ON THE HARMONIC OSCILLLATOR REPRESENTATION FOR A SMALL OSCILLLATOR RADIUS

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The use of the harmonic oscillator basis in nuclear problems for small values of oscillator radius r_0 is studied by the example of a short-range (Gauss) potential. Solutions obtained in the Algebraic Version of the Resonating Group Method (AVRGM) are analyzed and compared to a numerical solution of the Schrodinger equation. Phase shifts for the solutions belonging to the continuum spectrum calculated within different methods are presented.

Introduction

Using the expansion of a wave function in the harmonic oscillator basis for building the wave function which satisfies the Schrodinger equation, we should define the oscillator radius r_0 optimally. It was already noted [1] that real physical results do not depend on the choice of r_0 – this is the test for a calculating procedure. The second well-known reason concerns the convergence of the expansion series. It is formulated as a choice of such r_0 that provides the fastest convergence in the region where the asymptotics of a wave function is not yet true. In [2], it was shown that one can speed up convergence using r_0 less than the characteristic length of the potential energy of a system under consideration.

There is one more requirement essential for real calculations. It states that the choice of r_0 should provide the easiest algorithm for calculating matrix elements of the potential energy operator. In [3], it was shown that, for slowly decreasing potentials – Coulomb and one inversely proportional to the third power of hyperradius (the effective potential of the hyperspherical functions method) – potential energy becomes equivalent to a diagonal matrix for a large number of oscillator quanta. When the number of oscillator quanta is large, the algebraic equations for coefficients of a wave function expansion in the harmonic oscillator basis can be considered as those for the binding coefficients of trinomial recurrent relations for a finite number of quanta and asymptotic ones. Therefore the question was raised about the possibility to obtain such a simplification for short range potentials using a small oscillator length r_0 and transform the system of algebraic equations into recurrent relations and the condition of the completion for a small number of oscillator quanta.

We consider, as the example, the Schrodinger equation for a particle in the spherially symmetric Gauss potential. We will show that the positive answer can be given to the question raised. In the second section, we will recall the main statements concerning $3D$ harmonic oscillator basis states and the matrix elements of the Gauss potential on these states. There we will discuss a problem of non-uniform convergence of the wave function expansion in the harmonic oscillator basis and describe how one can find the actual number of basis functions needed to provide convergence for a predefined oscillator radius in the specified region. Also we will present some important results demonstrating the properties of the potential energy matrix when the oscillator radius is far less than the radius of nuclear forces. In the third section, we give the numerical results obtained using different methods for different r_0. All conclusions are given in the fourth section.

Basis and Matrix Elements

To find an eigenfunction

$$\Psi_{Elm}(r, \theta, \varphi) = R_l(r)\, Y_{lm}(\theta, \varphi) \qquad (1)$$

of the Hamiltonian $\hat{H} = \hat{T} + \hat{U}$ of a particle with kinetic energy $\hat{T}$ in a spherically symmetric potential $\hat{U} = U(r)$ in a state with energy E, orbital momentum l, and its projection m, we expand the radial part of the wave function as

$$R_{E,l}(r) = \sum_{n=0}^{\infty} C_{nl}^{E} R_{nl}(r). \qquad (2)$$

As usual, $Y_{lm}(\theta, \varphi)$-spherical harmonics, $R_{nl}(r)$ – radial harmonic oscillator basis functions, and C_{nl}^{E} – expansion coefficients we need to find. Instead of the Schrodinger equation for the function $\Psi_{Elm}(r, \theta, \varphi)$ in coordinate representation, we obtain the infinite

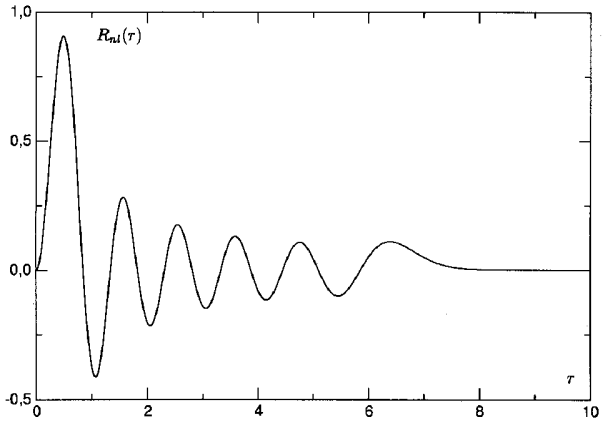

Fig. 1. Radial part $R_{nl}(r)$ of the basis function, $n = 10$, $l = 2$

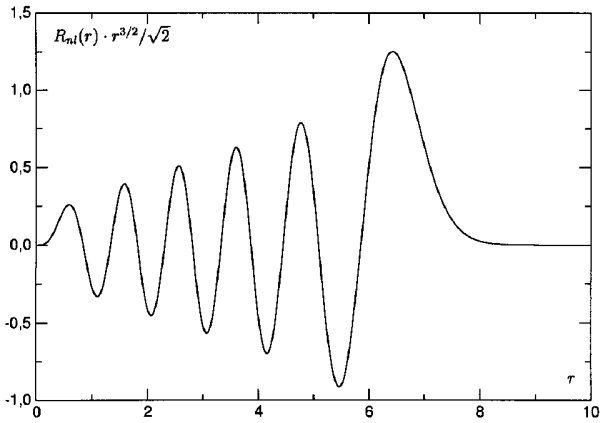

Fig. 2. δ-like behavior of the radial part $R_{nl}(r)$ of the basis function with multiplier $r^{3/2}/\sqrt{2}$, $n = 10$, $l = 2$

system of algebraic equations for C^E_{nl}:

$$\sum_{\tilde{n}=0}^{\infty} \{\langle n, l | \hat{H} | \tilde{n}, l\rangle - E\,\delta_{n,\tilde{n}}\}\, C^E_{\tilde{n}l} = 0, \qquad (3)$$

$n = 0, 1, 2, \ldots$

Before trying to solve system (3), we should analyze two following problems. First, we need to answer the question about the convergence type of (2), noting the fact that the asymptotics of any harmonic oscillator basis function decreases fast and differs from the asymptotics of bound states and continuum spectra. Second, we need the *a priori* procedure to solve the infinite system of algebraic equations (3).

1. Asymptotics of the Expansion Coefficients

It is well-known that the radial basis functions $R_{nl}(r)$ of a 3*D* harmonic oscillator can be expressed in terms of Laguerre polynomials $L_n^{l+1/2}(x^2)$ and $\exp(-x^2/2)$, so

$$R_{nl}(r) = \frac{N_{nl}}{r_0^{3/2}} x^l L_n^{l+1/2}(x^2) \exp(-x^2/2), \quad x = \frac{r}{r_0}. \qquad (4)$$

Every function has n modes in the interval $0 < r < r_t$, where $r_t(n) = r_0\sqrt{4n + 2l + 3}$ is the turning point. To the right from the turning point, these functions decrease as $\exp(-x^2/2)$. The typical dependence of R_{nl} on r is shown in Fig.1, where n is equal to 10 and $l = 2$. The remarkable feature of the functions $R_{nl}(r)$ is that they, being multiplied by $r^{3/2}$, become similar to δ-functions in the turning point region [6]. This is shown in Fig.2 for the case of $n = 10$, $l = 2$. The asymptotic limit of $r^{3/2} R_{nl}(r)$ for $n >> 1$ is given by the following equation:

$$r^{3/2} R_{nl}(r) \approx \sqrt{2}\,\delta(r - r_0\sqrt{4n + 2l + 3}). \qquad (5)$$

This statement is associated with the fact that the functions on the left and on the right of a turning point can be approximated in quasi-classical limit (e.g., for large n) by Airy functions [8]. Thus, there is a simple asymptotic relation between the coefficients C^E_{nl} and function $R_{nl}(r)$ at the points $r_t(n)$:

$$C^E_{nl} \approx R_{E,l}(r_0\sqrt{4n + 2l + 3})\,\sqrt{2}\,\sqrt{r_0}\,(4n + 2l + 3)^{1/4}. \qquad (6)$$

Of course, if $r_0\sqrt{4n + 2l + 3}$ is larger than the radius of nuclear forces b_0, then, for these values of $r_0\sqrt{4n + 2l + 3}$, the function $R_{E,l}(r)$ in coordinate representation has the well-known asymptotic form. With no Coulomb interaction for the states of continuum spectra, it has the form

$$R_{E,l}(r) \approx \cos\delta_l\, j_l(kr) - \sin\delta_l\, n_l(kr), \quad r > b_0, \qquad (7)$$

where $j_l(kr)$ spherical Bessel function, $n_l(kr)$ spherical Neumann function, $k = \sqrt{2mE/\hbar^2}$ momentum, m mass of a particle, δ_l phase shift. All we have to find is this phase shift. Solving the problem in coordinate representation assumes that the phase shift can be found using the conditions of equality of asymptotics (7) and the function found in the inner region at some intermediate point.

To solve the problem in harmonic oscillator representation, we also use asymptotics (7), but only to

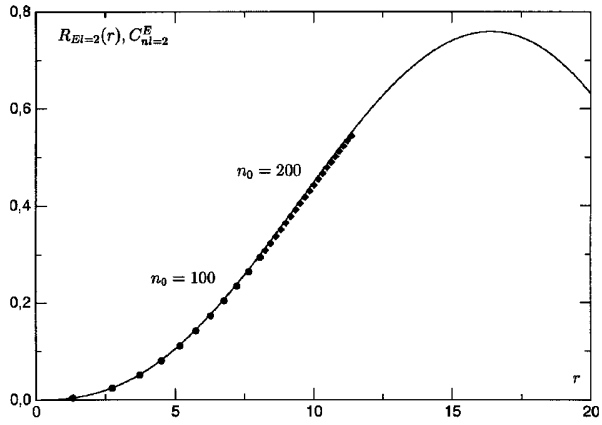

Fig. 3. Coeficients C^E_{nl} and exact solution $R_{E,\,l=2}(r)$ for $E = 1$ MeV, $l = 2$, $r_0 = 0.4$ fm, $n_0 = 100$, $n_0 = 200$

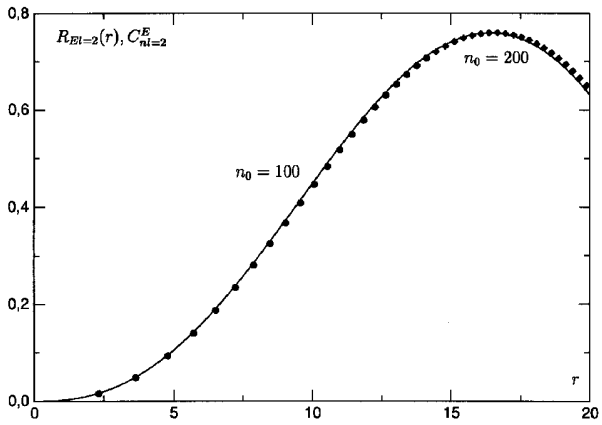

Fig. 4. The same as in Fig. 3 for $r_0 = 0.7$ fm

express all *a priori* unknown expansion coefficients in terms of phase shift. So, the equations

$$C^E_{nl} \approx \{\cos\delta_l j_l(kr_0\sqrt{4n+2l+3}) -$$

$$- \sin\delta_l n_l(kr_0\sqrt{4n+2l+3})\}\sqrt{2}\sqrt{r_0}\,(4n+2l+3)^{1/4},$$

$$n > n_0 \qquad (8)$$

allow us to transform the infinite system (3) into a finite system of algebraic equations for phase shift and unknown expansion coefficients C^E_{nl}, $n \le n_0$.

However, if $n >> 1$ and $r_0 < b_0$, then Eq. (6) is valid not only in the asymptotic region of $R_{E,l}(r)$, but also in the region where

$$r_0\sqrt{4n+2l+3} \approx b_0, \text{ and even } r_0\sqrt{4n+2l+3} < b_0.$$

Therefore, solving the system of algebraic equations for expansion coefficients C^E_{nl} gives us information about the behavior of the wave function immediately.

There is a question for what values of n Eq. (6) provides enough a high accuracy to be used in real calculations? To answer this, we refer to the system of algebraic equations with Gauss potential (3)

$$U(r) = V_0 \exp\left\{-\frac{2r_0^2}{b_0^2}x^2\right\},$$

$$V_0 = -100 \text{ MeV}, \quad b_0 = 1 \text{ fm}. \qquad (9)$$

E is equal to 1 MeV, and the oscillator radius r_0 has two different values: 0.7 and 0.4 fm.

Coefficients $\{C^E_{nl}\}$ of the state with energy $E = 1$ MeV and orbital momentum $l = 2$ were calculated for $n_0 = 100$, and then for $n_0 = 200$. To understand how these coefficients reproduce the behavior of the exact solution $R_{E,\,l=2}(r)$ of the equation

$$(\hat{T} + U(r))\,R_{E,l} = ER_{E,l} \qquad (10)$$

with the same potential (9) and energy, we found $R_{E,l=2}(r)$ within the standard numerical method, described in [9], and compared coefficients $\{C^E_{nl=2}\}$ with the function $\sqrt{2r}\,R_{E,l=2}(r)$. This is demonstrated in Fig. 3 for $r_0 = 0.4$ fm, and in Fig. 4 for $r_0 = 0.7$ fm. According to the stated above, coefficients $\{C^E_{nl=2}\}$ reproduce the exact solution accurately as long as

$$0 \le r_n \le r_0\sqrt{4n_0+7}.$$

In the region where $r_n \ge r_0\sqrt{4n_0+7}$, they can be reconstructed with Eq. (8).

2 . Non-uniform Convergence

On the ray $0 \le r < \infty$, series (2) does not converge uniformly. In other words, for any large n_0 the partial sum

$$R^{n_0}_l(r) = \sum_{n=0}^{n_0} C^E_{nl}R_{nl}(r) \qquad (11)$$

cannot approximate $R_l(r)$ with a predefined accuracy for all r, belonging this ray. But due to the completeness

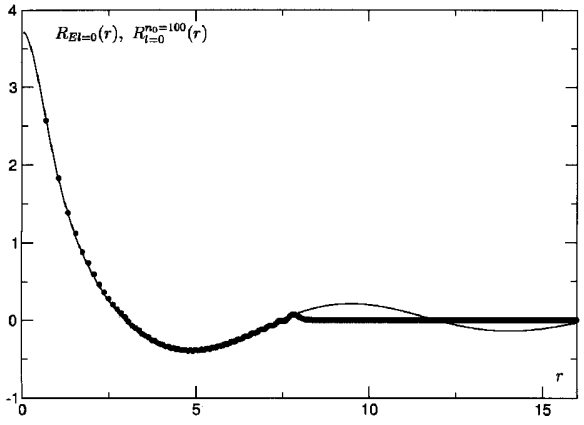

Fig. 5. Partial sum $R^{n_0}_{l=0}(r)$ and exact solution $R_{E,\,l=0}(r)$ for $E = 10$ MeV, $l = 0$, $r_0 = 0.4$ fm, $n_0 = 100$

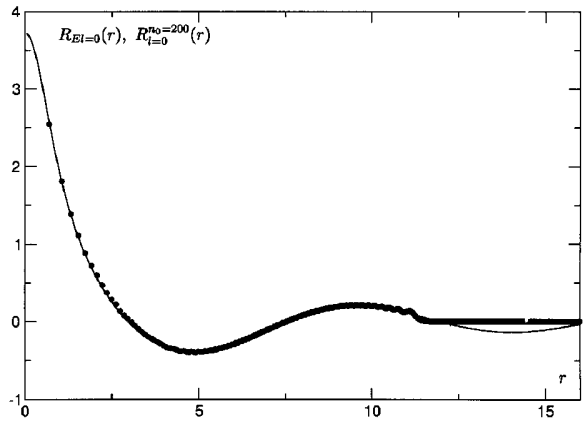

Fig. 6. The same as in Fig. 5 for $n_0 = 200$

of the system of radial basis functions $R_{nl}(r)$, for any finite interval $0 \le r \le r_{\max}$, one can specify such a

$$N_0 = N_0(\varepsilon, r_{\max}),$$

that provides the approximation with a predefined accuracy. Thus, for all r belonging to this interval, the inequality

$$|R_l(r) - \sum_{n=0}^{n_0} C^E_{nl} R_{nl}(r)| < \varepsilon$$

takes place if $n_0 > N_0$. There is a relation between values of $r_{\max}$, N_0, and oscillator radius r_0 (refer to [5]):

$$r_0 \sqrt{4N_0 + 3} \sim r_{\max}. \qquad (12)$$

Definitely, the lower limit for N_0 must be a little higher than the value given by (12).

To represent the dependence of the partial sum (11) on r, we calculated coefficients $C^E_{nl=0}$ in the state with energy $E = 10$ MeV for $r_0 = 0.4$ fm and then used their values in (11). The partial sum (11) and exact solution are represented in Fig. 5 for $n_0 = 100$ and in Fig. 6 for $n_0 = 200$. These figures show that the choice of n_0 is dictated only by the demand of transition of the wave function into the asymptotic region, where the phase shift totally determines the behavior of the solution.

3. Analysis of the System of Algebraic Equations

The key to the problem of solving the infinite system of equations (3) is the asymptotics of coefficients C^E_{nl} for large n. This is similar to solving the Schrodinger equation in coordinate representation and using the asymptotics of the wave function $R_l(r)$ for large r. Let's recall how the passage to the limit of large n in Eqs. (3) can be done. Since

$$\langle n, l | \hat{H} | \tilde{n}, l \rangle = \langle n, l | \hat{T} | \tilde{n}, l \rangle + \langle n, l | U(r) | \tilde{n}, l \rangle,$$

we consider the behavior of a sum

$$\sum_{\tilde{n}=0}^{\infty} \langle n, l | U(r) | \tilde{n}, l \rangle C^E_{nl},$$

when $n >> 1$. Within this limit, the following relations are true:

$$\sum_{\tilde{n}=0}^{\infty} \langle nl | U(r) | \tilde{n}\, l \rangle \tilde{C}^E_{\tilde{n}l} = \int_0^{\infty} R_{nl}(r)\, U(r) \times$$

$$\times \sum_{\tilde{n}=0}^{\infty} R_{\tilde{n}l} \tilde{C}^E_{\tilde{n}l}\, r^2\, dr =$$

$$= \int_0^{\infty} R_{nl}(r)\, r^{3/2}\, r^{1/2}\, U(r)\, R^E_l(r)\, dr =$$

$$= \int_0^{\infty} \delta(r - r_0\sqrt{4n + 2l + 3})\, r^{1/2}\, U(r)\, R^E_l(r)\, dr =$$

$$= U(r_0\sqrt{4n + 3})\, R^E_l(r_0\sqrt{4n + 2l + 3}) \times$$

$$\times \sqrt{r_0\sqrt{4n + 2l + 3}} = U(r_0\sqrt{4n + 2l + 3})\, C^E_{nl}. \qquad (13)$$

There we use the fact ([6]) that

$$R_{nl}(r)\, r^{3/2} \to \delta\left(r - r_0\sqrt{4n + 2l + 3}\right), \text{ if } n \to \infty. \quad (14)$$

The asymptotic equations (3) take the form:

$$\frac{\hbar^2}{2r_0^2}\{-\sqrt{(n+1)(n+l+3/2)}\, C^E_{n+1,l} +$$

$$+ (2n + l + 3/2)\, C^E_{nl} - \sqrt{n(n+l+1/2)}\, C^E_{n-1,l}\} +$$

$$+ U(r_0\sqrt{4n+2l+3})\, C^E_{nl} = E C^E_{nl}. \quad (15)$$

The mass of a particle is equal to 1.

For the short-range potential that decreases fast for large $r_{nl} = r_0\sqrt{4n + 2l + 3}$, we can disregard the last term in the left part of (15) for large r_n beginning with some value of n. A solution of the limit equation (15) is the expansion coefficients C^E_{nl} of the free-motion wave function when $E > 0$. Therefore, complete similarity between the harmonic oscillator representation and coordinate representation exists. Similarly to the use of the regular solution asymptotics (Bessel functions $J_{l+1/2}(kr)$) and irregular solution asymptotics (Neumann functions $N_{l+1/2}(kr)$) in the outer region, in the harmonic oscillator representation for $n \gg 1$, two sets of asymptotic coefficients should be used. One set,

$$C^{E,\mathrm{reg}}_{nl} = J_{l+1/2}(kr_0\sqrt{4n+2l+3}), \quad (16)$$

represents the regular solution, $k = \sqrt{2E/\hbar^2}$, and another

$$C^{E,\mathrm{irreg}}_{nl} = N_{l+1/2}(kr_0\sqrt{4n+2l+3}) \quad (17)$$

the irregular one. It must be noted that, to calculate these coeffcients, it is enough to know the solution for the set of discrete points. Also, if $r > r_0\sqrt{4\bar{n} + 2l + 3}$, then

$$J_{l+1/2}(r) = \sum_{n=\bar{n}}^{\infty} J_{l+1/2}(kr_0\sqrt{4n+2l+3})\, R_{nl}(r), \quad (18)$$

$$N_{l+1/2}(r) = \sum_{n=\bar{n}}^{\infty} N_{l+1/2}(kr_0\sqrt{4n+2l+3})\, R_{nl}(r). \quad (19)$$

Next, we express C^E_{nl} (defined for $n \geq \bar{n}$ by (3)) using the phase shift δ_l and asymptotic limits (16) and (17):

$$C^E_{nl} = \cos\delta_l\, C^{E,\mathrm{reg}}_{nl} - \sin\delta_l\, C^{E,\mathrm{irreg}}_{nl}. \quad (20)$$

After that, the infinite system (3) becomes a system of $\bar{n} + 1$ equations where the unknowns are first $\bar{n}$ coefficients C^E_{nl}, $n = 0, 1, 2, \ldots, \bar{n} - 1$, and phase shift δ_l.

4. Potential Energy Matrix

Let's go back to the potential energy matrix. The relation

$$\sum_{\tilde{n}=0}^{\infty} \langle nl \mid U(r) \mid \tilde{n}\, l\rangle \tilde{C}^E_{\tilde{n}l} = U(r_0\sqrt{4n+2l+3})\, C^E_{nl} \quad (21)$$

introduced earlier takes place for large enough n. For a short-range potential when r_0 is about its radius, this relation allows one to neglect the potential energy terms in (3) for large n and find asymptotic coefficients. However, decreasing r_0, one can come to conditions when the limit relation takes place but the potential $U(r_0\sqrt{4n+2l+3})$ cannot be neglected. It means that the potential energy matrix is equivalent to a diagonal matrix, i.e.,

$$\langle nl \mid U(r) \mid \tilde{n}\, l\rangle \sim U(r_0\sqrt{4n+2l+3})\, \delta_{n,\tilde{n}}. \quad (22)$$

It does not mean, however, that the following quantities are equal:

$$\langle nl \mid U(r) \mid \tilde{n}\, l\rangle \text{ and } U(r_0\sqrt{4n+2l+3}).$$

So, we have Eqs. (15) where the influence of the potential $U(r_0\sqrt{4n+2l+3})$ on the asymptotic coefficients should be taken into account.

To illustrate the preceding statements, we consider the Gauss potential (9) once again. The matrix elements

$$\langle nl \mid V_0 \exp\{-2r^2\} \mid \tilde{n}\, l\rangle$$

of this potential (9) are well known. Next, we consider their sums:

$$\sum_{\tilde{n}=0}^{\infty} \langle nl \mid U(r) \mid \tilde{n}\, l\rangle = F(n, l; r_0).$$

With very good accuracy (about one per cent), the function $F(n, l; r_0)$ reproduces potential (9) at points $r_{nl} = r_0\sqrt{(4n+2l+3)}$, beginning with $n = 0$, unless $r_0 = 0.1$ or less. Then all equations of system (3) can be considered in the form of (15). Hence, to obtain a wave equation in harmonic oscillator representation, one does not need to refer to the potential energy matrix $\langle nl \mid U(r) \mid \tilde{n}\, l\rangle$ because it is sufficient to

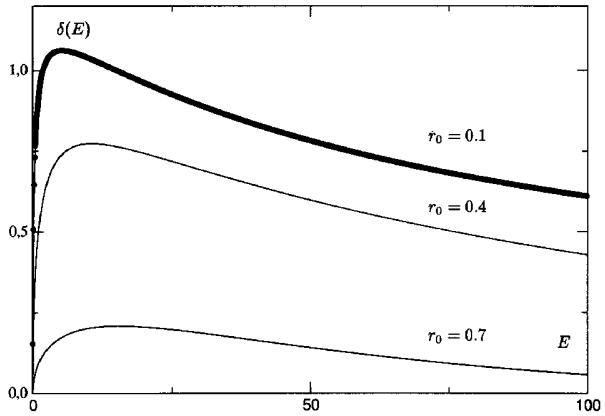

Fig. 7. Phase shift obtained within different methods for $r_0 = 0.1$, $r_0 = 0.4$, $r_0 = 0.7$ fm

consider the diagonal matrix $U(r_0\sqrt{4n+2l+3})\,\delta_{n,\tilde{n}}$. It is easy to formulate a recursive algorithm for solving this system of algebraic equations. Let's begin with such a large value of $\bar{n}$, that we can neglect the potential $U(r_0\sqrt{4\bar{n}+2l+3})$ in (15). Let

$$C^{E,\mathrm{reg}}_{\bar{n}+1,l} = J_{l+1/2}(kr_0\sqrt{4\bar{n}+2l+7}),$$

$$C^{E,\mathrm{reg}}_{\bar{n},l} = J_{l+1/2}(kr_0\sqrt{4\bar{n}+2l+3})\,. \qquad (23)$$

The value of $C^{E,\mathrm{reg}}_{\bar{n}-1,l}$ can be calculated from (15) when n is substituted by $\bar{n}$. Then (15) can be treated as trinomial recurent relations that allow one to 'climb down" from $C^{E,\mathrm{reg}}_{\bar{n},l}$ to $C^{E,\mathrm{reg}}_{1,l}$ and $C^{E,\mathrm{reg}}_{0,l}$. Similar actions lead to the calculation of the irregular coefficients $C^{E,\mathrm{irreg}}_{1,l}$ and $C^{E,\mathrm{irreg}}_{0,l}$. Of course,

$$C^{E}_{1,l} = \cos\delta_l\, C^{E,\mathrm{reg}}_{1,l} - \sin\delta_l\, C^{E,\mathrm{irreg}}_{1,l}, \qquad (24)$$

$$C^{E}_{0,l} = \cos\delta_l\, C^{E,\mathrm{reg}}_{0,l} - \sin\delta_l\, C^{E,\mathrm{irreg}}_{0,l}. \qquad (25)$$

The relation between $C^{E}_{1,l}$ and $C^{E}_{0,l}$ gives us the first, easiest equation of the system (15):

$$\frac{\hbar^2}{2r_0^2}\left\{-\sqrt{(l+3/2)}\,C^{E}_{1,l} + (l+3/2)\,C^{E}_{0,l}\right\} +$$

$$+\,U(r_0\sqrt{2l+3})\,C^{E}_{0,l} = E\,C^{E}_{0,l}. \qquad (26)$$

This relation determines the phase shift δ_l and coefficients C^{E}_{nl} for any given n.

The phase shift (as a function of energy) calculated with this simple algorithm cannot differ from that given by other methods. The only question is for what r_0 it is close to the exact phase shift.

Phase shift was calculated using different algorithms for potential (9) and zero angular momentum for different values of r_0, $0 < E < 100$ MeV. The results are shown in Fig. 7. The phase shift for $r_0 = 0{,}1$fm consists of the phase shift calculated by solving Schrodinger equation numerically [9] and phase shift calculated with standard procedures of AVRGM [6, 10].

Conclusion

In this paper, we examined non-uniform convergence of the expansion of the wave function $R^{E}_{l}(r)$ in the harmonic oscillator basis on a ray $0 \le r < \infty$ and showed how many basis functions we need to obtain uniform convergence on the finite interval $0 \le r \le r_{\max}$ for any given $r_{\max}$. Using the Gauss potential, we discovered a very important feature of the potential energy matrix $U(r)$. It implies that, for r_0 much less than the radius of a potential, this matrix is equivalent to a diagonal matrix $U(r_0\sqrt{4n+2l+3})\,\delta_{n,\tilde{n}}$, obtained by simple substitution of the argument r in the potential $U(r)$ by $r_0\sqrt{4n+2l+3}$. This results in reducing the algorithm of solving a system of algebraic equations for expansion coefficients of a wave function in the harmonic oscillator basis to a trivial recurrent procedure. Phase shifts, whose calculation was based on this algorithm and on the standard for the harmonic oscillator basis approach [7], almost do not differ. This confirms the statement [1] about independence of real physical results on the oscillator radius. Potentials with singularity at $r = 0$ require a special approach.

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