https://doi.org/10.15407/ujpe70.7.425

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FUNDAMENTALS OF THE ALGEBRAIC VERSION OF THE RESONATING-GROUP METHOD IN THE ONE-DIMENSIONAL CASE. I. ANALYTIC RESULTS

The features of analytic calculations in the framework of the algebraic version of the resonating-group method, which is based on expanding the wave function of a quantum system on the basis of oscillator functions, have been examined in the one-dimensional case. The construction of the Hamiltonian matrix elements using the technique of generating functions and generating matrix elements has been discussed in detail. The asymptotic behavior is found for the coefficients in the wave function expansion in the oscillator function basis as the oscillator quantum number tends to infinity in the continuous spectrum case. The asymptotic dependence of the potential-energy matrix elements on the oscillator quantum number has been obtained for a Gaussian potential.

K e y w o r d s: one-dimensional case, algebraic version of the resonating-group method, oscillator basis, matrix elements, asymptotics of coefficients.

1. Introduction

The fundamentals of the algebraic version of the resonating-group method (AVRGM) were initially formulated in works [1, 2]. This is a cluster approach, which is technically based on the expansion of the functions describing the relative motion of clusters in the oscillator function basis. From the very beginning, it was focused on describing the properties of the states in the discrete and continuous spectra of light atomic nuclei from the same viewpoint. This makes it especially interesting, because the research of the states in the continuous spectrum of light atomic nuclei has attracted attention of theorists and experimenters for many years. The corresponding explanation is simple: as a rule, these nuclei have only a small number of states in the discrete spectrum, whereas the overwhelming majority of their other states are in the continuous spectrum.

From the viewpoint of its useful application, the AVRGM has already demonstrated itself. Over the years, since its appearance, a very large number of works devoted to the study of the states in the discrete spectrum of light atomic nuclei, single- and multichannel reactions involving light atomic nuclei, the relation between the collective and cluster modes of motion, the influence of taking the Pauli principle into account on the properties of light atomic nuclei, the study of the properties of hypernuclei, and so forth have been published [3–12]. Unfortunately, we cannot provide references to a plenty of works performed in the AVRGM framework due to their large number, which does not reduce their significance. It should be

Citation: Filippov G.F., Soloha-Klymchak M.D., Nesterov A.V. Fundamentals of the algebraic version of the resonating-group method in the one-dimensional case. I. Analytic results. *Ukr. J. Phys.* **70**, No. 7, 425 (2025). https://doi.org/10.15407/ujpe70.7.425.

noted at once that, along with the works dealing with the development and application of the AVRGM, one should get acquainted with works [13–16], which are closely related to this method.

In order to understand more easily the possibilities of using the AVRGM, it is desirable to study, in more details, the features of working with the oscillator function basis, which the AVRGM is based on. Accordingly, the aim of this work is to help the reader, via using one-dimensional examples (which does not reduce the generality of consideration), penetrate deeper into the "secrets" of using the oscillator function basis in order to describe the states in both the discrete and continuous spectra of quantum systems. For this purpose, we consider one-dimensional quantum mechanical model problems with the presence of bound or quasi-stationary states with Gaussian-type potentials. This is not a very strong restriction on the systems that can be analyzed, because the basis composed of Gaussian functions is complete so that any potential can be represented with a reasonable accuracy as a superposition of Gaussians.

Today, we know about only two works, where the possibility of using the oscillator function basis to describe the states in the continuous spectrum of one-dimensional quantum systems was demonstrated [17,18]. The main difference of our work from those two works consists in that we pay considerable attention to the demonstration of the analytic calculation technique developed in the AVRGM framework. The idea of this work belongs to G.F. Filippov, who left his notes on this topic.

So, we have to solve the Schrödinger equation

$$\hat{H}\Psi(x) = E\Psi(x),$$

where

$$\hat{H} = \hat{T} + \hat{V},$$
$$\hat{T} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2},$$

and $\hat{V}(x)$ is given as a Gaussian function in the form $V_0 \exp\left(-x^2/r_0^2\right)$ or a superposition of Gaussian functions. As can be seen, our potential is always an even function. As a result, our problem practically becomes split into two problems: with positive and negative parity. Note that, in what follows, for the sake of brevity and clarity, most formulas for positive parity will be written down. All necessary expressions for negative parity can be obtained similarly to those for positive parity, or they can be obtained from the formulas for positive parity by simply redefining the indices. Specific calculations in both cases will be presented in the continuation of this paper.

Instead of solving the differential equation for the wave function $\Psi(x)$, let us represent this function in the form of a series expansion in Hermite functions

$$\Psi(x) = \sum_{m=0}^{\infty} C_m \phi_m(x),$$
$$\phi_m(x) = \frac{1}{\sqrt{2^m m!\, r_0 \sqrt{\pi}}} H_m(x) \exp\left(-\frac{x^2}{2}\right), \tag{1}$$

where the dimensionless variable x is normalized by the oscillator radius r_0. In this case, m is even or odd, if even or odd, respectively, states are considered, which is determined by the parity properties of Hermite polynomials. All the above brings us to a system of algebraic equations in the form

$$\sum_{\tilde{n}}^{\infty} \langle n|\hat{H}|\tilde{n}\rangle . C_{\tilde{n}} = EC_n,$$

which can be solved by considering the states in both the discrete and continuous spectra, setting the appropriate boundary conditions, determining the set of coefficients that represent the wave function of the problem in the oscillator representation, and finding the energies of the bound states or the parameters of the scattering process. It is obvious that our system of equations can be elementary rewritten in the matrix form. In other words, when working in the AVRGM framework, we are in the framework of matrix quantum mechanics. The applied representation is usually called the energy (or n-) representation.

2. Calculation of Hamiltonian Matrix Elements, Generating Functions, and Generating Matrix Elements

The matrix elements of the kinetic energy operator $\hat{T}$, being calculated on oscillator functions, are known. In our case, being expressed in $\hbar^2/\left(mr_0^2\right)$ units, they look like

$$\langle 2n|\hat{T}|2n-1\rangle = -\frac{\sqrt{2n(2n-1)}}{4},$$
$$\langle 2n|\hat{T}|2n\rangle = n + \frac{1}{4}, \tag{2}$$
$$\langle 2n|\hat{T}|2n+1\rangle = -\frac{\sqrt{(2n+1)(2n+2)}}{4}.$$

Here, in accordance with our previous agreement, we have written out the matrix elements of the kinetic energy operator only for the case of positive parity. What we need to pay attention to is that the kinetic energy matrix is tridiagonal, i.e., a Jacobi matrix (or J-matrix). The methods of matrix quantum mechanics where the kinetic energy is tridiagonal are often called the J-matrix methods; this also concerns the AVRGM.

Since, in practice, the calculation of the matrix elements of the kinetic energy operator usually does not cause difficulties, we will focus our attention on the calculation of the matrix elements of the potential energy operator. For this purpose, we need to calculate integrals in the form

$$\langle 2n|\,\hat{V}|2\tilde{n}\rangle = V_0 \int\limits_{-\infty}^{\infty} \phi^*_{2n}\,(x) \exp\left(-\frac{x^2}{b_0^2}\right) \phi_{2\tilde{n}}\,(x)\,dx.$$

Formulas for calculating such integrals are known (see, for example, work [19]). Therefore, we can immediately write down that

$$\langle 2n|\,\hat{V}|2\tilde{n}\rangle = (-1)^{n+\tilde{n}}\,V_0 z^{1/2}\,(1-z)^{n+\tilde{n}} \times$$

$$\times \sqrt{\frac{(2n-1)!!(2\tilde{n}-1)!!}{(2n)!!(2\tilde{n})!!}}\, {}_2F_1\left\{-n, -\tilde{n}; \frac{1}{2}; \left(\frac{z}{1-z}\right)^2\right\}, \quad (3)$$

or, in the expanded form,

$$\langle 2n|\,\hat{V}|2\tilde{n}\rangle = (-1)^{n+\tilde{n}}\,V_0 z^{1/2} (1-z)^{n+\tilde{n}} \sqrt{\frac{(2n)!(2\tilde{n})!}{2^{2n}2^{2\tilde{n}}}} \times$$

$$\times \sum_{k=0}^{\min\{n,\tilde{n}\}} \frac{2^{2k}}{(n-k)!\,(\tilde{n}-k)!\,(2k)!} \left(\frac{z}{1-z}\right)^{2k}, \quad (4)$$

where

$$\frac{1}{z} = 1 + \frac{r_0^2}{b_0^2}.$$

A good test for the validity of formulas (3) and (4) is the choice of unity as the potential energy operator. In our case, this is achieved by enlarging b_0 to infinity, which transforms z to unity. This operation should lead to the transformation of the potential energy matrix into a diagonal matrix with the matrix elements equal to V_0 due to the orthonormality of Hermite functions.

It may seem that the problem of calculating the matrix elements in the Hamiltonian has been solved. However, when dealing with real physical problems, one has to consider much more complicated expressions for the matrix elements and operate with matrix equations with large dimensions, where the situation becomes not so simple. Therefore, in order to calculate the matrix elements of the Hamiltonian, a special technique has been developed. It was called the technique of generating functions and generating matrix elements [20, 21], being closely related to the Bargmann representation for oscillator functions.

Let us consider the derivative function for Hermite functions in the notation that coincides by its form with the notation for the modified Bloch–Brink orbital. Namely,

$$\Phi_x\,(R) = \frac{1}{\sqrt[4]{\pi} r_0^{1/2}} \exp\left\{-\frac{x^2}{2} + \sqrt{2}Rx - \frac{R^2}{2}\right\} =$$

$$= \sum_{n=0}^{\infty} \frac{1}{\sqrt{n!}} R^n \frac{1}{\sqrt{2^n n! \sqrt{\pi}}} H_n\,(x) \exp\left(-\frac{x^2}{2}\right). \quad (5)$$

The last expansion associates every Hermitian function with the expression

$$\phi_n\,(R) = \frac{1}{\sqrt{n!}} R^n,$$

which can be considered as an image of the oscillator function in the representation of generating parameters. The choice of the coefficient $1/\sqrt{n!}$ allows us to work with normalized functions.

In order to calculate the generating matrix elements of some operator $\widehat{O}(x)$, let us introduce another orbital in form (5) where the generating parameter R is substituted by the generating parameter S,

$$\Phi_x\,(S) = \frac{1}{\sqrt[4]{\pi} r_0^{1/2}} \exp\left\{-\frac{x^2}{2} + \sqrt{2}Sx - \frac{S^2}{2}\right\} =$$

$$= \sum_{n=0}^{\infty} \frac{1}{\sqrt{n!}} S^n \frac{1}{\sqrt{2^2 n! \sqrt{\pi}}} H_n\,(x) \exp\left(-\frac{x^2}{2}\right). \quad (6)$$

Integral

$$O_{RS} = \int \Phi_x\,(R)\,\widehat{O}\,(x)\,\Phi_x\,(S)\,dx$$

is called the generating matrix element of the operator $\widehat{O}(x)$. This is so, because it can be represented as

the expansion

$$O_{RS} = \sum_{n=0}^{\infty}\sum_{\tilde{n}=0}^{\infty} \langle n|\widehat{O}(x)|\tilde{n}\rangle \frac{1}{\sqrt{n!}} R^n \frac{1}{\sqrt{\tilde{n}!}} S^{\tilde{n}}.$$

Whence one can see that the expansion coefficients of the generating matrix element in the functions $\phi_n(R)$ and $\phi_{\tilde{n}}(S)$ are the sought matrix elements of the operator $\widehat{O}(x)$ as the coefficients in front of $\phi_n(R)\phi_{\tilde{n}}(S)$. It is evident that, in full accordance with the definition of generating function, this is equivalent to the fact that, by differentiating the last expression, a required number of times with respect to R and S and, afterward, by zeroing R and S, we can obtain any required matrix element, which is calculated in the oscillator function basis.

Having obtained the basic relationships for calculating the generating matrix elements, it is necessary to recall that if we have functions given in the space of generator variables, then, according to the canons of quantum mechanics, we can write down the operators of physical quantities in terms of the same variables. In some cases, it can be easily done.

In particular, in $\hbar\omega$ units, the Hamiltonian operator of a harmonic oscillator takes the form

$$\hat{H}_{occ} = R\frac{\partial}{\partial R} + \frac{1}{2}.$$

This expression follows from the obvious fact that R can be considered as the creation operator of an oscillator quantum, and the derivative $\partial/\partial R$ as its annihilation operator, because

$$R\phi_n(R) = \sqrt{n+1}\phi_{n+1}, \quad \frac{\partial}{\partial R}\phi_n = \sqrt{n}\phi_{n-1},$$

and

$$\hat{H}_{occ}\phi_n(R) = \left(R\frac{\partial}{\partial R} + \frac{1}{2}\right)\phi_n(R) = \left(n+\frac{1}{2}\right)\phi_n(R).$$

It turns out that the operator

$$\hat{k} = -i\frac{d}{dx} \Rightarrow -\frac{i}{\sqrt{2}}\left(\frac{d}{dR} - R\right)$$

and, accordingly, the operator

$$\frac{\hat{k}^2}{2} = \frac{d^2}{2dx^2} \Rightarrow \frac{1}{4}\left(\frac{d}{dR} - R\right)^2 = \\ = \frac{1}{4}\left(\frac{d^2}{dR^2} - 2R\frac{d}{dR} - 1 + R^2\right)$$

are the momentum and kinetic energy operators, respectively. That is,

$$-\frac{\hat{k}^2}{2}\phi_n(R) = -\frac{1}{4}\sqrt{n(n-1)}\phi_{n-2}(R) + \\ + \frac{1}{2}\left(n+\frac{1}{2}\right)\phi_n(R) - \frac{1}{4}\sqrt{(n+1)(n+2)}\phi_{n+2}(R).$$

Let us write down explicit forms for three generating matrix elements, which are of interest to us, and their formal expansions. These are:

• the integral of overlapping with the unit operator, or the normalization integral,

$$I_{RS} = \exp(RS) = \sum_{n=0}^{\infty}\frac{1}{n!}R^n S^{\tilde{n}} = \sum_{n=0}^{\infty}\frac{1}{\sqrt{n!}}R^n\frac{1}{\sqrt{n!}}S^{\tilde{n}} = \\ = \sum_{n=0}^{\infty}\phi_n(R)\phi_n(S) = \sum_{n=0,\tilde{n}=0}^{\phi_n}(R)\phi_{\tilde{n}}(S)\delta_{n,\tilde{n}}. \qquad (7)$$

• the generative matrix element of kinetic energy,

$$T_{RS} = 1/2\exp(RS)\left(-1+(R-S)^2\right) = \\ = \sum_{n=0,\tilde{n}=0}^{\infty}\phi_n(R)\phi_{\tilde{n}}(S)\delta_{n,\tilde{n}} = \\ = \frac{1}{2}\left(-1+(R-S)^2\right)\sum_{n=0}^{\infty}\phi_n(R)\phi_n(S). \qquad (8)$$

• and the matrix generator of the potential energy operator,

$$V_{RS} = V_0 z^{1/2}\exp\left\{zRS - \frac{1-z}{2}\left(R^2+S^2\right)\right\} = \\ = \sum_{n=0}^{\infty}\sum_{\tilde{n}=0}^{\infty}\langle n|\hat{V}|\tilde{n}\rangle\phi_n(R)\phi_{\tilde{n}}(S). \qquad (9)$$

From these expressions, it is clear that the matrix of overlapping with unity is a unit matrix, which is obvious because the eigenfunctions of a harmonic oscillator are orthonormalized. The matrix of the kinetic energy operator is tridiagonal, with its elements given by Eq. (5). Surely, when considering $\langle n|\hat{V}|\tilde{n}\rangle$ with the positive parity, we obtain the matrix element in the form (3) or (4).

The generating matrix elements (7)–(9) do not have the parity property. But they can be projected onto a state with a certain parity following the standard way. In our case, this can be done already at the level

of generating matrix elements, in particular, using the fact that the generating functions of form (5) or (6) are constructed in such a way that the substitution of x by $-x$ in them is equivalent to the substitution of R by $-R$. Let us demonstrate this result by the example of the generating matrix elements of the potential energy operator,

$$V^{+}_{RS} = z^{1/2}\mathrm{ch}\,(zRS)\exp\left\{-\frac{(1-z)}{2}\left(R^2+S^2\right)\right\} =$$
$$= z^{1/2}\sum_{n=0,\tilde{n}=0}^{\infty}\langle 2n|\hat{V}|2\tilde{n}\rangle\,\phi_{2n}\,(R)\,\tilde{\phi}_{2\tilde{n}}\,(S),$$
$$V^{-}_{RS} = z^{1/2}\mathrm{sh}\,(zRS)\exp\left\{-\frac{(1-z)}{2}\left(R^2+S^2\right)\right\} =$$
$$= z^{1/2}\sum_{n=0,\tilde{n}=0}^{\infty}\langle 2n+1|\hat{V}|2\tilde{n}+1\rangle\,\phi_{2n+1}\,(R)\,\tilde{\phi}_{2\tilde{n}+1}\,(S).$$

Such a projection can not be done, but, in this case, it is necessary to remember all the time the parity peculiarities of Hermite polynomials.

The development of the AVRGM has reached a level at which the consideration of multicluster problems is possible. Here, given the enormous complexity of direct formulas for calculating the matrix elements of potential energy, practically the only way to calculate them is the application of recurrent relationships, and the source of the latter can be the method of derivative functions and derivatives of matrix elements. Below, using a simple example, we will try to outline the basic principles of their derivation in the framework of the indicated method

$$V_{RS} = V_0 z^{1/2}\exp\left\{zRS-\frac{1-z}{2}\left(R^2+S^2\right)\right\} =$$
$$=\sum_{n=0}^{\infty}\sum_{\tilde{n}=0}^{\infty}\langle n|\hat{V}\,|\tilde{n}\rangle\,\phi_n\,(R)\,\phi_{\tilde{n}}\,(S). \qquad (10)$$

Let us consider Eq. (9) for the generating matrix element and apply the quantum annihilation operator $\partial/\partial R$ to the right- and left-hand sides of tus equality. We obtain

$$\frac{\partial V_{RS}}{\partial R} = \sum_{n,\tilde{n}}\langle n|\hat{V}\,|\tilde{n}\rangle\,\sqrt{n}\phi_{n-1}\,(R)\,\phi_{\tilde{n}}\,(S)$$

and

$$\frac{\partial V_{RS}}{\partial R} = \{zS-(1-z)\,R\}\,V_{RS} =$$
$$=\sum_{n,\tilde{n}}\langle n|\,\hat{V}\,|\tilde{n}\rangle\Big\{z\sqrt{\tilde{n}+1}\phi_n\,(R)\,\phi_{\tilde{n}+1}\,(S)\,-$$
$$-\,(1-z)\,\sqrt{n+1}\phi_{n+1}\,(R)\,\phi_{\tilde{n}}\,(S)\Big\}.$$

By equating the last two expressions and comparing the coefficients at the same functions, we obtain the following recurrence relationship for the matrix elements of the potential energy operator:

$$\langle n|\,\hat{V}\,|\tilde{n}\rangle = \frac{1}{\sqrt{n}}\Big\{z\sqrt{\tilde{n}}\,\langle n-1|\,\hat{V}\,|\tilde{n}-1\rangle\,-$$
$$-\sqrt{n-1}\,(1-z)\,\langle n-2|\,\hat{V}\,|\tilde{n}\rangle\Big\}. \qquad (11)$$

A peculiarity of this recurrence relationship is that it does not work, if $n=0$, i.e., for the first row of the Hamiltonian matrix with the positive parity. Therefore, we have to supplement our first recurrence relationship with at least one more, which eliminates this drawback and gives us a complete set of recurrence relationships.

Let us apply the quantum annihilation operator $\partial/\partial R$ to the right- and left-hand sides of Eq. (10). Then, we obtain

$$\langle n|\,\hat{V}\,|\tilde{n}\rangle = \frac{1}{\sqrt{\tilde{n}}}\Big\{z\sqrt{n}\,\langle n-1|\,\hat{V}\,|\tilde{n}-1\rangle\,-$$
$$-\sqrt{\tilde{n}-1}\,(1-z)\,\langle n|\,\hat{V}\,|\tilde{n}-2\rangle\Big\}. \qquad (12)$$

Recurrence relationships (11) and (12) are enough to obtain the elements of the full potential energy matrix, if the simplest of them are given by direct formulas to start the recurrence sequence.

Sometimes the obtained recurrence relationships are not very convenient for numerical calculations. Then, provided that we have their complete set, it is possible to construct their linear combinations, which are more interesting. With the help of our recurrence relationships, we can do the following.

1. Multiply both parts of recurrence relationship (11) by $\sqrt{n/\tilde{n}}$.

2. Multiply both parts of recurrence relation (12) by $\sqrt{n/\tilde{n}}$.

3. Subtract the latter result from the former one; then we get a new recurrence relationship,

$$\left(\sqrt{\frac{n}{\tilde{n}}}-\sqrt{\frac{\tilde{n}}{n}}\right)\langle n|\,\hat{V}\,|\tilde{n}\rangle = (1-z)\times$$
$$\times\left(\sqrt{\frac{\tilde{n}-1}{n}}\,\langle n|\,\widehat{V}\,|\tilde{n}-1\rangle-\sqrt{\frac{n-1}{\tilde{n}}}\,\langle n-2|\,\widehat{V}\,|\tilde{n}\rangle\right).$$

It is symmetric with respect to the permutation of n and $\tilde{n}$ and allows us to calculate all matrix elements of the potential energy operator matrix, except the diagonal ones. One can also see that all non-diagonal matrix elements vanish at $z = 1$.

4. Sum up the results of steps 1) and 2) and put $\tilde{n} = n$; then, we obtain

$$\langle n|\,\hat{V}\,|n\rangle = z\,\langle n-1|\,\widehat{V}\,|n-1\rangle - \\ -(1-z)\sqrt{\frac{n-1}{n}}\,\langle n-2|\,\widehat{V}\,|n\rangle.$$

This recurrence relationship allows us to calculate those matrix elements of the potential energy operator that are located on the main diagonal. At $z = 1$, all matrix elements are equal to V_0 according to the orthonormality of Hermite functions.

By acting in such a way, we can obtain other recurrence relationships. For example, using the operators $\partial^2/\partial R^2$, $\partial^2/\partial S^2$, and $\partial^2/(\partial R \partial S)$, it is possible to find a complete set consisting of three recurrence relationships. Note that the obtained recurrence relationships are not the "children" of the method of generating functions and generating matrix elements, but a direct consequence of the properties of Hermite functions. The only question is: In which representation, the coordinate representation or the representation of generating parameters, should they be determined? Interesting information about the relevant properties of Hermite functions can be found in book [22].

3. Asymptotic Relationships

It is known how important the knowledge of the asymptotic wave function behavior is when performing quantum mechanical calculations in the coordinate representation. The same picture is observed when an expansion in the oscillator function basis is made, especially if it concerns the study of the states in the continuous spectrum, when the role of the wave function, as for the states in the discrete spectrum, is played by the set of coefficients $\{C_n\}$ in the expansion of the wave function in the oscillator function basis. The property of the oscillator expansion is as follows: the larger the value of the quantum number n, the larger the distances from the coordinate origin corresponding to the contribution given by the basis function $\phi_n(x)$. Therefore, we are interested in the asymptotic behavior of the expansion coefficients $\{C_n\}$ and some other quantities at large n-values.

The Schrödinger equation in the coordinate representation looks like

$$\left\{-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - \exp\left(-\frac{x^2}{b^2}\right)\right\}\Psi(x) = E\Psi(x).$$

As $|x|$ increases, this equation becomes simpler and transforms into the wave equation for free motion,

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\Psi(x) = E\Psi(x). \tag{13}$$

The general solution to this equation can be written as a superposition of the even and odd solutions,

$$\Psi(x) = A\sin kx + B\cos kx,$$

where

$$k = \sqrt{\frac{2mE}{\hbar^2}}.$$

In the discrete representation, owing to the principle of correspondence between the discrete and continuous representations, the same has to occur. Then, the limit transition to the equations

$$\sum_{\tilde{n}}^{\infty}\langle n|\,\hat{T}\,|\tilde{n}\rangle C_{\tilde{n}} = E_n C_n \tag{14}$$

is natural. Before proceeding to the analysis of this system of equations and in order to better understand the logic of our further speculations, let us consider the asymptotic behavior of the coefficients on the basis of the properties of Hermite polynomials when $n \gg 1$.

Let us consider the integral

$$C_{2n} = \int_{-\infty}^{+\infty}\phi_{2n}(x)\cos(kx)\,dx.$$

Its calculation gives us the coefficients in the expansion of the free-motion function. It is known that the Hermite polynomials satisfy the integral equation (see, for example, work [23])

$$e^{-\frac{x^2}{2}}H_{2n}(x) = (-1)^n\sqrt{\frac{2}{\pi}}\int_0^{\infty}e^{-\frac{t^2}{2}}H_{2n}(t)\cos(xt)\,dt.$$

This remarkable equality means, in particular, the invariance of Hermite functions with respect to the

Fourier transform. It also immediately brings us to the relationship

$$C_{2n} = Ar_0 (-1)^n \sqrt{2\pi} H_{2n} (kr_0) e^{-\frac{k^2 r_0^2}{2}}, \qquad (15)$$

where A is the normalization factor (for its explicit expression, see formula (1)).

After having found exact expressions for the coefficients of the $\cos(kx)$ expansion in the oscillator function basis, we should demonstrate whether it is realistic, in practice, to expand the free-motion wave function in a finite number of oscillator functions. For this purpose, let us consider the task of the numerical reconstruction of a continuous-spectrum function using the expansion coefficients obtained in a predetermined region of argument variation. The results of such a numerical experiment are shown in Fig. 1. The segment with the endpoints at -50 and 50 fm was taken as the range of independent variable x. The results are presented for three calculation variants corresponding to different numbers of basis functions $n = 50$, 100, and 200.

The depicted plots demonstrate that it is quite easy to describe the function of free particle motion using the expansion in oscillator functions. At an energy of 10 MeV, we have to use even functions with $n = 50$ in order to describe the free-motion function to a distance of approximately 25 fm, $n = 100$ to a distance of 40 fm, and $n = 200$ to distances more than 50 fm. Note that, from the viewpoint of the AVRGM, where the interaction of light atomic nuclei is usually considered, the distances exhibited in Fig. 1 are rather large, even if we take long-range Coulomb interaction into account, and the asymptotics are different. Here, we simply tried to demonstrate as well as possible some possibilities of expanding the free-motion function in the oscillator function basis.

The change to the asymptotic expression of Hermite polynomials in formula (1) can be performed using the asymptotic equality (see, for example, work [23])

$$H_n(x) = \sqrt{2} \left(\frac{2n}{e}\right)^{\frac{n}{2}} e^{\frac{x^2}{2}} \left[\cos\left(Nx - \frac{n\pi}{2}\right) + \right.$$

$$\left. + O\left(\frac{1}{n}\right) + O\left(n^{-\frac{1}{4}} |x|^{\frac{5}{2}}\right)\right], \qquad (16)$$

where $N = \sqrt{2n+1}$. Here, we should emphasize at once that the applicability of this formula largely depends on the ratio between the values of the quantities n and $|x|$.

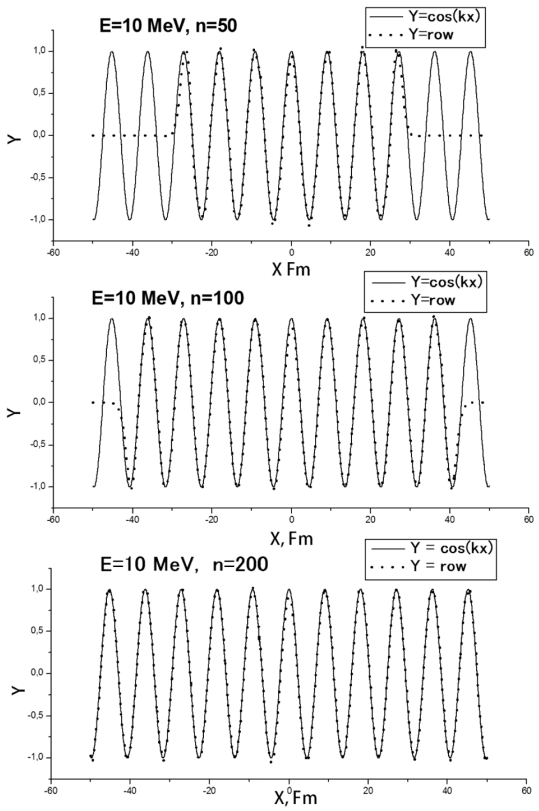

Fig. 1. Presentation of the free-motion function as a series expansion in the harmonic oscillator eigenfunctions

Using relationships (15) and (16), and applying Stirling's formula to simplify the expression for the normalizing factor, we arrive at the final expression, which can be written down in the form

$$C_{2n} = \frac{2r_0}{r_0^{1/2} \sqrt[4]{4n+1}} \cos\left(kr_0\sqrt{4n+1}\right). \qquad (17)$$

Attention should be paid to that the quantity $N = r_0\sqrt{4n+1}$ is the coordinate of the quasiclassical turning point for a one-dimensional harmonic oscillator. This point plays a very important role in the theory of harmonic oscillator; namely, the oscillator wave function density increases near the turning points as the oscillator quantum number grows. At $n \to \infty$, the behavior of the wave function acquires a δ-like character. An interpretation of this fact can already be given in the framework of classical concepts: it is clear that if the oscillator energy is large, the particle

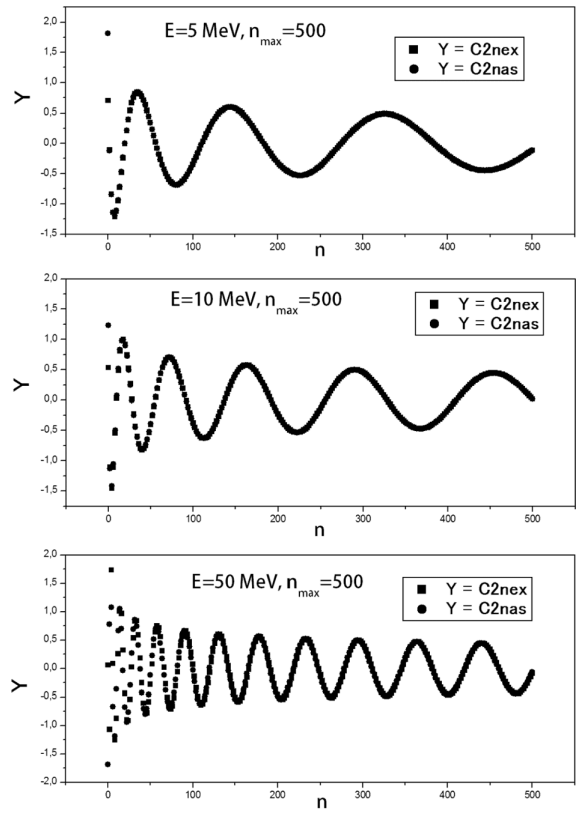

Fig. 2. Comparison of the exact values of the coefficients in the expansion of the free-motion function in the basis of oscillator functions with their asymptotic values at various energy values

passes the equilibrium point at a high velocity and spends the longest time near the turning points.

Let us look at obtaining the asymptotic expressions from the other side and return to Eqs. (14). They are discrete equations of the type

$$-\frac{1}{2}\sqrt{n\left(n-\frac{1}{2}\right)}C_{2n-2}+\left[\frac{1}{2}\left(2n+\frac{1}{2}\right)+\frac{1}{2}k^2r_0^2\right]\times$$
$$\times C_{2n}-\frac{1}{2}\sqrt{(n+1)\left(n+\left(\frac{1}{2}\right)\right)}C_{2n+2}=0.$$

At large n-values, we can consider the expansion coefficients C_{2n} as the values of a function of the continuous variable $2n$,

$$C_{2n}=C\left(2n\right).$$

In this case, we may write that $C(2n\pm 2)\ \rightarrow$ $\rightarrow C(x\pm\Delta x)$, i.e., $x=2n$ and $\Delta x=2$, and use the Taylor series expansion

$$C\left(x\pm\Delta x\right)\approx C\left(x\right)\pm\Delta x\frac{dC\left(x\right)}{dx}+\frac{1}{2}\left(\Delta x\right)^2\frac{d^2C\left(x\right)}{dx^2},$$

which makes it possible to transform the algebraic equation into a differential one,

$$-\frac{1}{2}\sqrt{n\left(n-\frac{1}{2}\right)}\left[C\left(x\right)-2\frac{dC\left(x\right)}{dx}+2\frac{d^2C\left(x\right)}{dx^2}\right]+$$
$$+\left[\frac{1}{2}\left(2n+\frac{1}{2}\right)+\frac{1}{2}k^2r_0^2\right]C\left(x\right)-$$
$$+\frac{1}{2}\sqrt{(n+1)\left(n+\left(\frac{1}{2}\right)\right)}\times$$
$$\times\left[C\left(x\right)+2\frac{dC\left(x\right)}{dx}+2\frac{d^2C\left(x\right)}{dx^2}\right]=0.$$

On the basis of previous experience, let us introduce a new variable R_n instead of the variable $x=2n$,

$$R_n=\sqrt{4n+1}=\sqrt{2x+1}.$$

Converting the derivatives and the coefficients in the equation to new variables and expanding the result in a power series of $1/R_n$ up to and including the fourth power of this quantity, we arrive at the equation

$$R_n^2\frac{d^2C\left(R_n\right)}{dR_n^2}+R_n\frac{dC\left(R_n\right)}{dR_n}+$$
$$+\left[-\frac{1}{4}+R_n^2k^2r_0^2\right]C\left(R_n\right)=0.$$

Hence, as a result of all transformations, we obtained the Bessel equation of order $1/2$. The solutions of this equation are the functions $J_{1/2}\left(\sqrt{kr_0\left(4n+1\right)}\right)$ and $N_{1/2}\left(\sqrt{kr_0\left(4n+1\right)}\right)$; the latter coincides with expression (17) to an accuracy of the coefficient and notations.

Let us illustrate by specific examples when the coefficients in the expansion of the free-motion function in the oscillator function basis can be replaced by their asymptotic expressions. For this purpose, let us refer to Fig. 2, where a comparison of the exact values of the coefficients in the expansion of the free-motion function in the oscillator function basis with their asymptotic values is made for various energy values. The results shown in the figure testify that the coefficients in the expansion of the free-motion

function become close to their asymptotic values at various quantum number values depending on the incident particle energy. The larger this energy is, the more oscillator functions should be involved for this purpose. This is easy to understand if you refer to the comment on formula (16).

At the end of this section, let us consider the behavior of the matrix elements of the potential energy in the course of the transition to large n- and $\tilde{n}$-values. For this purpose, we will use formula (3). For simplicity, we assume that $z = 1/2$. Accordingly, we obtain

$$\left(\frac{z}{1-z}\right)^2 = 1$$

and

$${}_2F_1\left\{-n, -\tilde{n}; \frac{1}{2}; \left(\frac{z}{1-z}\right)^2\right\} =$$

$$= {}_2F_1\left\{-n, -\tilde{n}; \frac{1}{2}; 1\right\} = \frac{\Gamma(1/2)\,\Gamma(n+\tilde{n}+1/2)}{\Gamma(n+1/2)\,\Gamma(\tilde{n}+1/2)}.$$

So, the matrix element of the potential energy operator with the Gaussian dependence acquires the form

$$\langle 2n|\,\hat{V}\,|2\tilde{n}\rangle = (-1)^{n+\tilde{n}}\,V_0\left(\frac{1}{2}\right)^{n+\tilde{n}+\frac{1}{2}} \times$$

$$\times\sqrt{\frac{(2n-1)!!\,(2\tilde{n}-1)!!}{(2n)!!\,(2\tilde{n})!!}}\,\frac{\Gamma(1/2)\,\Gamma(n+\tilde{n}+1/2)}{\Gamma(n+1/2)\,\Gamma(\tilde{n}+1/2)}. \quad (18)$$

By applying Stirling's formulas in the examined case, we obtain the following relationship:

$$\langle 2n|\,\hat{V}\,|2\tilde{n}\rangle \approx \frac{1}{2}V_0\left(-\frac{1}{2}\right)^{n+\tilde{n}} \times$$

$$\times\sqrt{\frac{1}{\pi\sqrt{n\tilde{n}}}}\left(1+\frac{\tilde{n}}{n}\right)^n\left(1+\frac{n}{\tilde{n}}\right)^{\tilde{n}}. \quad (19)$$

This formula shows that the matrix elements at the main diagonal decrease according to the law $1/\sqrt{n}$ as n increases, which can be seen from the relationship

$$\langle 2n|\,\hat{V}\,|2\tilde{n}\rangle \approx \frac{V_0}{2\sqrt{\pi n}}.$$

At the same time, the matrix elements of the kinetic energy operator grow proportionally to n. That is, at some stage of matrix expansion, we can neglect the matrix elements of the potential energy in comparison with the matrix elements of the kinetic energy and further assume that the Hamiltonian matrix is tridiagonal.

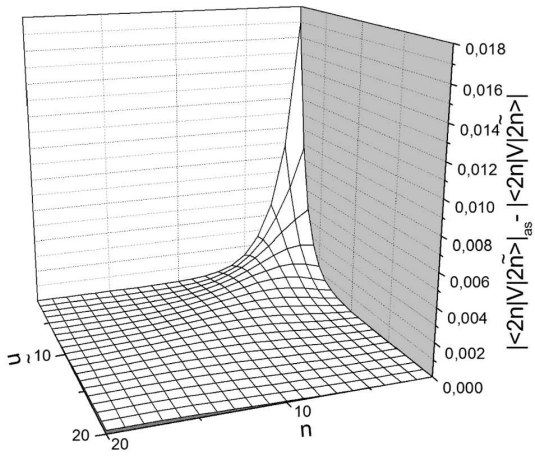

Fig. 3. Comparison of the exact and asymptotic values of the matrix elements of potential energy

A comparison of the calculation results obtained for the matrix elements using formulas (18) and (19) is illustrated in Fig. 3. The figure demonstrates the differences between the absolute values of the indicated matrix elements. An analysis shows that, as the quantum numbers of the lef and right functions increase, the exact values of matrix elements rather quickly attain their asymptotic values.

4. Conclusions

The aim of this work was to demonstrate techniques that can be used when constructing the Hamiltonian matrix in the framework of the algebraic version of the resonating-group method. For illustration, we considered the one-dimensional case, which is relatively noncumbersome from the analytic viewpoint. We also showed how the asymptotic behavior of the coefficients of the wave function expansion in the basis of oscillator functions, when the oscillator quantum number tends to infinity can be obtained by considering the states of the continuous spectrum. We demonstrated the convergence of the matrix elements of the potential energy to their asymptotic values.

We express our gratitude to V. Vasylevskyi for useful discussions of the obtained results. This work was partially supported by the Fundamental Research Pro-

gram of the Physics and Astronomy Department of the National Academy of Sciences of Ukraine (project No. 0122U000889) and by the Simons Foundation.

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Received 02.05.25.
Translated from Ukrainian by O.I. Voitenko

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ОСНОВНІ ПОЛОЖЕННЯ АЛГЕБРАЇЧНОЇ ВЕРСІЇ МЕТОДУ РЕЗОНУЮЧИХ ГРУП У РАЗІ ОДНОВИМІРНОГО ВИПАДКУ. І. АНАЛІТИЧНІ РЕЗУЛЬТАТИ

На прикладі одновимірного випадку розглядаються особливості проведення аналітичних розрахунків в межах Алгебраїчної версії методу резонуючих груп, яка ґрунтується на розкладі хвильової функції квантової системи по осциляторному базису. Детально обговорено побудову матричних елементів гамільтоніана за допомогою техніки твірних функцій та твірних матричних елементів. Знайдено асимптотичну поведінку коефіцієнтів розкладу хвильової функції по осциляторному базису при прямуванні осциляторного квантового числа до нескінченності у випадку неперервного спектра. Отримана асимптотична залежність матричних елементів потенціальної енергії від осциляторного квантового числа з гаусівським потенціалом.

Ключові слова: одновимірний випадок, алгебраїчна версії методу резонуючих груп, осциляторний базис, матричні елементи, асимптотика коефіцієнтів.