Gdansk University of Technology

Faculty of Theoretical Physics and Applied Mathematics

Dmitry Ponomarev

M. Sc. Thesis

Electronic states in zero-range potential models of nanostructures with a cyclic symmetry

Supervisor: prof. Sergey Leble

Gdansk

June 2010

Gdansk University of Technology

Faculty of Theoretical Physics and Applied Mathematics

Dmitry Ponomarev

M. Sc. Thesis

Electronic states in zero-range potential models of nanostructures with a cyclic symmetry

....

student signature   supervisor signature

Statement of the author

Aware of legal responsibility, I declare that the present work was done by myself and does not contain any content obtained in a manner inconsistent with the applicable regulations.

I also declare that the paper version is identical to the electronic version attached.

Date Signature

Contents

1 Introduction

In the present work we make an attempt to model certain symmetrical objects of nanoscale size. Our particular focus is on quantum rings with further generalization to quantum tubes, the structures that can be of high importance due to constantly growing interest to nanotechnologies and promising prospectives of amazing properties exhibited by nanoobjects.

Our approach is based on treating the mentioned atomic structures by means of so-called zero-range potentials which idea was originated by Enrico Fermi [11] and roughly can be viewed as a natural extension of the Dirac delta-function distribution to higher dimensions (though their application is not limited only to this). Within this basic model we describe each atom of the molecule as a point structure neglecting electrical interactions as well as movements of atoms with respect to each other. However, in spite of its simplicity, the zero-range potential method is known to be a very efficient tool in grasping effects of geometrical structure on the object properties [3, 5, 7, 10]. Using the zero-range potentials nanotubes and their properties has been recently studied [2, 19]. Though, in addition to this method, another approach of improving obtained solutions and potentials of the corresponding problem can be useful. Namely, the Darboux transformations [6, 9, 16, 21], with the parameters to be tuned in order to have coincidence with experimental data, might be applied (see [15] for the demonstration of success of this idea).

The aim of the work is to provide theoretical description of molecules possessing discrete rotational (cyclic) symmetry and, in the case of a quantum tube, additionally symmetry of translations. For the quantum ring case, both bounded state and scattering problems were considered.

The present section serves as a brief introductory part whereas the rest of the work is structured as given below. The second section gives self-containing description of the Darboux transformations that is followed by their few applications to classical quantum mechanical problem with delta-well potential in Cartesian coordinate system in the Section 3. The fourth section contains motivation for the zero-range potential method considering, in particular, three-dimensional point-potential. Here also we obtain the broader class of solvable potentials by means of application of the Darboux transformations. In the Section 5 the problem of a quantum ring is formulated and gradually solved: starting from particular cases to the general result. Besides discrete spectrum problem with bounded state and corresponding energies found, axial scattering on the ring is considered as well. The Section 6 describes generalization of results obtained for quantum ring to the case of quantum wire. Obtained results allow to calculate energy bands and bounded states of infinitely long tube having the rings in its cross-sections. The last section sums up the work that has been done and declares the directions of ongoing and further research. Finally, in the Appendix we list some programs written in order to help finding solution for the particular case in quantum ring problem (with further generalization furnished). They are given for instructive reasons, since they combine power of MATLAB and MAPLE in simplification of symbolic expressions at the different parts of calculations. These are non-typical computations and such experience might be also useful out of the topic of the present work.

2 Basic ideas of the Darboux transformations

Consider a solvable problem with classical Sturm-Liouville equation

$$-\psi''(x) + u(x)\psi(x) = \lambda\psi(x) \tag{1}$$

that is convenient to write in the form

$$L\psi = \lambda\psi, \tag{2}$$

where

$$L = -\frac{d^2}{dx^2} + u(x). \tag{3}$$

Let us choose a linear transformation D so that for some operator $L^{[1]}$ it satisfies the intertwining condition

$$DL = L^{[1]}D. \tag{4}$$

Application of this transformation to (2) yields

$$\underbrace{DL}_{=L^{[1]}D}\,\psi = \lambda D\psi \qquad \Rightarrow \qquad L^{[1]}\underbrace{(D\psi)}_{=\psi^{[1]}} = \lambda\underbrace{(D\psi)}_{=\psi^{[1]}}.$$

Thus, we arrived at the transformed equation

$$L^{[1]}\psi^{[1]} = \lambda\psi^{[1]}, \tag{5}$$

where we introduced transformed solution $\psi^{[1]} = D\psi$.

If we take transformation D in the form

$$D = \frac{d}{dx} - \sigma(x), \tag{6}$$

then $\sigma(x)$ can be chosen in a way that $L^{[1]}$ is covariant to L, i.e.

$$L^{[1]} = -\frac{d^2}{dx^2} + u^{[1]}(x). \tag{7}$$

Moreover, we will demonstrate that the potential is transformed as

$$u^{[1]}(x) = u(x) - 2\sigma'(x). \tag{8}$$

This is the statement of the Darboux theorem. Let us show it in a straightforward way.

Plugging (6) directly into the intertwining condition (4) applied to an arbitrary solution $\psi(x)$, we perform elementary algebraic manipulations with elimination of all second derivatives due to equation (1) and come to

$$\left(u - u^{[1]} - 2\sigma'\right)\psi' + \left(u' + u^{[1]}\sigma - u\sigma - \sigma''\right)\psi = 0.$$

Due to arbitrariness of $\psi(x)$, the following equations must hold true

$$\begin{cases} \left(u - u^{[1]} - 2\sigma'\right) = 0, \\ \left(u' + u^{[1]}\sigma - u\sigma - \sigma''\right) = 0. \end{cases} \tag{9}$$

The first of this two conditions is equivalent to (8) and the second one after feeding expressed $u^{[1]}$ into yields

$$u' - 2\sigma\sigma' - \sigma'' = 0 \qquad \Rightarrow \qquad \frac{d}{dx}\left(u - \sigma^2 - \sigma'\right) = 0.$$

Thereby, we come to Ricatti equation (with c_0 being an arbitrary constant)

$$\sigma' = -\sigma^2 + u + c_0, \tag{10}$$

that can be solved with substitution

$$\sigma = \frac{\psi_1'}{\psi_1}.$$

This gives

$$\frac{\psi_1''}{\psi_1} = u + c_0.$$

One can notice that by choosing $c_0 = -\lambda_1$ the last equation turns into

$$-\psi_1'' + u\psi_1 = \lambda_1\psi_1$$

and, therefore, is satisfied automatically for the solution ψ_1 corresponding to the eigenvalue λ_1 of the original equation (2).

Thus, once a particular solution $\psi_1(x)$ of (2) is known, we can use it to construct Darboux transformation $D = \frac{d}{dx} - \underbrace{\frac{\psi_1'}{\psi_1}}_{=\sigma(x)}$ such that $D\psi = \psi^{[1]}$ gives solution to the transformed (so-called dressed) problem (5).

The same procedure can be done by taking any other solution of original problem in lieu of $\psi_1(x)$ and, thereby, obtain all solutions of the transformed problem with new potential $u^{[1]}(x)$ that we will refer to as the dressed one.

Now moving towards more general case, we consider double application of Darboux transformation

$$\psi^{[2]} = \underbrace{\left(\frac{d}{dx} - \sigma_1\right)}_{=D^{[1]}}\psi^{[1]} = \underbrace{\left(\frac{d}{dx} - \frac{\left(\psi_2^{[1]}\right)'}{\psi_2^{[1]}}\right)}_{=D^{[1]}}\underbrace{\left(\frac{d}{dx} - \frac{\psi_1'}{\psi_1}\right)}_{=D}\psi,$$

where $\psi_2^{[1]}(x)$ denotes a particular solution of the once transformed problem (5).

Under this transformation potential changes as it follows

$$u^{[2]} = u^{[1]} - 2\sigma_1' = u - 2\underbrace{(\log\psi_1)''}_{=\sigma'} - 2\left(\log\psi_2^{[1]}\right)'' = u - 2\frac{d^2}{dx^2}\left[\log\left(\psi_2^{[1]}\psi_1\right)\right].$$

A particular solution $\psi_2^{[1]}(x)$ of (5) can be obtained from another solution $\psi_2(x)$ of the original problem (2)

$$\psi_2^{[1]} = D\psi_2 = \psi_2' - \psi_2\sigma = \frac{\psi_1\psi_2' - \psi_1'\psi_2}{\psi_1}.$$

Feeding this into the previous expression we arrive at

$$u^{[2]} = u - 2\frac{d^2}{dx^2}\left[\log\underbrace{(\psi_1\psi_2' - \psi_1'\psi_2)}_{=W(\psi_1,\,\psi_2)}\right],$$

where we rewrote the expression in round brackets as Wronskian of two solutions of the original equation (2).

According to Crum's theorem, it turns out (and we will show it at the end of the paragraph) that after N applications of Darboux transformation the dressing of original potential will have the same structure (see, for instance, [16])

$$u^{[N]} = u - 2\frac{d^2}{dx^2}\left[\log W(\psi_1,\,\ldots,\,\psi_N)\right]. \tag{11}$$

The solution of the corresponding N-dressed problem is expressed as a linear combination of derivatives of solution of the original problem with functional coefficients

$$\psi^{[N]} = D^{[N]}\psi = \psi^{(N)} + s_1\psi^{(N-1)} + \ldots + s_N\psi, \tag{12}$$

where $s_1(x), \ldots, s_N(x)$ can also be expressed in terms of particular solutions of the original problem $\psi_1, \ldots, \psi_N$.

Indeed, we can notice that

$$D^{[N]}\psi\Big|_{\psi=\psi_1, \psi_2^{[1]}, \ldots, \psi_N^{[N-1]}} = \left(\frac{d}{dx} - \frac{\left(\psi_N^{[N-1]}\right)'}{\psi_N^{[N-1]}}\right) \ldots \left(\frac{d}{dx} - \frac{\left(\psi_2^{[1]}\right)'}{\psi_2^{[1]}}\right)\left(\frac{d}{dx} - \frac{\psi_1'}{\psi_1}\right)\psi\Bigg|_{\psi=\psi_1, \psi_2^{[1]}, \ldots, \psi_N^{[N-1]}} = 0,$$

where $\psi_{k+1}^{[k]}(x)$ is a solution of $L^{[k]}\psi^{[k]} = \lambda\psi^{[k]}$ for $k = 1, \ldots, N$.

Moreover,

$$\begin{cases} D^{[N]}\psi_1 = 0, \\ D^{[N]}\psi_2 = \left(\frac{d}{dx} - \frac{\left(\psi_N^{[N-1]}\right)'}{\psi_N^{[N-1]}}\right) \ldots \left(\frac{d}{dx} - \frac{\left(\psi_2^{[1]}\right)'}{\psi_2^{[1]}}\right) \underbrace{\left(\frac{d}{dx} - \frac{(\psi_1)'}{\psi_1}\right)\psi_2}_{=D\psi_2=\psi_2^{[1]}} = 0, \\ D^{[N]}\psi_3 = \left(\frac{d}{dx} - \frac{\left(\psi_N^{[N-1]}\right)'}{\psi_N^{[N-1]}}\right) \ldots \left(\frac{d}{dx} - \frac{\left(\psi_3^{[2]}\right)'}{\psi_3^{[2]}}\right) \underbrace{\left(\frac{d}{dx} - \frac{\left(\psi_2^{[1]}\right)'}{\psi_2^{[1]}}\right) \underbrace{\left(\frac{d}{dx} - \frac{(\psi_1)'}{\psi_1}\right)\psi_3}_{=D\psi_3=\psi_3^{[1]}}}_{=D\psi_3^{[1]}=\psi_3^{[2]}} = 0, \\ \ldots \\ D^{[N]}\psi_N = \left(\frac{d}{dx} - \frac{\left(\psi_N^{[N-1]}\right)'}{\psi_N^{[N-1]}}\right) \underbrace{\ldots \left(\frac{d}{dx} - \frac{\left(\psi_2^{[1]}\right)'}{\psi_2^{[1]}}\right)\left(\frac{d}{dx} - \frac{(\psi_1)'}{\psi_1}\right)\psi_N}_{=\ldots=D\psi_N^{[N-2]}=\psi_N^{[N-1]}} = 0. \end{cases}$$

Thus, plugging here (12), we come to the system of linear equations for $s_1(x), \ldots, s_N(x)$. Determinant of the system is exactly Wronskian $W(\psi_1, \ldots, \psi_N)$. So, according to the Cramer's rule one has

$$s_k = -\frac{W_k(\psi_1, \ldots, \psi_N)}{W(\psi_1, \ldots, \psi_N)}, \tag{13}$$

where $k = 1, \ldots, N$ and $W_k(\psi_1, \ldots, \psi_N)$ is the determinant obtained from the Wronski matrix by replacing k-th column with the vector $(\psi_1^{(N)}, \ldots, \psi_N^{(N)})^T$.

In particular, $s_1(x)$ can be easily found.

If one computes

$$\frac{d}{dx}W(\psi_1,\ldots,\psi_N)=\frac{d}{dx}\begin{vmatrix}\psi_1 & \psi_1' & \ldots & \psi_1^{(N-2)} & \psi_1^{(N-1)}\\ \vdots & \vdots & \ddots & \vdots & \vdots\\ \psi_N & \psi_N' & \ldots & \psi_N^{(N-2)} & \psi_N^{(N-1)}\end{vmatrix}=$$

$$=\underbrace{\begin{vmatrix}\psi_1' & \psi_1' & \ldots & \psi_1^{(N-2)} & \psi_1^{(N-1)}\\ \vdots & \vdots & \ddots & \vdots & \vdots\\ \psi_N' & \psi_N' & \ldots & \psi_N^{(N-2)} & \psi_N^{(N-1)}\end{vmatrix}}_{=0}+\underbrace{\ldots}_{\text{(N-2) terms }=0}+\underbrace{\begin{vmatrix}\psi_1 & \psi_1' & \ldots & \psi_1^{(N-2)} & \psi_1^{(N)}\\ \vdots & \vdots & \ddots & \vdots & \vdots\\ \psi_N & \psi_N' & \ldots & \psi_N^{(N-2)} & \psi_N^{(N)}\end{vmatrix}}_{=-s_1W(\psi_1,\ldots,\psi_N)}$$

using the rule for differentiation determinants, then it immediately follows that

$$s_1(x)=-\frac{\frac{d}{dx}W(\psi_1,\ldots,\psi_N)}{W(\psi_1,\ldots,\psi_N)}=-\frac{d}{dx}\log W(\psi_1,\ldots,\psi_N). \tag{14}$$

As one can notice, the expression for N-fold transformation (12) can be rewritten as the ratio of two Wronskians

$$\psi^{[N]}=D^{[N]}\psi=\frac{W(\psi_1,\ldots,\psi_N,\psi)}{W(\psi_1,\ldots,\psi_N)}. \tag{15}$$

Indeed, using the Laplace expansion we have

$$\begin{aligned}\psi^{[N]} &= \frac{1}{W(\psi_1,\ldots,\psi_N)}\begin{vmatrix}\psi_1 & \psi_1' & \ldots & \psi_1^{(N-1)} & \psi_1^{(N)}\\ \vdots & \vdots & \ddots & \vdots & \vdots\\ \psi & \psi' & \ldots & \psi^{(N-1)} & \psi^{(N)}\end{vmatrix}=\\ &= \psi\cdot\frac{(-1)^{N+2}}{W(\psi_1,\ldots,\psi_N)}\underbrace{\underbrace{\begin{vmatrix}\psi_1' & \psi_1^{(2)} & \ldots & \psi_1^{(N-1)} & \psi_1^{(N)}\\ \vdots & \vdots & \ddots & \vdots & \vdots\\ \psi_N' & \psi_N^{(2)} & \ldots & \psi_N^{(N-1)} & \psi_N^{(N)}\end{vmatrix}}_{=(-1)^{N-1}\begin{vmatrix}\psi_1^{(N)} & \psi_1' & \ldots & \psi_1^{(N-2)} & \psi_1^{(N-1)}\\ \vdots & \vdots & \ddots & \vdots & \vdots\\ \psi_N^{(N)} & \psi_N' & \ldots & \psi_N^{(N-2)} & \psi_N^{(N-1)}\end{vmatrix}}}_{=s_N}+\end{aligned}$$

$$
\begin{aligned}
&+ \quad \psi' \cdot \frac{(-1)^{N+3}}{W(\psi_1,\,\ldots,\,\psi_N)} \underbrace{\underbrace{\begin{vmatrix} \psi_1 & \psi_1^{(2)} & \ldots & \psi_1^{(N-1)} & \psi_1^{(N)} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \psi_N & \psi_N^{(2)} & \ldots & \psi_N^{(N-1)} & \psi_N^{(N)} \end{vmatrix}}_{=(-1)^{N-2}\begin{vmatrix} \psi_1 & \psi_1^{(N)} & \ldots & \psi_1^{(N-2)} & \psi_1^{(N-1)} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \psi_N & \psi_N^{(N)} & \ldots & \psi_N^{(N-2)} & \psi_N^{(N-1)} \end{vmatrix}}}_{=s_{N-1}} \qquad + \\
&+ \quad \ldots + \psi^{(N)} \cdot \underbrace{\frac{(-1)^{2N+2}}{W(\psi_1,\,\ldots,\,\psi_N)} \begin{vmatrix} \psi_1 & \psi_1' & \ldots & \psi_1^{(N-2)} & \psi_1^{(N-1)} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \psi_N & \psi_N' & \ldots & \psi_N^{(N-2)} & \psi_N^{(N-1)} \end{vmatrix}}_{=1} \\
&= \quad \psi^{(N)} + s_1\psi^{(N-1)} + \ldots + s_N\psi
\end{aligned}
$$

Now, employing the representation (15), we can obtain the expression (11) for the transformation of a potential

$$
\begin{aligned}
u^{[N]} &= u^{[N-1]} - 2\frac{d^2}{dx^2}\log\psi_N^{[N-1]} = u^{[N-2]} - 2\frac{d^2}{dx^2}\log\left(\psi_N^{[N-1]}\cdot\psi_{N-1}^{[N-2]}\right) = \ldots = \\
&= u - 2\frac{d^2}{dx^2}\log\left(\psi_N^{[N-1]}\cdot\psi_{N-1}^{[N-2]}\cdot\ldots\cdot\psi_2^{[1]}\cdot\psi_1\right) = \\
&= u - 2\frac{d^2}{dx^2}\log\left(\frac{W(\psi_1,\,\ldots,\,\psi_{N-1},\,\psi_N)}{W(\psi_1,\,\ldots,\psi_{N-2},\,\psi_{N-1})}\cdot\frac{W(\psi_1,\,\ldots,\,\psi_{N-2},\,\psi_{N-1})}{W(\psi_1,\,\ldots,\,\psi_{N-3},\,\psi_{N-2})}\cdot\ldots\cdot\frac{W(\psi_1,\,\psi_2)}{\psi_1}\cdot\psi_1\right) = \\
&= u - 2\frac{d^2}{dx^2}\log W(\psi_1,\,\ldots,\,\psi_{N-1},\,\psi_N),
\end{aligned}
$$

where we used formulas (8) for single transformations.

The last formula taking into account expression (14) can be also written as

$$
u^{[N]}(x) = u(x) + 2s_1'(x). \tag{16}
$$

3 Demonstration of the Darboux transformation

3.1 Point-potential in Cartesian coordinates

Consider the Sturm-Liouville equation (1) with the potential proportional to the Dirac delta-function

$$u(x) = -\alpha\delta(x). \tag{17}$$

In order to obtain appropriate boundary condition, let us integrate the equation in 2ε-neighborhood of $x = 0$

$$\int_{-\varepsilon}^{\varepsilon} -\psi''(x)dx - \int_{-\varepsilon}^{\varepsilon} -\delta(x)\psi(x)dx = \lambda \int_{-\varepsilon}^{\varepsilon} \psi(x)dx$$

$$-\left(\psi'(\varepsilon) - \psi'(-\varepsilon)\right) - \alpha\psi(0) = 2\varepsilon\lambda\psi(\xi).$$

Taking limit as $\varepsilon \to 0$, we obtain

$$\psi_r'(0) = \psi_l'(0) - \alpha\psi(0),$$

where $\psi_l(x)$, $\psi_r(x)$ denote solutions to the left and to the right of the singularity, respectively.

3.2 Discrete spectrum dressing

First, let us consider discrete spectrum of the problem (1) with the potential (17)

$$\psi(x) = \begin{cases} \psi_l(x) = Ae^{\kappa x} + Be^{-\kappa x}, & x < 0, \\ \psi_r(x) = Ce^{\kappa x} + De^{-\kappa x}, & x > 0, \end{cases}$$

where $\kappa = \sqrt{\lambda} > 0$.

Boundary conditions at $x = 0$ (which are simply continuity condition and derived above jump condition) read

$$\begin{cases} \psi_l(0) = \psi_r(0), \\ \psi_r'(x) = \psi_l'(0) - \alpha\psi(0). \end{cases} \tag{18}$$

Therefore

$$\begin{cases} 2(A-C)\kappa = \alpha(A+B), \\ 2(B-D)\kappa = -\alpha(A+B). \end{cases} \tag{19}$$

Bounded state of the Schrodinger equation problem corresponds to the case when $B=0$, $C=0$. Then from (19) it follows that

$$\begin{cases} \kappa = \frac{1}{2}\alpha \equiv \kappa_0, \\ A = D \equiv A_0. \end{cases}$$

And the bounded state is given by[1]

$$\psi_0(x) = A_0\left(e^{\kappa_0 x}\theta(-x) + e^{-\kappa_0 x}\theta(x)\right) = A_0\left(e^{\kappa_0 x} - e^{-\kappa_0 x}\right)\theta(-x) + A_0 e^{-\kappa_0 x}. \tag{20}$$

Now consider dressing using a general form solution taken from discrete spectrum.

$$\sigma(x) = \kappa\left[\frac{Ae^{\kappa x} - Be^{-\kappa x}}{Ae^{\kappa x} + Be^{-\kappa x}} - \frac{Ce^{\kappa x} - De^{-\kappa x}}{Ce^{\kappa x} + De^{-\kappa x}}\right]\theta(-x) + \kappa\frac{Ce^{\kappa x} - De^{-\kappa x}}{Ce^{\kappa x} + De^{-\kappa x}}, \tag{21}$$

$$\begin{aligned} \sigma'(x) \quad = \quad & \underbrace{-\kappa\delta(x)\underbrace{\left(\frac{A-B}{A+B} - \frac{C-D}{C+D}\right)}_{=\frac{A-B+D-C}{A+B}=\frac{\alpha}{\kappa}}}_{=\alpha\delta(x)} + \kappa^2\underbrace{[\ldots]}_{=0} - \kappa^2\left[\underbrace{\frac{\left(Ae^{\kappa x} - Be^{-\kappa x}\right)^2}{\left(Ae^{\kappa x} + Be^{-\kappa x}\right)^2}}_{=\frac{-4AB}{\left(Ae^{\kappa x} + Be^{-\kappa x}\right)^2}} - \underbrace{\frac{\left(Ce^{\kappa x} - De^{-\kappa x}\right)^2}{\left(Ce^{\kappa x} + De^{-\kappa x}\right)^2}}_{=\frac{-4CD}{\left(Ce^{\kappa x} + De^{-\kappa x}\right)^2}}\right]\theta(-x) + \\ & + \kappa^2\underbrace{\frac{\left(Ce^{\kappa x} + De^{-\kappa x}\right)^2 - \left(Ce^{\kappa x} - De^{-\kappa x}\right)^2}{\left(Ce^{\kappa x} + De^{-\kappa x}\right)^2}}_{=\frac{4CD}{\left(Ce^{\kappa x} + De^{-\kappa x}\right)^2}}, \end{aligned}$$

where we used boundary conditions (19) in order to simplify the expressions.

Then we can write dressed potential in the symmetric form (though one understands that coefficients A, B, C, D are not independent, they linked by (19))

[1] Now and later on through the work we use the notion of Heaviside step-function $\theta(x)$ to write solutions in compact form suitable for further calculations.

$$u^{[1]}(x) = -\alpha\delta(x) - 2\sigma'(x) = \alpha\delta(x) - \frac{8AB}{(Ae^{\kappa x} + Be^{-\kappa x})^2}\kappa^2\theta(-x) - \frac{8CD}{(Ce^{\kappa x} + De^{-\kappa x})^2}\kappa^2\underbrace{(1-\theta(-x))}_{=\theta(x)}.$$

Let us dress this way the bounded state (20)

$$\begin{aligned}
\psi_0^{[1]}(x) &= \left(\frac{d}{dx} - \sigma(x)\right)\psi_0(x) = A_0\kappa_0\left(e^{\kappa_0 x}\theta(-x) - e^{-\kappa_0 x}\theta(x)\right) + \underbrace{(A_0 - A_0)\delta(x)}_{=0} - \\
&\quad -A_0\kappa e^{\kappa_0 x}\left(\frac{Ae^{\kappa x} - Be^{-\kappa x}}{Ae^{\kappa x} + Be^{-\kappa x}}\right)\theta(-x) - A_0\kappa e^{-\kappa_0 x}\left(\frac{Ce^{\kappa x} - De^{-\kappa x}}{Ce^{\kappa x} + De^{-\kappa x}}\right)\theta(x) = \\
&= A_0\kappa_0 e^{\kappa_0 x}\left[1 - \frac{\kappa}{\kappa_0}\left(\frac{Ae^{\kappa x} - Be^{-\kappa x}}{Ae^{\kappa x} + Be^{-\kappa x}}\right)\right]\theta(-x) - A_0\kappa_0 e^{-\kappa_0 x}\left[1 + \frac{\kappa}{\kappa_0}\left(\frac{Ce^{\kappa x} - De^{-\kappa x}}{Ce^{\kappa x} + De^{-\kappa x}}\right)\right]\theta(x).
\end{aligned}$$

3.3 Bounded state dressing with a continuous spectrum solution

Now, we consider continuous spectrum solutions

$$\psi(x) = \begin{cases} \psi_l(x) = Ae^{ikx} + Be^{-ikx}, & x < 0, \\ \psi_r(x) = Ce^{ikx} + De^{-ikx}, & x > 0, \end{cases}$$

where $k = \sqrt{|\lambda|} > 0$ satisfying the boundary conditions (18)

$$\begin{cases} 2(A - C)ik = \alpha(A + B), \\ 2(B - D)ik = -\alpha(A + B). \end{cases} \tag{22}$$

Consider the dressing with this general solution from continuous spectrum.

$$\sigma(x) = ik\left[\frac{Ae^{ikx} - Be^{-ikx}}{Ae^{ikx} + Be^{-ikx}}\right]\theta(-x) + ik\left[\frac{Ce^{ikx} - De^{-ikx}}{Ce^{ikx} + De^{-ikx}}\right]\theta(x),$$

$$\sigma'(x) = -ik\delta(x)\left(\frac{A-B}{A+B}-\frac{C-D}{C+D}\right)-k^2\left[\frac{\left(Ae^{ikx}+Be^{-ikx}\right)^2-\left(Ae^{ikx}-Be^{-ikx}\right)^2}{\left(Ae^{ikx}+Be^{-ikx}\right)^2}\right]\theta(-x)-$$
$$-k^2\left[\frac{\left(Ce^{ikx}+De^{-ikx}\right)^2-\left(Ce^{ikx}-De^{-ikx}\right)^2}{\left(Ce^{ikx}+De^{-ikx}\right)^2}\right]\theta(x).$$

Then the potential is transformed as follows

$$u^{[1]}(x) = -\alpha\delta(x)-2\sigma'(x)=\left(-\alpha+2ik\left(\frac{A-B}{A+B}-\frac{C-D}{C+D}\right)\right)\delta(x)+$$
$$+\frac{8AB}{\left(Ae^{ikx}+Be^{-ikx}\right)^2}k^2\theta(-x)+\frac{8CD}{\left(Ce^{ikx}+De^{-ikx}\right)^2}k^2\left(1-\theta(-x)\right).$$

In order for Schrodinger equation scattering problem has traditional physical sense (with Hamiltonian being a self-adjoint operator), the potential must be real. Obviously, to satisfy this requirement it is sufficient to impose the conditions

$$\begin{cases} A=B, \\ C=D. \end{cases}$$

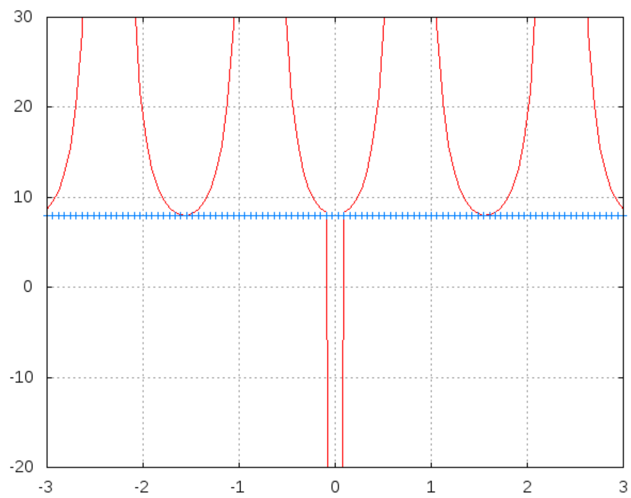
Then, employing boundary conditions (22), we simply have

$$A=B=C=D.$$

Therefore

$$u^{[1]}(x)=-\alpha\delta(x)+\frac{2k^2}{\cos^2(kx)}.$$

This potential is roughly sketched on the figure below



The horizontal line depicts $2k^2$-level whereas the vertical asymptotes, besides $x = 0$, are also k-dependent: $x = \dfrac{\pi}{4k}(1+2n)$, for any integer n.

Next, let us apply this dressing to the bounded state.

$$\sigma(x) = ikA\underbrace{\left[\frac{e^{ikx}-e^{-ikx}}{e^{ikx}+e^{-ikx}}\right]}_{=i\tan(kx)}\theta(-x) + ikA\underbrace{\left[\frac{e^{ikx}-e^{-ikx}}{e^{ikx}+e^{-ikx}}\right]}_{=i\tan(kx)}\theta(x) = -Ak\tan(kx), \tag{23}$$

$$\begin{aligned}\psi_0^{[1]}(x) &= \left(\frac{d}{dx}-\sigma(x)\right)\psi_0(x) = A_0\kappa_0\left(e^{\kappa_0 x}\theta(-x) - e^{-\kappa_0 x}\theta(x)\right) + \underbrace{(A_0-A_0)\delta(x)}_{=0} + \\ &\quad +A_0Ake^{\kappa_0 x}\tan(kx)\,\theta(-x) + A_0Ake^{-\kappa_0 x}\tan(kx)\,\theta(x) = \\ &= AA_0\kappa_0 e^{\kappa_0 x}\left[1+\frac{k}{\kappa_0}\tan(kx)\right]\theta(-x) - AA_0\kappa_0 e^{-\kappa_0 x}\left[1-\frac{k}{\kappa_0}\tan(kx)\right]\theta(x).\end{aligned}$$

3.4 Dressing of a continuous spectrum solution

Let us consider a solution as plain wave coming from $x=-\infty$ and being scattered on the delta-potential at $x=0$

$$\psi_0(x) = \begin{cases}\psi_l(x) = A_0e^{ik_0x}+B_0e^{-ik_0x}, & x<0,\\ \psi_r(x) = C_0e^{ik_0x}, & x>0.\end{cases}$$

The boundary conditions (22) in this case yield

$$B_0 = \frac{i\alpha}{2k_0-i\alpha}A_0,$$

$$C_0 = \frac{2k_0}{2k_0 - i\alpha} A_0.$$

Then

$$\psi_0(x) = A_0 \left(e^{ik_0 x} + \frac{i\alpha}{2k_0 - i\alpha} e^{-ik_0 x} \right) \theta(-x) + A_0 \frac{2k_0}{2k_0 - i\alpha} e^{ik_0 x} \theta(x),$$

$$\psi_0'(x) = A_0 i k_0 \left(e^{ik_0 x} - \frac{i\alpha}{2k_0 - i\alpha} e^{-ik_0 x} \right) \theta(-x) + A_0 \frac{2ik_0^2}{2k_0 - i\alpha} e^{ik_0 x} \theta(x).$$

Dressing with a solution from continuous spectrum (i.e. taking (23) in the transformation (6)) gives

$$\begin{aligned} \psi_0^{[1]}(x) &= A_0 \left[ik_0 \left(1 - iA\frac{k}{k_0} \tan(kx) \right) e^{ik_0 x} + \frac{\alpha k_0}{2k_0 - i\alpha} \left(1 + iA\frac{k}{k_0} \tan(kx) \right) e^{-ik_0 x} \right] \theta(-x) + \\ &+ A_0 \frac{2ik_0^2}{2k_0 - i\alpha} \left(1 - iA\frac{k}{k_0} \tan(kx) \right) e^{ik_0 x} \theta(x). \end{aligned}$$

On the other hand, performing dressing by using a solution from discrete spectrum (i.e. employing (21) in the Darboux transformation), we obtain

$$\begin{aligned} \psi_0^{[1]}(x) &= A_0 \left[ik_0 \left(1 + i\frac{\kappa}{k_0} \left(\frac{Ae^{\kappa x} - Be^{-\kappa x}}{Ae^{\kappa x} + Be^{-\kappa x}} \right) \right) e^{ik_0 x} + \frac{\alpha k_0}{2k_0 - i\alpha} \left(1 - i\frac{\kappa}{k_0} \left(\frac{Ce^{\kappa x} - De^{-\kappa x}}{Ce^{\kappa x} + De^{-\kappa x}} \right) \right) e^{-ik_0 x} \right] \theta(-x) + \\ &+ A_0 \frac{2ik_0^2}{2k_0 - i\alpha} \left(1 + i\frac{\kappa}{k_0} \left(\frac{Ce^{\kappa x} - De^{-\kappa x}}{Ce^{\kappa x} + De^{-\kappa x}} \right) \right) e^{ik_0 x} \theta(x). \end{aligned}$$

4 Single point-potential in spherical coordinates

4.1 Idea of zero-range potentials

It is often the case when model with short-range interaction can be well-described by point interactions. In one-dimensional Cartesian case, as it is well-known, this can be simply done with use of the conventional Dirac delta-function potential considered above, however the extensions to higher dimensions or different geometry is not straightforward. So-called zero-range potentials (or often referred as Fermi pseudopotentials) were originally introduced in [11]. The idea of the method is to replace real interaction potential, that is completely unknown, with some effective singular potential giving the same long-range behavior in a scattering problem at low energies.

We start with considering the Schrodinger equation in free space outside the range of potential-center placed in the origin $r = 0$

$$-\frac{\hbar^2}{2\mu}\underbrace{\left(\frac{1}{r^2}\frac{\partial}{\partial r}\left(\frac{1}{r^2}\frac{\partial\psi}{\partial r}\right)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right)+\frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2}\right)}_{=\Delta\psi}=E\psi, \tag{24}$$

where μ, E are mass and energy of a particle, respectively, $\hbar$ is the Planck's constant.

A standard procedure of separation of variables is

$$\psi(r,\,\theta,\,\phi)=\psi(r)Y_l^m(\theta,\,\phi),$$

where now we denote the radial wave function as $\psi(r)$.

The main point of our interest will be the radial Schrodinger equation

$$-\frac{\hbar^2}{2\mu}\left(\psi''+\frac{2}{r}\psi'\right)+\frac{l\,(l+1)\,\hbar^2}{2\mu r^2}\psi=E\psi.$$

This can be rewritten as

$$\underbrace{-\underbrace{\left(\psi''+\frac{2}{r}\psi'\right)}_{=\Delta_r\psi}+\frac{l\,(l+1)}{r^2}\psi}_{=-\Delta\psi}=k^2\psi, \tag{25}$$

where $k^2=\frac{2\mu E}{\hbar^2}$.

To demonstrate idea the most easily, we consider for now only partial s-waves, that is setting $l = 0$, and generalization will be given later.

Since for $r\psi(r)$ (25) is just one-dimensional Helmholtz equation, we can write general solution in the conventional form

$$\psi(r) = \frac{C_0}{kr}\left(\sin kr + \tan\eta_0 \cos kr\right), \tag{26}$$

where constants η_0, C_0 are determined by the form of potential and normalization condition, respectively.

Note that, alternatively, one can write the last equation as

$$\psi(r) = \frac{\tilde{C}_0}{kr}\left(s_0 \exp\left(ikr\right) - \exp\left(-ikr\right)\right), \tag{27}$$

with $s_0 = \exp\left(2i\eta_0\right)$ terming a scattering matrix.

Next step is to introduce a point-potential that gives the same behavior far from the center as this free space solution. However, since the solution is irregular in $r = 0$, the potential should also be singular.

Since for finite energies the solution at $r = 0$ behaves as

$$\psi(r) \approx C_0\left(1 + \frac{\tan\eta_0}{kr}\right) \approx C_0\frac{\tan\eta_0}{kr} \tag{28}$$

we can employ the identity (which validity can be easily verified by means of integration over a ball and applying the Gauss' theorem)

$$-\Delta\frac{1}{r} = 4\pi\delta(\vec{r})$$

and calculate

$$-\Delta\psi = 4\pi C_0\frac{\tan\eta_0}{k}\delta(\vec{r}).$$

Now, taking into account that the term $k^2\psi$ is less singular than $\Delta\psi$ at $r = 0$, we can introduce into the Schrodinger equation a source term leading to the desired behavior of solution (characterized by the parameter η_0) at the origin. Hence, the equation valid for the whole space should be

$$-\Delta\psi - k^2\psi = 4\pi C_0\frac{\tan\eta_0}{k}\delta(\vec{r}). \tag{29}$$

It remains only to eliminate normalization constant C_0 from the asymptotic behavior of the solution at the center (28). This can be done by applying the appropriate operator

$$C_0 = \frac{d}{dr}\left(r\psi\right)\bigg|_{r=0}. \tag{30}$$

Therefore, (29) results in

$$\left(-\Delta - 4\pi \frac{\tan \eta_0}{k} \delta(\vec{r}) \frac{d}{dr} r \right) \psi = k^2 \psi. \tag{31}$$

Denoting

$$a_0 = -\frac{\tan \eta_0}{k} \tag{32}$$

(that is an independent of k quantity for small energies, as it will be shown later), we bring the equation (31) back to the form of the original Schrodinger equation

$$\left(-\frac{\hbar^2}{2\mu}\Delta + \underbrace{2\pi \frac{a_0 \hbar^2}{\mu} \delta(\vec{r}) \frac{d}{dr} r}_{=U_0} \right) \psi = E\psi. \tag{33}$$

Thus, we can conclude that given the scattering characteristic of a potential, we can introduce singular point-center pseudopotential as operator $U_0 = 2\pi \frac{a_0 \hbar^2}{\mu} \delta(\vec{r}) \frac{d}{dr} r$ into the Schrodinger equation that is valid now in the whole space.

Alternatively, we can consider free-space solution having an appropriate asymptotic behavior at the origin, that can be formulated as a boundary condition.

Indeed, to eliminate the normalization constant C_0 and express the potential parameter η_0, we can form a combination

$$\left.\frac{\frac{d}{dr}(r\psi)}{r\psi}\right|_{r=0} = \frac{k}{\tan \eta_0} = -1/a_0. \tag{34}$$

This is consistent with the fact that interaction between particles can be described by the only parameter [5, 7] - the value of the logarithmic derivative $\frac{d \log(r\psi)}{dr} = \frac{1}{r\psi} \frac{d(r\psi)}{dr}$.

For bounded states we can write

$$\left.\frac{\frac{d}{dr}(r\psi)}{r\psi}\right|_{r=0} = -\beta, \tag{35}$$

where $\beta \equiv 1/a_0 > 0$ is the s-wave inverse scattering length.

In this form it can be seen as a sewing condition on the boundary of some infinitely deep and narrow potential well with the admissible (decaying, for a bounded state) solution at infinity.

Next we will give overview of more general potentials with possibilities of their extensions, however, taking into account that the partial s-wave gives the most contribution, it is usually enough to use spherically symmetric zero-range potentials described by the ZRP condition (35), and this is what we are going to employ onwards.

4.2 Generalized zero-range potentials

The same idea for the case $l > 0$ yields so-called generalized zero-range potentials. Although, this case was treated quite a long time ago [13, 12], it was not until recently when the situation started to become clear as the mistakes in Huang's works were corrected and different approaches were proposed [8, 18, 14]. However, to avoid possible ambiguity, the final expressions for pseudopotential given in those works still should be understood in an appropriate mathematical sense [17].

It is well-known that the general solution of the radial Schrodinger equation (25) can be formed as a linear combination of spherical Bessel and Neumann functions, $j_l(kr)$ and $y_l(kr)$, respectively,

$$\psi(r) = C_l \left(j_l(kr) - \tan\eta_l y_l(kr)\right), \tag{36}$$

or as a combination of spherical Hankel functions

$$\psi(r) = \tilde{C}_l \left(s_l h_l^{(1)}(kr) - h_l^{(2)}(kr)\right), \tag{37}$$

with $s_l = \exp(2i\eta_l)$ being a scattering matrix.

Taking into account the following asymptotes at $kr \to 0$ [1]

$$j_l(kr) \approx \frac{(kr)^l}{(2l+1)!!}, \tag{38}$$

$$y_l(kr) \approx -\frac{(2l-1)!!}{(kr)^{l+1}}, \tag{39}$$

written with notion of the odd factorial $(2l+1)!! = (2l+1)\cdot(2l-1)\cdot\ldots\cdot 3\cdot 1$, we obtain asymptotic behavior of finite-energy solution at the origin

$$\psi(r) \approx C_l \left(\frac{(kr)^l}{(2l+1)!!} + \tan\eta_l \frac{(2l-1)!!}{(kr)^{l+1}}\right) \approx C_l \tan\eta_l \frac{(2l-1)!!}{(kr)^{l+1}}. \tag{40}$$

From here, the constant C_l can be expressed as

$$C_l = \frac{(2l+1)!!}{k^l\,(2l+1)!}\,\frac{d^{2l+1}}{dr^{2l+1}}\left(r^{l+1}\psi\right)\Big|_{r=0}. \tag{41}$$

Following the same approach as for the case of $l=0$, we define pseudopotential as

$$U_l = \frac{\hbar^2}{2\mu} \lim_{r\to 0} \left(\Delta + k^2\right)\psi. \tag{42}$$

Since for finite energies the term with k^2 is obviously smaller than exacerbated by the differential operator

$$\Delta = \underbrace{\frac{1}{r^2}\frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r}}_{=\Delta_r} - \frac{l\left(l+1\right)}{r^2}$$

singular behavior of the solution (40) at the origin, it remains to obtain properly an effect of $\Delta \frac{1}{r^{l+1}}$. In order to do it, we form a combination $r^l \Delta \frac{1}{r^{l+1}}$ and consider it separately in a sense that multiplication by a spherical harmonic $Y_{lm}(\theta,\,\phi)$ is not implied, and integrate it over a small (such that asymptotic expressions are valid) ball in coordinates $(r'=r,\,\theta',\,\phi')$ (where we have $\Delta' = \Delta_r$ due to absence of dependencies on angular variables marked with prime and chosen volume of integration, that is a ball)

$$\begin{aligned}
\int_{V_\epsilon} r^l \Delta \frac{1}{r^{l+1}} dV' &= \int_{V_\epsilon} r^l \left(\Delta' \frac{1}{r^{l+1}} - \frac{l\left(l+1\right)}{r^2}\cdot\frac{1}{r^{l+1}}\right) dV' = \\
&= \int_{V_\epsilon} \left(r^l \Delta' \frac{1}{r^{l+1}} - \frac{1}{r^{l+1}}\Delta' r^l\right) + \underbrace{\int_{V_\epsilon} \frac{1}{r^{l+1}}\Delta' r^l dV' - \int_{V_\epsilon} r^l \frac{l\left(l+1\right)}{r^2}\cdot\frac{1}{r^{l+1}} dV'}_{=0} = \\
&= \int_{S_\epsilon} \left(r^l \nabla \frac{1}{r^{l+1}} - \frac{1}{r^{l+1}}\nabla r^l\right) d\vec{S}' = \left[-\left(l+1\right) - l\right] \int_{S_\epsilon} \frac{1}{r^2} dS' = -4\pi\left(2l+1\right)
\end{aligned}$$

where we have employed one of the Green's identities and straightforward calculation $\Delta' r^l = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r} r^l\right) = l\left(l+1\right) r^{l-2}$.

Therefore, we conclude that

$$\Delta \frac{1}{r^{l+1}} = -4\pi\left(2l+1\right)\frac{1}{r^l}\delta(\vec{r}') = -4\pi\left(2l+1\right)\frac{1}{r^{l+2}}\delta(r),$$

where the last part of the equality should be understood in a proper distributional sense (cf. chain of discussions [12, 18, 8, 14, 17]).

Eventually, combining this result with the previous expressions (42), (41), we obtain

$$U_l\psi = -2\pi\underbrace{(2l+1)\,(2l-1)!!}_{=(2l+1)!!}\underbrace{\frac{(2l+1)!!}{(2l+1)!}}_{=\frac{1}{2^l l!}}\frac{\hbar^2}{\mu}\frac{\tan\eta_l}{k^{2l+1}}\frac{1}{r^{l+2}}\delta(r)\frac{\partial^{2l+1}}{\partial r^{2l+1}}\left(r^{l+1}\psi\right). \tag{43}$$

As before, an alternative to pseudopotential approach (and less ambiguous) is to impose boundary condition similar to (34) that can be readily found from the asymptote of the solution (40). The desired combination allowing to eliminate C_l yields

$$\frac{1}{r^{l+1}\psi}\frac{\partial^{2l+1}}{\partial r^{2l+1}}\left(r^{l+1}\psi\right)\Big|_{r=0} = \underbrace{\frac{(2l+1)!}{(2l+1)!!}}_{=2^l l!}\cdot\frac{1}{(2l-1)!!}\cdot\frac{k^{2l+1}}{\tan\eta_l} = -\frac{2^l l!}{(2l-1)!!}1/a_l^{2l+1}, \tag{44}$$

where we introduced

$$a_l^{2l+1} = -\frac{\tan\eta_l}{k^{2l+1}}. \tag{45}$$

Before when writing (32) we have already stated that this quantity does not depend on k at its low values.

Let us analyze this more general combination and give postponed justification for the particular case of $l = 0$.

At the zero energy (i.e. $k = 0$) the radial Schrodinger equation (25) admits the following general solution

$$\psi(r) = A_1 r^l + A_2\frac{1}{r^{l+1}}. \tag{46}$$

On the other hand, we can consider solutions (36) for non-zero but small energies such that the small argument spherical function expansions (38), (39) can be used. Thus, by imposing requirement of matching (36) and (46), we conclude

$$A_1 \approx C_l^0\frac{k^l}{(2l+1)!!},$$

$$A_2 \approx -C_l^0\tan\eta_l\frac{(2l-1)!!}{k^{l+1}}.$$

Therefore

$$\tan\eta_l \approx \underbrace{-A_2/A_1\frac{1}{(2l+1)!!\,(2l-1)!!}}_{=\mathrm{const}}k^{2l+1}.$$

The quantity (45) is termed as the Wigner's threshold scattering length.

This allows to rewrite the expression (43) once again, hence the resulting pseudopotential to be introduced into the radial Schrodinger equation is

$$U_l = 2\pi \frac{(2l+1)!!}{2^l l!} \frac{a_l^{2l+1}\hbar^2}{\mu} \frac{\delta(r)}{r^{l+2}} \frac{\partial^{2l+1}}{\partial r^{2l+1}} r^{l+1}. \tag{47}$$

4.3 Even more general potentials obtained by dressing

First of all, we notice that the radial Schrodinger equation (25) can be brought to the form (1) eligible for direct application of obtained formulas. Namely, performing substitution $\psi = \chi/r$, we readily obtain

$$-\chi'' + \underbrace{\frac{l(l+1)}{r^2}}_{=u_l(r)} \chi = k^2 \chi. \tag{48}$$

That is to say, that we can apply Darboux transformation to the equation (25) meaning that all original wave functions ψ should be multiplied by r whereas the potential term

$$u_l(r) = \frac{l(l+1)}{r^2} \tag{49}$$

remains unchanged.

We start by choosing a spherical Bessel function as the seed solution

$$\psi_l(r) = C j_l(kr) \tag{50}$$

and apply N-th order Darboux transformation by taking spherical Hankel functions with specific parameters κ_m as prop functions

$$\phi_m(r) = C h_l^{(1)}(-i\kappa_m r), \qquad m = 1, \ldots, N. \tag{51}$$

Note that we denote here and later on C as generic constant without specific value, so that it can absorb constant multipliers (where their meaning is not important) without changing notations.

We can employ Crum's formula (15) and write the transformed solution

$$\psi_l^{[N]}(r) = C \frac{W(r\phi_1, \ldots, r\phi_N, r\psi_l)}{rW(r\phi_1, \ldots, r\phi_N)}. \tag{52}$$

The Wronskians can be computed if we consider asymptotic behavior of spherical functions at $r \to \infty$

$$j_l(kr) \approx \frac{\sin(kr - l\pi/2)}{kr}, \tag{53}$$

$$y_l(kr) \approx -\frac{\cos(kr - l\pi/2)}{kr}, \tag{54}$$

$$h_l^{(1)}(kr) = j_l(kr) + iy_l(kr) \approx (-i)^{l+1} \frac{\exp(ikr)}{kr}, \tag{55}$$

$$h_l^{(2)}(kr) = j_l(kr) - iy_l(kr) \approx i^{l+1} \frac{\exp(-ikr)}{kr}. \tag{56}$$

Then the Wronskians turn into Vandermond determinants, hence,

$$\psi_l^{[N]}(r) = C\left[(-i)^l \frac{\exp(ikr)}{kr} \frac{\Delta(\kappa_1, \ldots, \kappa_N, ik)}{\Delta(\kappa_1, \ldots, \kappa_N)} - i^l \frac{\exp(-ikr)}{kr} \frac{\Delta(\kappa_1, \ldots, \kappa_N, -ik)}{\Delta(\kappa_1, \ldots, \kappa_N)}\right]. \tag{57}$$

The Vandermond determinant can be computed by noticing that $k = -i\kappa_m$ (for $m = 1, \ldots, N$) are the roots of polynomial with respect to k equation that is obvious from the form of the matrix (replacement $ik \to \kappa_m$ yields its zero determinant due to linear dependencies of the rows), thereby allowing the following factorization

$$\Delta(\kappa_1, \ldots, \kappa_N, ik) = \begin{vmatrix} 1 & \kappa_1 & \kappa_1^2 & \ldots & \kappa_1^N \\ 1 & \kappa_2 & \kappa_2 & \ldots & \kappa_2^N \\ \ldots & \ldots & \ldots & \ldots & \ldots \\ 1 & \kappa_N & \kappa_N^2 & \ldots & \kappa_N^N \\ 1 & ik & (ik)^2 & \ldots & (ik)^N \end{vmatrix} = C\prod_{m=1}^{N}(\kappa_m - ik).$$

Denoting

$$s_l = \prod_{m=1}^{N} \frac{(\kappa_m - ik)}{(\kappa_m + ik)}, \tag{58}$$

we recognize in (57) the asymptotes of spherical Hankel functions, hence

$$\psi_l^{[N]}(r) = C\left[s_l h_l^{(1)}(kr) - h_l^{(2)}(kr)\right]. \tag{59}$$

According to (11), the corresponding to this solution effective potential is transformed from (49) into

$$u_l^{[N]} = \frac{l\,(l+1)}{r^2} - 2\frac{d^2}{dr^2}\log \underbrace{W\left(rh_l^{(1)}(-i\kappa_1 r),\,\ldots,\,rh_l^{(1)}(-i\kappa_N r)\right)}_{\equiv W}. \tag{60}$$

From this expression, due to the asymptotes (55), (56), we can observe that the Darboux transformation does not change the behavior of the potential at $r\to\infty$

$$u_l^{[N]} \approx \frac{l\,(l+1)}{r^2} = u_l,$$

whereas singular behavior at the origin is changed.

Indeed, using the asymptote at $r\to 0$

$$h_l^{(1)}(\kappa r) \approx -i\frac{(2l-1)!!}{(\kappa r)^{l+1}} - \frac{1}{2}\frac{(2l-1)!!}{(\kappa r)^{l}}, \tag{61}$$

where, in fact, particular values of constants in these terms are not important for us, due to further Wronskian calculations at the right-hand side of the equation (60) which result is affected only by total power of r in the expression (however, due to cancelations in the first order, next term needs to be taken into account).

Eventually, we arrive at the transformed effective finite-range potential behavior in vicinity of the origin

$$u_l^{[N]} \approx \begin{cases} \frac{1}{r^2}\left[l\,(l+1) - (N+1)\,(N-2) - 2Nl\right], & N>1,\\ \frac{1}{r^2}\left[l\,(l+1) - 2l\right], & N=1. \end{cases} \tag{62}$$

Connection with generalized zero-range potentials

In particular, one can notice that the expression (59) coincides with (37) if

$$\exp\left(2i\eta_l\right) = \prod_{m=1}^{N}\frac{(\kappa_m - ik)}{(\kappa_m + ik)}, \tag{63}$$

or, taking into account (45),

$$\tan\eta_l = -a_l^{2l+1}k^{2l+1} = -i\frac{\prod_{m=1}^{N}(\kappa_m - ik) - \prod_{m=1}^{N}(\kappa_m + ik)}{\prod_{m=1}^{N}(\kappa_m - ik) + \prod_{m=1}^{N}(\kappa_m + ik)}. \tag{64}$$

And we conclude that for the direct correspondence $N = 2l+1$ should be taken.

Since

$$\prod_{m=1}^{N}\left(\kappa_m+ik\right)=\prod_{m=1}^{N}\kappa_m+ik\sum_{n=1}^{N}\prod_{\substack{m=1\\ m\neq n}}^{N}\kappa_m+\left(ik\right)^2\sum_{j=1}^{N}\sum_{n<j}^{N}\prod_{\substack{m=1\\ m\neq n,\, m\neq j}}^{N}\kappa_m+\ldots+\left(ik\right)^{N-1}\sum_{n=1}^{N}\kappa_n+\left(ik\right)^N,$$

we continue the last equality as

$$a_l^{2l+1}k^{2l+1}=-i\frac{ik\sum_{n=1}^{2l+1}\prod_{\substack{m=1\\ m\neq n}}^{2l+1}\kappa_m+\ldots+\left(ik\right)^{2l+1}}{\prod_{m=1}^{2l+1}\kappa_m+\ldots+\left(ik\right)^{2l}\sum_{n=1}^{2l+1}\kappa_n}. \tag{65}$$

We can see that by matching coefficients at the same powers of k (namely, by setting all terms but the first one and the last one in denominator and numerator, respectively, equal to zero, and $\prod_{m=1}^{N}\kappa_m=-i\left(i/a_l\right)^{2l+1}=\left(-1\right)^l/a_l^{2l+1}$) we obtain a set of equations allowing to determine all the transformation parameters κ_m.

However, one can use an alternative and more convenient approach of choosing κ_m.

Given some quantity $a=|a|\,e^{i\phi_a}$, the parameters $\kappa_1,\,\ldots,\,\kappa_{2l+1}$ needs to be chosen in a way that

$$\prod_{m=1}^{2l+1}\left(\kappa_m+ik\right)=\left(ik\right)^{2l+1}-a. \tag{66}$$

This is equivalent to the $ik=-\kappa_m$ $(m=1,\,\ldots,\,2l+1)$ being the roots of the equation

$$\left(ik\right)^{2l+1}=a,$$

that is to say $-\kappa_m=\sqrt[(2l+1)]{a}$, or

$$-\kappa_m=|a|^{1/(2l+1)}\exp\left(i\frac{\left(\phi_a+2\pi m\right)}{2l+1}\right),\qquad m=1,\,\ldots,\,2l+1. \tag{67}$$

Following the same procedure, we can write (simply by replacing $ik\to-ik$)

$$\prod_{m=1}^{2l+1}\left(\kappa_m-ik\right)=\left(-ik\right)^{2l+1}-a. \tag{68}$$

Substitution of (66), (68) into (64) results in

$$a_l^{2l+1}k^{2l+1}=\underbrace{i^{2l+2}}_{=(-1)^{l+1}}\frac{1}{a}k^{2l+1}\qquad\Rightarrow\qquad a=\left(-1\right)^{l+1}/a_l^{2l+1}.$$

Therefore, providing a_l is a real number, (67) yields

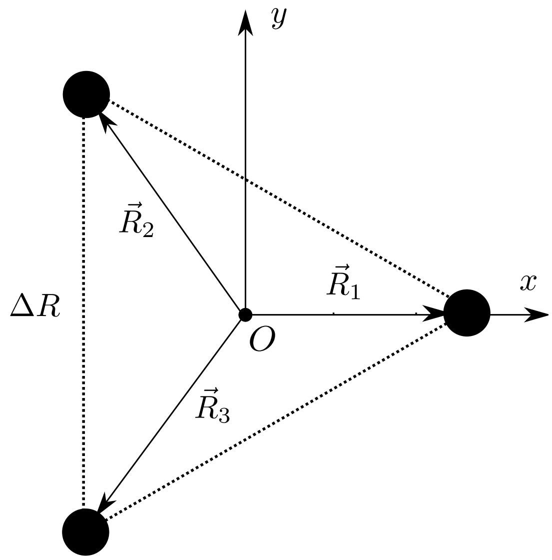
$$\kappa_m = -1/a_l \cdot \exp\left(i\pi\frac{l+2m+1}{2l+1}\right), \qquad m = 1, \ldots, 2l+1. \tag{69}$$

To sum up, the Darboux transformations significantly broadening the range of solvable potentials, in particular, give a possibility to tune a free-space solution to correspond to potential scattering characteristics, whilst the same transformation of the solution at the origin yields generalized zero-range potentials behavior.

5 Problem with plane symmetric multiple point-center potential

5.1 Toy problem with 3 point-centers - discrete spectrum

Let us start with considering a problem of finding bounded states of the potential describing symmetrical structure with 3 fixed point-centers (i.e. their positions constitute the cyclic group C_3).



Due to linearity of the Schrodinger equation, the superposition principle can be applied and, therefore, bounded state solution (33) is written in the form

$$\psi(\vec{r}) = C_1 \frac{e^{-\kappa\left|\vec{r}-\vec{R}_1\right|}}{\left|\vec{r}-\vec{R}_1\right|} + C_2 \frac{e^{-\kappa\left|\vec{r}-\vec{R}_2\right|}}{\left|\vec{r}-\vec{R}_2\right|} + C_3 \frac{e^{-\kappa\left|\vec{r}-\vec{R}_3\right|}}{\left|\vec{r}-\vec{R}_3\right|}, \tag{70}$$

where $\kappa = \sqrt{-\dfrac{2\mu E}{\hbar^2}}$.

This solution must satisfy zero-range potential conditions (35) at each center

$$\left.\frac{\partial \log\left(\left|\vec{r}-\vec{R}_i\right| \cdot \psi(\vec{r})\right)}{\partial\left|\vec{r}-\vec{R}_i\right|}\right|_{\left|\vec{r}-\vec{R}_i\right|=0} = -\beta, \qquad i = 1,\, 2,\, 3.$$

We expand on calculation and existence of these derivatives while discussing general case of N point-centers in the next section.

Taking into account that $\left|\vec{R}_2-\vec{R}_1\right| = \left|\vec{R}_3-\vec{R}_1\right| = \left|\vec{R}_3-\vec{R}_2\right| \equiv \Delta R$, these conditions give

$$\begin{cases} -\kappa + \dfrac{C_2 + C_3}{C_1} \cdot \dfrac{e^{-\kappa\Delta R}}{\Delta R} = -\beta, \\ -\kappa + \dfrac{C_1 + C_3}{C_2} \cdot \dfrac{e^{-\kappa\Delta R}}{\Delta R} = -\beta, \\ -\kappa + \dfrac{C_1 + C_2}{C_3} \cdot \dfrac{e^{-\kappa\Delta R}}{\Delta R} = -\beta. \end{cases}$$

In the matrix form this reads

$$\begin{pmatrix} (\beta-\kappa)\Delta R \cdot e^{\kappa\Delta R} & 1 & 1 \\ 1 & (\beta-\kappa)\Delta R \cdot e^{\kappa\Delta R} & 1 \\ 1 & 1 & (\beta-\kappa)\Delta R \cdot e^{\kappa\Delta R} \end{pmatrix} \begin{pmatrix} C_1 \\ C_2 \\ C_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}.$$

Compatibility condition of this system is

$$d_3 \equiv \begin{vmatrix} a & 1 & 1 \\ 1 & a & 1 \\ 1 & 1 & a \end{vmatrix} = a \cdot d_2 - 2b_2 = (a-1)^2(a+2) = 0,$$

where

$$d_2 = \begin{vmatrix} a & 1 \\ 1 & a \end{vmatrix} = a^2 - 1,$$

$$b_2 \equiv \begin{vmatrix} 1 & 1 \\ 1 & a \end{vmatrix} = a - 1,$$

$$a \equiv (\beta - \kappa)\Delta R \cdot e^{\kappa\Delta R}.$$

This leads to two possibilities

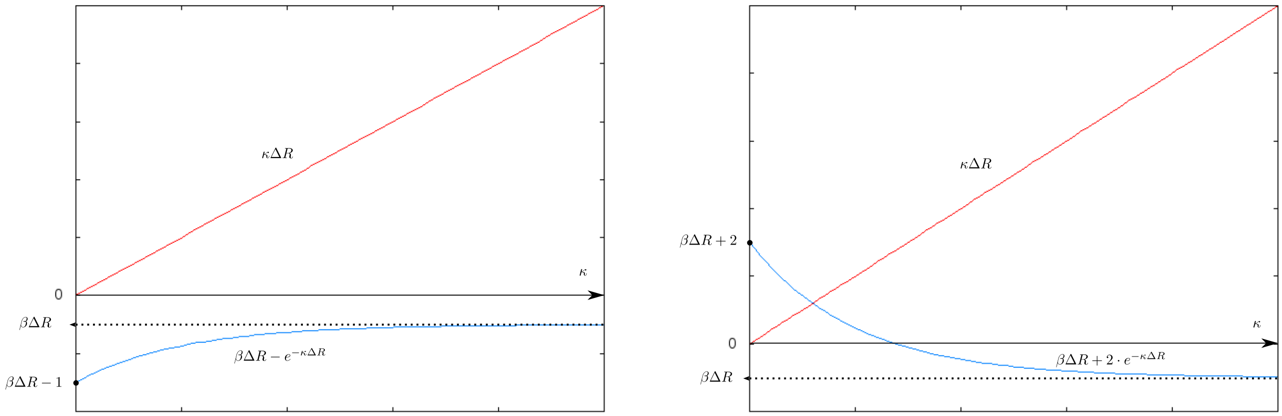
$$(\beta-\kappa)\Delta R \cdot e^{\kappa\Delta R} = 1, \tag{71}$$

in case if $\beta > \dfrac{1}{\Delta R}$, and

$$(\beta-\kappa)\Delta R \cdot e^{\kappa\Delta R} = -2 \tag{72}$$

providing $\beta > -\dfrac{2}{\Delta R}$.

Existence conditions $\beta > \dfrac{1}{\Delta R}$ and $\beta > -\dfrac{2}{\Delta R}$ for (71) and (72), respectively, are apparent from plotting with respect to κ the both sides of the equations $\kappa\Delta R = \beta\Delta R - e^{-\kappa\Delta R}$ and $\kappa\Delta R = \beta\Delta R + 2 \cdot e^{-\kappa\Delta R}$.



Solution corresponding to the last condition (72), i.e. $a = -2$, can be found using the Cramer's rule.

Take, for example, $C_3 \equiv C_0$ as a free variable and consider two of the equations

$$\begin{pmatrix} a & 1 \\ 1 & a \end{pmatrix} \begin{pmatrix} C_1 \\ C_2 \end{pmatrix} = \begin{pmatrix} -C_0 \\ -C_0 \end{pmatrix}.$$

Then the Cramer's formulas yield

$$C_1 = C_2 = -C_0 \frac{b_2}{d_2} = -C_0 \frac{1}{a+1} = C_0.$$

Thus, in this case we have predictable from the symmetry properties result $C_1 = C_2 = C_3 = C_0$ where C_0 is simply a normalization constant.

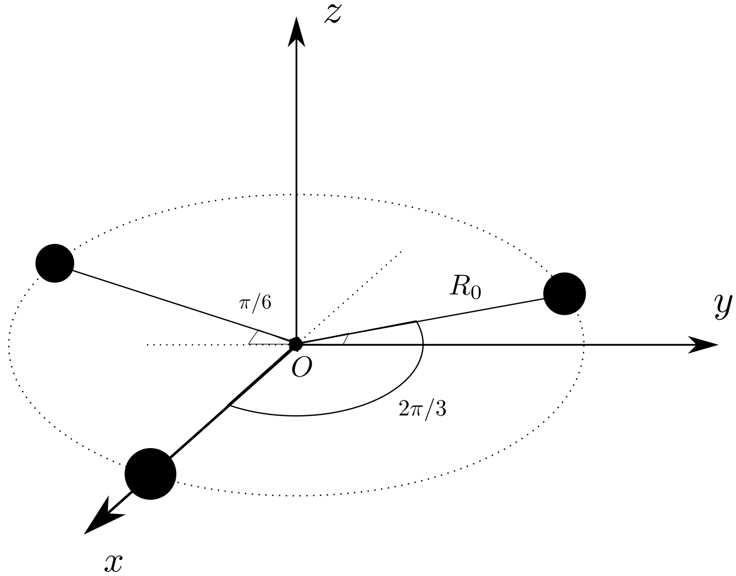
The first case, (71), allows to have any values of C_1, C_2, C_3 satisfying the only condition

$$C_1 + C_2 + C_3 = 0,$$

that is obvious from the direct substitution of $a = 1$ into the set of equations.

Let us consider this case in more detail. The solution (106) yields

$$\psi(\vec{r}) = C_1 \frac{e^{-\kappa\left|\vec{r}-\vec{R}_1\right|}}{\left|\vec{r}-\vec{R}_1\right|} + C_2 \frac{e^{-\kappa\left|\vec{r}-\vec{R}_2\right|}}{\left|\vec{r}-\vec{R}_2\right|} - (C_1 + C_2) \frac{e^{-\kappa\left|\vec{r}-\vec{R}_3\right|}}{\left|\vec{r}-\vec{R}_3\right|}.$$



However, due to symmetry in positions of centers, only those solutions which are symmetric must be realized. This is to say that given an energy level, all corresponding states must possess the symmetry of the problem. Mathematically it means that all Hamiltonian eigenstates must also be eigenfunctions (with eigenvalues of the complex exponential form $e^{i\phi_0}$, multiplication on which is known not to change a state of the system) of an appropriate rotation operator.

To employ this symmetry considerations in a convenient way, we choose coordinate system such that all centers are lying in the plane $z = 0$ (i.e. $\theta = \pi/2$, see the figure), and formulate an eigenvalue problem for the operator T_3 that performs rotation of the coordinates around z-axis on $2\pi/3$ angle

$$T_3\psi(\vec{r}) = \lambda C_1 \frac{e^{-\kappa\left|\vec{r}-\vec{R}_1\right|}}{\left|\vec{r}-\vec{R}_1\right|} + \lambda C_2 \frac{e^{-\kappa\left|\vec{r}-\vec{R}_2\right|}}{\left|\vec{r}-\vec{R}_2\right|} - \lambda(C_1+C_2) \frac{e^{-\kappa\left|\vec{r}-\vec{R}_3\right|}}{\left|\vec{r}-\vec{R}_3\right|}.$$

On the other hand, since in our case the rotation results simply in the transposition $\vec{R}_1 \to \vec{R}_2$, $\vec{R}_2 \to \vec{R}_3$, $\vec{R}_3 \to \vec{R}_1$, we have

$$T_3\psi(\vec{r}) = C_1 \frac{e^{-\kappa\left|\vec{r}-\vec{R}_2\right|}}{\left|\vec{r}-\vec{R}_2\right|} + C_2 \frac{e^{-\kappa\left|\vec{r}-\vec{R}_3\right|}}{\left|\vec{r}-\vec{R}_3\right|} - (C_1+C_2) \frac{e^{-\kappa\left|\vec{r}-\vec{R}_1\right|}}{\left|\vec{r}-\vec{R}_1\right|}.$$

From the last two expressions it follows that

$$\left[C_1(\lambda+1)+C_2\right] \frac{e^{-\kappa\left|\vec{r}-\vec{R}_1\right|}}{\left|\vec{r}-\vec{R}_1\right|} + \left[\lambda C_2 - C_1\right] \frac{e^{-\kappa\left|\vec{r}-\vec{R}_2\right|}}{\left|\vec{r}-\vec{R}_2\right|} - \left[C_1\lambda + C_2(\lambda+1)\right] \frac{e^{-\kappa\left|\vec{r}-\vec{R}_3\right|}}{\left|\vec{r}-\vec{R}_3\right|} = 0. \tag{73}$$

However, we note that due to the order (symmetry) in positions of point-centers $\vec{R}_i$, the functions $\dfrac{e^{-\kappa\left|\vec{r}-\vec{R}_i\right|}}{\left|\vec{r}-\vec{R}_i\right|}$, $i = 1,\, 2,\, 3$ can not be considered as independent.

Assuming an observation point to be arbitrary but close to the origin of the symmetrical structure, i.e. $r \ll R_0$ where $R_0 = \left|\vec{R}_1\right| = \left|\vec{R}_2\right| = \left|\vec{R}_3\right|$, we can do approximation $e^{-\kappa\left|\vec{r}-\vec{R}_i\right|} \approx e^{-\kappa R_0}$, $i = 1,\, 2,\, 3$ and write the following expansions

$$\frac{1}{\left|\vec{r}-\vec{R}_i\right|} = \sum_{l=0}^{\infty} \frac{r^l}{R_0^{l+1}} P_l\left(\cos\gamma_i\right), \qquad i = 1,\, 2,\, 3,$$

where $\cos\gamma_i = \dfrac{\vec{r}\cdot\vec{R}_i}{|\vec{r}|\cdot R_0}$.

Now we utilize the addition theorem for spherical harmonics (see, for instance, [4]) that gives

$$P_l\left(\cos\gamma_1\right) = \frac{4\pi}{2l+1} \sum_{m=-l}^{l} (-1)^m\, Y_l^m(\theta,\, \phi)\, Y_l^{-m}(\pi/2,\, 0),$$

$$P_l\left(\cos\gamma_2\right) = \frac{4\pi}{2l+1} \sum_{m=-l}^{l} (-1)^m\, Y_l^m(\theta,\, \phi)\, \underbrace{Y_l^{-m}(\pi/2,\, 2\pi/3)}_{=Y_l^{-m}(\pi/2,0)\cdot e^{-i\frac{2\pi}{3}m}}\,,$$

$$P_l\left(\cos\gamma_3\right) = \frac{4\pi}{2l+1} \sum_{m=-l}^{l} (-1)^m\, Y_l^m(\theta,\, \phi)\, \underbrace{Y_l^{-m}(\pi/2,\, 4\pi/3)}_{=Y_l^{-m}(\pi/2,0)\cdot e^{-i\frac{4\pi}{3}m}}\,.$$

Taking these expansions into account, the expression (73) leads us to

$$\sum_{l=0}^{\infty} \frac{4\pi}{2l+1}\cdot\frac{r^l}{R_0^{l+1}} \sum_{m=-l}^{l} (-1)^m\, Y_l^{-m}(\pi/2,\, 0) \Big[\left(C_1 - \lambda C_2\right) e^{-i\frac{2\pi}{3}m} + \\ + \left(\lambda C_1 + C_2\left(\lambda+1\right)\right) e^{-i\frac{4\pi}{3}m} - C_1\left(\lambda+1\right) - C_2\Big]\, Y_l^m(\theta,\, \phi) = 0.$$

Due to the independence of different spherical harmonics, we readily conclude that the expression in square brackets should be equal to zero for each m. Because of periodicity of the complex exponents, this condition is reduced to be valid only for $m = 0,\, \pm 1,\, \pm 2,\, \pm 3$.

Thus,

$$\left(C_1 - \lambda C_2\right) e^{-i\frac{2\pi}{3}m} + \left(\lambda C_1 + C_2\left(\lambda+1\right)\right) e^{-i\frac{4\pi}{3}m} - C_1\left(\lambda+1\right) - C_2 = 0, \qquad |m| = 0,\, \ldots,\, 3. \tag{74}$$

Obviously, for $m = 0$ the condition is automatically satisfied, so we consider the case $m = \pm 1$ and, later on, it remains to check that the result is consistent with fulfillment of the conditions for $m = \pm 2, \pm 3$.

For the case $m = \pm 1$ we require

$$\begin{cases} \left(-1 - \lambda + e^{-i\frac{2\pi}{3}} + \lambda e^{-i\frac{4\pi}{3}}\right) C_1 + \left(-1 - \lambda e^{-i\frac{2\pi}{3}} + (1+\lambda)\, e^{-i\frac{4\pi}{3}}\right) C_2 = 0, \\ \left(-1 - \lambda + e^{i\frac{2\pi}{3}} + \lambda e^{i\frac{4\pi}{3}}\right) C_1 + \left(-1 - \lambda e^{i\frac{2\pi}{3}} + (1+\lambda)\, e^{i\frac{4\pi}{3}}\right) C_2 = 0. \end{cases}$$

To have a non-zero solution, the characteristic equation of the system matrix must hold true.

Skipping tedious intermediate calculations, the characteristic equation simplifies to

$$\lambda^2 + \lambda + 1 = 0.$$

This gives

$$\lambda_1 = e^{i\frac{2\pi}{3}}, \qquad \lambda_2 = e^{i\frac{4\pi}{3}} = e^{-i\frac{2\pi}{3}}.$$

It is a natural result due to commutation of the rotation operator T_3 and the Hamiltonian of the system, as it was mentioned before.

By finding the corresponding set of constants C_1, C_2 (calculations are purely algebraic and quite cumbersome to be given here), we end up with the following eigenstates corresponding to λ_1, λ_2, respectively,

$$\psi_1(\vec{r}) = C_{01} \cdot \left(e^{-i\frac{\pi}{3}} \frac{e^{-\kappa|\vec{r}-\vec{R}_1|}}{\left|\vec{r}-\vec{R}_1\right|} - \frac{e^{-\kappa|\vec{r}-\vec{R}_2|}}{\left|\vec{r}-\vec{R}_2\right|} + e^{i\frac{\pi}{3}} \frac{e^{-\kappa|\vec{r}-\vec{R}_3|}}{\left|\vec{r}-\vec{R}_3\right|} \right),$$

$$\psi_2(\vec{r}) = C_{02} \cdot \left(e^{i\frac{\pi}{3}} \frac{e^{-\kappa|\vec{r}-\vec{R}_1|}}{\left|\vec{r}-\vec{R}_1\right|} - \frac{e^{-\kappa|\vec{r}-\vec{R}_2|}}{\left|\vec{r}-\vec{R}_2\right|} + e^{-i\frac{\pi}{3}} \frac{e^{-\kappa|\vec{r}-\vec{R}_3|}}{\left|\vec{r}-\vec{R}_3\right|} \right),$$

where C_{01}, C_{02} are normalization constants.

In order to make further generalization possible, it is convenient to redefine constants $C_{01} \to C_{01} \cdot e^{i\frac{\pi}{3}}$, $C_{02} \to C_{02} \cdot e^{-i\frac{\pi}{3}}$ and rewrite the last expressions as it follows

$$\psi_1(\vec{r}) = C_{01} \cdot \left(\frac{e^{-\kappa|\vec{r}-\vec{R}_1|}}{\left|\vec{r}-\vec{R}_1\right|} + e^{-i\frac{2\pi}{3}} \frac{e^{-\kappa|\vec{r}-\vec{R}_2|}}{\left|\vec{r}-\vec{R}_2\right|} + e^{i\frac{2\pi}{3}} \frac{e^{-\kappa|\vec{r}-\vec{R}_3|}}{\left|\vec{r}-\vec{R}_3\right|} \right), \tag{75}$$

$$\psi_2(\vec{r}) = C_{02} \cdot \left(\frac{e^{-\kappa\left|\vec{r}-\vec{R}_1\right|}}{\left|\vec{r}-\vec{R}_1\right|} + e^{i\frac{2\pi}{3}} \frac{e^{-\kappa\left|\vec{r}-\vec{R}_2\right|}}{\left|\vec{r}-\vec{R}_2\right|} + e^{-i\frac{2\pi}{3}} \frac{e^{-\kappa\left|\vec{r}-\vec{R}_3\right|}}{\left|\vec{r}-\vec{R}_3\right|} \right). \tag{76}$$

These states (that are, in fact, complex conjugated) corresponding to the eigenvalue with the energy determined from (71), along with the state

$$\psi_3(\vec{r}) = C_{03} \cdot \left(\frac{e^{-\kappa\left|\vec{r}-\vec{R}_1\right|}}{\left|\vec{r}-\vec{R}_1\right|} + \frac{e^{-\kappa\left|\vec{r}-\vec{R}_2\right|}}{\left|\vec{r}-\vec{R}_2\right|} + \frac{e^{-\kappa\left|\vec{r}-\vec{R}_3\right|}}{\left|\vec{r}-\vec{R}_3\right|} \right), \tag{77}$$

having the energy to be found from (72), make up the complete set of solutions for the 3 point-center symmetrical potential case.

Also we note that each of these solutions is an eigenfunction of the rotation operator T_3 (with eigenvalues $e^{i\frac{2\pi}{3}}$, $e^{i\frac{4\pi}{3}}$, 1, respectively) and, therefore, obey to the symmetry of the problem.

5.2 Case of N point-center plane symmetric potential

Now we continue with generalization of the previous case by considering the potential describing a symmetrical structure with point-centers forming the cyclic group C_N in space.

As before, we write solution as

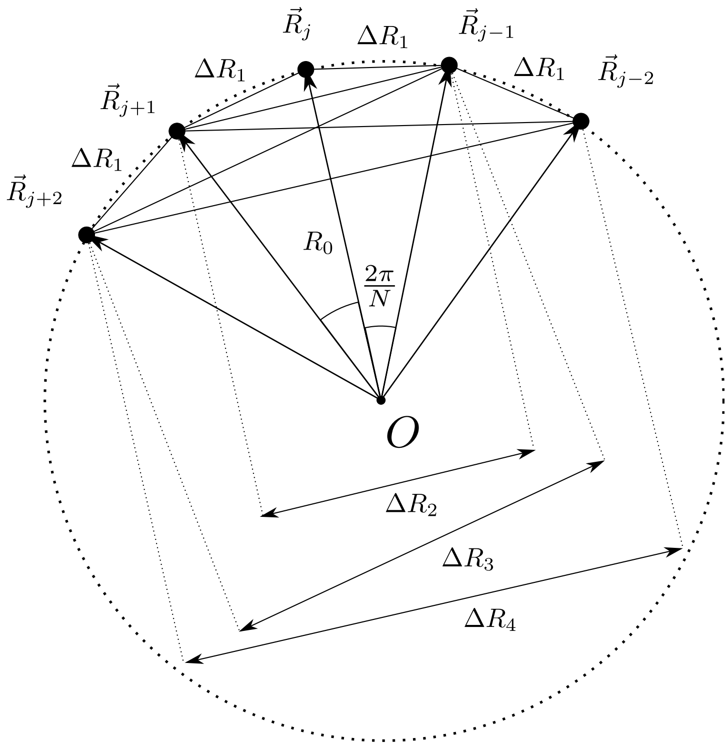
$$\psi(\vec{r}) = \sum_{k=1}^{N} C_k \frac{e^{-\kappa\left|\vec{r}-\vec{R}_k\right|}}{\left|\vec{r}-\vec{R}_k\right|}, \tag{78}$$

subject to the conditions

$$\left. \frac{\partial \log\left(\left|\vec{r}-\vec{R}_i\right| \cdot \psi(\vec{r})\right)}{\partial \left|\vec{r}-\vec{R}_i\right|} \right|_{\left|\vec{r}-\vec{R}_i\right|=0} = -\beta, \tag{79}$$

where $i = 1, \ldots, N$.

Let us introduce the following notation. We will denote a distance between nearest neighboring centers as ΔR_1, between every second center from each given one - ΔR_2, every third - ΔR_3, and so on.



From simple geometrical considerations it follows that

$$\Delta R_j = 2R_0 \sin\left(\frac{2\pi}{N} \cdot \frac{j}{2}\right) = 2R_0 \sin\left(\phi_{j+1}/2\right), \tag{80}$$

for $j = 1, \ldots, [N/2]$, where $[\cdot]$ marks integer part of an argument (i.e. the floor function), $\phi_j = \dfrac{2\pi}{N}(j-1)$ azimuthal angle coordinate of a j-th point-center.

We develop conditions (79) to show the existence of such derivatives

$$\begin{aligned}
\left.\frac{\partial \log\left(\left|\vec{r}-\vec{R}_i\right| \cdot \psi(\vec{r})\right)}{\partial\left|\vec{r}-\vec{R}_i\right|}\right|_{\left|\vec{r}-\vec{R}_i\right|=0} \quad &= \quad \frac{1}{C_i}\left[\left(\ldots + C_{i-1} \cdot \frac{e^{-\kappa \Delta R_1}}{\Delta R_1} - C_i \cdot \kappa + C_{i+1} \cdot \frac{e^{-\kappa \Delta R_1}}{\Delta R_1} + \ldots\right) + \right. \\
&\left. + \left|\vec{r}-\vec{R}_i\right| \cdot \left.\frac{\partial\left(\psi(\vec{r}) - \frac{e^{-\kappa\left|\vec{r}-\vec{R}_i\right|}}{\left|\vec{r}-\vec{R}_i\right|}\right)}{\partial\left|\vec{r}-\vec{R}_i\right|}\right|_{\left|\vec{r}-\vec{R}_i\right|=0}\right].
\end{aligned}$$

To show that the last term in the square bracketed expression is well-defined and equal to zero due to the presence of the multiplier $\left|\vec{r}-\vec{R}_i\right|$, we first note that $\psi(\vec{r}) - \frac{e^{-\kappa\left|\vec{r}-\vec{R}_i\right|}}{\left|\vec{r}-\vec{R}_i\right|}$ is a function of the arguments $\left|\vec{r}-\vec{R}_k\right|$ for $k = 1, \ldots, N$, $k \neq i$, which does not lead to a singularity when computed at $\left|\vec{r}-\vec{R}_i\right| = 0$. Thus, due to the chain rule, it remains to demonstrate that the derivatives $\frac{\partial\left|\vec{r}-\vec{R}_k\right|}{\partial\left|\vec{r}-\vec{R}_i\right|}$ do not blow up at $\left|\vec{r}-\vec{R}_i\right|=0$. This can be done in a straightforward manner as it follows

$$
\begin{aligned}
\frac{\partial\left|\vec{r}-\vec{R}_k\right|}{\partial\left|\vec{r}-\vec{R}_i\right|} &= \frac{\partial\left|\vec{r}-\vec{R}_i+\Delta\vec{R}_{ik}\right|}{\partial\left|\vec{r}-\vec{R}_i\right|} = \frac{\partial\sqrt{\left|\vec{r}-\vec{R}_i\right|^2+2\cdot\left(\Delta\vec{R}_{ik},\,\vec{r}-\vec{R}_i\right)+\left|\Delta\vec{R}_{ik}\right|^2}}{\partial\left|\vec{r}-\vec{R}_i\right|} = \\
&= \frac{1}{\left|\vec{r}-\vec{R}_k\right|}\left(\left|\vec{r}-\vec{R}_i\right|+\frac{d\left(\Delta\vec{R}_{ik},\,\vec{r}-\vec{R}_i\right)}{d\left|\vec{r}-\vec{R}_i\right|}\right),
\end{aligned}
$$

where $\Delta\vec{R}_{ik}=\vec{R}_i-\vec{R}_k$.

Taking into account that

$$
\left.\frac{d\left(\Delta\vec{R}_{ik},\,\vec{r}-\vec{R}_i\right)}{d\left|\vec{r}-\vec{R}_i\right|}\right|_{\left|\vec{r}-\vec{R}_i\right|=0} = \lim_{\left|\vec{\delta}\right|\to 0}\frac{\left(\Delta\vec{R}_{ik},\,\vec{\delta}\right)-0}{\left|\vec{\delta}\right|} = \left|\Delta\vec{R}_{ik}\right|\cdot\cos\Phi_0,
$$

where $\cos\Phi_0=\frac{\left(\Delta\vec{R}_{ik},\,\vec{\delta}\right)}{\left|\Delta\vec{R}_{ik}\right|\cdot\left|\vec{\delta}\right|}$, we conclude

$$
\left.\frac{\partial\left|\vec{r}-\vec{R}_k\right|}{\partial\left|\vec{r}-\vec{R}_i\right|}\right|_{\left|\vec{r}-\vec{R}_i\right|=0} = \cos\Phi_0
$$

That is, we have shown required boundedness

$$
-1 \le \left.\frac{\partial\left|\vec{r}-\vec{R}_k\right|}{\partial\left|\vec{r}-\vec{R}_i\right|}\right|_{\left|\vec{r}-\vec{R}_i\right|=0} \le 1,
$$

Therefore

$$
\left.\frac{\partial\log\left(\left|\vec{r}-\vec{R}_i\right|\cdot\psi(\vec{r})\right)}{\partial\left|\vec{r}-\vec{R}_i\right|}\right|_{\left|\vec{r}-\vec{R}_i\right|=0} = \frac{1}{C_i}\left(\ldots+C_{i-1}\cdot\frac{e^{-\kappa\Delta R_1}}{\Delta R_1}-C_i\cdot\kappa+C_{i+1}\cdot\frac{e^{-\kappa\Delta R_1}}{\Delta R_1}+\ldots\right)=-\beta.
$$

Next, due to peculiar differences, we consider separately the cases when N is even and odd.

5.2.1 Case of even number of point-centers formulation

Consider first the case where the number of point-centers N is even.

Conditions (79) yield

$$
\begin{cases}
(\beta-\kappa)\,C_1+\dfrac{e^{-\kappa\Delta R_1}}{\Delta R_1}C_2+\dfrac{e^{-\kappa\Delta R_2}}{\Delta R_2}C_3+\ldots+\dfrac{e^{-\kappa\Delta R_{N/2-1}}}{\Delta R_{N/2-1}}C_{N/2}+\dfrac{e^{-\kappa\Delta R_{N/2}}}{\Delta R_{N/2}}C_{N/2+1} \quad + & \\
\qquad + \quad \dfrac{e^{-\kappa\Delta R_{N/2-1}}}{\Delta R_{N/2-1}}C_{N/2+2}+\ldots+\dfrac{e^{-\kappa\Delta R_2}}{\Delta R_2}C_{N-1}+\dfrac{e^{-\kappa\Delta R_1}}{\Delta R_1}C_N & =0,\\
\dfrac{e^{-\kappa\Delta R_1}}{\Delta R_1}C_1+(\beta-\kappa)\,C_2+\dfrac{e^{-\kappa\Delta R_1}}{\Delta R_1}C_3+\ldots+\dfrac{e^{-\kappa\Delta R_{N/2-1}}}{\Delta R_{N/2-1}}C_{N/2+1}+\dfrac{e^{-\kappa\Delta R_{N/2}}}{\Delta R_{N/2}}C_{N/2+2} \quad + & \\
\qquad + \quad \dfrac{e^{-\kappa\Delta R_{N/2-1}}}{\Delta R_{N/2-1}}C_{N/2+3}+\ldots+\dfrac{e^{-\kappa\Delta R_3}}{\Delta R_3}C_{N-1}+\dfrac{e^{-\kappa\Delta R_2}}{\Delta R_2}C_N & =0,\\
\ldots \quad \ldots \quad \ldots \quad \ldots \quad \ldots \quad \ldots \quad \ldots \quad \ldots \quad \ldots & \\
\ldots \quad \ldots \quad \ldots \quad \ldots \quad \ldots \quad \ldots \quad \ldots \quad \ldots \quad \ldots &
\end{cases}
\tag{81}
$$

In the matrix form we can rewrite this set of algebraic linear equations as

$$
\begin{pmatrix}
(\beta-\kappa) & \chi_1 & \cdots & \chi_{N/2-1} & \chi_{N/2} & \chi_{N/2-1} & \cdots & \chi_2 & \chi_1\\
\chi_1 & (\beta-\kappa) & \cdots & \chi_{N/2-2} & \chi_{N/2-1} & \chi_{N/2} & \cdots & \chi_3 & \chi_2\\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots\\
\chi_2 & \chi_3 & \cdots & \chi_{N/2} & \chi_{N/2-1} & \chi_{N/2-2} & \cdots & (\beta-\kappa) & \chi_1\\
\chi_1 & \chi_2 & \cdots & \chi_{N/2-1} & \chi_{N/2} & \chi_{N/2-1} & \cdots & \chi_1 & (\beta-\kappa)
\end{pmatrix}
\begin{pmatrix} C_1\\ C_2\\ \vdots\\ C_{N-1}\\ C_N \end{pmatrix}
=
\begin{pmatrix} 0\\ 0\\ \vdots\\ 0\\ 0 \end{pmatrix},
$$

where we utilize notation $\chi_j \equiv \dfrac{e^{-\kappa\Delta R_j}}{\Delta R_j}$ for $j=1,\,\ldots,\,N/2$.

5.2.2 Case of odd number of point-centers formulation

Now we proceed with the odd number N of point-centers.

In this case in similar fashion as before we employ (79) and obtain

$$
\begin{cases}
(\beta-\kappa)\,C_1+\dfrac{e^{-\kappa\Delta R_1}}{\Delta R_1}C_2+\dfrac{e^{-\kappa\Delta R_2}}{\Delta R_2}C_3+\ldots+\dfrac{e^{-\kappa\Delta R_{(N-1)/2}}}{\Delta R_{(N-1)/2}}C_{(N+1)/2} \quad + \\
\qquad + \quad \dfrac{e^{-\kappa\Delta R_{(N-1)/2}}}{\Delta R_{(N-1)/2}}C_{(N+1)/2+1}+\ldots+\dfrac{e^{-\kappa\Delta R_2}}{\Delta R_2}C_{N-1}+\dfrac{e^{-\kappa\Delta R_1}}{\Delta R_1}C_N \quad =0, \\
\dfrac{e^{-\kappa\Delta R_1}}{\Delta R_1}C_1+(\beta-\kappa)\,C_2+\dfrac{e^{-\kappa\Delta R_1}}{\Delta R_1}C_3+\ldots+\dfrac{e^{-\kappa\Delta R_{(N-1)/2}}}{\Delta R_{(N-1)/2}}C_{(N+1)/2+1} \quad + \\
\qquad + \quad \dfrac{e^{-\kappa\Delta R_{(N-1)/2}}}{\Delta R_{(N-1)/2}}C_{(N+1)/2+2}+\ldots+\dfrac{e^{-\kappa\Delta R_3}}{\Delta R_3}C_{N-1}+\dfrac{e^{-\kappa\Delta R_2}}{\Delta R_2}C_N \quad =0, \\
\ldots \quad \ldots \quad \ldots \quad \ldots \quad \ldots \quad \ldots \quad \ldots \quad \ldots \quad \ldots \\
\ldots \quad \ldots \quad \ldots \quad \ldots \quad \ldots \quad \ldots \quad \ldots \quad \ldots \quad \ldots
\end{cases}
\tag{82}
$$

In the matrix form this reads

$$
\begin{pmatrix}
(\beta-\kappa) & \chi_1 & \cdots & \chi_{(N-1)/2} & \chi_{(N-1)/2} & \chi_{(N-1)/2-1} & \cdots & \chi_2 & \chi_1 \\
\chi_1 & (\beta-\kappa) & \cdots & \chi_{(N-1)/2-1} & \chi_{(N-1)/2} & \chi_{(N-1)/2} & \cdots & \chi_3 & \chi_2 \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\chi_2 & \chi_3 & \cdots & \chi_{(N-1)/2} & \chi_{(N-1)/2} & \chi_{(N-1)/2-1} & \cdots & (\beta-\kappa) & \chi_1 \\
\chi_1 & \chi_2 & \cdots & \chi_{(N-1)/2-1} & \chi_{(N-1)/2} & \chi_{(N-1)/2} & \cdots & \chi_1 & (\beta-\kappa)
\end{pmatrix}
\begin{pmatrix} C_1 \\ C_2 \\ \vdots \\ C_{N-1} \\ C_N \end{pmatrix}
=
\begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ 0 \end{pmatrix},
$$

where again we denote $\chi_j \equiv \dfrac{e^{-\kappa\Delta R_j}}{\Delta R_j}$ for $j=1,\,\ldots,\,(N-1)\,/2$.

5.2.3 General case formulation

Formally, we can combine both previous cases into one (though in quite awkward manner, utilizing again notion of $[\cdot]$ for separating integer part of an argument) and write

$$
\begin{cases}
(\beta-\kappa)\,C_1+\dfrac{e^{-\kappa\Delta R_1}}{\Delta R_1}C_2+\dfrac{e^{-\kappa\Delta R_2}}{\Delta R_2}C_3+\ldots+\dfrac{e^{-\kappa\Delta R_{[(N-1)/2]}}}{\Delta R_{[(N-1)/2]}}C_{[(N-1)/2]+1}+\dfrac{e^{-\kappa\Delta R_{[N/2]}}}{\Delta R_{[N/2]}}C_{[(N-1)/2]+2} \quad + \\
\qquad + \quad \dfrac{e^{-\kappa\Delta R_{[(N-1)/2]+[N/2]-[(N+1)/2]}}}{\Delta R_{[(N-1)/2]+[N/2]-[(N+1)/2]}}C_{[(N-1)/2]+3}+\ldots+\dfrac{e^{-\kappa\Delta R_2}}{\Delta R_2}C_{N-1}+\dfrac{e^{-\kappa\Delta R_1}}{\Delta R_1}C_N \qquad =0, \\
\dfrac{e^{-\kappa\Delta R_1}}{\Delta R_1}C_1+(\beta-\kappa)\,C_2+\dfrac{e^{-\kappa\Delta R_1}}{\Delta R_1}C_3+\ldots+\dfrac{e^{-\kappa\Delta R_{[(N-1)/2]}}}{\Delta R_{[(N-1)/2]}}C_{[(N-1)/2]+2}+\dfrac{e^{-\kappa\Delta R_{[N/2]}}}{\Delta R_{[N/2]}}C_{[(N-1)/2]+3} \quad + \\
\qquad + \quad \dfrac{e^{-\kappa\Delta R_{[(N-1)/2]+[N/2]-[(N+1)/2]}}}{\Delta R_{[(N-1)/2]+[N/2]-[(N+1)/2]}}C_{[(N-1)/2]+4}+\ldots+\dfrac{e^{-\kappa\Delta R_3}}{\Delta R_3}C_{N-1}+\dfrac{e^{-\kappa\Delta R_2}}{\Delta R_2}C_N \qquad =0, \\
\ldots \quad \ldots \quad \ldots \quad \ldots \quad \ldots \quad \ldots \quad \ldots \quad \ldots \quad \ldots \\
\ldots \quad \ldots \quad \ldots \quad \ldots \quad \ldots \quad \ldots \quad \ldots \quad \ldots \quad \ldots
\end{cases}
\tag{83}
$$

5.2.4 Particular cases $N = 4$ and $N = 5$ solutions

Before we will be able to come up with the solution of the general case, we get back to few particular cases that help us to make an important observation allowing to proceed with generalization.

Case $N = 4$

We immediately start with the zero-range potential conditions (79) in the matrix form

$$\begin{pmatrix} (\beta-\kappa) & \chi_1 & \chi_2 & \chi_1 \\ \chi_1 & (\beta-\kappa) & \chi_1 & \chi_2 \\ \chi_2 & \chi_1 & (\beta-\kappa) & \chi_1 \\ \chi_1 & \chi_2 & \chi_1 & (\beta-\kappa) \end{pmatrix} \begin{pmatrix} C_1 \\ C_2 \\ C_3 \\ C_4 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}.$$

Two roots of the characteristic equation can be easily guessed. One of them follows from the trivial symmetry consequence stating that the state with $C_1 = C_2 = C_3 = C_4$ is a solution. This is consistent with the condition above providing the energy level solves the following transcendent equation

$$\kappa - \beta = 2\chi_1(\kappa) + \chi_2(\kappa). \tag{84}$$

By inspection, one can see the second solution corresponding to

$$\kappa - \beta = -\chi_2(\kappa), \tag{85}$$

since, indeed, $\beta - \kappa = \chi_1$ turns determinant of the matrix to zero (due to linear dependencies of rows).

From the characteristic equation it is seen that this eigenvalue has multiplicity 2 and the last energy level corresponds to solution of

$$\kappa - \beta = -2\chi_1(\kappa) + \chi_2(\kappa). \tag{86}$$

As before, analyzing behavior of both hand sides of the equations, we conclude that fulfillment of the conditions (84), (85), (86) is guaranteed in case if $\beta > -\left(\frac{2}{\Delta R_1} + \frac{1}{\Delta R_2}\right)$, $\beta > \frac{1}{\Delta R_2}$, $\beta > \left(\frac{2}{\Delta R_1} - \frac{1}{\Delta R_2}\right)$, respectively.

From the linear set of algebraic equations we find that $C_2 = C_4 = -C_3 = -C_1$ for (86), while (85) gives just $C_3 = -C_1$, $C_4 = -C_2$. The uncertainty of choosing constants in latter case is reduced by imposing condition of symmetry of solution, i.e. a solution must be an eigenfunction of the appropriate rotational operator.

Therefore we solve eigenvalue problem for the operator T_4 that performs rotation around z-axis over angle $\pi/2$. As for the case of $N=3$, this yields

$$(C_1 - \lambda C_2)\, e^{-i\frac{\pi}{2}m} + (C_2 + \lambda C_1)\, e^{-i\pi m} + (-C_1 + \lambda C_2)\, e^{-i\frac{3\pi}{2}m} - C_2 - \lambda C_1 = 0, \qquad |m| = 0, \ldots, 4.$$

It is sufficient to solve

$$C_1 \left(e^{-i\frac{\pi}{2}m} + \lambda e^{-i\pi m} - e^{-i\frac{3\pi}{2}m} - \lambda \right) + C_2 \left(-\lambda e^{-i\frac{\pi}{2}m} + e^{-i\pi m} + \lambda e^{-i\frac{3\pi}{2}m} - 1 \right) = 0, \qquad m = \pm 1,$$

and check validity of the result for all other m.

This gives

$$\lambda_1 = e^{i\frac{\pi}{2}}, \qquad \lambda_2 = e^{i\frac{3\pi}{2}} = e^{-i\frac{\pi}{2}},$$

corresponding to the relations $C_2 = -iC_1$ and $C_2 = iC_1$, respectively.

Therefore[2]

$$\psi_1(\vec{r}) = C_{01} \cdot \left(\frac{e^{-\kappa|\vec{r}-\vec{R}_1|}}{\left|\vec{r}-\vec{R}_1\right|} + e^{-i\frac{\pi}{2}} \frac{e^{-\kappa|\vec{r}-\vec{R}_2|}}{\left|\vec{r}-\vec{R}_2\right|} + e^{i\pi} \frac{e^{-\kappa|\vec{r}-\vec{R}_3|}}{\left|\vec{r}-\vec{R}_3\right|} + e^{i\frac{\pi}{2}} \frac{e^{-\kappa|\vec{r}-\vec{R}_4|}}{\left|\vec{r}-\vec{R}_4\right|} \right), \tag{87}$$

$$\psi_2(\vec{r}) = C_{02} \cdot \left(\frac{e^{-\kappa|\vec{r}-\vec{R}_1|}}{\left|\vec{r}-\vec{R}_1\right|} + e^{i\frac{\pi}{2}} \frac{e^{-\kappa|\vec{r}-\vec{R}_2|}}{\left|\vec{r}-\vec{R}_2\right|} + e^{-i\pi} \frac{e^{-\kappa|\vec{r}-\vec{R}_3|}}{\left|\vec{r}-\vec{R}_3\right|} + e^{-i\frac{\pi}{2}} \frac{e^{-\kappa|\vec{r}-\vec{R}_4|}}{\left|\vec{r}-\vec{R}_4\right|} \right). \tag{88}$$

Also we write two other solutions corresponding to spectral conditions (84), (86) that we found

$$\psi_3(\vec{r}) = C_{03} \cdot \left(\frac{e^{-\kappa|\vec{r}-\vec{R}_1|}}{\left|\vec{r}-\vec{R}_1\right|} + \frac{e^{-\kappa|\vec{r}-\vec{R}_2|}}{\left|\vec{r}-\vec{R}_2\right|} + \frac{e^{-\kappa|\vec{r}-\vec{R}_3|}}{\left|\vec{r}-\vec{R}_3\right|} + \frac{e^{-\kappa|\vec{r}-\vec{R}_4|}}{\left|\vec{r}-\vec{R}_4\right|} \right), \tag{89}$$

$$\psi_4(\vec{r}) = C_{04} \cdot \left(\frac{e^{-\kappa|\vec{r}-\vec{R}_1|}}{\left|\vec{r}-\vec{R}_1\right|} + e^{-i\pi} \frac{e^{-\kappa|\vec{r}-\vec{R}_2|}}{\left|\vec{r}-\vec{R}_2\right|} + \frac{e^{-\kappa|\vec{r}-\vec{R}_3|}}{\left|\vec{r}-\vec{R}_3\right|} + e^{i\pi} \frac{e^{-\kappa|\vec{r}-\vec{R}_4|}}{\left|\vec{r}-\vec{R}_4\right|} \right), \tag{90}$$

and note that they can be represented as complex conjugated (this fact is predictable since the potential in Schrodinger equation is real) and realize the eigenvalues of T_4 operator $\lambda_3 = 1$, $\lambda_4 = e^{i\pi}$, accordingly.

[2]Here and afterwards we use notation that might be not the most compact, but the one that makes easy to see further generalization.

Case $N = 5$

Omitting details here we act in a similar fashion as we did before in cases $N = 3$ and $N = 4$.

As usually, we start with

$$\begin{pmatrix} (\beta-\kappa) & \chi_1 & \chi_2 & \chi_2 & \chi_1 \\ \chi_1 & (\beta-\kappa) & \chi_1 & \chi_2 & \chi_2 \\ \chi_2 & \chi_1 & (\beta-\kappa) & \chi_1 & \chi_2 \\ \chi_2 & \chi_2 & \chi_1 & (\beta-\kappa) & \chi_1 \\ \chi_1 & \chi_2 & \chi_2 & \chi_1 & (\beta-\kappa) \end{pmatrix} \begin{pmatrix} C_1 \\ C_2 \\ C_3 \\ C_4 \\ C_5 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} . \tag{91}$$

Since it becomes more difficult even to solve the characteristic equation, we make use of symbolic computation and employ both MAPLE and MATLAB software for performing different parts of calculations and analysis of relations between constants $C_1, \ldots, C_5$, resorting the task to an auxiliary problem of finding matrix eigenvectors. This reveals that we have two pairs of complex conjugated solutions

$$\psi_1(\vec{r}) = C_{01} \cdot \left(\frac{e^{-\kappa|\vec{r}-\vec{R}_1|}}{\left|\vec{r}-\vec{R}_1\right|} + e^{-i\frac{2\pi}{5}} \frac{e^{-\kappa|\vec{r}-\vec{R}_2|}}{\left|\vec{r}-\vec{R}_2\right|} + e^{-i\frac{4\pi}{5}} \frac{e^{-\kappa|\vec{r}-\vec{R}_3|}}{\left|\vec{r}-\vec{R}_3\right|} + e^{i\frac{4\pi}{5}} \frac{e^{-\kappa|\vec{r}-\vec{R}_4|}}{\left|\vec{r}-\vec{R}_4\right|} + e^{i\frac{2\pi}{5}} \frac{e^{-\kappa|\vec{r}-\vec{R}_5|}}{\left|\vec{r}-\vec{R}_5\right|} \right), \tag{92}$$

$$\psi_2(\vec{r}) = C_{02} \cdot \left(\frac{e^{-\kappa|\vec{r}-\vec{R}_1|}}{\left|\vec{r}-\vec{R}_1\right|} + e^{i\frac{2\pi}{5}} \frac{e^{-\kappa|\vec{r}-\vec{R}_2|}}{\left|\vec{r}-\vec{R}_2\right|} + e^{i\frac{4\pi}{5}} \frac{e^{-\kappa|\vec{r}-\vec{R}_3|}}{\left|\vec{r}-\vec{R}_3\right|} + e^{-i\frac{4\pi}{5}} \frac{e^{-\kappa|\vec{r}-\vec{R}_4|}}{\left|\vec{r}-\vec{R}_4\right|} + e^{-i\frac{2\pi}{5}} \frac{e^{-\kappa|\vec{r}-\vec{R}_5|}}{\left|\vec{r}-\vec{R}_5\right|} \right), \tag{93}$$

and

$$\psi_3(\vec{r}) = C_{03} \cdot \left(\frac{e^{-\kappa|\vec{r}-\vec{R}_1|}}{\left|\vec{r}-\vec{R}_1\right|} + e^{-i\frac{4\pi}{5}} \frac{e^{-\kappa|\vec{r}-\vec{R}_2|}}{\left|\vec{r}-\vec{R}_2\right|} + e^{i\frac{2\pi}{5}} \frac{e^{-\kappa|\vec{r}-\vec{R}_3|}}{\left|\vec{r}-\vec{R}_3\right|} + e^{-i\frac{2\pi}{5}} \frac{e^{-\kappa|\vec{r}-\vec{R}_4|}}{\left|\vec{r}-\vec{R}_4\right|} + e^{i\frac{4\pi}{5}} \frac{e^{-\kappa|\vec{r}-\vec{R}_5|}}{\left|\vec{r}-\vec{R}_5\right|} \right), \tag{94}$$

$$\psi_4(\vec{r}) = C_{04} \cdot \left(\frac{e^{-\kappa|\vec{r}-\vec{R}_1|}}{\left|\vec{r}-\vec{R}_1\right|} + e^{i\frac{4\pi}{5}} \frac{e^{-\kappa|\vec{r}-\vec{R}_2|}}{\left|\vec{r}-\vec{R}_2\right|} + e^{-i\frac{2\pi}{5}} \frac{e^{-\kappa|\vec{r}-\vec{R}_3|}}{\left|\vec{r}-\vec{R}_3\right|} + e^{i\frac{2\pi}{5}} \frac{e^{-\kappa|\vec{r}-\vec{R}_4|}}{\left|\vec{r}-\vec{R}_4\right|} + e^{-i\frac{4\pi}{5}} \frac{e^{-\kappa|\vec{r}-\vec{R}_5|}}{\left|\vec{r}-\vec{R}_5\right|} \right), \tag{95}$$

as well as the obvious solution

$$\psi_5(\vec{r}) = C_{05} \cdot \left(\frac{e^{-\kappa\left|\vec{r}-\vec{R}_1\right|}}{\left|\vec{r}-\vec{R}_1\right|} + \frac{e^{-\kappa\left|\vec{r}-\vec{R}_2\right|}}{\left|\vec{r}-\vec{R}_2\right|} + \frac{e^{-\kappa\left|\vec{r}-\vec{R}_3\right|}}{\left|\vec{r}-\vec{R}_3\right|} + \frac{e^{-\kappa\left|\vec{r}-\vec{R}_4\right|}}{\left|\vec{r}-\vec{R}_4\right|} + \frac{e^{-\kappa\left|\vec{r}-\vec{R}_5\right|}}{\left|\vec{r}-\vec{R}_5\right|} \right). \tag{96}$$

The states (92), (93) correspond to the energy to be found from

$$\beta - \kappa = \frac{1}{2}\left(\chi_1(\kappa) + \chi_2(\kappa)\right) + \frac{\sqrt{5}}{2}\left(\chi_2(\kappa) - \chi_1(\kappa)\right). \tag{97}$$

Existence of the solution is guaranteed if $\beta > \frac{1}{2}\left(\frac{1}{\Delta R_1} + \frac{1}{\Delta R_2}\right) + \frac{\sqrt{5}}{2}\left(\frac{1}{\Delta R_2} - \frac{1}{\Delta R_1}\right)$.

The other pair of states (94), (95) possess the energy solving the similar transcendent equation

$$\beta - \kappa = \frac{1}{2}\left(\chi_1(\kappa) + \chi_2(\kappa)\right) - \frac{\sqrt{5}}{2}\left(\chi_2(\kappa) - \chi_1(\kappa)\right). \tag{98}$$

Fulfillment of the condition $\beta > \frac{1}{2}\left(\frac{1}{\Delta R_1} + \frac{1}{\Delta R_2}\right) - \frac{\sqrt{5}}{2}\left(\frac{1}{\Delta R_2} - \frac{1}{\Delta R_1}\right)$ helps to ensure these states exist.

The last state (96) with energy bringing solution to

$$\beta - \kappa = 2\left(\chi_1(\kappa) + \chi_2(\kappa)\right) \tag{99}$$

surely exists if $\beta > 2\left(\frac{1}{\Delta R_1} + \frac{1}{\Delta R_2}\right)$.

From symmetrical point of view, in order for a solution to be an eigenfunction of rotation operator T_5 (and, therefore, possess required symmetry), constants C_1, …, C_5 defining the state must satisfy

$$\begin{aligned} C_1\left(-\lambda + e^{-i\frac{2\pi}{5}m}\right) + C_2\left(-\lambda e^{-i\frac{2\pi}{5}m} + e^{-i\frac{4\pi}{5}m}\right) + C_3\left(-\lambda e^{-i\frac{4\pi}{5}m} + e^{-i\frac{6\pi}{5}m}\right) \quad + \\ + \quad C_4\left(-\lambda e^{-i\frac{6\pi}{5}m} + e^{-i\frac{8\pi}{5}m}\right) + C_5\left(-\lambda e^{-i\frac{8\pi}{5}m} + 1\right) \quad = 0, \qquad |m| = 0, \ldots, 5. \end{aligned} \tag{100}$$

Among these equations only two couples of them are effectively used: $m = \pm 1$ for determining constants in the solution (92), (93) and $m = \pm 2$ in finding the states (94), (95).

Note that the states (92), (93), (94), (95) realize the operator T_5 eigenvalues $\lambda_1 = e^{i\frac{2\pi}{5}}$, $\lambda_2 = e^{i\frac{8\pi}{5}} = e^{-i\frac{2\pi}{5}}$, $\lambda_3 = e^{i\frac{4\pi}{5}}$, $\lambda_4 = e^{i\frac{6\pi}{5}} = e^{-i\frac{4\pi}{5}}$, respectively, while the obvious symmetrical solution (96) corresponds to the trivial eigenvalue $\lambda_5 = 1$.

5.2.5 General case solutions

Having obtained solutions for simple cases, we are now able to see general patterns.

Since with increasing of number of point-centers, the ZRP conditions matrix grows and becomes extremely difficult to tackle, we change our point of view and start solving the problem immediately using the symmetrical considerations. That is to say that, for example, in case of $N = 5$ instead of solving ZRP conditions system (91) it is better to begin with the set of equations (100), knowing that all eigenvalues of T_N operator performing rotation on $2\pi/N$ angle are realized and can be found without solving corresponding characteristic equation:

$$[T_N]^N = 1 \qquad \Rightarrow \qquad \lambda_j = e^{i\frac{2\pi}{N}j}, \qquad j = 0,\, \ldots,\, N-1.$$

Now we make use of previously obtained results regarding the fact that complex conjugated states with the same energy level realize complex conjugated eigenvalues λ of T_N and consider only eigenvalues $\lambda_j = e^{i\phi_j}$ with $0 \leq \phi_j \leq \pi$ where $\phi_j = \frac{2\pi}{N}j$, $j = 0,\, \ldots,\, [N/2]$.

Next, according to our observation based on cases $N = 3,\, 4,\, 5$, we state that the constants $C_1,\, \ldots,\, C_N$ in (78) determining the state with λ_j are obtained by successive multiplication by $e^{-i\phi_j}$ of some initial normalization constant value C_{0j} so that

$$\begin{aligned}\psi_j(\vec{r}) \quad &= \quad C_{0j} \cdot \left(\frac{e^{-\kappa\left|\vec{r}-\vec{R}_1\right|}}{\left|\vec{r}-\vec{R}_1\right|} + e^{-i\phi_j}\frac{e^{-\kappa\left|\vec{r}-\vec{R}_2\right|}}{\left|\vec{r}-\vec{R}_2\right|} + e^{-2i\phi_j}\frac{e^{-\kappa\left|\vec{r}-\vec{R}_3\right|}}{\left|\vec{r}-\vec{R}_3\right|} + \right. \\ &\left. + \ldots + e^{-i(N-2)\phi_j}\frac{e^{-\kappa\left|\vec{r}-\vec{R}_{N-1}\right|}}{\left|\vec{r}-\vec{R}_{N-1}\right|} + e^{-i(N-1)\phi_j}\frac{e^{-\kappa\left|\vec{r}-\vec{R}_N\right|}}{\left|\vec{r}-\vec{R}_N\right|} \right), \end{aligned} \tag{101}$$

and its complex conjugated

$$\begin{aligned}\bar{\psi}_j(\vec{r}) \quad &= \quad C_{0j} \cdot \left(\frac{e^{-\kappa\left|\vec{r}-\vec{R}_1\right|}}{\left|\vec{r}-\vec{R}_1\right|} + e^{i\phi_j}\frac{e^{-\kappa\left|\vec{r}-\vec{R}_2\right|}}{\left|\vec{r}-\vec{R}_2\right|} + e^{2i\phi_j}\frac{e^{-\kappa\left|\vec{r}-\vec{R}_3\right|}}{\left|\vec{r}-\vec{R}_3\right|} + \right. \\ &\left. + \ldots + e^{i(N-2)\phi_j}\frac{e^{-\kappa\left|\vec{r}-\vec{R}_{N-1}\right|}}{\left|\vec{r}-\vec{R}_{N-1}\right|} + e^{i(N-1)\phi_j}\frac{e^{-\kappa\left|\vec{r}-\vec{R}_N\right|}}{\left|\vec{r}-\vec{R}_N\right|} \right). \end{aligned} \tag{102}$$

As it was pointed out, the both states possess the same level of energy to be found by solving transcendental equation with respect to κ. This spectral condition can be obtained by substituting the set of constants for one of these states into the ZRP conditions. Namely, it results after the substitution $C_1, \ldots, C_N$ relations into one of the equation from the set (83).

Summarizing the obtained results, we generally write bounded states as

$$\psi^{(n)}(\vec{r}) = C_{0n} \sum_{j=1}^{N} e^{i(j-1)\phi_n} \frac{e^{-\kappa\left|\vec{r}-\vec{R}_j\right|}}{\left|\vec{r}-\vec{R}_j\right|}, \tag{103}$$

where $\phi_n = \frac{2\pi}{N}(n-1)$, $n = 1, \ldots, N$ with the corresponding energy $E^{(n)} = -\frac{\kappa^2\hbar^2}{2\mu}$ to be found from solution of

$$\beta - \kappa + \sum_{j=2}^{N} e^{i(j-1)\phi_n} \frac{e^{-\kappa\left|\vec{R}_j-\vec{R}_1\right|}}{\left|\vec{R}_j-\vec{R}_1\right|} = 0 \tag{104}$$

or, alternatively rewritten (taking into account that $\left|\vec{R}_j - \vec{R}_1\right| = R_0\sqrt{2\left(1-\cos\phi_j\right)} = 2R_0\sin\left(\phi_j/2\right)$),

$$\beta - \kappa + \frac{1}{2R_0} \sum_{j=2}^{N} e^{i(j-1)\phi_n} \frac{e^{-2\kappa R_0 \sin(\phi_j/2)}}{\sin\left(\phi_j/2\right)} = 0. \tag{105}$$

However this numeration ($n = 1, \ldots, N$) corresponds to complete set of energy values including repetitions, since we keep in mind that all energy levels except $n = 1$ and possibly (if N is even) $n = [N/2]+1$ are degenerated having multiplicity 2, as it was discussed above.

Additionally, for the sake of further simplification of the expressions (101), (102), we again consider separately cases of even and odd number of point-centers.

5.2.6 Even number of point-centers case solution

In order to express the spectral condition in a simple form, we take, for instance, the first equation from the set (81)

$$\kappa - \beta = \sum_{j=1}^{N/2-1} \chi_j(\kappa) \cdot \left(C_{j+1} + C_{N-j+1}\right) + \chi_{N/2}(\kappa) \cdot C_{N/2+1}.$$

If we consider the set of constants corresponding to $\lambda_1 = e^{i\frac{2\pi}{N}}$, i.e. $\phi_1 = \dfrac{2\pi}{N}$,

$$C_{j+1} = e^{-i\frac{2\pi}{N}j}, \qquad C_{N-j+1} = \bar{C}_{j+1} = e^{i\frac{2\pi}{N}j}, \qquad j = 1, \ldots, N/2-1,$$

$$C_{N/2+1} = e^{-i\pi},$$

then this spectral condition simplifies to

$$\kappa - \beta = 2 \sum_{j=1}^{N/2-1} \chi_j(\kappa) \cdot \cos\left(\frac{2\pi}{N} j\right) - \chi_{N/2}(\kappa).$$

The existence of solution for this transcendental equation is guaranteed by graphical means if

$$\beta > -2 \sum_{j=1}^{N/2-1} \frac{1}{\Delta R_j} \cdot \cos\left(\frac{2\pi}{N} j\right) + \frac{1}{\Delta R_{N/2}}.$$

In this case we are also able to write down the relevant solution in a point $\vec{r}$ is such that $y = 0$

$$\psi_1(\vec{r}) = \bar{\psi}_1(\vec{r}) = C_{01} \cdot \left(\frac{e^{-\kappa\left|\vec{r}-\vec{R}_1\right|}}{\left|\vec{r}-\vec{R}_1\right|} + 2 \sum_{j=1}^{N/2-1} \cos\left(\frac{2\pi}{N} j\right) \cdot \frac{e^{-\kappa\left|\vec{r}-\vec{R}_{j+1}\right|}}{\left|\vec{r}-\vec{R}_{j+1}\right|} - \frac{e^{-\kappa\left|\vec{r}-\vec{R}_{N/2+1}\right|}}{\left|\vec{r}-\vec{R}_{N/2+1}\right|} \right).$$

If we additionally set $x = 0$, we obviously have $\left|\vec{r}-\vec{R}_1\right| = \left|\vec{r}-\vec{R}_2\right| = \ldots = \left|\vec{r}-\vec{R}_N\right| \equiv \left|\vec{r}-\vec{R}\right| = \sqrt{z^2+R_0^2}$, so we are able to obtain solution along z-axis in even more simple form

$$\psi_1(\vec{r}) = \bar{\psi}_1(\vec{r}) = C_{01} \cdot \frac{e^{-\kappa\left|\vec{r}-\vec{R}\right|}}{\left|\vec{r}-\vec{R}\right|} \cdot \left(2 \sum_{j=1}^{N/2-1} \cos\left(\frac{2\pi}{N} j\right) \right) = C_{01} \cdot \left(\frac{\sin\left((N-1)\cdot \pi/N\right)}{\sin\left(\pi/N\right)} - 1 \right) \cdot \frac{e^{-\kappa\left|\vec{r}-\vec{R}\right|}}{\left|\vec{r}-\vec{R}\right|},$$

where we have used the Dirichlet summation formula

$$\sum_{j=-M}^{M} e^{ijx} = 1 + 2\sum_{j=1}^{M} \cos\left(jx\right) = \frac{\sin\left((2M+1)\cdot x/2\right)}{\sin\left(x/2\right)}$$

5.2.7 Odd number of point-centers case solution

In this case (82) yields the following spectral condition

$$\kappa - \beta = \sum_{j=1}^{(N-1)/2} \chi_j(\kappa) \cdot \left(C_{j+1} + C_{N-j+1}\right).$$

Again we consider the state with $\lambda_1 = e^{i\frac{2\pi}{N}}$, i.e.

$$C_{j+1} = e^{-i\frac{2\pi}{N} j}, \qquad C_{N-j+1} = \bar{C}_{j+1} = e^{i\frac{2\pi}{N} j}, \qquad j = 1, \ldots, (N-1)/2,$$

that results in simplification of the spectral condition

$$\kappa - \beta = 2 \sum_{j=1}^{(N-1)/2} \chi_j(\kappa) \cdot \cos\left(\frac{2\pi}{N} j\right)$$

and the corresponding state itself

$$\psi_1(\vec{r}) = \bar{\psi}_1(\vec{r}) = C_{01} \cdot \left(\frac{e^{-\kappa\left|\vec{r}-\vec{R}_1\right|}}{\left|\vec{r}-\vec{R}_1\right|} + 2 \sum_{j=1}^{(N-1)/2} \cos\left(\frac{2\pi}{N} j\right) \cdot \frac{e^{-\kappa\left|\vec{r}-\vec{R}_{j+1}\right|}}{\left|\vec{r}-\vec{R}_{j+1}\right|} \right)$$

when computed at $y = 0$.

Note that on the z-axis (i.e. additionally setting $x = 0$ in the last expression) we have

$$\psi_1(\vec{r}) = \bar{\psi}_1(\vec{r}) = C_{01} \cdot \frac{e^{-\kappa\left|\vec{r}-\vec{R}\right|}}{\left|\vec{r}-\vec{R}\right|} \cdot \left(1 + 2 \sum_{j=1}^{(N-1)/2} \cos\left(\frac{2\pi}{N} j\right) \right) = C_{01} \cdot \frac{\sin\left(N \cdot \pi/N\right)}{\sin\left(\pi/N\right)} \cdot \frac{e^{-\kappa\left|\vec{r}-\vec{R}\right|}}{\left|\vec{r}-\vec{R}\right|} = 0.$$

The sufficient condition for existence of this state is

$$\beta > -2 \sum_{j=1}^{(N-1)/2} \frac{1}{\Delta R_j} \cdot \cos\left(\frac{2\pi}{N} j\right).$$

5.2.8 Infinite number of point-centers

Now we consider a limiting case when number of point-centers is infinitely large. So we define their linear density ρ_0 and replace summation over point-center contributions with integral over the ring arc where they lie. In this case there is no crucial importance of direction of x-axis so the expressions obtained above, in fact, define radial dependence in xy-plane

$$\psi_1(\vec{r}) = \bar{\psi}_1(\vec{r}) = 2C_{01}\rho_0 \int_0^\pi \cos\phi \frac{e^{-\kappa\left|\vec{r}-\vec{R}\right|}}{\left|\vec{r}-\vec{R}\right|} R_0 d\phi,$$

where $\vec{R} = \left(R_0 \cos\phi,\, R_0 \sin\phi,\, 0\right)^T$.

Assume the observation point is deep inside the symmetrical structure, that is $r \ll R_0$ where $r = \left|\left(\vec{r}\cdot\vec{e}_x,\, \vec{r}\cdot\vec{e}_y,\, 0\right)^T\right|$.

Then $e^{-\kappa\left|\vec{r}-\vec{R}\right|} \approx e^{-\kappa R_0}$ and using generating function technique for Legendre polynomials we can perform expansion

$$\frac{1}{\left|\vec{r}-\vec{R}\right|} = \sum_{l=0}^{\infty} \frac{r^l}{R_0^{l+1}} \cdot P_l(\cos\phi).$$

Therefore

$$\psi_1(\vec{r}) = 2C_{01}\rho_0 e^{-\kappa R_0} \sum_{l=0}^{\infty} \left(\frac{r}{R_0}\right)^l \int\limits_0^{\pi} P_l(\cos\phi)\cos\phi \cdot d\phi.$$

Due to orthogonality of Legendre polynomials, among all terms in summation only the one with $l = 1$ remains.

Thus, finally we arrive at

$$\psi_1(\vec{r}) = C_{01}\frac{\pi\rho_0}{R_0}e^{-\kappa R_0}r,$$

when $z = 0$.

5.3 Scattering on N point-centers - continuous spectrum problem

Now we consider the scattering of plane wave incident axially on the N-center potential plane symmetrical structure under question.

We write the solution to the Schrodinger equation as

$$\psi(\vec{r}) = A_0 e^{ikz} + \sum_{j=1}^{N} C_j \frac{e^{ik\left|\vec{r}-\vec{R}_j\right|}}{\left|\vec{r}-\vec{R}_j\right|}, \tag{106}$$

where $k = \sqrt{\dfrac{2\mu E}{\hbar^2}}$ and A_0 is an amplitude of the incident plane wave.

As before (and using previously described notation), at each center (scatterer) the solution must satisfy the ZRP condition (79)

$$\left.\frac{\partial \log\left(\left|\vec{r}-\vec{R}_j\right|\cdot\psi(\vec{r})\right)}{\partial\left|\vec{r}-\vec{R}_j\right|}\right|_{\left|\vec{r}-\vec{R}_j\right|=0} = \frac{1}{C_j}\left(A_0 + \ldots + C_{j-1}\cdot\frac{e^{ik\Delta R_1}}{\Delta R_1} + C_j\cdot ik + C_{j+1}\cdot\frac{e^{ik\Delta R_1}}{\Delta R_1} + \ldots\right) = -\beta.$$

This results in the set of linear equations

$$\begin{pmatrix} \beta+ik & \chi_1 & \ldots & \chi_2 & \chi_1 \\ \chi_1 & \beta+ik & \ldots & \chi_3 & \chi_2 \\ \ldots & \ldots & \ddots & \ldots & \ldots \\ \chi_2 & \chi_3 & \ldots & \beta+ik & \chi_1 \\ \chi_1 & \chi_2 & \ldots & \chi_1 & \beta+ik \end{pmatrix} \begin{pmatrix} C_1 \\ C_2 \\ \vdots \\ C_{N-1} \\ C_N \end{pmatrix} = -A_0 \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \\ 1 \end{pmatrix},$$

where we now denote $\chi_j = \dfrac{e^{ik\Delta R_j}}{\Delta R_j}$, $j = 1, \ldots, [N/2]$ employing the floor function $[x]$.

This set obviously has the solution corresponding to trivial symmetry of the system

$$C_1 = \ldots = C_N \equiv C_{0N}.$$

For odd number of scatterers we have

$$C_{0N} = -\frac{A_0}{\beta + ik + 2\sum_{j=1}^{(N-1)/2} \chi_j}. \tag{107}$$

For even number of scatterers:

$$C_{0N} = -\frac{A_0}{\beta + ik + 2\sum_{j=1}^{N/2-1} \chi_j + \chi_{N/2}}. \tag{108}$$

These results can be unified in the following manner

$$C_{0N} = -\frac{A_0}{\beta + ik + 2\sum_{j=1}^{(N+g_N)/2-1} \chi_j + g_{N-1} \cdot \chi_{N/2}}, \tag{109}$$

where $g_N = \frac{N/2-[N/2]}{N/2-[(N-1)/2]}$ is an indicator of parity of number of scatterers.

When calculating C_{0N}, it might be useful to recall (80) and rewrite the sum as

$$\sum_{j=1}^{(N+g_N)/2-1} \chi_j = \frac{1}{2R_0} \sum_{j=1}^{(N+g_N)/2-1} \frac{\exp\left(2ikR_0 \sin\left(\phi_{j+1}/2\right)\right)}{\sin\left(\phi_{j+1}/2\right)} = \frac{1}{2R_0} \sum_{j=1}^{(N+g_N)/2-1} \frac{\exp\left(2ikR_0 \sin\left(\pi j/N\right)\right)}{\sin\left(\pi j/N\right)}.$$

Having obtained that, and taking into account expansion $\left|\vec{r} - \vec{R}_j\right| \underset{r\to\infty}{\approx} r - \frac{\vec{r}}{r} \cdot \vec{R}_j$, we can present the solution (106) as

$$\psi(\vec{r}) = A_0 \left(e^{ikz} + f(\theta, \phi) \frac{e^{ikr}}{r} \right), \tag{110}$$

where the scattering amplitude at long distances in direction $\vec{n} = \vec{r}/r = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)^T$ is given by

$$f(\theta, \phi) = C_{0N}/A_0 \sum_{j=1}^{N} e^{-ik\vec{n}\cdot\vec{R}_j} = C_{0N}/A_0 \sum_{j=1}^{N} \exp\left\{-ikR_0 \sin\theta \cos\left(\phi - \phi_j\right)\right\}. \tag{111}$$

From here differential cross-section can be determined

$$\frac{d\sigma}{d\Omega} = |f(\theta,\, \phi)|^2\,, \tag{112}$$

as well as the integral scattering cross-section

$$\sigma = \int_0^{2\pi} \int_0^{\pi} |f(\theta,\, \phi)|^2 \sin\theta d\theta d\phi. \tag{113}$$

For a large number of scatterers one can pass to the limit $N \to \infty$ by introducing linear density of point scatterers ρ_0 on a ring. Then the expression (109) can be rewritten as

$$C_0 = -A_0 \left(\beta + ik + \frac{\rho_0}{R_0} \int_0^{\pi} \frac{\exp\left\{2ikR_0 \sin\left(\phi'/2\right)\right\}}{\sin\left(\phi'/2\right)} d\phi' \right)^{-1} \tag{114}$$

and further substituted into the modified expression (111)

$$f(\theta,\, \phi) = \rho_0 C_0 / A_0 \int_0^{2\pi} \exp\left\{-ikR_0 \sin\theta \cos\left(\phi - \phi'\right)\right\} d\phi'. \tag{115}$$

Afterwards, the expressions (112), (113) can be employed to calculate scattering cross-sections.

Moreover, in case of elastic scattering one might employ the optical theorem stating that the total scattering cross-section can be expressed as

$$\sigma = \frac{4\pi}{k} \mathrm{Im}\left[f(0,\, \phi)\right]. \tag{116}$$

Therefore,

$$\sigma \quad = \quad \frac{4\pi N}{k} \mathrm{Im}\left[C_{0N}/A_0\right] = \frac{4\pi N}{k} \frac{k + P}{(k+P)^2 + (\beta + Q)^2}, \tag{117}$$

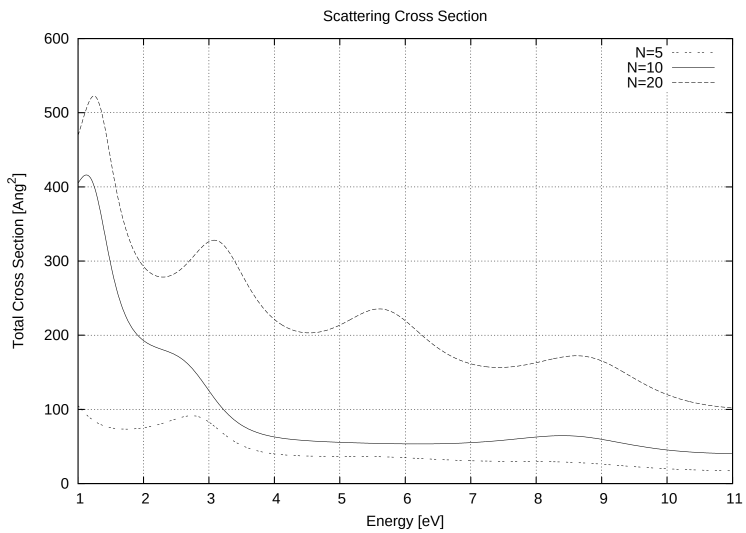
where we denote

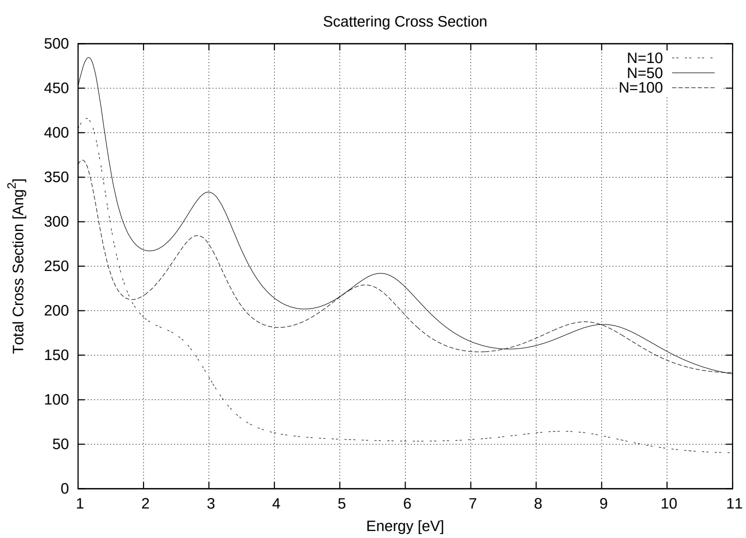
$$P \equiv \frac{1}{R_0} \left[\sum_{j=1}^{(N+g_N)/2-1} \frac{\sin\left(2kR_0 \sin\left(\pi j/N\right)\right)}{\sin\left(\pi j/N\right)} + \frac{g_{N-1}}{2} \cdot \sin\left(2kR_0\right) \right],$$

$$Q \equiv \frac{1}{R_0} \left[\sum_{j=1}^{(N+g_N)/2-1} \frac{\cos\left(2kR_0 \sin\left(\pi j/N\right)\right)}{\sin\left(\pi j/N\right)} + \frac{g_{N-1}}{2} \cdot \cos\left(2kR_0\right) \right].$$

On the figures below we present total scattering cross sections dependence on energy $E = (\hbar k)^2 / (2\mu)$ obtained for different number of scatterers N as given by (117). However, this can serve only as a demonstration of the model rather than a source of valuable results.

Within the model, we observe reasonable decay of total scattering cross section as energy grows whilst change of this dependence with respect to number of scatterers is not uniform (see the second figure).



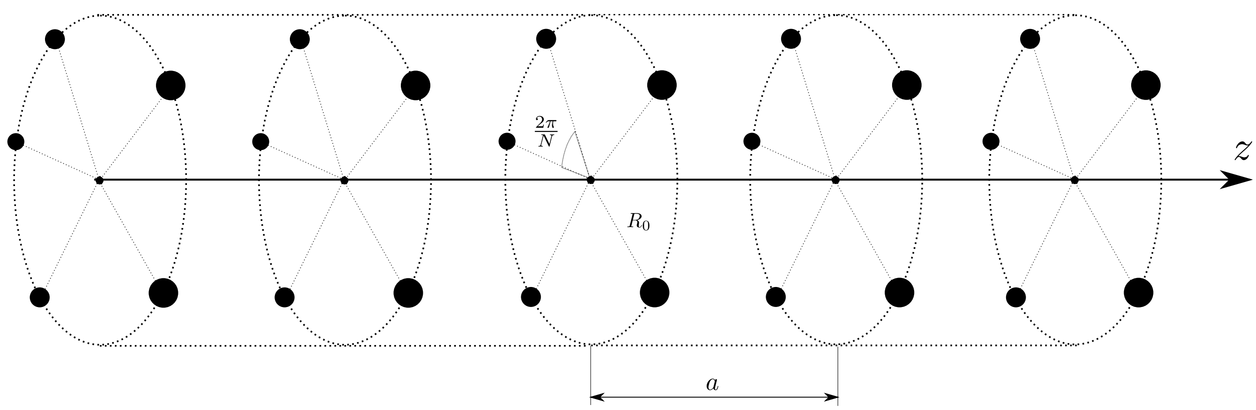


When plotting, the following values of parameters were used: $\beta = 0.5\,[\mathrm{Ang}^{-1}]$, $R_0 = 10.0\,[\mathrm{Ang}]$.

6 Cylindrical tube made of point-centers

More realistic structure is the long tube with cross-sections periodically filled with point-centers forming symmetrical structures.

We focus on bounded state solutions for an infinitely long tube made of plane N-fold symmetrical structures considered before by means of unidirectional translation.



General form of the solution is

$$\psi(\vec{r}) = \sum_{m=-\infty}^{+\infty} \sum_{j=1}^{N} C_{mj} \frac{e^{-\kappa \left|\vec{r}-\vec{R}_{mj}\right|}}{\left|\vec{r}-\vec{R}_{mj}\right|}, \tag{118}$$

where the first sum (index m) is carried over cross-section planes with centers while the second sum (index j) is over centers in a plane numerated, as before, from 1 to N, and positions of centers are

$$\vec{R}_{mj} = \vec{R}_j + m\vec{a}, \tag{119}$$

with $\vec{a} = a\vec{e}_z$ being a shift vector corresponding to distances between the nearest cross-section planes with centers and $\vec{R}_j$ denoting positions of centers in a plane orthogonal to z-axis.

Coefficients C_{mj} are to be determined from ZRP conditions as before

$$\left. \frac{\partial \log \left(\left|\vec{r}-\vec{R}_{mj}\right| \cdot \psi(\vec{r}) \right)}{\partial \left|\vec{r}-\vec{R}_{mj}\right|} \right|_{\left|\vec{r}-\vec{R}_{mj}\right|=0} = -\beta, \tag{120}$$

however because of symmetry this task is simplified.

Owing to the translational periodicity of the potential, the Bloch theorem states that

$$\psi(\vec{r}) \equiv \psi_k(\vec{r}) = U(\vec{r}) e^{ik\vec{e}_z \cdot \vec{r}},$$

where $U(\vec{r} + n\vec{a}) = U(\vec{r})$ for any integer n.

Therefore,

$$\psi(\vec{r} + n\vec{a}) = e^{ikna}\psi(\vec{r}).$$

On the other hand, from (118) and (119) it follows

$$\psi(\vec{r} + n\vec{a}) = \sum_{m=-\infty}^{+\infty} \sum_{j=1}^{N} C_{mj} \frac{e^{-\kappa\left|\vec{r} - \vec{R}_{(m-n)j}\right|}}{\left|\vec{r} - \vec{R}_{(m-n)j}\right|} = \sum_{m=-\infty}^{+\infty} \sum_{j=1}^{N} C_{(m+n)j} \frac{e^{-\kappa\left|\vec{r} - \vec{R}_{mj}\right|}}{\left|\vec{r} - \vec{R}_{mj}\right|}.$$

Hence, we conclude that

$$C_{(m+n)j} = e^{ikna} C_{mj},$$

and, given an origin plane, we can write

$$C_{mj} = e^{ikma} C_{0j} \equiv e^{ikma} C_j.$$

Now, the solution (118) reduces to

$$\psi(\vec{r}) = \sum_{m=-\infty}^{+\infty} e^{ikma} \sum_{j=1}^{N} C_j \frac{e^{-\kappa\left|\vec{r} - \vec{R}_{mj}\right|}}{\left|\vec{r} - \vec{R}_{mj}\right|}. \tag{121}$$

It is straightforward to see that combined operations of rotation and translation form an Abelian group.

Indeed, consider group element $g_{jm} = (A_j,\, a_m)$ where

$$A_j = \begin{pmatrix} \cos\phi_j & \sin\phi_j & 0 \\ -\sin\phi_j & \cos\phi_j & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

is rotation operator acting on $\vec{r} = (x,\, y,\, z)^T$ with $\phi_j = \frac{2\pi}{N} j$, $j = 0,\, \dots,\, N-1$ and

$$a_m = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & T_m \end{pmatrix},$$

with T_m denoting scalar translation operator acting such that $T_m z = z + ma$, $m \in \mathbb{Z}$.

In this form it is easily visible that

$$g_{jm} \cdot g_{j'm'} = \begin{pmatrix} \cos\phi_j \cos\phi_{j'} - \sin\phi_j \sin\phi_{j'} & \cos\phi_j \sin\phi_{j'} + \sin\phi_j \cos\phi_{j'} & 0 \\ -\sin\phi_j \cos\phi_{j'} - \cos\phi_j \sin\phi_{j'} & -\sin\phi_j \sin\phi_{j'} + \cos\phi_j \cos\phi_{j'} & 0 \\ 0 & 0 & T_m T_{m'} \end{pmatrix} = g_{j'm'} \cdot g_{jm},$$

since obviously $T_m T_{m'} = T_{m'} T_m$.

So we can state that translational symmetry does not interfere N-fold rotational invariance of the problem, and, hence, consider the coefficients C_j to be known from the previously solved problem. Namely, they are

$$C_j^{(n)} = e^{i(j-1)\phi_n} C_0, \qquad \text{where} \qquad \phi_n = \frac{2\pi}{N}(n-1), \qquad n = 1,\, \dots,\, N. \tag{122}$$

Therefore, we obtain the complete set of bounded states solutions

$$\psi_k^{(n)}(\vec{r}) = C_0 \sum_{m=-\infty}^{+\infty} e^{ikma} \sum_{j=1}^{N} e^{i(j-1)\phi_n} \frac{e^{-\kappa\left|\vec{r} - \vec{R}_{mj}\right|}}{\left|\vec{r} - \vec{R}_{mj}\right|}.$$

The corresponding energy $E_k^{(n)}$ can be found from (120), but before performing substitution of (122) let us first develop that condition in detail.

For the sake of brevity, we will make use of notation $\chi_{mj}^{m'j'} \equiv \dfrac{e^{-\kappa\left|\vec{R}_{m'j'} - \vec{R}_{mj}\right|}}{\left|\vec{R}_{m'j'} - \vec{R}_{mj}\right|} = \dfrac{e^{-\kappa\left|\vec{R}_{j'} - \vec{R}_j + (m'-m)\vec{a}\right|}}{\left|\vec{R}_{j'} - \vec{R}_j + (m'-m)\vec{a}\right|}$ to write the ZRP condition at the center $\vec{R}_{m'j'}$

$$\frac{1}{C_{j'} e^{ikm'a}} \left[\sum_{m=-\infty}^{+\infty} e^{ikma} \sum_{\substack{j=1 \\ j\neq j'}}^{N} C_j \chi_{mj}^{m'j'} + \sum_{\substack{m=-\infty \\ m\neq m'}}^{+\infty} e^{ikma} C_{j'} \chi_{mj'}^{m'j'} - e^{ikm'a} C_{j'} \kappa \right] = -\beta.$$

That is equivalent to

$$\sum_{m=-\infty}^{+\infty} e^{ikma} \sum_{\substack{j=1 \\ j\neq j'}}^{N} C_j \chi_{mj}^{m'j'} + \sum_{\substack{m=-\infty \\ m\neq m'}}^{+\infty} e^{ikma} C_{j'} \chi_{mj'}^{m'j'} + (\beta-\kappa)\, e^{ikm'a} C_{j'} = 0.$$

By multiplying the both sides of the last equation by $e^{-ikm'a}$ and changing summation index $m-m' \to m$, we have

$$\sum_{\substack{j=1 \\ j\neq j'}}^{N} C_j \sum_{m=-\infty}^{+\infty} e^{ikma} \frac{e^{-\kappa\left|\vec{R}_{j'}-\vec{R}_j+m\vec{a}\right|}}{\left|\vec{R}_{j'}-\vec{R}_j+m\vec{a}\right|} + C_{j'} \left(\beta-\kappa+\sum_{\substack{m=-\infty \\ m\neq m'}}^{+\infty} e^{ikma} \frac{e^{-\kappa|m|a}}{|m|\,a}\right) = 0. \tag{123}$$

The series in the last term

$$\sum_{\substack{m=-\infty \\ m\neq m'}}^{+\infty} e^{ikma} \frac{e^{-\kappa|m|a}}{|m|\,a} = \sum_{m=1}^{+\infty} \frac{e^{-(\kappa-ik)ma}}{ma} + \sum_{m=1}^{+\infty} \frac{e^{-(\kappa+ik)ma}}{ma} \tag{124}$$

can be summed up as it follows.

Denoting $\lambda_{\pm} = e^{-(\kappa\pm ik)a}$, we notice that $|\lambda_{\pm}| < 1$. This allows us to write

$$\sum_{m=1}^{+\infty} \frac{\lambda^m}{m} = \sum_{m=1}^{+\infty} \int_0^{\lambda} \tilde{\lambda}^{m-1} d\tilde{\lambda} = \int_0^{\lambda} \underbrace{\sum_{m=0}^{+\infty} \tilde{\lambda}^m}_{=\frac{1}{1-\tilde{\lambda}}} d\tilde{\lambda} = -\log\left(1-\lambda\right).$$

Therefore, (124) becomes

$$\begin{aligned} \sum_{\substack{m=-\infty \\ m\neq m'}}^{+\infty} e^{ikma} \frac{e^{-\kappa|m|a}}{|m|\,a} &= -\frac{1}{a}\log\left[\left(1-\lambda_-\right)\left(1-\lambda_+\right)\right] = -\frac{1}{a}\log\left[\left(1-e^{-\kappa a}\cos ka\right)^2 + e^{-2\kappa a}\sin^2 ka\right] = \\ &= -\frac{1}{a}\log\left[2e^{-\kappa a}\left(\cosh\kappa a-\cos ka\right)\right] = -\frac{1}{a}\log\left[2\left(\cosh\kappa a-\cos ka\right)\right] + \kappa. \end{aligned}$$

Plugging this into (123) yields

$$\sum_{\substack{j=1 \\ j\neq j'}}^{N} C_j \sum_{m=-\infty}^{+\infty} e^{ikma} \frac{e^{-\kappa\left|\vec{R}_{j'}-\vec{R}_j+m\vec{a}\right|}}{\left|\vec{R}_{j'}-\vec{R}_j+m\vec{a}\right|} + C_{j'} \left(\beta-\frac{1}{a}\log\left[2\left(\cosh\kappa a-\cos ka\right)\right]\right) = 0.$$

Additionally, without a loss of generality, we can set $j'=1$ and feed into here (122) to find a state energy $E_k^{(n)}$

$$\sum_{j=2}^{N} e^{i(j-1)\phi_n} \sum_{m=-\infty}^{+\infty} e^{ikma} \frac{e^{-\kappa\left|\vec{R}_1-\vec{R}_j+m\vec{a}\right|}}{\left|\vec{R}_1-\vec{R}_j+m\vec{a}\right|} + \left(\beta - \frac{1}{a}\log\left[2\left(\cosh\kappa a-\cos ka\right)\right]\right) = 0, \qquad (125)$$

that can be alternatively rewritten as

$$\sum_{j=2}^{N} e^{i(j-1)\phi_n} \sum_{m=-\infty}^{+\infty} e^{ikma} \frac{e^{-\kappa\sqrt{2R_0^2(1-\cos\phi_j)+m^2a^2}}}{\sqrt{2R_0^2\left(1-\cos\phi_j\right)+m^2a^2}} + \left(\beta - \frac{1}{a}\log\left[2\left(\cosh\kappa a-\cos ka\right)\right]\right) = 0, \qquad (126)$$

or

$$\sum_{j=2}^{N} e^{i(j-1)\phi_n} \sum_{m=-\infty}^{+\infty} e^{ikma} \frac{e^{-\kappa\sqrt{4R_0^2\sin^2(\phi_j/2)+m^2a^2}}}{\sqrt{4R_0^2\sin^2\left(\phi_j/2\right)+m^2a^2}} + \left(\beta - \frac{1}{a}\log\left[2\left(\cosh\kappa a-\cos ka\right)\right]\right) = 0. \qquad (127)$$

Solving the transcendental equation with respect to $\kappa = \sqrt{-\left(2\mu/\hbar^2\right) E_k^{(n)}}$, one can find dependence $E_k^{(n)}(k)$ for the n-th bounded state.

7 Conclusions

Within the framework of the present work, after giving an instructive overview of the Darboux transformation and zero-range potential (and beyond) methods, quantum ring and quantum wire problems were considered.

In the Sections 5 and 6 we obtained the main results of the work. Namely, for arbitrary N-fold discrete symmetry, there were obtained formulas for bounded states for the case of quantum ring and quantum wire, respectively. In some particular case, transition (by means of limit passing to the case $N \to \infty$) to continuous symmetry was discussed as well. Energy corresponding to the given states can be calculated numerically by solving the transcendent equations that were obtained. In case of the quantum ring, solution to scattering problem can also be further simplified depending on the range of interest in terms of the energy of the incident wave: either the stationary phase method can be used to estimate the resulting integral in high-energy range or simply small-argument direct series expansion for the case of large wavelengths in comparison with the size of the ring. Eventually computed scattering cross-section might be used in estimates of electrical conductivity of solids that contain these quantum rings structures as inclusions or surface additions.

The improvement of obtained solutions can be further done by application of the Moutard transformation (see, for instance, [9, 21]), that is a two-dimensional counterpart of the Darboux transformation. Alternatively, a passage to limit of small distances between centers (as rotational symmetry order increases $N \to \infty$ whereas distance between the nearest cross-section planes with point-centers decreases $a \to 0$) can be performed and, hence, one-dimensional model of a cylindrical quantum tube can be obtained. In this case, a dressing of the solution by means of the Darboux transformation can be done, however the result of the problem itself is interesting to be compared with the one that can be obtained by solving a model with initially chosen cylindrical zero-range potential [20].

Given spectral equations in the form of transcendent equations to be solved numerically, density of states can also be obtained and further used for estimating such material properties as conductance [2, 19].

Appendix

Here we list some of the programs for symbolic computation software that were produced in order to obtain results for the case of $N = 5$ point-center potential and, hence, to help making further generalization possible.

The given codes are:

- **C5_prematlab.mws** (pre-processing in MAPLE Classical Worksheet)
- **C5_matrix.m** (main calculation in MATLAB)
- **C5_postmatlab1.mw** (post-processing first pair of solutions in MAPLE)
- **C5_postmatlab2.mw** (post-processing second pair of solutions in MAPLE)

```
> ##### C5_prematlab.mws #####
>
>
>
> assume(h1 > 0, h2 > 0) :
> with(LinearAlgebra):
```

```
> B0:=<<0, h1, h2, h2, h1>|<h1, 0, h1, h2, h2>|<h2, h1, 0, h1,
h2>|<h2, h2, h1, 0, h1>|<h1, h2, h2, h1, 0>>;
```

$$B0 := \begin{bmatrix} 0 & h1\sim & h2\sim & h2\sim & h1\sim \\ h1\sim & 0 & h1\sim & h2\sim & h2\sim \\ h2\sim & h1\sim & 0 & h1\sim & h2\sim \\ h2\sim & h2\sim & h1\sim & 0 & h1\sim \\ h1\sim & h2\sim & h2\sim & h1\sim & 0 \end{bmatrix} \quad (1)$$

```
> (Evalues, EVecs):=Eigenvectors(B0):
> Evalues;
```

$$\begin{bmatrix} -\frac{1}{2}\,h1\sim - \frac{1}{2}\,h2\sim - \frac{1}{2}\sqrt{5}\,h1\sim + \frac{1}{2}\sqrt{5}\,h2\sim \\ -\frac{1}{2}\,h1\sim - \frac{1}{2}\,h2\sim - \frac{1}{2}\sqrt{5}\,h1\sim + \frac{1}{2}\sqrt{5}\,h2\sim \\ -\frac{1}{2}\,h1\sim - \frac{1}{2}\,h2\sim + \frac{1}{2}\sqrt{5}\,h1\sim - \frac{1}{2}\sqrt{5}\,h2\sim \\ -\frac{1}{2}\,h1\sim - \frac{1}{2}\,h2\sim + \frac{1}{2}\sqrt{5}\,h1\sim - \frac{1}{2}\sqrt{5}\,h2\sim \\ 2\,h1\sim + 2\,h2\sim \end{bmatrix} \quad (2)$$

```
> EVecs:=simplify(EVecs);
```

$$EVecs := \Big[\Big[\big(2\,\big(h1\sim^3\sqrt{5} - 4\,h1\sim^2\,h2\sim\sqrt{5} + 4\,h1\sim\,h2\sim^2\sqrt{5} - h2\sim^3\sqrt{5} + 3\,h1\sim^3 \quad (3)$$

$$- 8\,h2\sim\,h1\sim^2 + h2\sim^3\big)\big) \Big/ \big(\big(h1\sim + h2\sim + \sqrt{5}\,h1\sim - \sqrt{5}\,h2\sim\big)\,\big(-2\,h1\sim^2 + 3\,h1\sim\sqrt{5}\,h2\sim$$

$$- h1\sim\,h2\sim + h2\sim^2 - \sqrt{5}\,h2\sim^2\big)\big), -\big(4\,\big(-2\,h1\sim^5 - 5\,h2\sim\,h1\sim^4 + h1\sim^4\sqrt{5}\,h2\sim$$

$$+ 21\,h2\sim^2\,h1\sim^3 + h1\sim^3\sqrt{5}\,h2\sim^2 + 22\,h2\sim^3\,h1\sim^2 - 12\,h1\sim^2\,h2\sim^3\sqrt{5} - 19\,h1\sim\,h2\sim^4$$

$$+ 7\,h1\sim\,h2\sim^4\sqrt{5} + 3\,h2\sim^5 - h2\sim^5\sqrt{5}\big)\big) \Big/ \big(\big(h1\sim + h2\sim + \sqrt{5}\,h1\sim - \sqrt{5}\,h2\sim\big)\,\big(-h1\sim^2$$

$$+ h1\sim^2 \sqrt{5} + 3\, h1\sim \sqrt{5}\, h2\sim - h1\sim h2\sim + 2\, h2\sim^2\big) \big(-2\, h1\sim^2 + 3\, h1\sim \sqrt{5}\, h2\sim - h1\sim h2\sim$$

$$+ h2\sim^2 - \sqrt{5}\, h2\sim^2\big)\big)\big), -\big(2\,\big(h1\sim^3 \sqrt{5} - 4\, h1\sim^2 h2\sim \sqrt{5} + 4\, h1\sim h2\sim^2 \sqrt{5}$$

$$- h2\sim^3 \sqrt{5} - 3\, h1\sim^3 + 8\, h2\sim h1\sim^2 - h2\sim^3\big)\big) \Big/ \big(\big(-h1\sim - h2\sim + \sqrt{5}\, h1\sim$$

$$- \sqrt{5}\, h2\sim\big) \big(2\, h1\sim^2 + 3\, h1\sim \sqrt{5}\, h2\sim + h1\sim h2\sim - \sqrt{5}\, h2\sim^2 - h2\sim^2\big)\big), -\big(4\,\big(2\, h1\sim^5$$

$$+ h1\sim^4 \sqrt{5}\, h2\sim + 5\, h2\sim h1\sim^4 - 21\, h2\sim^2 h1\sim^3 + h1\sim^3 \sqrt{5}\, h2\sim^2 - 22\, h2\sim^3 h1\sim^2$$

$$- 12\, h1\sim^2 h2\sim^3 \sqrt{5} + 19\, h1\sim h2\sim^4 + 7\, h1\sim h2\sim^4 \sqrt{5} - 3\, h2\sim^5 - h2\sim^5 \sqrt{5}\big)\big) \Big/ \big(\big(-h1\sim$$

$$- h2\sim + \sqrt{5}\, h1\sim - \sqrt{5}\, h2\sim\big) \big(h1\sim^2 + h1\sim^2 \sqrt{5} + 3\, h1\sim \sqrt{5}\, h2\sim + h1\sim h2\sim$$

$$- 2\, h2\sim^2\big) \big(2\, h1\sim^2 + 3\, h1\sim \sqrt{5}\, h2\sim + h1\sim h2\sim - \sqrt{5}\, h2\sim^2 - h2\sim^2\big)\big), 1\big],$$

$$\Bigg[-\frac{h1\sim^2 \sqrt{5} - h1\sim \sqrt{5}\, h2\sim + h1\sim^2 - 7\, h1\sim h2\sim + 2\, h2\sim^2}{-2\, h1\sim^2 + 3\, h1\sim \sqrt{5}\, h2\sim - h1\sim h2\sim + h2\sim^2 - \sqrt{5}\, h2\sim^2}, \big(4\,\big(-h1\sim^4 - 4\, h2\sim h1\sim^3$$

$$+ h1\sim^3 \sqrt{5}\, h2\sim + 4\, h1\sim^2 \sqrt{5}\, h2\sim^2 + 2\, h2\sim^2 h1\sim^2 - h1\sim h2\sim^3 \sqrt{5} + 4\, h2\sim^3 h1\sim - h2\sim^4\big)\big)$$

$$\Big/ \big(\big(-h1\sim^2 + h1\sim^2 \sqrt{5} + 3\, h1\sim \sqrt{5}\, h2\sim - h1\sim h2\sim + 2\, h2\sim^2\big) \big(-2\, h1\sim^2 + 3\, h1\sim \sqrt{5}\, h2\sim$$

$$- h1\sim h2\sim + h2\sim^2 - \sqrt{5}\, h2\sim^2\big)\big),$$

$$-\frac{h1\sim^2 \sqrt{5} - h1\sim \sqrt{5}\, h2\sim - h1\sim^2 + 7\, h1\sim h2\sim - 2\, h2\sim^2}{2\, h1\sim^2 + 3\, h1\sim \sqrt{5}\, h2\sim + h1\sim h2\sim - \sqrt{5}\, h2\sim^2 - h2\sim^2}, -\big(4\,\big(h1\sim^4 + 4\, h2\sim h1\sim^3$$

$$+ h1\sim^3 \sqrt{5}\, h2\sim + 4\, h1\sim^2 \sqrt{5}\, h2\sim^2 - 2\, h2\sim^2 h1\sim^2 - h1\sim h2\sim^3 \sqrt{5} - 4\, h2\sim^3 h1\sim + h2\sim^4\big)\big)$$

$$\Big/ \big(\big(h1\sim^2 + h1\sim^2 \sqrt{5} + 3\, h1\sim \sqrt{5}\, h2\sim + h1\sim h2\sim - 2\, h2\sim^2\big) \big(2\, h1\sim^2 + 3\, h1\sim \sqrt{5}\, h2\sim$$

$$+ h1\sim h2\sim - \sqrt{5}\, h2\sim^2 - h2\sim^2\big)\big), 1\big],$$

$$\Bigg[-1, -\frac{2\, h1\sim^2 + h1\sim \sqrt{5}\, h2\sim + 7\, h1\sim h2\sim + \sqrt{5}\, h2\sim^2 + h2\sim^2}{-h1\sim^2 + h1\sim^2 \sqrt{5} + 3\, h1\sim \sqrt{5}\, h2\sim - h1\sim h2\sim + 2\, h2\sim^2}, -1,$$

$$-\frac{-2\, h1\sim^2 + h1\sim \sqrt{5}\, h2\sim - 7\, h1\sim h2\sim - h2\sim^2 + \sqrt{5}\, h2\sim^2}{h1\sim^2 + h1\sim^2 \sqrt{5} + 3\, h1\sim \sqrt{5}\, h2\sim + h1\sim h2\sim - 2\, h2\sim^2}, 1 \Bigg],$$

$$\big[0, 1, 0, 1, 1\big],$$

$$\big[1, 0, 1, 0, 1\big]\big]$$

```
> simplify(EVecs(1..-1,2));
```

$$[[-(4(-2h1\sim^5-5h2\sim h1\sim^4+h1\sim^4\sqrt{5}\,h2\sim+21h2\sim^2h1\sim^3+h1\sim^3\sqrt{5}\,h2\sim^2+22h2\sim^3h1\sim^2-12h1\sim^2h2\sim^3\sqrt{5}-19h1\sim h2\sim^4+7h1\sim h2\sim^4\sqrt{5}+3h2\sim^5-h2\sim^5\sqrt{5}))\Big/((h1\sim+h2\sim+\sqrt{5}\,h1\sim-\sqrt{5}\,h2\sim)(-h1\sim^2+h1\sim^2\sqrt{5}+3h1\sim\sqrt{5}\,h2\sim-h1\sim h2\sim+2h2\sim^2)(-2h1\sim^2+3h1\sim\sqrt{5}\,h2\sim-h1\sim h2\sim+h2\sim^2-\sqrt{5}\,h2\sim^2))],$$

$$[(4(-h1\sim^4-4h2\sim h1\sim^3+h1\sim^3\sqrt{5}\,h2\sim+4h1\sim^2\sqrt{5}\,h2\sim^2+2h2\sim^2h1\sim^2-h1\sim h2\sim^3\sqrt{5}+4h2\sim^3h1\sim-h2\sim^4))\Big/((-h1\sim^2+h1\sim^2\sqrt{5}+3h1\sim\sqrt{5}\,h2\sim-h1\sim h2\sim+2h2\sim^2)(-2h1\sim^2+3h1\sim\sqrt{5}\,h2\sim-h1\sim h2\sim+h2\sim^2-\sqrt{5}\,h2\sim^2))],$$

$$\left[-\frac{2h1\sim^2+h1\sim\sqrt{5}\,h2\sim+7h1\sim h2\sim+\sqrt{5}\,h2\sim^2+h2\sim^2}{-h1\sim^2+h1\sim^2\sqrt{5}+3h1\sim\sqrt{5}\,h2\sim-h1\sim h2\sim+2h2\sim^2}\right],$$

$$\left[1\right],$$

$$\left[0\right]] \qquad (4)$$

```
> B1:=<<a, h1, h2, h2, h1>|<h1, a, h1, h2, h2>|<h2, h1, a, h1,
  h2>|<h2, h2, h1, a, h1>|<h1, h2, h2, h1, a>>;
```

$$B1:=\begin{bmatrix} a & h1\sim & h2\sim & h2\sim & h1\sim \\ h1\sim & a & h1\sim & h2\sim & h2\sim \\ h2\sim & h1\sim & a & h1\sim & h2\sim \\ h2\sim & h2\sim & h1\sim & a & h1\sim \\ h1\sim & h2\sim & h2\sim & h1\sim & a \end{bmatrix} \qquad (5)$$

```
> B2:=eval(B1, a=-Evalues(1));
```

$$B2:=\left[\left[\frac{1}{2}\,h1\sim+\frac{1}{2}\,h2\sim+\frac{1}{2}\sqrt{5}\,h1\sim-\frac{1}{2}\sqrt{5}\,h2\sim, h1\sim, h2\sim, h2\sim, h1\sim\right],\right.$$

$$\left[h1\sim, \frac{1}{2}\,h1\sim+\frac{1}{2}\,h2\sim+\frac{1}{2}\sqrt{5}\,h1\sim-\frac{1}{2}\sqrt{5}\,h2\sim, h1\sim, h2\sim, h2\sim\right],$$

$$\left[h2\sim, h1\sim, \frac{1}{2}\,h1\sim+\frac{1}{2}\,h2\sim+\frac{1}{2}\sqrt{5}\,h1\sim-\frac{1}{2}\sqrt{5}\,h2\sim, h1\sim, h2\sim\right],$$

$$\left[h2\sim, h2\sim, h1\sim, \frac{1}{2}\,h1\sim+\frac{1}{2}\,h2\sim+\frac{1}{2}\sqrt{5}\,h1\sim-\frac{1}{2}\sqrt{5}\,h2\sim, h1\sim\right],$$

$$\left.\left[h1\sim, h2\sim, h2\sim, h1\sim, \frac{1}{2}\,h1\sim+\frac{1}{2}\,h2\sim+\frac{1}{2}\sqrt{5}\,h1\sim-\frac{1}{2}\sqrt{5}\,h2\sim\right]\right] \qquad (6)$$

```
> sols:=LinearSolve(B2, <0, 0, 0, 0, 0>, free='C');
```

$$sols := \begin{bmatrix} C_1 \\ -C_5 - \frac{1}{2} C_1 \sqrt{5} - \frac{1}{2} C_1 \\ \frac{1}{2} \left(\sqrt{5}+1\right) \left(C_5 + C_1\right) \\ -\frac{1}{2} C_5 - C_1 - \frac{1}{2} C_5 \sqrt{5} \\ C_5 \end{bmatrix} \quad (7)$$

```
> B2:=eval(B1, a=-Evalues(3));
```

$$B2 := \left[\left[\frac{1}{2} h1\sim + \frac{1}{2} h2\sim - \frac{1}{2}\sqrt{5}\, h1\sim + \frac{1}{2}\sqrt{5}\, h2\sim, h1\sim, h2\sim, h2\sim, h1\sim\right],\right.$$
$$\left[h1\sim, \frac{1}{2} h1\sim + \frac{1}{2} h2\sim - \frac{1}{2}\sqrt{5}\, h1\sim + \frac{1}{2}\sqrt{5}\, h2\sim, h1\sim, h2\sim, h2\sim\right],$$
$$\left[h2\sim, h1\sim, \frac{1}{2} h1\sim + \frac{1}{2} h2\sim - \frac{1}{2}\sqrt{5}\, h1\sim + \frac{1}{2}\sqrt{5}\, h2\sim, h1\sim, h2\sim\right],$$
$$\left[h2\sim, h2\sim, h1\sim, \frac{1}{2} h1\sim + \frac{1}{2} h2\sim - \frac{1}{2}\sqrt{5}\, h1\sim + \frac{1}{2}\sqrt{5}\, h2\sim, h1\sim\right],$$
$$\left.\left[h1\sim, h2\sim, h2\sim, h1\sim, \frac{1}{2} h1\sim + \frac{1}{2} h2\sim - \frac{1}{2}\sqrt{5}\, h1\sim + \frac{1}{2}\sqrt{5}\, h2\sim\right]\right] \quad (8)$$

```
> sols:=LinearSolve(B2, <0, 0, 0, 0, 0>, free='C');
```

$$sols := \begin{bmatrix} C_1 \\ -C_5 - \frac{1}{2} C_1 + \frac{1}{2} C_1 \sqrt{5} \\ -\frac{1}{2} \left(-1+\sqrt{5}\right) \left(C_5 + C_1\right) \\ -\frac{1}{2} C_5 - C_1 + \frac{1}{2} C_5 \sqrt{5} \\ C_5 \end{bmatrix} \quad (9)$$

```
> B2:=eval(B1, a=-Evalues(5));
```

$$B2 := \begin{bmatrix} -2\,h1\sim - 2\,h2\sim & h1\sim & h2\sim & h2\sim & h1\sim \\ h1\sim & -2\,h1\sim - 2\,h2\sim & h1\sim & h2\sim & h2\sim \\ h2\sim & h1\sim & -2\,h1\sim - 2\,h2\sim & h1\sim & h2\sim \\ h2\sim & h2\sim & h1\sim & -2\,h1\sim - 2\,h2\sim & h1\sim \\ h1\sim & h2\sim & h2\sim & h1\sim & -2\,h1\sim - 2\,h2\sim \end{bmatrix} \quad (10)$$

```
> sols:=LinearSolve(B2, <0, 0, 0, 0, 0>, free='C');
```

$$sols := \begin{bmatrix} C_5 \\ C_5 \\ C_5 \\ C_5 \\ C_5 \end{bmatrix} \quad \textbf{(11)}$$

C5_matrix.m


```
clear;
syms m lmb a h1 h2 C1 C2 C3 C4 C5;
B=[a h1 h2 h2 h1; h1 a h1 h2 h2; h2 h1 a h1 h2; h2 h2 h1 a h1; h1 h2 h2 h1 a];
B0=subs(B, a, 0);

B0_vals=eig(B0);
-B0_vals

[B0_vec,B0_val]=eig(B0);

B0_vec=simplify(B0_vec)

gen_eq='C1*(-lmb+exp(-i*2*pi/5*m))+C2*(-lmb*exp(-i*2*pi/5*m)+exp(-i*4*pi/5*m))+C3*(-lmb*exp(-i*4*pi/5*m)+exp(-
i*6*pi/5*m))+C4*(-lmb*exp(-i*6*pi/5*m)+exp(-i*8*pi/5*m))+C5*(-lmb*exp(-i*8*pi/5*m)+1)'


% First H-eigenvalue pair

C2_gen='-(sqrt(5)+1)/2*C1-C5';
C3_gen='(sqrt(5)+1)/2*(C1+C5)';
C4_gen='-C1-(sqrt(5)+1)/2*C5';

eq1=subs(gen_eq, {'C2', 'C3', 'C4'}, {C2_gen, C3_gen, C4_gen})

gen_matr=[subs(eq1, {'C1', 'C5', 'm'}, {1, 0, -2}) subs(eq1, {'C1', 'C5', 'm'}, {0, 1, -2});
    subs(eq1, {'C1', 'C5', 'm'}, {1, 0, 2}) subs(eq1, {'C1', 'C5', 'm'}, {0, 1, 2})]

det_matr=simplify(det(gen_matr))
lmbs1=simplify(solve(det_matr, 'lmb'))
eval(abs(lmbs1(1)))
eval(real(lmbs1(1)))
eval(atan(imag(lmbs1(1))/real(lmbs1(1)))/(2*pi/5))
eval(abs(lmbs1(2)))
eval(real(lmbs1(2)))
eval(atan(imag(lmbs1(2))/real(lmbs1(2)))/(2*pi/5))

C5_sol1=simplify(solve(subs(eq1, {'C1', 'lmb', 'm'}, {1, lmbs1(1), 2}), 'C5'))
eval(abs(C5_sol1))
eval(real(C5_sol1))
eval(imag(C5_sol1))
% eval(atan(imag(C5_sol1)/real(C5_sol1))/(2*pi/5))

C2_sol1=subs(C2_gen, {'C1', 'C5'}, {1, C5_sol1})
eval(abs(C2_sol1))
eval(real(C2_sol1))
% eval(atan(imag(C2_sol1)/real(C2_sol1))/(2*pi/5))
C3_sol1=subs(C3_gen, {'C1', 'C5'}, {1, C5_sol1})
eval(abs(C3_sol1))
% eval(atan(imag(C3_sol1)/real(C3_sol1))/(2*pi/5))
eval(real(C3_sol1))
C4_sol1=subs(C4_gen, {'C1', 'C5'}, {1, C5_sol1})
eval(abs(C4_sol1))
% eval(atan(imag(C4_sol1)/real(C4_sol1))/(2*pi/5))
eval(real(C4_sol1))

C5_sol2=simplify(solve(subs(eq1, {'C1', 'lmb', 'm'}, {1, lmbs1(2), -2}), 'C5'))
eval(abs(C5_sol2))
eval(real(C5_sol2))
eval(imag(C5_sol2))
% eval(atan(imag(C5_sol2)/real(C5_sol2))/(2*pi/5))

C2_sol2=subs(C2_gen, {'C1', 'C5'}, {1, C5_sol2})
eval(abs(C2_sol2))
eval(real(C2_sol2))
% eval(atan(imag(C2_sol2)/real(C2_sol2))/(2*pi/5))
C3_sol2=subs(C3_gen, {'C1', 'C5'}, {1, C5_sol2})
eval(abs(C3_sol2))
% eval(atan(imag(C3_sol2)/real(C3_sol2))/(2*pi/5))
eval(real(C3_sol2))
C4_sol2=subs(C4_gen, {'C1', 'C5'}, {1, C5_sol2})
eval(abs(C4_sol2))
% eval(atan(imag(C4_sol2)/real(C4_sol2))/(2*pi/5))
```

```
eval(real(C4_sol2))


% Second H-eigenvalue pair

C2_gen='(sqrt(5)-1)/2*C1-C5';
C3_gen='-(sqrt(5)-1)/2*(C1+C5)';
C4_gen='-C1+(sqrt(5)-1)/2*C5';

eq2=subs(gen_eq, {'C2', 'C3', 'C4'}, {C2_gen, C3_gen, C4_gen})

gen_matr=[subs(eq2, {'C1', 'C5', 'm'}, {1, 0, -1}) subs(eq2, {'C1', 'C5', 'm'}, {0, 1, -1});
    subs(eq2, {'C1', 'C5', 'm'}, {1, 0, 1}) subs(eq2, {'C1', 'C5', 'm'}, {0, 1, 1})]

det_matr=simplify(det(gen_matr))
lmbs2=simplify(solve(det_matr, 'lmb'))
eval(abs(lmbs2(1)))
eval(real(lmbs2(1)))
eval(atan(imag(lmbs2(1))/real(lmbs2(1)))/(2*pi/5))
eval(abs(lmbs2(2)))
eval(real(lmbs2(2)))
eval(atan(imag(lmbs2(2))/real(lmbs2(2)))/(2*pi/5))

C5_sol1=simplify(solve(subs(eq2, {'C1', 'lmb', 'm'}, {1, lmbs2(1), 1}), 'C5'))
eval(abs(C5_sol1))
eval(real(C5_sol1))
eval(imag(C5_sol1))
% eval(atan(imag(C5_sol1)/real(C5_sol1))/(2*pi/5))

C2_sol1=subs(C2_gen, {'C1', 'C5'}, {1, C5_sol1})
eval(abs(C2_sol1))
eval(real(C2_sol1))
% eval(atan(imag(C2_sol1)/real(C2_sol1))/(2*pi/5))
C3_sol1=subs(C3_gen, {'C1', 'C5'}, {1, C5_sol1})
eval(abs(C3_sol1))
% eval(atan(imag(C3_sol1)/real(C3_sol1))/(2*pi/5))
eval(real(C3_sol1))
C4_sol1=subs(C4_gen, {'C1', 'C5'}, {1, C5_sol1})
eval(abs(C4_sol1))
% eval(atan(imag(C4_sol1)/real(C4_sol1))/(2*pi/5))
eval(real(C4_sol1))

C5_sol2=simplify(solve(subs(eq2, {'C1', 'lmb', 'm'}, {1, lmbs2(2), -1}), 'C5'))
eval(abs(C5_sol2))
eval(real(C5_sol2))
eval(imag(C5_sol2))
% eval(atan(imag(C5_sol2)/real(C5_sol2))/(2*pi/5))

C2_sol2=subs(C2_gen, {'C1', 'C5'}, {1, C5_sol2})
eval(abs(C2_sol2))
eval(real(C2_sol2))
% eval(atan(imag(C2_sol2)/real(C2_sol2))/(2*pi/5))
C3_sol2=subs(C3_gen, {'C1', 'C5'}, {1, C5_sol2})
eval(abs(C3_sol2))
% eval(atan(imag(C3_sol2)/real(C3_sol2))/(2*pi/5))
eval(real(C3_sol2))
C4_sol2=subs(C4_gen, {'C1', 'C5'}, {1, C5_sol2})
eval(abs(C4_sol2))
% eval(atan(imag(C4_sol2)/real(C4_sol2))/(2*pi/5))
eval(real(C4_sol2))
```

```
> ##### C5_postmatlab1.mw #####
>
>
>
> with(MTM) :
> C5_sol1 := (16*3125^(1/2) - 9300*5^(1/2) + 1050*(-2*5^(1/2) - 10)^(1/2)
    + 2100*(2*5^(1/2) - 10)^(1/2) + 1250*(-10*5^(1/2) - 50)^(1/2) - 50
    *(10*5^(1/2) - 50)^(1/2) - 25*(150 - 50*5^(1/2))^(1/2) - 525*(50*5^(1
    /2) + 150)^(1/2) + 30*(-50*5^(1/2) - 250)^(1/2) + 310*(50*5^(1/2)
    - 250)^(1/2) + 20*(750 - 250*5^(1/2))^(1/2) - 100*(250*5^(1/2) + 750)
    ^(1/2) + 50*(-200*5^(1/2) - 1000)^(1/2) + 170*(-250*5^(1/2) - 1250)
    ^(1/2) + 20*(250*5^(1/2) - 1250)^(1/2) + 5*(3750 - 1250*5^(1/2))^(1/2)
    + 5*(1250*5^(1/2) + 3750)^(1/2) + 20*(-1000*5^(1/2) - 5000)^(1/2) - 5
    *(1000*5^(1/2) - 5000)^(1/2) - 5*(5000*5^(1/2) - 25000)^(1/2) - 15500)
    /(5000*5^(1/2) - 10*(150 - 50*5^(1/2))^(1/2) + 410*(50*5^(1/2) + 150)
    ^(1/2) - 20*(750 - 250*5^(1/2))^(1/2) + 180*(250*5^(1/2) + 750)^(1/2)
    - 2*(3750 - 1250*5^(1/2))^(1/2) + 2*(1250*5^(1/2) + 3750)^(1/2)
    + 33800) :
>
> C5_sol1 := simplify(C5_sol1);
```

$C5_{sol1} :=$ **(1)**

$$\frac{1}{80}\,\frac{1}{5+\sqrt{5}}\left(-120\sqrt{5}+17\,\mathrm{I}\sqrt{2\sqrt{5}+10}+34\,\mathrm{I}\sqrt{-2\sqrt{5}+10}+23\,\mathrm{I}\sqrt{5}\,\sqrt{2\sqrt{5}+10}-200\right)$$

\> $\mathrm{Re}(C5_{sol1});$

$$\frac{1}{80}\,\frac{-120\sqrt{5}-200}{5+\sqrt{5}} \qquad \textbf{(2)}$$

\> $\mathrm{Im}(C5_{sol1});$

$$\frac{1}{80}\,\frac{17\sqrt{2\sqrt{5}+10}+34\sqrt{-2\sqrt{5}+10}+23\sqrt{5}\,\sqrt{2\sqrt{5}+10}}{5+\sqrt{5}} \qquad \textbf{(3)}$$

\> $\mathit{evalf}(\mathrm{abs}(C5_{sol1}));$

$$0.9999999999 \qquad \textbf{(4)}$$

\> $\mathit{evalf}\left(\dfrac{\mathrm{atan}\left(\mathit{evalf}\left(\dfrac{\mathrm{Im}(C5_{sol1})}{\mathrm{Re}(C5_{sol1})}\right)\right)}{\dfrac{2\cdot\mathrm{Pi}}{5}}\right);$

$$-0.4999999999 \qquad \textbf{(5)}$$

```
> C2_sol1 := - 5^(1/2)/2 - (16*3125^(1/2) - 9300*5^(1/2) + 1050*(-2*5^(1/2)
    - 10)^(1/2) + 2100*(2*5^(1/2) - 10)^(1/2) + 1250*(-10*5^(1/2) - 50)^(1
    /2) - 50*(10*5^(1/2) - 50)^(1/2) - 25*(150 - 50*5^(1/2))^(1/2) - 525*(50
    *5^(1/2) + 150)^(1/2) + 30*(-50*5^(1/2) - 250)^(1/2) + 310*(50*5^(1
```

```
/2) - 250)^(1/2) + 20*(750 - 250*5^(1/2))^(1/2) - 100*(250*5^(1/2)
+ 750)^(1/2) + 50*(- 200*5^(1/2) - 1000)^(1/2) + 170*(- 250*5^(1/2)
- 1250)^(1/2) + 20*(250*5^(1/2) - 1250)^(1/2) + 5*(3750 - 1250*5^(1/2))
^(1/2) + 5*(1250*5^(1/2) + 3750)^(1/2) + 20*(- 1000*5^(1/2) - 5000)^(1
/2) - 5*(1000*5^(1/2) - 5000)^(1/2) - 5*(5000*5^(1/2) - 25000)^(1/2)
- 15500)/(5000*5^(1/2) - 10*(150 - 50*5^(1/2))^(1/2) + 410*(50*5^(1
/2) + 150)^(1/2) - 20*(750 - 250*5^(1/2))^(1/2) + 180*(250*5^(1/2)
+ 750)^(1/2) - 2*(3750 - 1250*5^(1/2))^(1/2) + 2*(1250*5^(1/2) + 3750)
^(1/2) + 33800) - 1/2:
```

> $C2_{sol1} := simplify(C2_{sol1});$

$$C2_{sol1} := -\frac{1}{80}\,\frac{1}{5+\sqrt{5}}\left(200+120\sqrt{5}+17\,I\sqrt{2\sqrt{5}+10}+34\,I\sqrt{-2\sqrt{5}+10}+23\,I\sqrt{5}\,\sqrt{2\sqrt{5}+10}\right) \tag{6}$$

> $\mathrm{Re}(C2_{sol1});$

$$-\frac{1}{80}\,\frac{200+120\sqrt{5}}{5+\sqrt{5}} \tag{7}$$

> $\mathrm{Im}(C2_{sol1});$

$$-\frac{1}{80}\,\frac{17\sqrt{2\sqrt{5}+10}+34\sqrt{-2\sqrt{5}+10}+23\sqrt{5}\,\sqrt{2\sqrt{5}+10}}{5+\sqrt{5}} \tag{8}$$

> $evalf(\mathrm{abs}(C2_{sol1}));$

$$0.9999999999 \tag{9}$$

> $evalf\left(\frac{\mathrm{atan}\left(evalf\left(\frac{\mathrm{Im}(C2_{sol1})}{\mathrm{Re}(C2_{sol1})}\right)\right)}{\frac{2\cdot \mathrm{Pi}}{5}}\right);$

$$0.4999999999 \tag{10}$$

> $C3_{sol1}$:= (5^(1/2)/2 + 1/2)*((16*3125^(1/2) - 9300*5^(1/2) + 1050*(- 2*5^(1

```
/2) - 10)^(1/2) + 2100*(2*5^(1/2) - 10)^(1/2) + 1250*(- 10*5^(1/2)
- 50)^(1/2) - 50*(10*5^(1/2) - 50)^(1/2) - 25*(150 - 50*5^(1/2))^(1/2)
- 525*(50*5^(1/2) + 150)^(1/2) + 30*(- 50*5^(1/2) - 250)^(1/2) + 310
*(50*5^(1/2) - 250)^(1/2) + 20*(750 - 250*5^(1/2))^(1/2) - 100*(250*5
^(1/2) + 750)^(1/2) + 50*(- 200*5^(1/2) - 1000)^(1/2) + 170*(- 250*5
^(1/2) - 1250)^(1/2) + 20*(250*5^(1/2) - 1250)^(1/2) + 5*(3750 - 1250*5
^(1/2))^(1/2) + 5*(1250*5^(1/2) + 3750)^(1/2) + 20*(- 1000*5^(1/2)
- 5000)^(1/2) - 5*(1000*5^(1/2) - 5000)^(1/2) - 5*(5000*5^(1/2) - 25000)
^(1/2) - 15500)/(5000*5^(1/2) - 10*(150 - 50*5^(1/2))^(1/2) + 410*(50
*5^(1/2) + 150)^(1/2) - 20*(750 - 250*5^(1/2))^(1/2) + 180*(250*5^(1
/2) + 750)^(1/2) - 2*(3750 - 1250*5^(1/2))^(1/2) + 2*(1250*5^(1/2)
+ 3750)^(1/2) + 33800) + 1):
```

> $C3_{sol1} := simplify(C3_{sol1});$

$$C3_{sol1} := \frac{1}{160}\,\frac{1}{5+\sqrt{5}}\left(\left(\sqrt{5}+1\right)\left(-40\sqrt{5}+17\,\mathrm{I}\sqrt{2\sqrt{5}+10}+34\,\mathrm{I}\sqrt{-2\sqrt{5}+10}+23\,\mathrm{I}\sqrt{5}\,\sqrt{2\sqrt{5}+10}+200\right)\right) \quad \textbf{(11)}$$

> Re($C3_{sol1}$);

$$\frac{\left(\frac{1}{160}\sqrt{5}+\frac{1}{160}\right)\left(-40\sqrt{5}+200\right)}{5+\sqrt{5}} \quad \textbf{(12)}$$

> Im($C3_{sol1}$);

$$\frac{\left(\frac{1}{160}\sqrt{5}+\frac{1}{160}\right)\left(17\sqrt{2\sqrt{5}+10}+34\sqrt{-2\sqrt{5}+10}+23\sqrt{5}\,\sqrt{2\sqrt{5}+10}\right)}{5+\sqrt{5}} \quad \textbf{(13)}$$

> *evalf*(abs($C3_{sol1}$));

$$1.000000000 \quad \textbf{(14)}$$

> $evalf\left(\frac{\operatorname{atan}\left(evalf\left(\frac{\operatorname{Im}(C3_{sol1})}{\operatorname{Re}(C3_{sol1})}\right)\right)}{\frac{2\cdot \mathrm{Pi}}{5}}\right)$;

$$0.9999999992 \quad \textbf{(15)}$$

> $C4_{sol1}$:= - ((5^(1/2)/2 + 1/2) * (16 * 3125^(1/2) - 9300 * 5^(1/2) + 1050 * (- 2 * 5^(1/2) - 10)^(1/2) + 2100 * (2 * 5^(1/2) - 10)^(1/2) + 1250 * (- 10 * 5^(1/2) - 50)^(1/2) - 50 * (10 * 5^(1/2) - 50)^(1/2) - 25 * (150 - 50 * 5^(1/2))^(1/2) - 525 * (50 * 5^(1/2) + 150)^(1/2) + 30 * (- 50 * 5^(1/2) - 250)^(1/2) + 310 * (50 * 5^(1/2) - 250)^(1/2) + 20 * (750 - 250 * 5^(1/2))^(1/2) - 100 * (250 * 5^(1/2) + 750)^(1/2) + 50 * (- 200 * 5^(1/2) - 1000)^(1/2) + 170 * (- 250 * 5^(1/2) - 1250)^(1/2) + 20 * (250 * 5^(1/2) - 1250)^(1/2) + 5 * (3750 - 1250 * 5^(1/2))^(1/2) + 5 * (1250 * 5^(1/2) + 3750)^(1/2) + 20 * (- 1000 * 5^(1/2) - 5000)^(1/2) - 5 * (1000 * 5^(1/2) - 5000)^(1/2) - 5 * (5000 * 5^(1/2) - 25000)^(1/2) - 15500)) / (5000 * 5^(1/2) - 10 * (150 - 50 * 5^(1/2))^(1/2) + 410 * (50 * 5^(1/2) + 150)^(1/2) - 20 * (750 - 250 * 5^(1/2))^(1/2) + 180 * (250 * 5^(1/2) + 750)^(1/2) - 2 * (3750 - 1250 * 5^(1/2))^(1/2) + 2 * (1250 * 5^(1/2) + 3750)^(1/2) + 33800) - 1 :

> $C4_{sol1}$:= *simplify*($C4_{sol1}$);

$$C4_{sol1} := -\frac{1}{80}\,\frac{1}{5+\sqrt{5}}\left(20\,\mathrm{I}\sqrt{5}\,\sqrt{2\sqrt{5}+10}+17\,\mathrm{I}\sqrt{5}\,\sqrt{-2\sqrt{5}+10}+66\,\mathrm{I}\sqrt{2\sqrt{5}+10}-80\sqrt{5}+17\,\mathrm{I}\sqrt{-2\sqrt{5}+10}\right) \quad \textbf{(16)}$$

> Re($C4_{sol1}$);

$$\frac{\sqrt{5}}{5+\sqrt{5}} \quad \textbf{(17)}$$

> Im($C4_{sol1}$);

$$-\frac{1}{80}\,\frac{1}{5+\sqrt{5}}\left(20\sqrt{5}\,\sqrt{2\sqrt{5}+10}+17\sqrt{-2\sqrt{5}+10}\,\sqrt{5}+66\sqrt{2\sqrt{5}+10}+17\sqrt{-2\sqrt{5}+10}\right) \quad \textbf{(18)}$$

> $evalf(\mathrm{abs}(C4_{sol1}));$

$$0.9999999999 \quad \textbf{(19)}$$

> $evalf\left(\frac{\mathrm{atan}\left(evalf\left(\frac{\mathrm{Im}(C4_{sol1})}{\mathrm{Re}(C4_{sol1})}\right)\right)}{\frac{2\cdot \mathrm{Pi}}{5}}\right);$

$$-0.9999999992 \quad \textbf{(20)}$$

>

> $C5_{sol2}$:= -(9300 * 5^(1/2) - 16 * 3125^(1/2) + 1050 * (- 2 * 5^(1/2) - 10)^(1/2) + 2100 * (2 * 5^(1/2) - 10)^(1/2) + 1250 * (- 10 * 5^(1/2) - 50)^(1/2) - 50 * (10 * 5^(1/2) - 50)^(1/2) + 25 * (150 - 50 * 5^(1/2))^(1/2) + 525 * (50 * 5^(1/2) + 150)^(1/2) + 30 * (- 50 * 5^(1/2) - 250)^(1/2) + 310 * (50 * 5^(1/2) - 250)^(1/2) - 20 * (750 - 250 * 5^(1/2))^(1/2) + 100 * (250 * 5^(1/2) + 750)^(1/2) + 50 * (- 200 * 5^(1/2) - 1000)^(1/2) + 170 * (- 250 * 5^(1/2) - 1250)^(1/2) + 20 * (250 * 5^(1/2) - 1250)^(1/2) - 5 * (3750 - 1250 * 5^(1/2))^(1/2) - 5 * (1250 * 5^(1/2) + 3750)^(1/2) + 20 * (- 1000 * 5^(1/2) - 5000)^(1/2) - 5 * (1000 * 5^(1/2) - 5000)^(1/2) - 5 * (5000 * 5^(1/2) - 25000)^(1/2) + 15500) / (5000 * 5^(1/2) - 10 * (150 - 50 * 5^(1/2))^(1/2) + 410 * (50 * 5^(1/2) + 150)^(1/2) - 20 * (750 - 250 * 5^(1/2))^(1/2) + 180 * (250 * 5^(1/2) + 750)^(1/2) - 2 * (3750 - 1250 * 5^(1/2))^(1/2) + 2 * (1250 * 5^(1/2) + 3750)^(1/2) + 33800) :

> $C5_{sol2} := simplify(C5_{sol2});$

$$C5_{sol2} := -\frac{1}{80}\,\frac{1}{5+\sqrt{5}}\left(200+120\sqrt{5}+17\,\mathrm{I}\sqrt{2\sqrt{5}+10}+34\,\mathrm{I}\sqrt{-2\sqrt{5}+10}+23\,\mathrm{I}\sqrt{5}\,\sqrt{2\sqrt{5}+10}\right) \quad \textbf{(21)}$$

> $\mathrm{Re}(C5_{sol2});$

$$-\frac{1}{80}\,\frac{200+120\sqrt{5}}{5+\sqrt{5}} \quad \textbf{(22)}$$

> $\mathrm{Im}(C5_{sol2});$

$$-\frac{1}{80}\,\frac{17\sqrt{2\sqrt{5}+10}+34\sqrt{-2\sqrt{5}+10}+23\sqrt{5}\,\sqrt{2\sqrt{5}+10}}{5+\sqrt{5}} \quad \textbf{(23)}$$

> $evalf(\mathrm{abs}(C5_{sol2}));$

$$0.9999999999 \quad \textbf{(24)}$$

$$> evalf\left(\frac{\mathrm{atan}\left(evalf\left(\frac{\mathrm{Im}(C5_{sol2})}{\mathrm{Re}(C5_{sol2})}\right)\right)}{\frac{2\cdot \mathrm{Pi}}{5}}\right);$$

$$0.4999999999 \tag{25}$$

```
> C2_sol2 := (9300*5^(1/2) - 16*3125^(1/2) + 1050*(- 2*5^(1/2) - 10)^(1/2)
    + 2100*(2*5^(1/2) - 10)^(1/2) + 1250*(- 10*5^(1/2) - 50)^(1/2) - 50
    *(10*5^(1/2) - 50)^(1/2) + 25*(150 - 50*5^(1/2))^(1/2) + 525*(50*5^(1
    /2) + 150)^(1/2) + 30*(- 50*5^(1/2) - 250)^(1/2) + 310*(50*5^(1/2)
    - 250)^(1/2) - 20*(750 - 250*5^(1/2))^(1/2) + 100*(250*5^(1/2) + 750)
    ^(1/2) + 50*(- 200*5^(1/2) - 1000)^(1/2) + 170*(- 250*5^(1/2) - 1250)
    ^(1/2) + 20*(250*5^(1/2) - 1250)^(1/2) - 5*(3750 - 1250*5^(1/2))^(1/2)
    - 5*(1250*5^(1/2) + 3750)^(1/2) + 20*(- 1000*5^(1/2) - 5000)^(1/2) - 5
    *(1000*5^(1/2) - 5000)^(1/2) - 5*(5000*5^(1/2) - 25000)^(1/2) + 15500)
    /(5000*5^(1/2) - 10*(150 - 50*5^(1/2))^(1/2) + 410*(50*5^(1/2) + 150)
    ^(1/2) - 20*(750 - 250*5^(1/2))^(1/2) + 180*(250*5^(1/2) + 750)^(1/2)
    - 2*(3750 - 1250*5^(1/2))^(1/2) + 2*(1250*5^(1/2) + 3750)^(1/2)
    + 33800) - 5^(1/2)/2 - 1/2 :
```

$$> C2_{sol2} := simplify(C2_{sol2});$$

$$C2_{sol2} := \frac{1}{80}\,\frac{1}{5+\sqrt{5}}\left(-120\sqrt{5}+17\,\mathrm{I}\sqrt{2\sqrt{5}+10}+34\,\mathrm{I}\sqrt{-2\sqrt{5}+10}+23\,\mathrm{I}\sqrt{5}\,\sqrt{2\sqrt{5}+10}-200\right) \tag{26}$$

$$> \mathrm{Re}(C2_{sol2});$$

$$\frac{1}{80}\,\frac{-120\sqrt{5}-200}{5+\sqrt{5}} \tag{27}$$

$$> \mathrm{Im}(C2_{sol2});$$

$$\frac{1}{80}\,\frac{17\sqrt{2\sqrt{5}+10}+34\sqrt{-2\sqrt{5}+10}+23\sqrt{5}\,\sqrt{2\sqrt{5}+10}}{5+\sqrt{5}} \tag{28}$$

$$> evalf(\mathrm{abs}(C2_{sol2}));$$

$$0.9999999999 \tag{29}$$

$$> evalf\left(\frac{\mathrm{atan}\left(evalf\left(\frac{\mathrm{Im}(C2_{sol2})}{\mathrm{Re}(C2_{sol2})}\right)\right)}{\frac{2\cdot \mathrm{Pi}}{5}}\right);$$

$$-0.4999999999 \tag{30}$$

```
> C3_sol2 := -(5^(1/2)/2 + 1/2)*((9300*5^(1/2) - 16*3125^(1/2) + 1050*(- 2*5
    ^(1/2) - 10)^(1/2) + 2100*(2*5^(1/2) - 10)^(1/2) + 1250*(- 10*5^(1/2)
    - 50)^(1/2) - 50*(10*5^(1/2) - 50)^(1/2) + 25*(150 - 50*5^(1/2))^(1/2)
    + 525*(50*5^(1/2) + 150)^(1/2) + 30*(- 50*5^(1/2) - 250)^(1/2) + 310
```

```
* (50 * 5^(1/2) - 250)^(1/2) - 20 * (750 - 250 * 5^(1/2))^(1/2) + 100 * (250 * 5
^(1/2) + 750)^(1/2) + 50 * (- 200 * 5^(1/2) - 1000)^(1/2) + 170 * (- 250 * 5
^(1/2) - 1250)^(1/2) + 20 * (250 * 5^(1/2) - 1250)^(1/2) - 5 * (3750 - 1250 * 5
^(1/2))^(1/2) - 5 * (1250 * 5^(1/2) + 3750)^(1/2) + 20 * (- 1000 * 5^(1/2)
- 5000)^(1/2) - 5 * (1000 * 5^(1/2) - 5000)^(1/2) - 5 * (5000 * 5^(1/2) - 25000)
^(1/2) + 15500) / (5000 * 5^(1/2) - 10 * (150 - 50 * 5^(1/2))^(1/2) + 410 * (50
* 5^(1/2) + 150)^(1/2) - 20 * (750 - 250 * 5^(1/2))^(1/2) + 180 * (250 * 5^(1
/2) + 750)^(1/2) - 2 * (3750 - 1250 * 5^(1/2))^(1/2) + 2 * (1250 * 5^(1/2)
+ 3750)^(1/2) + 33800) - 1) :
```

> $C3_{sol2} := simplify(C3_{sol2});$

$$C3_{sol2} := -\frac{1}{160}\,\frac{1}{5+\sqrt{5}}\left(\left(\sqrt{5}+1\right)\left(40\sqrt{5}+17\,\mathrm{I}\sqrt{2\sqrt{5}+10}+34\,\mathrm{I}\sqrt{-2\sqrt{5}+10}+23\,\mathrm{I}\sqrt{5}\sqrt{2\sqrt{5}+10}-200\right)\right) \quad \textbf{(31)}$$

> $\mathrm{Re}(C3_{sol2});$

$$\frac{\left(-\frac{1}{160}\sqrt{5}-\frac{1}{160}\right)\left(40\sqrt{5}-200\right)}{5+\sqrt{5}} \quad \textbf{(32)}$$

> $\mathrm{Im}(C3_{sol2});$

$$\frac{\left(-\frac{1}{160}\sqrt{5}-\frac{1}{160}\right)\left(17\sqrt{2\sqrt{5}+10}+34\sqrt{-2\sqrt{5}+10}+23\sqrt{5}\sqrt{2\sqrt{5}+10}\right)}{5+\sqrt{5}} \quad \textbf{(33)}$$

> $evalf(\mathrm{abs}(C3_{sol2}));$

$$1.000000000 \quad \textbf{(34)}$$

> $evalf\left(\frac{\mathrm{atan}\left(evalf\left(\frac{\mathrm{Im}(C3_{sol2})}{\mathrm{Re}(C3_{sol2})}\right)\right)}{\frac{2\cdot\mathrm{Pi}}{5}}\right);$

$$-0.9999999992 \quad \textbf{(35)}$$

> $C4_{sol2}$:= ((5^(1/2)/2 + 1/2) * (9300 * 5^(1/2) - 16 * 3125^(1/2) + 1050 * (- 2 * 5^(1

```
/2) - 10)^(1/2) + 2100 * (2 * 5^(1/2) - 10)^(1/2) + 1250 * (- 10 * 5^(1/2)
- 50)^(1/2) - 50 * (10 * 5^(1/2) - 50)^(1/2) + 25 * (150 - 50 * 5^(1/2))^(1/2)
+ 525 * (50 * 5^(1/2) + 150)^(1/2) + 30 * (- 50 * 5^(1/2) - 250)^(1/2) + 310
* (50 * 5^(1/2) - 250)^(1/2) - 20 * (750 - 250 * 5^(1/2))^(1/2) + 100 * (250 * 5
^(1/2) + 750)^(1/2) + 50 * (- 200 * 5^(1/2) - 1000)^(1/2) + 170 * (- 250 * 5
^(1/2) - 1250)^(1/2) + 20 * (250 * 5^(1/2) - 1250)^(1/2) - 5 * (3750 - 1250 * 5
^(1/2))^(1/2) - 5 * (1250 * 5^(1/2) + 3750)^(1/2) + 20 * (- 1000 * 5^(1/2)
- 5000)^(1/2) - 5 * (1000 * 5^(1/2) - 5000)^(1/2) - 5 * (5000 * 5^(1/2) - 25000)
^(1/2) + 15500)) / (5000 * 5^(1/2) - 10 * (150 - 50 * 5^(1/2))^(1/2) + 410 * (50
* 5^(1/2) + 150)^(1/2) - 20 * (750 - 250 * 5^(1/2))^(1/2) + 180 * (250 * 5^(1
/2) + 750)^(1/2) - 2 * (3750 - 1250 * 5^(1/2))^(1/2) + 2 * (1250 * 5^(1/2)
+ 3750)^(1/2) + 33800) - 1 :
```

> $C4_{sol2} := simplify(C4_{sol2});$

$$C4_{sol2} := \frac{1}{80}\,\frac{1}{5+\sqrt{5}}\Big(20\,\mathrm{I}\sqrt{5}\,\sqrt{2\sqrt{5}+10}+17\,\mathrm{I}\sqrt{5}\,\sqrt{-2\sqrt{5}+10}+66\,\mathrm{I}\sqrt{2\sqrt{5}+10}+80\sqrt{5}+17\,\mathrm{I}\sqrt{-2\sqrt{5}+10}\Big) \quad \textbf{(36)}$$

> $\mathrm{Re}(C4_{sol2});$

$$\frac{\sqrt{5}}{5+\sqrt{5}} \quad \textbf{(37)}$$

> $\mathrm{Im}(C4_{sol2});$

$$\frac{1}{80}\,\frac{1}{5+\sqrt{5}}\Big(20\sqrt{5}\,\sqrt{2\sqrt{5}+10}+17\sqrt{-2\sqrt{5}+10}\,\sqrt{5}+66\sqrt{2\sqrt{5}+10}+17\sqrt{-2\sqrt{5}+10}\Big) \quad \textbf{(38)}$$

> $evalf(\mathrm{abs}(C4_{sol2}));$

$$0.9999999999 \quad \textbf{(39)}$$

> $evalf\left(\dfrac{\mathrm{atan}\left(evalf\left(\dfrac{\mathrm{Im}(C4_{sol2})}{\mathrm{Re}(C4_{sol2})}\right)\right)}{\dfrac{2\cdot \mathrm{Pi}}{5}}\right);$

$$0.9999999992 \quad \textbf{(40)}$$

>

```
> ##### C5_postmatlab2.mw #####
>
>
>
> with(MTM) :
> C5_sol1 := - (8900 * 5^(1/2) + 2100 * ( - 2 * 5^(1/2) - 10)^(1/2) - 1050 * (2 * 5^(1/2)
    - 10)^(1/2) + 50 * ( - 10 * 5^(1/2) - 50)^(1/2) + 1250 * (10 * 5^(1/2) - 50)^(1
    /2) + 525 * (150 - 50 * 5^(1/2))^(1/2) + 25 * (50 * 5^(1/2) + 150)^(1/2) + 310
    * ( - 50 * 5^(1/2) - 250)^(1/2) - 30 * (50 * 5^(1/2) - 250)^(1/2) - 100 * (750
    - 250 * 5^(1/2))^(1/2) + 20 * (250 * 5^(1/2) + 750)^(1/2) - 50 * (200 * 5^(1/2)
    - 1000)^(1/2) - 20 * ( - 250 * 5^(1/2) - 1250)^(1/2) + 170 * (250 * 5^(1/2)
    - 1250)^(1/2) - 5 * (3750 - 1250 * 5^(1/2))^(1/2) - 5 * (1250 * 5^(1/2) + 3750)
    ^(1/2) + 5 * ( - 1000 * 5^(1/2) - 5000)^(1/2) + 20 * (1000 * 5^(1/2) - 5000)^(1
    /2) - 5 * ( - 5000 * 5^(1/2) - 25000)^(1/2) - 15500) / (5000 * 5^(1/2) + 410
    * (150 - 50 * 5^(1/2))^(1/2) - 10 * (50 * 5^(1/2) + 150)^(1/2) - 180 * (750
    - 250 * 5^(1/2))^(1/2) + 20 * (250 * 5^(1/2) + 750)^(1/2) + 2 * (3750 - 1250 * 5
    ^(1/2))^(1/2) - 2 * (1250 * 5^(1/2) + 3750)^(1/2) - 33800) :
>
> C5_sol1 := simplify(C5_sol1);
```

$$C5_{sol1} := -\frac{1}{80}\,\frac{1}{\sqrt{5}-5}\left(-17\,\mathrm{I}\sqrt{-2\sqrt{5}+10}+23\,\mathrm{I}\sqrt{5}\,\sqrt{-2\sqrt{5}+10}+120\sqrt{5}+34\,\mathrm{I}\sqrt{2\sqrt{5}+10}-200\right) \tag{1}$$

```
> Re(C5_sol1);
```

$$-\frac{1}{80}\,\frac{120\sqrt{5}-200}{\sqrt{5}-5} \tag{2}$$

```
> Im(C5_sol1);
```

$$-\frac{1}{80}\,\frac{-17\sqrt{-2\sqrt{5}+10}+23\sqrt{5}\,\sqrt{-2\sqrt{5}+10}+34\sqrt{2\sqrt{5}+10}}{\sqrt{5}-5} \tag{3}$$

```
> evalf(abs(C5_sol1));
```

$$0.9999999994 \tag{4}$$

$$> evalf\left(\frac{\mathrm{atan}\left(evalf\left(\frac{\mathrm{Im}(C5_{sol1})}{\mathrm{Re}(C5_{sol1})}\right)\right)}{\frac{2\cdot\mathrm{Pi}}{5}}\right);$$

$$1.000000000 \tag{5}$$

```
> C2_sol1 := 5^(1/2)/2 + (8900 * 5^(1/2) + 2100 * ( - 2 * 5^(1/2) - 10)^(1/2) - 1050
    * (2 * 5^(1/2) - 10)^(1/2) + 50 * ( - 10 * 5^(1/2) - 50)^(1/2) + 1250 * (10 * 5
    ^(1/2) - 50)^(1/2) + 525 * (150 - 50 * 5^(1/2))^(1/2) + 25 * (50 * 5^(1/2)
    + 150)^(1/2) + 310 * ( - 50 * 5^(1/2) - 250)^(1/2) - 30 * (50 * 5^(1/2) - 250)
    ^(1/2) - 100 * (750 - 250 * 5^(1/2))^(1/2) + 20 * (250 * 5^(1/2) + 750)^(1/2)
```

- 50 * (200 * 5^(1/2) - 1000)^(1/2) - 20 * (- 250 * 5^(1/2) - 1250)^(1/2) + 170 * (250 * 5^(1/2) - 1250)^(1/2) - 5 * (3750 - 1250 * 5^(1/2))^(1/2) - 5 * (1250 * 5^(1/2) + 3750)^(1/2) + 5 * (- 1000 * 5^(1/2) - 5000)^(1/2) + 20 * (1000 * 5 ^(1/2) - 5000)^(1/2) - 5 * (- 5000 * 5^(1/2) - 25000)^(1/2) - 15500) / (5000 * 5 ^(1/2) + 410 * (150 - 50 * 5^(1/2))^(1/2) - 10 * (50 * 5^(1/2) + 150)^(1/2) - 180 * (750 - 250 * 5^(1/2))^(1/2) + 20 * (250 * 5^(1/2) + 750)^(1/2) + 2 * (3750 - 1250 * 5^(1/2))^(1/2) - 2 * (1250 * 5^(1/2) + 3750)^(1/2) - 33800) - 1/2 :

> $C2_{sol1} := simplify(C2_{sol1});$

$$C2_{sol1} := \frac{1}{80} \frac{1}{\sqrt{5}-5}\left(200-120\sqrt{5}-17\,\mathrm{I}\sqrt{-2\sqrt{5}+10}+23\,\mathrm{I}\sqrt{5}\sqrt{-2\sqrt{5}+10}+34\,\mathrm{I}\sqrt{2\sqrt{5}+10}\right) \tag{6}$$

> $\mathrm{Re}(C2_{sol1});$

$$\frac{1}{80}\frac{200-120\sqrt{5}}{\sqrt{5}-5} \tag{7}$$

> $\mathrm{Im}(C2_{sol1});$

$$\frac{1}{80}\frac{-17\sqrt{-2\sqrt{5}+10}+23\sqrt{5}\sqrt{-2\sqrt{5}+10}+34\sqrt{2\sqrt{5}+10}}{\sqrt{5}-5} \tag{8}$$

> $evalf(\mathrm{abs}(C2_{sol1}));$

$$0.9999999994 \tag{9}$$

> $evalf\left(\frac{\mathrm{atan}\left(evalf\left(\frac{\mathrm{Im}(C2_{sol1})}{\mathrm{Re}(C2_{sol1})}\right)\right)}{\frac{2\cdot\mathrm{Pi}}{5}}\right);$

$$-1.000000000 \tag{10}$$

> $C3_{sol1}$:= ((8900 * 5^(1/2) + 2100 * (- 2 * 5^(1/2) - 10)^(1/2) - 1050 * (2 * 5^(1/2) - 10)^(1/2) + 50 * (- 10 * 5^(1/2) - 50)^(1/2) + 1250 * (10 * 5^(1/2) - 50)^(1 /2) + 525 * (150 - 50 * 5^(1/2))^(1/2) + 25 * (50 * 5^(1/2) + 150)^(1/2) + 310 * (- 50 * 5^(1/2) - 250)^(1/2) - 30 * (50 * 5^(1/2) - 250)^(1/2) - 100 * (750 - 250 * 5^(1/2))^(1/2) + 20 * (250 * 5^(1/2) + 750)^(1/2) - 50 * (200 * 5^(1/2) - 1000)^(1/2) - 20 * (- 250 * 5^(1/2) - 1250)^(1/2) + 170 * (250 * 5^(1/2) - 1250)^(1/2) - 5 * (3750 - 1250 * 5^(1/2))^(1/2) - 5 * (1250 * 5^(1/2) + 3750) ^(1/2) + 5 * (- 1000 * 5^(1/2) - 5000)^(1/2) + 20 * (1000 * 5^(1/2) - 5000)^(1 /2) - 5 * (- 5000 * 5^(1/2) - 25000)^(1/2) - 15500) / (5000 * 5^(1/2) + 410 * (150 - 50 * 5^(1/2))^(1/2) - 10 * (50 * 5^(1/2) + 150)^(1/2) - 180 * (750 - 250 * 5^(1/2))^(1/2) + 20 * (250 * 5^(1/2) + 750)^(1/2) + 2 * (3750 - 1250 * 5 ^(1/2))^(1/2) - 2 * (1250 * 5^(1/2) + 3750)^(1/2) - 33800) - 1) * (5^(1/2)/2 - 1/2) :

> $C3_{sol1} := simplify(C3_{sol1});$

(11)

$$C3_{sol1} := \frac{1}{160}\,\frac{1}{\sqrt{5}-5}\Big(\Big(-17\,\mathrm{I}\sqrt{-2\sqrt{5}+10}+23\,\mathrm{I}\sqrt{5}\,\sqrt{-2\sqrt{5}+10}+40\sqrt{5}+34\,\mathrm{I}\sqrt{2\sqrt{5}+10}+200\Big)\big(\sqrt{5}-1\big)\Big) \qquad \textbf{(11)}$$

> $\mathrm{Re}(C3_{sol1})$;

$$\frac{\left(\frac{1}{160}\sqrt{5}-\frac{1}{160}\right)\left(40\sqrt{5}+200\right)}{\sqrt{5}-5} \qquad \textbf{(12)}$$

> $\mathrm{Im}(C3_{sol1})$;

$$\frac{\left(\frac{1}{160}\sqrt{5}-\frac{1}{160}\right)\left(-17\sqrt{-2\sqrt{5}+10}+23\sqrt{5}\,\sqrt{-2\sqrt{5}+10}+34\sqrt{2\sqrt{5}+10}\right)}{\sqrt{5}-5} \qquad \textbf{(13)}$$

> $\mathit{evalf}(\mathrm{abs}(C3_{sol1}))$;

$$0.9999999994 \qquad \textbf{(14)}$$

> $\mathit{evalf}\left(\dfrac{\mathrm{atan}\left(\mathit{evalf}\left(\dfrac{\mathrm{Im}(C3_{sol1})}{\mathrm{Re}(C3_{sol1})}\right)\right)}{\dfrac{2\cdot\mathrm{Pi}}{5}}\right)$;

$$0.4999999996 \qquad \textbf{(15)}$$

> $C4_{sol1}$:= - ((5^(1/2)/2 - 1/2) * (8900 * 5^(1/2) + 2100 * (- 2 * 5^(1/2) - 10)^(1/2) - 1050 * (2 * 5^(1/2) - 10)^(1/2) + 50 * (- 10 * 5^(1/2) - 50)^(1/2) + 1250 * (10 * 5^(1/2) - 50)^(1/2) + 525 * (150 - 50 * 5^(1/2))^(1/2) + 25 * (50 * 5^(1/2) + 150)^(1/2) + 310 * (- 50 * 5^(1/2) - 250)^(1/2) - 30 * (50 * 5^(1/2) - 250)^(1/2) - 100 * (750 - 250 * 5^(1/2))^(1/2) + 20 * (250 * 5^(1/2) + 750)^(1/2) - 50 * (200 * 5^(1/2) - 1000)^(1/2) - 20 * (- 250 * 5^(1/2) - 1250)^(1/2) + 170 * (250 * 5^(1/2) - 1250)^(1/2) - 5 * (3750 - 1250 * 5^(1/2))^(1/2) - 5 * (1250 * 5^(1/2) + 3750)^(1/2) + 5 * (- 1000 * 5^(1/2) - 5000)^(1/2) + 20 * (1000 * 5^(1/2) - 5000)^(1/2) - 5 * (- 5000 * 5^(1/2) - 25000)^(1/2) - 15500))/(5000 * 5^(1/2) + 410 * (150 - 50 * 5^(1/2))^(1/2) - 10 * (50 * 5^(1/2) + 150)^(1/2) - 180 * (750 - 250 * 5^(1/2))^(1/2) + 20 * (250 * 5^(1/2) + 750)^(1/2) + 2 * (3750 - 1250 * 5^(1/2))^(1/2) - 2 * (1250 * 5^(1/2) + 3750)^(1/2) - 33800) - 1 :

> $C4_{sol1} := \mathit{simplify}(C4_{sol1})$;

$$C4_{sol1} := \frac{1}{80}\,\frac{1}{\sqrt{5}-5}\Big(20\,\mathrm{I}\sqrt{5}\,\sqrt{-2\sqrt{5}+10}-66\,\mathrm{I}\sqrt{-2\sqrt{5}+10}-17\,\mathrm{I}\sqrt{5}\,\sqrt{2\sqrt{5}+10}+80\sqrt{5}+17\,\mathrm{I}\sqrt{2\sqrt{5}+10}\Big) \qquad \textbf{(16)}$$

> $\mathrm{Re}(C4_{sol1})$;

$$\frac{\sqrt{5}}{\sqrt{5}-5} \qquad \textbf{(17)}$$

> $\mathrm{Im}(C4_{sol1})$;

$$\frac{1}{80}\,\frac{1}{\sqrt{5}-5}\left(20\sqrt{5}\,\sqrt{-2\sqrt{5}+10}-66\sqrt{-2\sqrt{5}+10}-17\sqrt{2\sqrt{5}+10}\,\sqrt{5}+17\sqrt{2\sqrt{5}+10}\right) \quad \textbf{(18)}$$

> $evalf(\mathrm{abs}(C4_{sol1}));$

$$0.9999999999 \quad \textbf{(19)}$$

> $evalf\left(\dfrac{\mathrm{atan}\left(evalf\left(\dfrac{\mathrm{Im}(C4_{sol1})}{\mathrm{Re}(C4_{sol1})}\right)\right)}{\dfrac{2\cdot \mathrm{Pi}}{5}}\right);$

$$-0.4999999999 \quad \textbf{(20)}$$

>

> $C5_{sol2}$:= (2100 * (- 2 * 5^(1/2) - 10)^(1/2) - 8900 * 5^(1/2) - 1050 * (2 * 5^(1/2) - 10)^(1/2) + 50 * (- 10 * 5^(1/2) - 50)^(1/2) + 1250 * (10 * 5^(1/2) - 50)^(1/2) - 525 * (150 - 50 * 5^(1/2))^(1/2) - 25 * (50 * 5^(1/2) + 150)^(1/2) + 310 * (- 50 * 5^(1/2) - 250)^(1/2) - 30 * (50 * 5^(1/2) - 250)^(1/2) + 100 * (750 - 250 * 5^(1/2))^(1/2) - 20 * (250 * 5^(1/2) + 750)^(1/2) - 50 * (200 * 5^(1/2) - 1000)^(1/2) - 20 * (- 250 * 5^(1/2) - 1250)^(1/2) + 170 * (250 * 5^(1/2) - 1250)^(1/2) + 5 * (3750 - 1250 * 5^(1/2))^(1/2) + 5 * (1250 * 5^(1/2) + 3750)^(1/2) + 5 * (- 1000 * 5^(1/2) - 5000)^(1/2) + 20 * (1000 * 5^(1/2) - 5000)^(1/2) - 5 * (- 5000 * 5^(1/2) - 25000)^(1/2) + 15500) / (5000 * 5^(1/2) + 410 * (150 - 50 * 5^(1/2))^(1/2) - 10 * (50 * 5^(1/2) + 150)^(1/2) - 180 * (750 - 250 * 5^(1/2))^(1/2) + 20 * (250 * 5^(1/2) + 750)^(1/2) + 2 * (3750 - 1250 * 5^(1/2))^(1/2) - 2 * (1250 * 5^(1/2) + 3750)^(1/2) - 33800)
:

> $C5_{sol2} := simplify(C5_{sol2});$

$$C5_{sol2} := \frac{1}{80}\,\frac{1}{\sqrt{5}-5}\left(200-120\sqrt{5}-17\,\mathrm{I}\sqrt{-2\sqrt{5}+10}+23\,\mathrm{I}\sqrt{5}\,\sqrt{-2\sqrt{5}+10}+34\,\mathrm{I}\sqrt{2\sqrt{5}+10}\right) \quad \textbf{(21)}$$

> $\mathrm{Re}(C5_{sol2});$

$$\frac{1}{80}\,\frac{200-120\sqrt{5}}{\sqrt{5}-5} \quad \textbf{(22)}$$

> $\mathrm{Im}(C5_{sol2});$

$$\frac{1}{80}\,\frac{-17\sqrt{-2\sqrt{5}+10}+23\sqrt{5}\,\sqrt{-2\sqrt{5}+10}+34\sqrt{2\sqrt{5}+10}}{\sqrt{5}-5} \quad \textbf{(23)}$$

> $evalf(\mathrm{abs}(C5_{sol2}));$

$$0.9999999994 \quad \textbf{(24)}$$

$$> evalf\left(\frac{\operatorname{atan}\left(evalf\left(\frac{\operatorname{Im}(C5_{sol2})}{\operatorname{Re}(C5_{sol2})}\right)\right)}{\frac{2\cdot\mathrm{Pi}}{5}}\right);$$

$$-1.000000000 \tag{25}$$

$> C2_{sol2}$:= 5^(1/2)/2 - (2100*(-2*5^(1/2) - 10)^(1/2) - 8900*5^(1/2) - 1050*(2*5^(1/2) - 10)^(1/2) + 50*(-10*5^(1/2) - 50)^(1/2) + 1250*(10*5^(1/2) - 50)^(1/2) - 525*(150 - 50*5^(1/2))^(1/2) - 25*(50*5^(1/2) + 150)^(1/2) + 310*(-50*5^(1/2) - 250)^(1/2) - 30*(50*5^(1/2) - 250)^(1/2) + 100*(750 - 250*5^(1/2))^(1/2) - 20*(250*5^(1/2) + 750)^(1/2) - 50*(200*5^(1/2) - 1000)^(1/2) - 20*(-250*5^(1/2) - 1250)^(1/2) + 170*(250*5^(1/2) - 1250)^(1/2) + 5*(3750 - 1250*5^(1/2))^(1/2) + 5*(1250*5^(1/2) + 3750)^(1/2) + 5*(-1000*5^(1/2) - 5000)^(1/2) + 20*(1000*5^(1/2) - 5000)^(1/2) - 5*(-5000*5^(1/2) - 25000)^(1/2) + 15500)/(5000*5^(1/2) + 410*(150 - 50*5^(1/2))^(1/2) - 10*(50*5^(1/2) + 150)^(1/2) - 180*(750 - 250*5^(1/2))^(1/2) + 20*(250*5^(1/2) + 750)^(1/2) + 2*(3750 - 1250*5^(1/2))^(1/2) - 2*(1250*5^(1/2) + 3750)^(1/2) - 33800) - 1/2 :

$> C2_{sol2} := simplify(C2_{sol2});$

$$C2_{sol2} := -\frac{1}{80}\,\frac{1}{\sqrt{5}-5}\left(-17\,\mathrm{I}\sqrt{-2\sqrt{5}+10}+23\,\mathrm{I}\sqrt{5}\,\sqrt{-2\sqrt{5}+10}+120\sqrt{5}+34\,\mathrm{I}\sqrt{2\sqrt{5}+10}-200\right) \tag{26}$$

$> \operatorname{Re}(C2_{sol2});$

$$-\frac{1}{80}\,\frac{120\sqrt{5}-200}{\sqrt{5}-5} \tag{27}$$

$> \operatorname{Im}(C2_{sol2});$

$$-\frac{1}{80}\,\frac{-17\sqrt{-2\sqrt{5}+10}+23\sqrt{5}\,\sqrt{-2\sqrt{5}+10}+34\sqrt{2\sqrt{5}+10}}{\sqrt{5}-5} \tag{28}$$

$> evalf(\operatorname{abs}(C2_{sol2}));$

$$0.9999999994 \tag{29}$$

$$> evalf\left(\frac{\operatorname{atan}\left(evalf\left(\frac{\operatorname{Im}(C2_{sol2})}{\operatorname{Re}(C2_{sol2})}\right)\right)}{\frac{2\cdot\mathrm{Pi}}{5}}\right);$$

$$1.000000000 \tag{30}$$

$> C3_{sol2}$:= -((2100*(-2*5^(1/2) - 10)^(1/2) - 8900*5^(1/2) - 1050*(2*5^(1/2) - 10)^(1/2) + 50*(-10*5^(1/2) - 50)^(1/2) + 1250*(10*5^(1/2) - 50)^(1/2) - 525*(150 - 50*5^(1/2))^(1/2) - 25*(50*5^(1/2) + 150)^(1/2) + 310*(-50*5^(1/2) - 250)^(1/2) - 30*(50*5^(1/2) - 250)^(1/2) + 100*(750

```
- 250*5^(1/2))^(1/2) - 20*(250*5^(1/2) + 750)^(1/2) - 50*(200*5^(1/2)
- 1000)^(1/2) - 20*(- 250*5^(1/2) - 1250)^(1/2) + 170*(250*5^(1/2)
- 1250)^(1/2) + 5*(3750 - 1250*5^(1/2))^(1/2) + 5*(1250*5^(1/2)
+ 3750)^(1/2) + 5*(- 1000*5^(1/2) - 5000)^(1/2) + 20*(1000*5^(1/2)
- 5000)^(1/2) - 5*(- 5000*5^(1/2) - 25000)^(1/2) + 15500)/(5000*5^(1/2)
+ 410*(150 - 50*5^(1/2))^(1/2) - 10*(50*5^(1/2) + 150)^(1/2) - 180
*(750 - 250*5^(1/2))^(1/2) + 20*(250*5^(1/2) + 750)^(1/2) + 2*(3750
- 1250*5^(1/2))^(1/2) - 2*(1250*5^(1/2) + 3750)^(1/2) - 33800) + 1)*(5
^(1/2)/2 - 1/2) :
```

> $C3_{sol2} := simplify(C3_{sol2});$

$$C3_{sol2} := -\frac{1}{160}\frac{1}{\sqrt{5}-5}\left(\left(-17\,\mathrm{I}\sqrt{-2\sqrt{5}+10}+23\,\mathrm{I}\sqrt{5}\sqrt{-2\sqrt{5}+10}-40\sqrt{5}+34\,\mathrm{I}\sqrt{2\sqrt{5}+10}-200\right)\left(\sqrt{5}-1\right)\right) \quad (31)$$

> $\mathrm{Re}(C3_{sol2});$

$$\frac{\left(-\frac{1}{160}\sqrt{5}+\frac{1}{160}\right)\left(-40\sqrt{5}-200\right)}{\sqrt{5}-5} \quad (32)$$

> $\mathrm{Im}(C3_{sol2});$

$$\frac{1}{\sqrt{5}-5}\left(\left(-\frac{1}{160}\sqrt{5}+\frac{1}{160}\right)\left(-17\sqrt{-2\sqrt{5}+10}+23\sqrt{5}\sqrt{-2\sqrt{5}+10}+34\sqrt{2\sqrt{5}+10}\right)\right) \quad (33)$$

> $evalf(\mathrm{abs}(C3_{sol2}));$

$$0.9999999994 \quad (34)$$

> $evalf\left(\frac{\mathrm{atan}\left(evalf\left(\frac{\mathrm{Im}(C3_{sol2})}{\mathrm{Re}(C3_{sol2})}\right)\right)}{\frac{2\cdot\mathrm{Pi}}{5}}\right);$

$$-0.4999999996 \quad (35)$$

> $C4_{sol2}$:= ((5^(1/2)/2 - 1/2)*(2100*(- 2*5^(1/2) - 10)^(1/2) - 8900*5^(1/2)

```
- 1050*(2*5^(1/2) - 10)^(1/2) + 50*(- 10*5^(1/2) - 50)^(1/2) + 1250
*(10*5^(1/2) - 50)^(1/2) - 525*(150 - 50*5^(1/2))^(1/2) - 25*(50*5^(1
/2) + 150)^(1/2) + 310*(- 50*5^(1/2) - 250)^(1/2) - 30*(50*5^(1/2)
- 250)^(1/2) + 100*(750 - 250*5^(1/2))^(1/2) - 20*(250*5^(1/2) + 750)
^(1/2) - 50*(200*5^(1/2) - 1000)^(1/2) - 20*(- 250*5^(1/2) - 1250)^(1
/2) + 170*(250*5^(1/2) - 1250)^(1/2) + 5*(3750 - 1250*5^(1/2))^(1/2)
+ 5*(1250*5^(1/2) + 3750)^(1/2) + 5*(- 1000*5^(1/2) - 5000)^(1/2) + 20
*(1000*5^(1/2) - 5000)^(1/2) - 5*(- 5000*5^(1/2) - 25000)^(1/2)
+ 15500))/(5000*5^(1/2) + 410*(150 - 50*5^(1/2))^(1/2) - 10*(50*5^(1
/2) + 150)^(1/2) - 180*(750 - 250*5^(1/2))^(1/2) + 20*(250*5^(1/2)
+ 750)^(1/2) + 2*(3750 - 1250*5^(1/2))^(1/2) - 2*(1250*5^(1/2) + 3750)
^(1/2) - 33800) - 1 :
```

```
> C4[sol2] := simplify(C4[sol2]);
```

$$C4_{sol2} := -\frac{1}{80}\,\frac{1}{\sqrt{5}-5}\Big(20\,\mathrm{I}\sqrt{5}\,\sqrt{-2\sqrt{5}+10} - 66\,\mathrm{I}\sqrt{-2\sqrt{5}+10} - 17\,\mathrm{I}\sqrt{5}\,\sqrt{2\sqrt{5}+10} - 80\sqrt{5} + 17\,\mathrm{I}\sqrt{2\sqrt{5}+10}\Big) \tag{36}$$

```
> Re(C4[sol2]);
```

$$\frac{\sqrt{5}}{\sqrt{5}-5} \tag{37}$$

```
> Im(C4[sol2]);
```

$$-\frac{1}{80}\,\frac{1}{\sqrt{5}-5}\Big(20\sqrt{5}\,\sqrt{-2\sqrt{5}+10} - 66\sqrt{-2\sqrt{5}+10} - 17\sqrt{2\sqrt{5}+10}\,\sqrt{5} + 17\sqrt{2\sqrt{5}+10}\Big) \tag{38}$$

```
> evalf(abs(C4[sol2]));
```

$$0.9999999999 \tag{39}$$

$$> \mathit{evalf}\left(\frac{\operatorname{atan}\left(\mathit{evalf}\left(\frac{\operatorname{Im}(C4_{sol2})}{\operatorname{Re}(C4_{sol2})}\right)\right)}{\frac{2\cdot\mathrm{Pi}}{5}}\right);$$

$$0.4999999999 \tag{40}$$

```
>
```

References

[1] Abramowitz M., Stegun I., "Handbook of mathematical functions with formulas, graphs, and mathematical tables", Dover, New York, 1964.

[2] Adamyan V., Tishchenko S., "One-electron states and interband optical absorption in single-wall carbon nanotubes", J. Phys.: Condens. Matter, 18, 2007.

[3] Albeverio S., Gesztesy F., Hoegh-Krohn R., Holden H., "Solvable models in quantum mechanics", Springer, New York, 1988.

[4] Arfken G. B., Weber H. J., "Mathematical methods for physicists", Elsevier, 2005.

[5] Baz' A. I., Zel'dovich Ya. B., Perelomov A. M., "Scattering, reactions, and decays in nonrelativistic mechanics" (in Russian), Nauka, Moscow, 1971.

[6] Darboux G., "Sur une proposition relative aux équations linéaires", C. R. Acad. Sci Paris, 94, 1456-1459, 1982.

[7] Demkov Yu. N., Ostrovskii V. N., "Zero-range potentials and their applications in atomic physics", Plenum Press, New York, 1988.

[8] Derevianko A., "Revised Huang-Yang multipolar pseudopotential", Phys. Rev. A, 72, 044701, 2005.

[9] Doktorov E. V., Leble S. B., "A dressing method in mathematical physics", Springer, London, 2006.

[10] Drukarev G., "The zero-range potential model and its application in atomic and molecular physics", Adv. Quantum Chem., 11, 251-274, 1979.

[11] Fermi E., "Sopra lo spostamento per pressione delle righe elevate delle serie spettrali", Il Nuovo Cimento, 11, 157-166, 1934.

[12] Huang K., "Statistical mechanics", Wiley, New York, 1963.

[13] Huang K., Yang C.N., "Quantum-mechanical many-body problem with hard-sphere interaction", Phys. Rev., 105, 767-775, 1957.

[14] Idziaszek Z., Callarco T., "Pseudopotential method for higher partial wave scattering", Phys. Rev. Lett., 96, 013201, 2006.

[15] Leble S. B., Yalunin S., "A dressing of zero-range potentials and electron–molecule scattering problem at low energies", Phys. Lett. A, 339, 83-88, 2005.

[16] Matveev V. B., Salle M. A., “Darboux transformations and solitons”, Springer-Verlag Berlin, Heidelberg, 1991.

[17] Stampfer F., Wagner P., “A mathematically rigorous formulation of the pseudopotential method”, J. Math. Anal. Appl., 342, 202-212, 2008.

[18] Stock R., Silberfarb A., Bolda E. L., Deutsch I. H., “Generalized Pseudopotentials for Higher Partial Wave Scattering”, Phys. Rev. Lett., 94, 023202, 2005.

[19] Tishchenko S., “Ballistic conductance and impedance of one-dimensional systems”, Ukrains’kyi Fizychnyi Zhurnal, 50, 980-985, 2005.

[20] Wodkiewicz K., “Fermi pseudopotentials in arbitrary dimensions”, Phys. Rev. A, 43, 68-76, 1991.

[21] Yurov A. V., “Darboux transformation in quantum mechanics” (in Russian), Kaliningrad University, Kaliningrad, 1998.