing auxiliary integration by parameter λ, one can represent the inverse operator in the form of an integral from product of independent differential operators:

$$\left(\Delta_{3N} - k^2\right)^{-1} = -\frac{1}{k^2} \int_0^{+\infty} \exp\{-\lambda\} \left(\prod_{j=1}^{3N} \hat{S}_j \right) d\lambda \, , \tag{3.11}$$

$$\hat{S}_j = \exp\left\{ \frac{\lambda}{k^2} \frac{\partial^2}{\partial z_j^2} \right\}. \tag{3.12}$$

Let's expand the operators (3.12) into the Taylors series. The inverse factorials that are constant multipliers at partial derivatives can be considered as the result of Laplace inverse transformation of complex arguments p_j in corresponding power with the arguments y_j of the original functions equal to unity:

$$\frac{1}{p_j^{n_j+1}} \leftrightarrow \frac{y_j^{n_j}}{n_j!}\Bigg|_{y_j=1} = \frac{1}{n_j!} \, . \tag{3.13}$$

It gives an opportunity to represent the operators (3.12) in the form of integral operators product:

$$\hat{S}_j = \sum_{n_j=0}^{\infty} \frac{\lambda^{n_j}}{n_j! k^{2n_j}} \left(\frac{\partial^2}{\partial z_j^2} \right)^{n_j} \leftrightarrow \sum_{n_j=0}^{\infty} \frac{\lambda^{n_j}}{p_j^{n_j+1} k^{2n_j}} \left(\frac{\partial^2}{\partial z_j^2} \right)^{n_j} =$$

$$= \frac{1}{p_j - \dfrac{\lambda}{k^2} \dfrac{\partial^2}{\partial z_j^2}} = \frac{\dfrac{k^2}{\lambda} \hat{t}_{j+} \hat{t}_{j-}}{\left(k\hat{t}_{j+} \sqrt{\dfrac{p_j}{\lambda}} - 1 \right) \left(k\hat{t}_{j-} \sqrt{\dfrac{p_j}{\lambda}} + 1 \right)} =$$

$$= -\frac{k^2}{\lambda} \hat{T}_{j+} \hat{T}_{j-} \, , \tag{3.14}$$

$$\hat{T}_{j+} = \sum_{m_j=0}^{\infty} \left(k\sqrt{\frac{p_j}{\lambda}} \right)^{m_j} \left(\hat{t}_{j+} \right)^{m_j+1} , \tag{3.15}$$

$$\hat{T}_{j-} = \sum_{m_j=0}^{\infty} (-1)^{m_j} \left(k\sqrt{\frac{p_j}{\lambda}} \right)^{m_j} \left(\hat{t}_{j-} \right)^{m_j+1} . \tag{3.16}$$

Using the expressions (3.11), (3.14), (2.3), (2.4) and inverse Laplace transforms with the argument of original functions equal to unity:

$$\exp\left\{-\alpha_j \sqrt{p_j}\right\} \leftrightarrow \frac{\alpha_j \exp\left\{-\dfrac{\alpha_j^2}{4y_j}\right\}}{2y_j\sqrt{\pi y_j}}\Bigg|_{y_j=1} = \frac{\alpha_j}{2\sqrt{\pi}} \exp\left\{-\frac{\alpha_j^2}{4}\right\}. \tag{3.17}$$

Then, from the equality (3.10) one gets the integral equation:

$$\varphi_N(\vec{z}) = \varphi_{0N}(\vec{z}) + \int_{(z_j)}^{(+\infty)} \int_{(-\infty)}^{(\xi_j)} g_N(\vec{\xi}) u \varphi(\vec{\eta}) d\vec{\eta} \, d\vec{\xi} \, , \tag{3.18}$$

$$\vec{\chi} = 2\vec{\xi} - \vec{z} - \vec{\eta} \, , \tag{3.19}$$

$$g_N = \left(\frac{4\pi}{k}\right)^{3N} G_{3N}(\chi) \prod_{j=1}^{3N} \chi_j \,. \qquad (3.20)$$

To verify the obtained equation (3.18), one can consider its one-dimensional case that looks like this:

$$\varphi_1(z_1) = \\ = \varphi_{01}(z_1) - \int_{z_j}^{+\infty} \int_{-\infty}^{\xi_j} \exp\{-k(2\xi_1 - z_1 - \eta_1)\} u\, \varphi(\eta_1)\, d\eta_1\, d\xi_1 \,. \qquad (3.21)$$

Taking the integral part in the right part of Eq. (3.21) and adding and subtracting the selected term, it is simple to obtain the equation (1.4).

4. Conclusions

For the wave function corresponding to the bound state of a particle system, we have obtained the kernel of the Fredholm type integral equation that is defined by the expressions (3.5) to (3.9). In the case of one particle, the found expression coincides with the known kernel for the one-particle function (1.3). Using the method of inversion of differential operators, we have constructed the equation (3.18) that in one-dimensional case coincides with the well-known Volterra type equation (1.4). The obtained integral equations allow expanding the possibilities to model nanostructure formation, to determine their energy spectrum and spatial distribution of particles.

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