Zero-range potentials and Darboux transformations

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General purposes

Physics: **Scattering and electronic multi-center problems; classic and generalized Zero-Range potentials configurations, symmetry group account.**

Math.: **Generation of ZRP via gauge-Matveev transformations, development of the generalized ZRP technique to nonzero orbital moment, multi-center problem applications. Group theory aspect. ZRP as distributions and Hermitian operator extensions**

E. Doktorov, S. Leble, Dressing method in mathematical physics. Springer, 2007.

55 udir convienmi ancor come l'essemplo
56 e l'essemplare non vanno d'un modo,
57 ché io per me indarno a ciò contemplo.

Dante Alighieri, *Divina Commedia*
Paradiso, Canto XXVIII

55 then I still have to hear just how the model
56 and copy do not share in one same plan
57 for by myself I think on this in vain.

Translated by A. Mandelbaum

Source publications: Leble, S. Yalunin, S.: (2003) Generalized zero-range potentials and multi-channel electron-molecule scattering, *Rad. Phys. Chem.* **68**, 181-186. Phys. lett.2005, Multiple scattering and electron-uracil collisions
at low energies EPJ v.144, 115-122,2007. E. Doktorov, S. Leble, Dressing method in mathematical physics. Springer, 2007. S. leble D. Ponomarev, Electronic states in zero-range potential models of nanostructures with a cyclic symmetry, ArXive 2010.

Introduction. On ZRP potentials.

- **History**

  F e r m i E. Sopra lo spostamento per pressione delle righe elevante delle serie spettrali//Nuovo Cimento.— 1934.— V. 11.— P. 157—166. F e r m i E. Sul moto dei neutroni nelle sostanze idrogenante//Ric. ScL— 1936.— V. 7.— P. 13-52.

- **General remarks and bibliography:**

  B S Pavlov, "The theory of extensions and explicitly-soluble models", RUSS MATH SURV, 1987, 42 (6), 127–168.

  Demkov Yu N, Ostrovsky V N (1988) Zero-Range Potentials and their Applications in Atomic Physics, Plenum, New York

  Albeverio S, Gesztesy F, Høegh-Krohn R and Holden H (1988) Solvable Models in Quantum Mechanics, Springer-Verlag, New York.

- **Pseudopotential method**

  F. Stampfer and P. Wagner. A mathematically rigorous formulation of the pseudopotential method. Journal of Mathematical Analysis and Applications, 342 (2008) 202-212. Recent applications examples: Analytical solutions for the system of two ultracold spin-polarized fermions interacting in p wave and confined in an axially symmetric harmonic trap.

  Zbigniew Idziaszek Phys. Rev. A 79, 062701 (2009) Atomistic pseudopotential simulation of nanometer sized CMOS (Complementary Metal Oxide Semiconductor) devices —. Lin-Wang Wang ...

  Parameter Modelling for High Order Transport Models Computational methods L.W. Wang, "Novel computational methods for nanostructure electronic structure calculations", Ann. Rev. Phys. Chem. 61, 19, (2010).

- **Radial equation, s - states.** Demkov, Ostrovskij, etc. s-wave dominates in low energy range

- $l \neq 0$ **problem discussion.**

  Discrepancy noted first by Roth, Feldmeyer 2001 Phys. Rev.

  Corrected in: A. Derevianko, Phys. Rev. A 67 (2003) 033607. Phys. Rev. A 72, 039901(E) (2005) [2 pages] Erratum: Anisotropic pseudopotential for polarized dilute quantum gases [Phys. Rev. A 67, 033607 (2003)] arXiv:0807.3111v1.

- *Darboux transformations* Schnizer W.A., Leeb H., Generalized Darboux transformations: classification of inverse scattering methods for the radial Schrödinger equation (1994) J.Phys. A: Math. Gen. 27:2605-2614.,

Radial equation

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

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

A standard procedure of separation of variables is

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

denote the radial wave function as $\psi(r)$, l=0 - s-wave, l=1 - p-wave, etc. This yields for $\psi(r)$

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

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

To demonstrate idea the most easily, we consider for now only partial s-waves, setting $l = 0$, generalization will be given later. Since for $r\psi(r)$ (1) is just one-dimensional Helmholtz equation, write general solution in the conventional form

$$\psi(r) = \frac{C_0}{kr} \left(\sin kr - \tan \eta_0 \cos kr\right), \qquad (2)$$

constants η_0, C_0 are determined by the form of potential and normalization condition, respectively. alternatively, one can write the last equation as

$$\psi(r) = \frac{\tilde{C}_0}{kr} \left(s_0 \exp\left(ikr\right) - \exp\left(-ikr\right)\right), \qquad (3)$$

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. Since the solution is irregular in $r = 0$, the potential should also be singular.

For finite energies the solution at $r = 0$ behaves as

$$\psi(r) \approx C_0 \left(1 - \frac{\tan \eta_0}{kr}\right) \approx C_0 \frac{\tan \eta_0}{kr} \qquad (4)$$

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

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

and calculate

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

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

$$-\Delta\psi - k^2\psi = 4\pi C_0 \frac{\tan\eta_0}{k}\delta(\vec{r}). \qquad (5)$$

It remains only to eliminate normalization constant C_0 from the asymptotic behavior of the solution at the center (4). This can be done by applying the appropriate operator

$$C_0 = \frac{d}{dr}(r\psi)\Big|_{r=0}. \qquad (6)$$

That leads to the *Statement*

$$\left(-\Delta - 4\pi\frac{\tan\eta_0}{k}\delta(\vec{r})\frac{d}{dr}r\right)\psi = k^2\psi. \qquad (7)$$

that fix form of the potential.

Remark. Denoting

$$a_0 = -\frac{\tan \eta_0}{k} \tag{8}$$

(that is an independent of k quantity for small energies, as it will be shown later), we bring the equation (7) back to the form of the original Schrodinger equation

$$\left(-\frac{\hbar^2}{2\mu}\Delta + \underbrace{2\pi\frac{a_0\hbar^2}{\mu}\delta(\vec{r})\frac{d}{dr}r}_{=U_0} \right)\psi = E\psi. \tag{9}$$

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

$$\left.\frac{\frac{d}{dr}(r\psi)}{r\psi}\right|_{r=0} = -\frac{k}{\tan\eta_0} = 1/a_0. \qquad (10)$$

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

For bounded states $a_0 < 0$, so we can write

$$\left.\frac{\frac{d}{dr}(r\psi)}{r\psi}\right|_{r=0} = -\beta, \qquad (11)$$

where $\beta \equiv -1/a_0$.

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 (11), and this is what we are going to employ onwards.

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 (Huang-Yang, Huang), recently started to become clear as the mistakes in Huang's works were corrected and different approaches were proposed (Derevianko,Stock,Idziaszek). To avoid possible ambiguity, the final expressions for pseudopotential given in those works still should be understood in an appropriate mathematical sense (Stampfer).

General solution of the radial equation (1) formed via spherical Bessel and Neumann functions - $j_l(kr)$ and $y_l(kr)$, ,

$$\psi(r) = C_l \left(j_l(kr) - \tan \eta_l y_l(kr) \right), \qquad (12)$$

or as a combination of spherical Hankel functions

$$\psi(r) = \tilde{C}_l \left(s_l h_l^{(1)}(kr) - h_l^{(2)}(kr) \right), \qquad (13)$$

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

Taking into account the following asymptotes at $kr \longrightarrow 0$

$$j_l(kr) \approx \frac{(kr)^l}{(2l+1)!!}, \tag{14}$$

$$y_l(kr) \approx -\frac{(2l-1)!!}{(kr)^{l+1}}, \tag{15}$$

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

$$\begin{gathered}\psi(r) \approx C_l\left(\frac{(kr)^l}{(2l+1)!!} + \tan\eta_l \frac{(2l-1)!!}{(kr)^{l+1}}\right) \approx \\ C_l \tan\eta_l \frac{(2l-1)!!}{(kr)^{l+1}}.\end{gathered} \tag{16}$$

From here, the constant C_l can be expressed as

$$C_l = \frac{(2l+1)!!}{k^l\,(2l+1)!}\,\frac{d^{2l+1}}{dr^{2l+1}}\left(r^{l+1}\psi\right)\Big|_{r=0}. \tag{17}$$

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

$$U_l = \frac{\hbar^2}{2\mu} \lim_{r \to 0} \left(\Delta + k^2 \right) \psi. \tag{18}$$

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

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

singular behavior of the solution (16) at the origin, it remains to obtain properly an effect of $\Delta \dfrac{1}{r^{l+1}}$.

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)

$$\begin{gathered}
\int_{V_\epsilon} r^l \Delta \frac{1}{r^{l+1}} dV' = \\
\int_{V_\epsilon} r^l \left(\Delta' \frac{1}{r^{l+1}} - \frac{l\,(l+1)}{r^2} \cdot \frac{1}{r^{l+1}} \right) dV' = \\
\int_{V_\epsilon} \left(r^l \Delta' \frac{1}{r^{l+1}} - \frac{1}{r^{l+1}} \Delta' r^l \right) = \\
\int_{S_\epsilon} \left(r^l \nabla \frac{1}{r^{l+1}} - \frac{1}{r^{l+1}} \nabla r^l \right) d\vec{S}' = \\
\left[-(l+1) - l \right] \int_{S_\epsilon} \frac{1}{r^2} dS' = \\
-4\pi\,(2l+1)
\end{gathered} \tag{19}$$

we employed Green identity and calculation

$$\Delta' r^l = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} r^l \right) = l\,(l+1)\, r^{l-2}.$$

Therefore, we conclude that

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

where the last part of the equality should be understood in a proper distributional sense (cf. chain of discussions (Huang,Stock,Derevianko,Idziaszek,Stampfer).

Combining this result with the previous expressions (18), (17), we obtain

STATEMENT

$$U_l\psi = -2\pi \underbrace{(2l+1)\,(2l-1)!!}_{=(2l+1)!!} \underbrace{\frac{(2l+1)!!}{(2l+1)!}}_{=\frac{1}{2^l l!}} \frac{\hbar^2}{\mu} \frac{\tan\eta_l}{k^{2l+1}} \frac{1}{r^{l+2}}\delta(r) \tag{20}$$

As before, an alternative to pseudopotential approach (less ambiguous) is to impose boundary condition similar to (10) that can be readily found from the asymptotic of the solution (16). The desired combination allowing to eliminate C_l yields

$$\frac{1}{r^{l+1}\psi}\frac{\partial^{2l+1}}{\partial r^{2l+1}}\left(r^{l+1}\psi\right)\Big|_{r=0} = \underbrace{\frac{(2l+1)!}{(2l+1)!!}}_{=2^l l!}\cdot\frac{1}{(2l-1)!!}\cdot\frac{k^{2l+1}}{\tan\eta_l} = -\frac{2^l l!}{(2l-1)!!}a_l^{2l+1}, \tag{21}$$

where we introduced

$$a_l^{2l+1} = -\frac{k^{2l+1}}{\tan\eta_l}. \tag{22}$$

Before when writing (8) 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 (1) admits the following general solution

$$\psi = A_1 r^l + A_2 \frac{1}{r^{l+1}}. \tag{23}$$

On the other hand, we can consider solutions (12) for non-zero but small energies such that the small argument spherical function expansions (14), (15) can be used. Thus, by imposing requirement of matching (12) and (23), 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

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

The quantity (22) is termed as the Wigner's threshold scattering length.

This allows to rewrite the expression (20) once again, hence the resulting pseudopotential to be introduced into the radial Schrodinger equation is

$$U_l = 2\pi \frac{(2l+1)!!}{2^l l!} \frac{a_l^{2l+1} \hbar^2}{\mu} \frac{\delta(r)}{r^{l+2}} \frac{\partial^{2l+1}}{\partial r^{2l+1}} r^{l+1}. \quad (24)$$

Even more general potentials obtained by dressing. First of all, we notice that the radial Schrodinger equation (1) can be brought to the form eligible for direct application of obtained formulas. Performing substitution $\psi = \chi/r$, we readily obtain

$$-\chi'' + \underbrace{\frac{l\,(l+1)}{r^2}}_{=u_l(r)}\chi = k^2\chi. \tag{25}$$

That is to say, that we can apply Darboux transformation to the equation (1) meaning that all original wave functions ψ should be multiplied by r whereas the potential term

$$u_l(r) = \frac{l\,(l+1)}{r^2} \tag{26}$$

remains unchanged.

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

$$\psi_l(r) = Cj_l\,(kr) \tag{27}$$

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

$$\phi_m(r) = C y_m(\kappa_m r), \qquad m = 1, \ldots, N. \tag{28}$$

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 employ Crum's formula and write the transformed solution

$$\psi_l^{[N]}(r) = C\frac{W\left(r\phi_1, \ldots, r\phi_N, r\psi_l\right)}{rW\left(r\phi_1, \ldots, r\phi_N\right)}. \qquad (29)$$

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

$$j_l(kr) \approx \frac{\sin\left(kr - l\pi/2\right)}{kr}, \qquad (30)$$

$$y_l(kr) \approx -\frac{\cos\left(kr - l\pi/2\right)}{kr}, \tag{31}$$

$$h_l^{(1)}(kr) = j_l(kr) + iy_l(kr) \approx (-i)^{l+1}\,\frac{\exp\left(ikr\right)}{kr}, \tag{32}$$

$$h_l^{(2)}(kr) = j_l(kr) - iy_l(kr) \approx i^{l+1}\frac{\exp\left(-ikr\right)}{kr}. \tag{33}$$

Then the Wronskians turn into Vandermond determinants, hence,

$$\psi_l^{[N]}(r) = C[(-i)^l\,\frac{\exp(ikr)}{kr}\frac{\Delta(\kappa_1,...,\kappa_N,ik)}{\Delta(\kappa_1,...,\kappa_N)} - i^l\frac{\exp(-ikr)}{kr}\frac{\Delta(\kappa_1,...,\kappa_N,-ik)}{\Delta(\kappa_1,...,\kappa_N)}]. \tag{34}$$

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 $ik \longrightarrow \kappa_m$ yields its zero determinant due to linear dependencies of the rows), thereby allowing the following factorization

$$\Delta\left(\kappa_1, \ldots, \kappa_N, ik\right) = \begin{vmatrix} 1 & \kappa_1 & \kappa_1^2 & \ldots & \kappa_1^N \\ 1 & \kappa_2 & \kappa_2 & \ldots & \kappa_2^N \\ \ldots & \ldots & \ldots & \ldots & \ldots \\ 1 & \kappa_N & \kappa_N^2 & \ldots & \kappa_N^N \\ 1 & ik & (ik)^2 & \ldots & (ik)^N \end{vmatrix} =$$

$$C \prod_{m=1}^{N} \left(\kappa_m - ik\right).$$

Denoting

$$s_l = \prod_{m=1}^{N} \frac{(\kappa_m - ik)}{(\kappa_m + ik)}, \tag{35}$$

we recognize in (34) the asymptotes of spherical Hankel functions, hence

$$\psi_l^{[N]}(r) = C\left[s_l h_l^{(1)}(kr) - h_l^{(2)}(kr)\right]. \tag{36}$$

Corresponding to this solution effective potential is transformed from (26) into

$$u_l^{[N]} = \frac{l\,(l+1)}{r^2} - 2\frac{d^2}{dr^2}\log \underbrace{W\left(rh_l^{(1)}(\kappa_1 r), \ldots, rh_l^{(1)}(\kappa_N r\right.}_{\equiv W} \tag{37}$$

Due to the asymptotes (32), (33), we can observe that the Darboux transformation does not change the behavior of the potential at $r \longrightarrow \infty$

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

whereas singular behavior at the origin is changed.

Main result for a potential V(x)

Indeed, using the asymptotic at $r \longrightarrow 0$

$$h_l^{(1)}(\kappa r) = -i\frac{(2l-1)!!}{(\kappa r)^{l+1}}, \tag{38}$$

we compute the Wronskian at the right hand side of the equation (37)

$$W \approx$$

$$-i\,(2l-1)!! \begin{pmatrix} (\kappa_1 r)^{-l} & -\frac{l}{r}\,(\kappa_1 r)^{-l} & \dots & (-1)^{N-1}\,\underline{l\,(l} \\ \dots & \dots & \dots & \\ (\kappa_N r)^{-l} & -\frac{l}{r}\,(\kappa_N r)^{-l} & \dots & (-1)^{N-1}\,\underline{l\,(l} \end{pmatrix}$$

Therefore

$$W \approx \frac{C}{r^{Nl} \cdot r^{N(N-1)/2}} \qquad \Rightarrow$$

$$\Rightarrow \qquad \log W \left(r h_l^{(1)}(\kappa_1 r), \ldots, r h_l^{(1)}(\kappa_N r) \right) \approx$$

$$-N \left(l + \frac{N-1}{2} \right) \log r + C.$$

Finally, the expression (37) yields the transformed effective finite-range potential

$$u_l^{[N]} \approx \frac{1}{r^2} \left[l\,(l+1) - N\,(2l+N-1) \right]. \qquad (39)$$

Connection with generalized zero-range potentials

In particular, one can notice that the expression (36) coincides with (13) if

$$\exp(2i\eta_l) = \prod_{m=1}^{N} \frac{(\kappa_m - ik)}{(\kappa_m + ik)}, \tag{40}$$

or, taking into account (22),

$$\tan\eta_l = -a_l^{2l+1}k^{2l+1} = -i\frac{\prod_{m=1}^{N}(\kappa_m - ik) - \prod_{m=1}^{N}(\kappa_m + ik)}{\prod_{m=1}^{N}(\kappa_m - ik) + \prod_{m=1}^{N}(\kappa_m + ik)}. \tag{41}$$

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

Since

$$\prod_{m=1}^{N}(\kappa_m + ik) =$$

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

$$(ik)^{N-1}\sum_{n=1}^{N}\kappa_n+(ik)^N,$$

we continue the last equality as

$$a_l^{2l+1}k^{2l+1}=i\frac{ik\sum_{n=1}^{2l+1}\prod_{\substack{m=1\\m\neq n}}^{2l+1}\kappa_m+\ldots+(ik)^{2l+1}}{\prod_{m=1}^{2l+1}\kappa_m+\ldots+(ik)^{2l}\sum_{n=1}^{2l+1}\kappa_n}. \tag{42}$$

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 $\prod_{m=1}^{N} \kappa_m = i\,(i/a_l)^{2l+1} = (-1)^{2l+1}/a_l^{2l+1}$) we obtain a set of equations allowing to determine all the transformation parameters κ_m.

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

Given some quantity $a = |a|\, e^{i\phi_a}$, we want to choose parameters $\kappa_1, \ldots, \kappa_{2l+1}$ in a way that

$$\prod_{m=1}^{2l+1} (\kappa_m + ik) = (ik)^{2l+1} - a. \qquad (43)$$

as solutions of algebraic problem

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

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

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

$$-\kappa_m = |a|^{1/(2l+1)} \exp\left(i\frac{(\phi_a + 2\pi m)}{2l+1}\right), \qquad m = 1, \ldots, 2 \tag{44}$$

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

$$\prod_{m=1}^{2l+1} (\kappa_m - ik) = (-ik)^{2l+1} - a. \tag{45}$$

Substitution of (43), (45) into (41) results in

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

$$a = (-1)^{l+1} / a_l^{2l+1}.$$

Kappa choice

Therefore, providing a_l is a real number, (44) yields

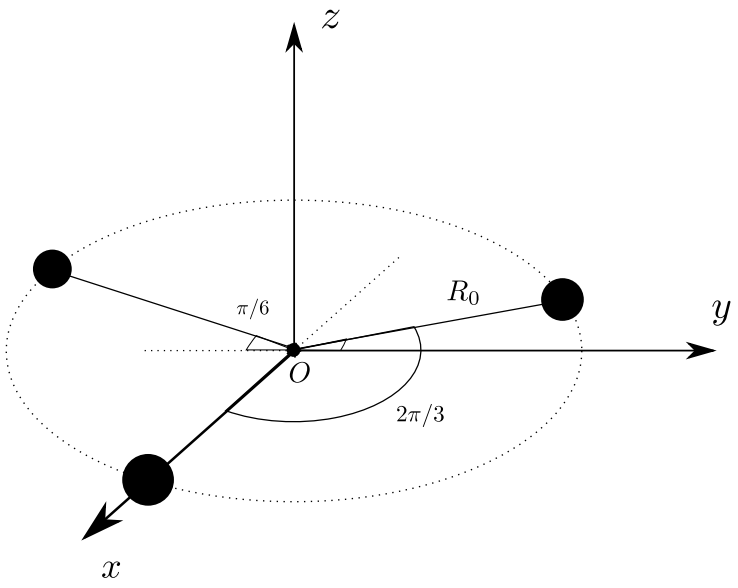
$$\kappa_m = -1/a_l \cdot \exp\left(i\pi \frac{l+2m+1}{2l+1}\right), \qquad m = 1, \ldots, 2l+1. \tag{46}$$

To sum up, the Darboux transformations significantly broadening the range of solvable (integrable) 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.

Problem with plane symmetric multiple point-center potential

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 (9) is written in the form

$$\psi(\vec{r}) = C_1 \frac{e^{-\kappa\left|\vec{r}-\vec{R}_1\right|}}{\left|\vec{r}-\vec{R}_1\right|} + C_2 \frac{e^{-\kappa\left|\vec{r}-\vec{R}_2\right|}}{\left|\vec{r}-\vec{R}_2\right|} + C_3 \frac{e^{-\kappa\left|\vec{r}-\vec{R}_3\right|}}{\left|\vec{r}-\vec{R}_3\right|}, \tag{47}$$

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

This solution must satisfy zero-range potential conditions (11) 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

$$\begin{pmatrix} (\beta - \kappa)\Delta R \cdot e^{\kappa \Delta R} & 1 & 1 \\ 1 & (\beta - \kappa)\Delta R \cdot e^{\kappa \Delta R} & 1 \\ 1 & 1 & (\beta - \kappa)\Delta R \cdot e^{\kappa} \end{pmatrix}$$

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

$$(\beta - \kappa)\Delta R \cdot e^{\kappa \Delta R} = 1, \qquad (48)$$

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

$$(\beta - \kappa)\Delta R \cdot e^{\kappa \Delta R} = -2 \tag{49}$$

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

Existence conditions $\beta > \dfrac{1}{\Delta R}$ and $\beta > -\dfrac{2}{\Delta R}$ for (48) and (49), 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 (49), 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.

or, finally The first case, (48), 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 (58) yields

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

The symmetric combination of functions.

Due to symmetry in positions of centers, only solutions which are representations in he correspondent eigenvalue subspace must be realized. It means that in nondegenerate case 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

$$[C_1(\lambda+1)+C_2]\frac{e^{-\kappa\left|\vec{r}-\vec{R}_1\right|}}{\left|\vec{r}-\vec{R}_1\right|}+ \tag{50}$$

$$[\lambda C_2-C_1]\frac{e^{-\kappa\left|\vec{r}-\vec{R}_2\right|}}{\left|\vec{r}-\vec{R}_2\right|}-$$

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

However, we note that due to the order (symmetry) in positions of point-centers $\vec{R}_i$, the functions $\frac{e^{-\kappa\left|\vec{r}-\vec{R}_i\right|}}{\left|\vec{r}-\vec{R}_i\right|}$, $i=1,2,3$ 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

$$P_l\left(\cos\gamma_1\right)=$$

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

$$P_l\left(\cos\gamma_2\right)=$$

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

$$P_l\left(\cos\gamma_3\right)=$$

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

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

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

$$+\left(\lambda C_1+C_2\left(\lambda+1\right)\right)e^{-i\frac{4\pi}{3}m}-C_1\left(\lambda+1\right)-C_2]Y_l^m(\theta,\,\phi)=0.$$

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,

$$\begin{aligned} &(C_1 - \lambda C_2)\, e^{-i\frac{2\pi}{3}m} + \\ &(\lambda C_1 + C_2\,(\lambda+1))\, e^{-i\frac{4\pi}{3}m} - C_1\,(\lambda+1) - C_2 = 0, \end{aligned} \quad + \tag{51}$$

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

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

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,

$$\psi_1(\vec{r}) =$$

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

$$\psi_2(\vec{r}) =$$

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

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

$$\psi_1(\vec{r}) = C_{01} \cdot \left(\frac{e^{-\kappa\left|\vec{r}-\vec{R}_1\right|}}{\left|\vec{r}-\vec{R}_1\right|} + e^{-i\frac{2\pi}{3}} \frac{e^{-\kappa\left|\vec{r}-\vec{R}_2\right|}}{\left|\vec{r}-\vec{R}_2\right|} + e^{i\frac{2\pi}{3}} \frac{e^{-\kappa\left|\vec{r}-\vec{R}\right.}}{\left|\vec{r}-\vec{R}\right.} \right. \tag{52}$$

$$\psi_2(\vec{r}) = C_{02} \cdot \left(\frac{e^{-\kappa\left|\vec{r}-\vec{R}_1\right|}}{\left|\vec{r}-\vec{R}_1\right|} + e^{i\frac{2\pi}{3}} \frac{e^{-\kappa\left|\vec{r}-\vec{R}_2\right|}}{\left|\vec{r}-\vec{R}_2\right|} + e^{-i\frac{2\pi}{3}} \frac{e^{-\kappa\left|\vec{r}-\vec{R}\right.}}{\left|\vec{r}-\vec{R}\right.} \right. \tag{53}$$

These states (that are, in fact, complex conjugated) corresponding to the eigenvalue with the energy determined from (48), along with the state

$$\psi_3(\vec{r}) = C_{03} \cdot \left(\frac{e^{-\kappa\left|\vec{r}-\vec{R}_1\right|}}{\left|\vec{r}-\vec{R}_1\right|} + \frac{e^{-\kappa\left|\vec{r}-\vec{R}_2\right|}}{\left|\vec{r}-\vec{R}_2\right|} + \frac{e^{-\kappa\left|\vec{r}-\vec{R}_3\right|}}{\left|\vec{r}-\vec{R}_3\right|} \right), \tag{54}$$

having the energy to be found from (49), 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.

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

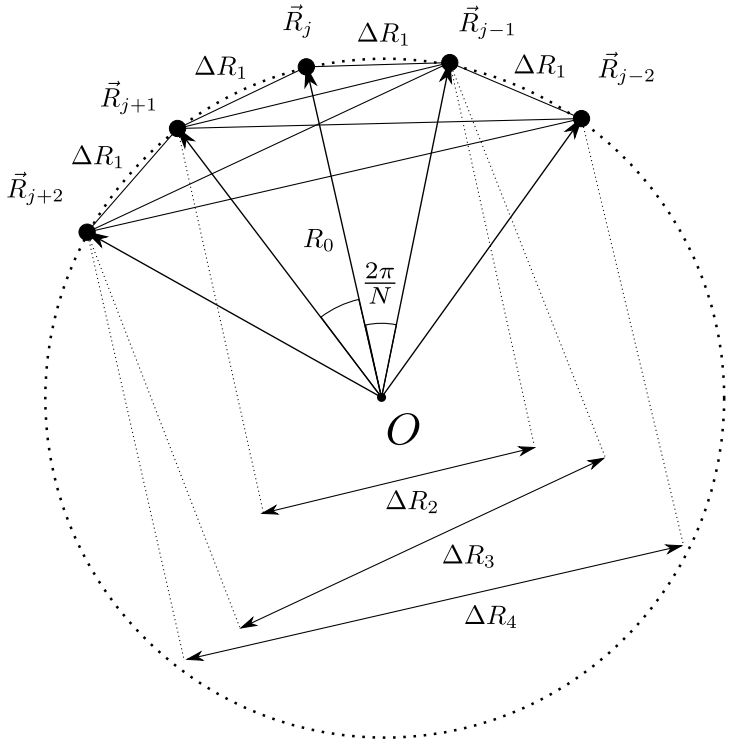
$$\psi(\vec{r}) = \sum_{k=1}^{N} C_k \frac{e^{-\kappa\left|\vec{r}-\vec{R}_k\right|}}{\left|\vec{r}-\vec{R}_k\right|}, \tag{55}$$

subject to the conditions

$$\left.\frac{\partial \log\left(\left|\vec{r}-\vec{R}_i\right| \cdot \psi(\vec{r})\right)}{\partial\left|\vec{r}-\vec{R}_i\right|}\right|_{\left|\vec{r}-\vec{R}_i\right|=0} = -\beta, \tag{56}$$

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

$$\Delta R_j = 2R_0 \sin\left(\frac{2\pi}{N}\cdot\frac{j}{2}\right) = 2R_0 \sin\left(\phi_{j+1}/2\right), \tag{57}$$

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

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

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

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

$$\psi_1(\vec{r}) = 2C_{01}\rho_0 e^{-\kappa R_0} \sum_{l=0}^{\infty} \left(\frac{r}{R_0}\right)^l \int_0^{\pi} P_l(\cos\phi)\cos\phi \cdot d\phi.$$

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 $z = 0$.

Scattering on N-centers - continuous spectrum problem

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

$$\psi(\vec{r}) = A_0 e^{ikz} + \sum_{j=1}^{N} C_j \frac{e^{ik\left|\vec{r}-\vec{R}_j\right|}}{\left|\vec{r}-\vec{R}_j\right|}, \qquad (58)$$

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

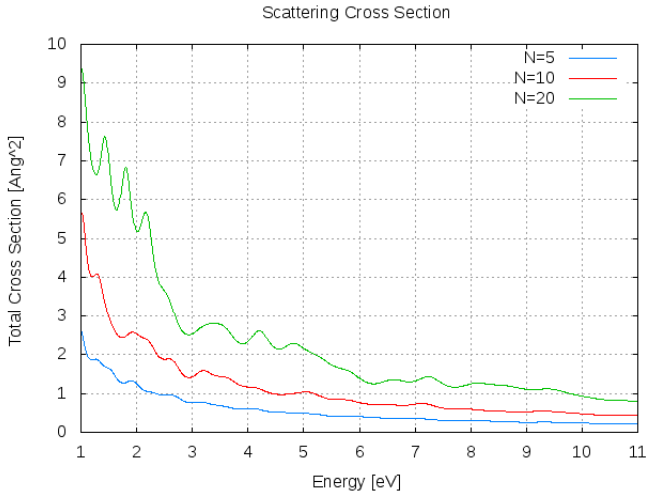
Using previously described notation, at each center (scatterer) the solution must satisfy the ZRP condition (56)

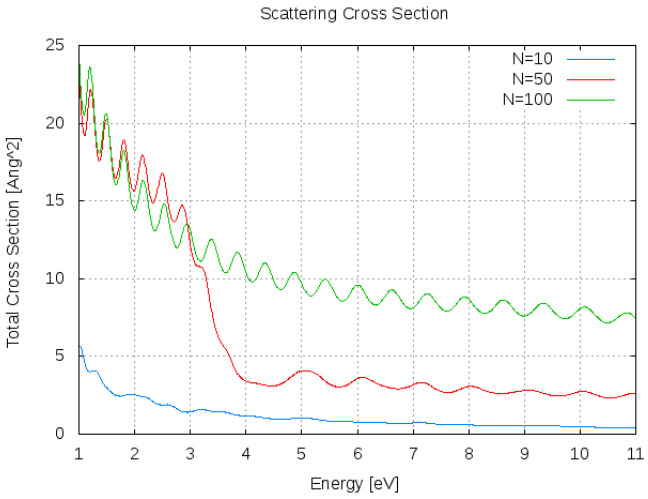
$$\left.\frac{\partial \log\left(\left|\vec{r}-\vec{R}_j\right| \cdot \psi(\vec{r})\right)}{\partial\left|\vec{r}-\vec{R}_j\right|}\right|_{\left|\vec{r}-\vec{R}_j\right|=0} = \frac{1}{C_j}\left(A_0 + \ldots\right.$$

$$+C_{j-1}\cdot\frac{e^{ik\Delta R_1}}{\Delta R_1}+C_j\cdot ik+C_{j+1}\cdot\frac{e^{ik\Delta R_1}}{\Delta R_1}+\ldots=-\beta.$$

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.

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:
$\kappa = 0.5\,[\mathrm{Ang}^{-1}]$, $R_0 = 5.0\,[\mathrm{Ang}]$.

Dressing in a multi-center problem The second observation is principal, it allows to built a zero-range potential eigenfunction in the multi-center problem. In a more general situation one can consider a system with a smooth potential plus a number of ZRP. If one knows the Green function for the smooth potential, then one can provide a solution for the problem with the ZRPs added. This was outlined in Demkov,Ostrovskij, where the case of a single ZRP was considered. Generalization to the case with an arbitrary number of ZRP is straightforward. On the contrary, our general idea is to "dress" a multicenter system without Green function consideration. This procedure gives simple formulas for partial phases and their corrections at low energies.

Let us consider scattering problem for a non-spherical potential U:

$$\left(-\frac{1}{2}\frac{\partial^2}{\partial r^2}-\frac{1}{r}\frac{\partial}{\partial r}+\frac{\hat{L}^2}{2r^2}+\hat{U}-E\right)\psi(\vec{r})=0, \quad (59)$$

where $\hat{L}^2$ is square of angular momentum operator, E describes the energy of particle. The asymptotic of wave function $\psi(\vec{r})$ looks like

$$\psi(\vec{r}) \overset{r\to\infty}{\sim} \exp(i\vec{k}\cdot\vec{r})+f(\theta)\frac{e^{ikr}}{r}, \quad (60)$$

where $f(\theta)$ is scattering amplitude, which depends on scattering angle θ. The operator $\widehat{L}^2$ commutes with all radial derivatives, in particular with $\partial = \partial/\partial r$.

In three-dimensional space the DT may be reduced to one-dimensional operator (or matrix) problem. The first order DT for Schrödinger equation (59) is

$$\begin{aligned} \psi^{(1)} &= (\partial - \widehat{s})\psi, \\ \widehat{U}^{(1)} &= \widehat{U} + 1/r^2 - \widehat{s}', \end{aligned} \tag{61}$$

and $\widehat{s}$ must be assumed as function of the operator variable $\widehat{L}^2$. The formula (61) gives non-local (over angles) potential which depends on $\widehat{L}^2$. In order to find operator $\widehat{s}$ we can use covariance principle for the equation (59).

The covariance principle formally yields explicit constraint for $\widehat{s}$, which gives

$$\widehat{s}' + \frac{2}{r}\widehat{s} + \widehat{s}^2 = \frac{\widehat{L}^2}{r^2} + 2\widehat{U} + K^2, \qquad (62)$$

It is supposed that the constant of integration (by r) $K = \sum_{n=0}^{\infty} K_n \widehat{L}^{2n}$ is the analytical function of $\widehat{L}^2$. The operator $\widehat{s}$ can be found as series $\sum_{n=0}^{\infty} s_n \widehat{L}^{2n}$ where the coefficients s_n depend only on r. It is easy to show that the equation leads to recursion relations for the coefficients s_n.

Thus, we have the algorithm that determine the operator $\widehat{s}$ and a dressed potential via the operator K. The choice $\widehat{s}' = 0$ at the infinity that corresponds the desirable case $\widehat{U^{(1)}} \to 0$ (61) yields $\widehat{s}(\infty) = K$. For our purpose (cross section evaluation) we need only partial phases or scattering amplitude related to operator K. In order to find the partial phases for a dressed potential we need to apply the DT to wave function. However, we have one trouble: in general DT modifies the plane wave $\exp(\mathrm{i}\vec{k}\cdot\vec{r})$. Thus, DT applied to wave function $\psi(\vec{r})$ with asymptotic (60) gives an another asymptotic. In some particular cases, special choice of the operator K allows to avoid this problem. Indeed, consider the partial wave asymptotics for a non-spherical potential $Demkov, Rudakov$

$$\psi_J(\vec{r}) \sim \frac{1}{2\mathrm{i}kr}(\mathrm{e}^{\mathrm{i}kr+\mathrm{i}\delta_J}\Lambda_J(\vec{n}) - \mathrm{e}^{-\mathrm{i}kr-\mathrm{i}\delta_J}\Lambda_J(-\vec{n})), \tag{63}$$

where $\vec{n}$ is unit vector directed as $\vec{r}$, δ_J denote partial shifts, and $\Lambda_J(\vec{n})$ are normalized eigenvectors of S-matrix operator (partial harmonics). The most simple formulas for the shifts $\delta_J^{(1)}$ for the potential $\widehat{U}^{(1)}$ result when partial harmonic Λ_J are also eigenvectors of operator K. For example, suppose all partial harmonic Λ_J are eigenvector of K but only Λ_0 has nonzero eigenvalue κ

$$K\Lambda_0(\vec{n}) = \kappa\Lambda_0(\vec{n}). \tag{64}$$

The asymptotic dressing is reduced to the action of the operator $\partial - K$ on asymptotic (63). It is easy to show by using expression

$$\ln\left(\frac{\kappa - \mathrm{i}k}{\kappa + \mathrm{i}k}\right) = -2\mathrm{i}\arctan(k/\kappa), \tag{65}$$

for real-valued variables k, κ, that DT changes only the partial shift δ_0 as

$$\delta_0^{(1)} = \delta_0 - \arctan(k/\kappa). \tag{66}$$

In this special case we add only one additional parameter. In the region $k \gg |\kappa|$ the second term of the equation (66) practically does not contribute to the partial cross section

$$\sigma_J = \frac{4\pi}{k^2}\sin^2\delta_J. \tag{67}$$

One observes an important contribution to the cross section when $k \approx |\kappa|$ and hence it can be considered as a correction at low energies.

Illustrations: X_n and YX_n structures

we consider the scattering problem for a dressed multi-center potential with a symmetry. The multi-center scattering within the framework of the ZRP model was investigated by Demkov and Rudakov, Szmytkowski, and others.

Suppose a structure X_n contains n identical scatterers, which involve only s-waves. Let R denote the distance between two nearest scatterers X-X. The partial waves and phase shifts can be classified with respect to symmetry group representation for the structures X_n (n=2,3,4), degeneracy being defined by the dimension of the representation $Demkov, Rudakov$.

The partial phases can be calculated by classical ZRP method $Demkov, Ostrovskij$

$$\tan\delta_J = \begin{cases} -a\frac{kR+(n-1)\sin(kR)}{R+(n-1)a\cos(kR)}, & J=0 \\ -a\frac{kR-\sin(kR)}{R-a\cos(kR)}, & J=\overline{1,n-1}. \end{cases} \quad (68)$$

In special case $n=4$, our result coincides with $Szmytkowski$

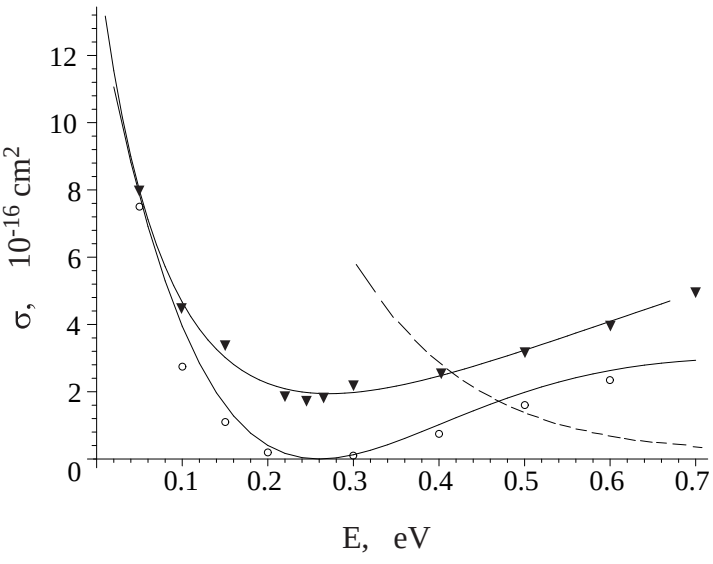
Consider **structures $\mathbf{YX_n}$**. For simplicity, suppose that the scatterers X are in vertices of a regular structure $\mathsf{X_n}$. Let D denotes the distance between scatterers Y-X and R denotes distance between X-X. Position of the scatterer Y perfectly fixed only if n=4 (geometric center of tetrahedron). We arrive at the constraint $R = 2\sqrt{\frac{2}{3}}D$. The partial phases derived analytically

$$\tan\delta_J = -a_{\mathsf{X}}\frac{kR - \sin(kR)}{R - a_{\mathsf{X}}\cos(kR)}, \qquad J = \overline{2,n}. \quad (69)$$

The $t = \tan\delta_{0,1}$ obeys the quadratic equation

$$(t + a_{\mathsf{Y}}k)\left(\frac{t}{n-1} + a_{\mathsf{X}}\left(\frac{k}{n-1} + \frac{\sin(kR)}{R} + t\frac{\cos(kR)}{R}\right)\right) = \frac{n}{n-1}a_{\mathsf{X}}a_{\mathsf{Y}}\left(\frac{\sin(kD)}{D} + t\frac{\cos(kD)}{D}\right)^2, \quad (70)$$

where $a_{\mathsf{X}}, a_{\mathsf{Y}}$, denote boundary parameters. For large distances we can interpret the parameters as scattering lengths of isolated atoms. Thus, in the limiting case when the distance D is very large, $\tan\delta_0$ tends to first equation of (68) and $\tan\delta_1 \sim -a_{\mathsf{Y}}k$. This situation corresponds to independent scattering on a molecule $\mathsf{X_n}$ and an atom Y.



Integral cross sections for electron-Silane scattering around the Ramsauer-Townsend minimum; upper line - least squares fitting to the experiment (Wan H. X., Moore J. H., Tossel J. A. (1989) J. Chem. Phys. 91:1340) (triangles); lower curve describes our model calculation for partial wave A_1; open circles denotes calculation for partial wave A_1 $Jain$; broken curve describes the calculation from $Gianturco$

Conclusions/Problems/Perspective

1. This approach allows to calculate quantum scattering parameters

2. Our procedure allows to combine dressing with ZRP actions.

3. Integrable potentials

4. Analyze SUSY partners,

5. **Further generalizations. Extension theory**

   Berezin F, Faddeev L. Note on Schrodinger equation with singular potential DAN 1961 - Extension of Neumenn.

   BS Pavlov TMF (Theor. Math. Phys) 1984 Internal structure via Hilbert space extensions.

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