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SOLUTION OF THE INVERSE SCATTERING PROBLEM AT FIXED ENERGY FOR POTENTIALS BEING ZERO BEYOND A FIXED RADIUS*

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Based on the relation between the m-function and the spectral function we construct an inverse quantum scattering procedure at fixed energy which can be applied to spherical radial potentials vanishing beyond a fixed radius a. To solve the Gelfand–Levitan–Marchenko integral equation for the transformation kernel, we determine the input symmetrical kernel by using a minimum norm method with moments defined by the input set of scattering phase shifts. The method applied to the box and Gauss potentials needs further practical developments regarding the treatment of bound states.

Keywords: Inverse quantum scattering; spectral problem.

1. Introduction

Starting from the partial wave radial Schrödinger equation with unknown potential $q(r)$ vanishing beyond the finite radius $r = a < \infty$, we transform both the wave function φ_l and the radial variable r to arrive at the standard Sturm–Liouville equation.

1.1. *Schrödinger equation on the finite interval* $0 \le r \le a < \infty$

Let us consider the radial Schrödinger equation

$$-\varphi_l''(r) + \left(\frac{l(l+1/2)}{r^2} + q(r) - k^2\right)\varphi_l(r) = 0 \tag{1}$$

with the boundary conditions $\varphi_l(r \to 0) \approx r^{l+1}$, and $\varphi_l(r \to \infty) \approx \sin(kr - l\pi/2 + \delta_l)$ with angular momentum quantum numbers $l = 0, 1, 2, \ldots$. Here $f \approx g$ means that

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there exists a constant $c \neq 0$ such that $f(r) = cg(r)(1 + \mathbf{o}(1))$. In Eq. (1) $q(r)$ is the 'effective' potential which is related to the 'physical' potential $V(r)$ by the relation $q(r) = V(r)/(\hbar^2/2m)$ with m being the reduced mass. We shall call $q(r)$ also potential or inverse potential if we speak, respectively, of the exact (test) potential or of the one constructed by the inverse procedure.

If the potential $q(r)$ is zero beyond a certain radius $r = a < \infty$,

$$q(r \geq a) = 0, \tag{2}$$

then the wave function can be written as a linear combination of the two independent free solutions:

$$\varphi_l(r \geq a) \approx \sqrt{r}\left(J_{l+\frac{1}{2}}(kr) - \tan(\delta_l(k))Y_{l+\frac{1}{2}}(kr)\right). \tag{3}$$

The input quantities for the inverse procedure are the set of phase shifts $\{\delta_l(k)\}$ which determine the logarithmic derivatives $\frac{\mathrm{d}}{\mathrm{d}r}\ln\varphi_l(a)$, $\quad l = 0, 1, \ldots, L \approx ka$ where the maximal angular momentum L is related to the wave number k and the range a of the potential.

1.2. *Transformed Schrödinger equation on the half line* $0 \leq x \leq \infty$

Performing the transformations

$$\varphi_l(r) = \sqrt{r}y_l(x), \quad r = a\exp(-x), \quad 0 \leq r \leq a \tag{4}$$

one obtains the transformed Schrödinger equation

$$-y_l''(x) + Q(x)y_l(x) = -(l + 1/2)^2\, y_l(x) \tag{5}$$

with the transformed potential[1]

$$Q(x) = r^2(q(r) - k^2), \quad 0 \leq x \leq \infty. \tag{6}$$

Formally, Eq. (5) is an eigenvalue equation on the half line with 'eigenvalues' at $\lambda = -(l + \frac{1}{2})^2$. The initial slope of these 'eigenfunctions' is known to be:

$$\frac{y_l'(0)}{y_l(0)} = \frac{1}{2} - a\frac{\varphi_l'(a)}{\varphi_l(a)} = -ka\frac{J_{l+1/2}'(ka) - \tan\delta_l Y_{l+1/2}'(ka)}{J_{l+1/2}(ka) - \tan\delta_l Y_{l+1/2}(ka)}. \tag{7}$$

Also, Eq. (5) can be considered as a Sturm–Liouville equation

$$-y''(x) + Q(x)y(x) = \lambda\, y(x) \tag{8}$$

whose inverse problem (that is, uniqueness of Q by the spectral function) is solved for a long time (see e.g. Refs. 2 and 3).

Let us remark that for bound states supported by the transformed $Q(x)$ the eigenvalues are negative, $\lambda < 0$, and we know from the above treatment that the values $\lambda = -(l + 1/2)^2$ are associated with different initial boundary conditions depending on l.

2. Inverse Spectral Problem

The inverse spectral problem will be solved using the given set of scattering phase shifts $\{\delta_l\}$, in order to recover the unknown potential $q(r)$.

2.1. *Spectral functions*

The inverse spectral problem for Eq. (8) is well known from the work of Levitan.[2] Let us consider the spectral problem given by the initial boundary conditions

$$Y_\lambda(0) = 1 \quad \text{and} \quad Y'_\lambda(0) = 0\,. \tag{9}$$

To this spectral problem there exits a spectral function $\rho(\lambda)$, $\lambda \in \mathbf{R}$ such that any element $f \in L_2(0, \infty, dx)$ can be transformed into the space with elements $\tilde{F} \in L_2(-\infty, \infty, d\rho)$ by a unitary operator, i.e.

$$\int_0^\infty |f(x)|^2\, dx = \int_{-\infty}^\infty |\tilde{F}(\lambda)|^2\, d\rho(\lambda)\,, \tag{10}$$

where

$$\tilde{F}(\lambda) = \int_0^\infty f(x)Y(x,\lambda)\, dx \quad \text{and} \quad f(x) = \int_{-\infty}^\infty \tilde{F}(\lambda)Y(x,\lambda)\, d\rho(\lambda)\,, \tag{11}$$

with $Y(x,\lambda) = Y_\lambda(x)$ being the solution function of the Sturm–Liouville equation (8) with boundary conditions (9).

If $Q(x) \equiv 0$ then the (free) solution corresponding to (9) is obtained from (8) as $Y_\lambda(x) = \cos\left(\sqrt{\lambda}x\right)$ and the related (free) spectral function is given by

$$\rho_0(\lambda) = \begin{cases} \dfrac{2}{\pi}\sqrt{\lambda}, & \lambda \geq 0\,, \\ 0, & \lambda < 0\,. \end{cases} \tag{12}$$

2.2. *Completeness relations*

The completeness relations are as follows:

$$\delta(x-t) = \int_{-\infty}^\infty Y(x,\lambda)Y(t,\lambda)\, d\rho(\lambda)\,, \tag{13}$$

$$\delta(x-t) = \int_{-\infty}^\infty \cos(\sqrt{\lambda}x)\cos(\sqrt{\lambda}t)\, d\rho_0(\lambda)\,. \tag{14}$$

These relations together with the Sturm–Liouville equation (8) can be used to solve[2] the inverse spectral problem, i.e. to determine $Q(x)$, if $\rho(\lambda)$ is given.

2.3. *The m-function and its connection to the spectral function*

In what follows we suppose that

$$rq(r) \in L_1(0, a)$$

which implies by (6) that

$$Q(x) \in L_1(0, \infty).$$

Let $y(x) = y(x, \lambda)$ be the L_2-solution of (8); from $Q \in L_1$ it follows that the operator (8) is in the limit point case, and then the L_2-solution of (8) is unique up to a constant factor (for every λ not belonging to the spectrum). The Weyl–Titchmarsh m-function is defined by

$$m(\lambda) = \frac{y'(0, \lambda)}{y(0, \lambda)}\,. \tag{15}$$

Since

$$y_l(x) = y(x, -(l + 1/2)^2) \approx \exp(-(l + 1/2)x) \quad x \to \infty\,,$$

we have $y_l \in L_2(0, \infty)$, so from (3) and (4) we infer that

$$m(-(l + 1/2)^2) = \frac{y'(0, -(l + 1/2)^2)}{y(0, -(l + 1/2)^2)} = -ka\frac{J'_{l+1/2}(ka) - \tan\delta_l Y'_{l+1/2}(ka)}{J_{l+1/2}(ka) - \tan\delta_l Y_{l+1/2}(ka)}\,. \tag{16}$$

The basis of our inversion method is the use of the theorem[2] that establishes a connection between the m-function and the spectral function:

$$\frac{1}{m(\lambda)} = \int_{-\infty}^{\infty} \frac{\mathrm{d}\rho(t)}{\lambda - t}\,. \tag{17}$$

Since the spectral function uniquely determines the potential,[2,3] our task is to recover $\rho(t)$ from the given $m(\lambda)$'s.

2.4. *The GLM equation and the inverse potential*

By the usual method [see e.g. Ref. 2] we arrive at the definition

$$F(x) = \int_{-\infty}^{\infty} \cos(\sqrt{\lambda}x)\; d\sigma(\lambda), \quad \text{with} \quad \sigma(\lambda) = \rho(\lambda) - \rho_0(\lambda)\,, \tag{18}$$

from which the input symmetrical kernel is obtained as

$$F(x, t) = \int_{-\infty}^{\infty} \cos(\sqrt{\lambda}x)\cos(\sqrt{\lambda}t)\; d\sigma(\lambda) = \frac{1}{2}(F(x + t) + F(|x - t|))\,. \tag{19}$$

Thus the spectral function determines the input kernel. Knowing the input kernel one can determine the transformation kernel $K(x,t)$ by solving the Gelfand–Levitan–Marchenko (GLM) equation:

$$0 = F(x,t) + K(x,t) + \int_0^x K(x,s)F(s,t)\mathrm{d}s \qquad (0 \le t \le x)\,. \tag{20}$$

From the transformation kernel one obtains the (transformed) potential as

$$Q(x) = 2\frac{d}{dx}K(x,x)\,, \tag{21}$$

which is related, at the fixed energy $E = \frac{\hbar^2}{2m}k^2$, to the inverse potential by the rule

$$q\,(r = a\exp(-x)) = \frac{Q(x)}{r^2} + k^2\,. \tag{22}$$

3. Solution Method

3.1. *Setting up a moment problem*

Introduce the moments

$$\mu_l = \int_0^\infty F(x)\exp(-(l+1/2)x)dx \quad l = 0,1,\dots \tag{23}$$

The integral is convergent if there are no eigenvalues of (8) and (9) with $\lambda \le -1/4$. The moments μ_l can be explicitly expressed by the phase shifts:

Lemma 1. *If the spectrum of the problem* $-y" + Q(x)y = \lambda y$, $y'(0) = 0$ *is contained in* $(-1/4, \infty)$, *then in* (23) *we have*

$$\mu_l = \frac{l+1/2}{ka}\,\frac{J_{l+1/2}(ka) - \tan\delta_l Y_{l+1/2}(ka)}{J'_{l+1/2}(ka) - \tan\delta_l Y'_{l+1/2}(ka)} - 1 \tag{24}$$

$$= \frac{J_{l+3/2}(ka) - \tan\delta_l Y_{l+3/2}(ka)}{J'_{l+1/2}(ka) - \tan\delta_l Y'_{l+1/2}(ka)}\,. \tag{25}$$

If there are eigenvalues $\lambda_j \le -1/4$ *then for the function*

$$\tilde F(x) = \int_{-1/4+0}^\infty \cos\sqrt{\lambda}x\, d\sigma(\lambda) \tag{26}$$

we have

$$\tilde F(x) = F(x) - \sum_{\lambda_j \le -1/4} \cosh\sqrt{-\lambda_j}x \cdot (\varrho(\lambda_j + 0) - \varrho(\lambda_j - 0))\,, \tag{27}$$

$$\int_0^\infty \tilde F(x)\exp(-(l+1/2)x)\,dx = \mu_l - \sum_{\lambda_j \le -1/4} \frac{l+1/2}{(l+1/2)^2 + \lambda_j} \cdot (\varrho(\lambda_j + 0) - \varrho(\lambda_j - 0))\,, \tag{28}$$

where the quantities μ_l *satisfy* (24), (25).

Proof. Suppose first that there are no eigenvalues $\leq -1/4$. We know from Levitan,[2] Chapter II that the convergence

$$\int_{-1/4+0}^{M} \cos\sqrt{\lambda}x\, d\sigma(\lambda) \to F(x) \quad M \to \infty$$

is locally bounded in x. Consequently

$$\begin{aligned}
&\int_0^N F(x)\exp(-(l+1/2)x)\,dx \\
&= \lim_{M\to\infty}\int_{-1/4+0}^{M}\left[\int_0^N \cos\sqrt{\lambda}x \exp(-(l+1/2)x)\,dx\right] d\sigma(\lambda) \\
&= \int_{-1/4+0}^{\infty}\left[\int_0^N \cos\sqrt{\lambda}x \exp(-(l+1/2)x)\,dx\right] d\sigma(\lambda) \\
&= \int_{-1/4+0}^{\infty}\left[\frac{\exp((i\sqrt{\lambda}-l-1/2)x)}{2(i\sqrt{\lambda}-l-1/2)} + \frac{\exp((-i\sqrt{\lambda}-l-1/2)x)}{2(-i\sqrt{\lambda}-l-1/2)}\right]_{x=0}^{N} d\sigma(\lambda) \\
&= \int_{-1/4+0}^{\infty}\frac{l+1/2}{(l+1/2)^2+\lambda} d\sigma(\lambda) \\
&\quad + \int_{-1/4+0}^{\infty}\frac{\sqrt{\lambda}\sin\sqrt{\lambda}N - (l+1/2)\cos\sqrt{\lambda}N}{(l+1/2)^2+\lambda}\exp(-(l+1/2)N)\,d\sigma(\lambda) \\
&= I_1 + I_2\,.
\end{aligned}$$

Since $\sigma(\lambda)$ is bounded (see (46) below), an integration by parts in I_2 gives that

$$I_2 = \mathbf{O}(N\exp(-(l+\delta)N) \to 0 \quad N \to \infty$$

for some $\delta > 0$. This implies that

$$\int_0^{\infty} F(x)\exp(-(l+1/2)x)dx = \int_{-1/4+0}^{\infty}\frac{l+1/2}{(l+1/2)^2+\lambda} d\sigma(\lambda).$$

From the formula (17) we derive by (16) that

$$\begin{aligned}
&\int_0^{\infty} F(x)\exp(-(l+1/2)x)dx = (l+1/2)\left(\frac{1}{m_0(-(l+1/2)^2)} - \frac{1}{m(-(l+1/2)^2)}\right) \\
&= -(l+1/2)\frac{y_l(0)}{y_l'(0)} - 1 = \frac{l+1/2}{ka}\;\frac{J_{l+1/2}(ka) - \tan\delta_l Y_{l+1/2}(ka)}{J'_{l+1/2}(ka) - \tan\delta_l Y'_{l+1/2}(ka)} - 1
\end{aligned}$$

which is (24). From the identity

$$\frac{\nu}{r}J_\nu(r) - J'_\nu(r) = J_{\nu+1}(r)$$

we get

$$\frac{l+1/2}{ka} J_{l+1/2}(ka) - J'_{l+1/2}(ka) = J_{l+3/2}(ka)$$

and analogously with Y instead of J, hence (24) implies (25). Now if there are eigenvalues $\leq 1/4$, then we start with (26) and obtain

$$\begin{aligned}\int_0^\infty \tilde{F}(x)\exp(-(l+1/2)x)dx &= \int_{-1/4+0}^\infty \frac{l+1/2}{(l+1/2)^2+\lambda} d\sigma(\lambda) \\ &= (l+1/2)\left(\frac{1}{m_0(-(l+1/2)^2)} - \frac{1}{m(-(l+1/2)^2)}\right) \\ &\quad - \sum_{\lambda_j \leq -1/4} \frac{l+1/2}{(l+1/2)^2+\lambda_j} \cdot (\varrho(\lambda_j+0) - \varrho(\lambda_j - 0))\end{aligned}$$

which is (28). □

3.2. *Minimum norm solutions*

In what follows we look for solutions of the moment problem (23) or (28) which are the most "economic" in the following sense:

Lemma 2. *If the functions $\varphi_n \in L_2(0,\infty), n = 0,\ldots,N$ are linearly independent then the solution of the moment problem*

$$\mu_n = \int_0^\infty h\varphi_n \quad n = 0,\ldots,N \tag{29}$$

of the smallest norm $\|h\|_{L_2}$ can be given by the formula

$$h = \sum_{n=0}^N c_n \varphi_n \tag{30}$$

where the coefficients c_n satisfy

$$\sum_{n=0}^N c_n < \varphi_n, \varphi_i >_{L_2} = \mu_i \quad i = 0,\ldots,N. \tag{31}$$

Proof. Substituting (30) into (29) we get (31). Since the φ_n are independent, the Gram matrix $(< \varphi_n, \varphi_i >)_{i,n=0}^N$ is nonsingular, so (31) has a unique solution. This means that the problem (29) has a unique solution in the linear hull $\mathcal{L}$ of the φ_n, $0 \leq n \leq N$ and it is given by (30), (31). For any other solution of (29) the $\mathcal{L}$-component satisfies (30), (31) and the component orthogonal to $\mathcal{L}$ will increase the L_2-norm. □

Corollary. *If* $F(x) = \mathbf{O}(\exp(d_0 x))$ *with some constant* $d_0 < 1/2$ *then the moment problem*

$$\int_0^\infty F(x)\exp(-(l+1/2)x)\,dx = \mu_l \quad l = 0,\dots,N \tag{32}$$

has a unique solution which minimizes the expression

$$\int_0^\infty F^2(x)\exp(-(d_0+1/2)x)\,dx. \tag{33}$$

This solution has the form

$$F(x) = \sum_{n=0}^{N} c_n \exp((d_0-n)x), \tag{34}$$

$$\sum_{n=0}^{N} \frac{c_n}{n+l+1/2-d_0} = \mu_l \quad l = 0,\dots,N. \tag{35}$$

Proof. Denote

$$\varphi_n(x) = \exp((1/2(d_0-1/2)-n)x),$$

then

$$\int_0^\infty F(x)\exp(-(l+1/2)x)\,dx = \int_0^\infty F(x)\exp(-1/2(d_0+1/2)x)\varphi_l(x)\,dx.$$

Hence Lemma 2 applies with $h(x) = F(x)\exp(-1/2(d_0+1/2)x)$ and with

$$< \varphi_n, \varphi_i >= \int_0^\infty \exp((d_0-1/2-n-i)x)\,dx = \frac{1}{n+i+1/2-d_0}.$$ □

This corollary motivated us to seek for $F(x)$ in the form (34) also in the general case if $F(x) = \mathbf{O}(\exp(d_0 x))$ with an arbitrary positive constant d_0. Now the expansion (34) can be interpreted as

$$F(x) = \sum_{n\le d_0-1/2} 2c_n\cosh((d_0-n)x) + \tilde{F}(x) \tag{36}$$

$$\tilde{F}(x) = \sum_{n>d_0-1/2} c_n\exp((d_0-n)x) - \sum_{n\le d_0-1/2} c_n\exp((n-d_0)x) \tag{37}$$

in analogy with (27). The moment problem (28) has the form

$$\int_0^\infty \tilde{F}(x)\exp(-(l+1/2)x)\,dx$$
$$= \mu_l - \sum_{n\le d_0-1/2} \frac{2c_n(l+1/2)}{(l+1/2)^2-(d_0-n)^2}, \qquad 0\le l\le N\,. \tag{38}$$

Substituting (37) into the integral of (38) we get the system (35) again. Thus the formulae (34), (35) are used to approximate F for arbitrary $d_0 > 0$.

Another way to approximate $F(x) = \mathbf{O}(\exp(d_0 x))$ is the "Ansatz"

$$F(x) = c_0 \exp(d_0 x) + c_1 + c_2 \exp(-x) + \ldots + c_N \exp(-(N-1)x)\,. \tag{39}$$

This can be written in the form

$$F(x) = 2c_0 \cosh(d_0 x) + \tilde{F}(x) \tag{40}$$

$$\tilde{F}(x) = -c_0 \exp(-d_0 x) + c_1 + \ldots + c_N \exp(-(N-1)x)\,, \tag{41}$$

so the moment problem (28) has the form

$$\int_0^\infty \tilde{F}(x) \exp(-(l+1/2)x)\, dx = \mu_l - \frac{2c_0(l+1/2)}{(l+1/2)^2 - d_0^2} \quad l = 0, \ldots, N\,. \tag{42}$$

If $d_0 < 1/2$, this is equivalent to (23). Substituting (41) into (42) gives

$$\frac{c_0}{l+1/2-d_0} + \sum_{n=1}^{N} \frac{c_n}{n+l-1/2} = \mu_l \quad l = 0, \ldots, N\,. \tag{43}$$

Lemma 3. *Suppose that*

$$F(x) = c_0 \exp(d_0 x) + \tilde{\tilde{F}}(x), \quad \tilde{\tilde{F}}(x) \exp(-x/4) \in L_2(0, \infty)\,. \tag{44}$$

Then the moment problem

$$\int_0^\infty \tilde{\tilde{F}}(x) \exp(-(l+1/2)x)\, dx = \mu_l - \frac{c_0}{l+1/2-d_0} \quad l = 0, \ldots, N-1 \tag{45}$$

has a unique solution for which

$$\int_0^\infty \tilde{\tilde{F}}^2(x) \exp(-x/2)\, dx$$

is minimal; this solution has the form

$$\tilde{\tilde{F}}(x) = c_1 + c_2 \exp(-x) + \ldots + c_N \exp(-(N-1)x)\,,$$

with

$$\sum_{n=1}^{N} \frac{c_n}{n+l-1/2} = \mu_l - \frac{c_0}{l+1/2-d_0}, \qquad l = 0, \ldots, N-1\,.$$

Proof. Apply Lemma 2 with $\varphi_l(x) = \exp(-(l+1/4)x)$ and $h(x) = \tilde{\tilde{F}}(x) \times \exp(-x/4)$. □

3.3. *Looking for the ground state*

Both representations (34) and (39) contain the unknown parameter $d_0 > 0$ where $\lambda_0 = -d_0^2$ is the ground state of the operator. The problem is how to get the ground state from the phase shifts. A heuristic method is based on the following fact:

Lemma 4. $F(0) = 0$.

Proof. By definition, $F(0) = 0$ means that

$$\int_{-\infty}^{\infty} d\sigma(\lambda) = 0.$$

From Levitan,[2] (2.1.8) we infer

$$\varrho(\lambda) = \frac{2}{\pi}\sqrt{\lambda} + \varrho(-\infty) + \mathbf{o}(1) \quad \lambda \to +\infty\,. \tag{46}$$

Thus, if $\varrho(\lambda)$ is continuous in λ_0,

$$\int_{-\infty}^{\lambda_0} d\sigma = \varrho(\lambda_0) - \varrho(-\infty) - \frac{2}{\pi}\sqrt{\lambda_0} = \mathbf{o}(1) \to 0 \quad \lambda_0 \to \infty\,. \qquad \square$$

By the representation (34) or (39), $F(0) = 0$ means that

$$c_0 + c_1 + \ldots + c_N = 0\,. \tag{47}$$

In both cases every c_i is a function of the ground state parameter d_0. Our strategy is to solve Eq. (47) in the variable d_0. In the case (39) the Eq. (47) is particularly simple: it is linear in d_0 (though the summands c_i are not linear):

Lemma 5. *Let $\gamma_0, \ldots, \gamma_N$ be different, $b_0, \ldots, b_N, L_0, \ldots, L_N$ be arbitrary real numbers. Then for the solution of the linear system*

$$\sum_{j=0}^{N} \frac{x_j}{L_j + \gamma_i} = b_i \quad i = 0, \ldots, N\,, \tag{48}$$

the expression $x_0 + \ldots + x_N$ is linear in L_j if the L_k, $k \neq j$ are fixed.

Proof. It is enough to prove the linearity of $X = x_0 + \ldots + x_N$ in the variable L_0. Putting $x_0 = X - x_1 - \ldots - x_N$ into (48) gives

$$\frac{X}{L_0 + \gamma_i} + \sum_{j=1}^{N} x_j \left[\frac{1}{L_j + \gamma_i} - \frac{1}{L_0 + \gamma_i}\right] = b_i,$$

or

$$X + \sum_{j=1}^{N} x_j \frac{L_0 - L_j}{L_j + \gamma_i} = b_i(L_0 + \gamma_i) \quad i = 0, \ldots, N.$$

Introducing the new variables $\tilde{x}_j = x_j(L_0 - L_j)$ we get

$$X + \sum_{j=1}^{N} \frac{\tilde{x}_j}{L_j + \gamma_i} = b_i(L_0 + \gamma_i) \quad i = 0, \ldots, N.$$

Solving this system by the Cramer's rule we see that $X(= x_0 + \ldots + x_N)$ and $\tilde{x}_j(= x_j(L_0 - L_j))$ are linear in L_0. □

Corollary. *If* $F(x)$ *is defined by* (39) *and* (43) *then*

$$F(0) = c_0 + \ldots + c_N$$

is a linear function of d_0*.*

4. Examples

4.1. *Test results for box potential of strength* q_0 *and range* a

In this section we apply the method defined by (34), (35) to the box potential

$$V(r) = \begin{cases} 0.5 & \text{if } 0 \leq r \leq a = \sqrt{2}\,, \\ 0 & \text{else}\,. \end{cases} \tag{49}$$

The results are shown in Fig. 1 and Table 1 at the particular scattering energy of $E = 0.5$ au. We have used eleven exact phase shifts ($L = 10$) as input data and obtained the values $|\sum c_i| = 7.9476E - 05$ for the approximate solution (47) and $\sqrt{-\lambda_0} = 0.3881$ for the bound state position supported by the transformed potential $Q(x)$. The values of the moments μ_l and the expansion coefficients c_l are also listed in table 1. We can observe some convergence of the these values but also a strong parity dependence of alternate sign which puts forward the neccessity of deep theoretical and numerical analysis of the proposed method. Nevertheless, in Fig. 1 we see that the method is capable of reproducing the constant potential within almost the whole range of interval $0 < r < a$ except for a narrow region at the origin where the break down is attributed to numerical imprecision of the extraction of the bound state value λ_0 of $Q(x)$ from the input phase shifts.

4.2. *Test results for Gauss potential*

As a next test example we consider the Gauss potential of the form

$$V(r) = -2e^{-r*r/0.2}\,. \tag{50}$$

The results are shown in Fig. 2 and Table 2 at the particular scattering energy of $E = 1.125$ au. We have used eight phase shifts as input data and obtained the values $|\sum c_i| = 0.000778349535$ for the approximate solution of (47) and

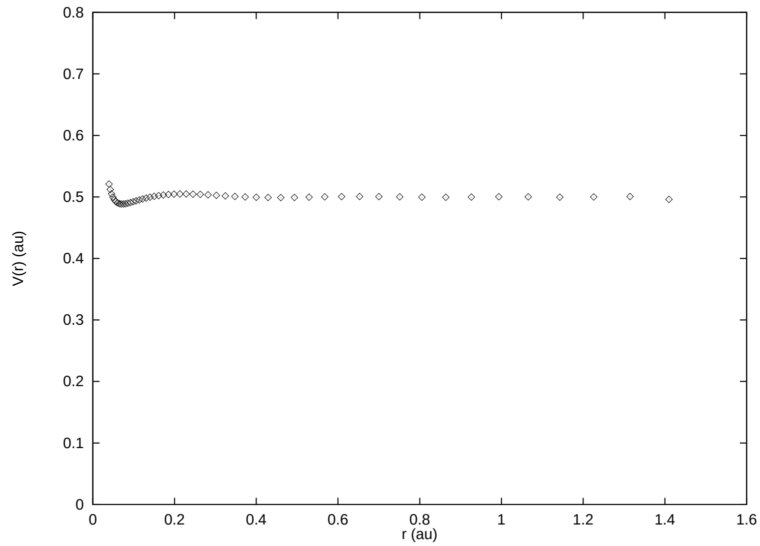

Fig. 1. Values of inversion potential $V(r) = q(r)/2$ at various points of r. The results denoted by dots are obtained with inversion of eleven phase shifts listed in Table 1 at the fixed energy of $E_{cm} = 0.5$ au ($k = 1$ au).

Table 1. Original phase shifts δ_l produced by the box potential (49) at scattering energy $E = 0.5$ au ($k = 1$ au). Moments μ_l (24), coefficients c_l coordinate x potential $Q(x)$, coordinate r, inverse potential $V(r) = q(r)/2$.

l	δ_l	μ_l	c_l	r	$V(r)$	x	$Q(x)$
0	−0.26787108	2.46301475	0.294588221	0.04	0.51	3.50	−0.88E-03
1	−0.0412087867	0.158049407	−8.32712136E-006	0.10	0.49	2.66	−0.49E-02
2	−0.00266860754	0.061258996	−0.142407159	0.15	0.50	2.24	−0.11E-01
3	−8.9958849E-005	0.0329292625	−0.72507853	0.30	0.50	1.54	−0.45E-01
4	−1.87764359E-006	0.0206405363	3.95075817	0.46	0.50	1.12	−0.11
5	−2.6793723E-008	0.0141723626	−15.5544656	0.61	0.50	0.84	−0.19
6	−2.78409534E-010	0.0103412551	38.154116	0.70	0.50	0.70	−0.24
7	−2.20235589E-012	0.007882243	−57.9791576	0.81	0.50	0.56	−0.32
8	−1.37123257E-014	0.00620882469	52.9974668	0.99	0.50	0.35	−0.49
9	−6.8964531E-017	0.00501805571	−26.6661648	1.14	0.50	0.21	−0.65
10	−2.86070009E-019	0.00414035976	5.67043232	1.41	0.50	0.00	−1.00

$\sqrt{-\lambda_0} = 2.0853656$ for the bound state position supported by the transformed potential $Q(x)$. The values of the moments μ_l and expansion coefficients c_l are listed in table 2 and we observe here also some parity dependence (alternating sign) of the method. In Fig. 2 we see also that the method reproduces well the Gauss potential within the interval $0.2 < r < a = 2.2$, except a for small region around the origin.

Table 2. Original phase shifts δ_l produced by the Gauss potential (50) at scattering energy $E = 1.125$ au ($k = 1.5$ au). Moments μ_l (24), coefficients c_l, coordinate r, inverse potential $V(r) = q(r)/2$, coordinate x potential $Q(x)$.

l	δ_l	μ_l	c_l	r	$V(r)$	x	$Q(x)$
0	0.232176185	−0.959479958	1.00099009	0.1	−0.38E+01	3.08	−0.57E-01
1	0.0153019948	−1.95222072	−0.0079578094	0.2	−0.36E+01	2.37	−0.23E+00
2	0.000655156119	2.22067925	0.14751958	0.4	−0.17E+01	2.65	−0.64E+00
3	2.07843498E-005	0.546233968	−1.2520096	0.59	−0.66E+00	1.26	−0.10E+01
4	5.17332799E-007	0.276018431	0.887810522	0.82	−0.13E+00	0.94	−0.16E+01
5	1.05616589E-008	0.17171037	−0.147292003	1.21	0.99E-02	0.55	−0.33E+01
6	1.83660135E-010	0.118605312	−1.21488495	1.6	0.29E-02	0.28	−0.57E+01
7	2.9692562E-012	0.0873778751	0.586602528	2.1	−0.33E-03	0	−0.99E+01

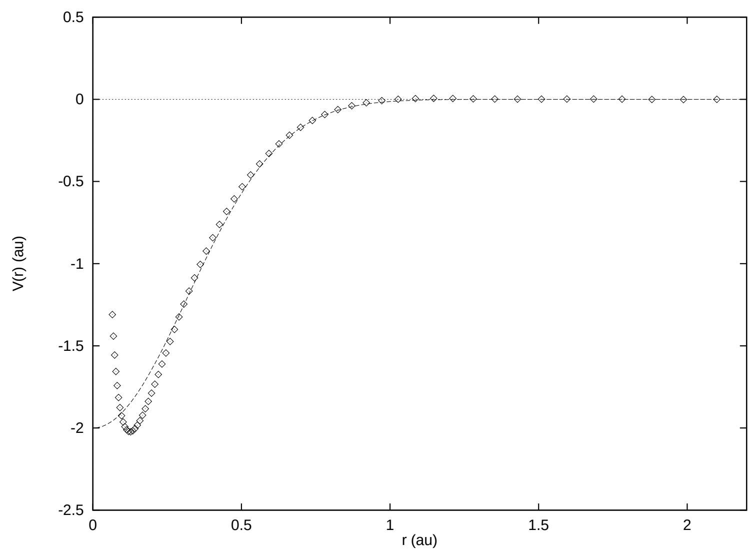

Fig. 2. Gauss potential results for the inversion of eight phase shifts at $E_{cm} = 1.125$ au ($k = 1.5$ au) using the inversion method of this work.

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