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Quasi-Sturmian functions in the continuum spectrum problems

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Purpose

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Description of quantum system continuum

Approaches

- Expansion on the basis of square integrable functions (J-matrix, CCC)
- Expansion on the generalized Sturmian functions (Sturmias approach)

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The problem formulation

Problem to be solved:

Two-body problem

Tasks:

- Construction of the basis functions with appropriate asymptotic behavior
- The basis set application to solving the scattering problem
- Efficiency of the numerical scheme based upon the expansion on basis set

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The problem formulation

Let us consider the motion of a particle of mass μ in a potential

$$V(r) = \frac{Z_1 Z_2}{r} + U(r), \tag{1}$$

The scattering wave function $\Psi_\ell^{(+)}$ satisfies the Schrödinger equation

$$\left[-\frac{1}{2\mu}\left(\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2}\right) + V(r) - E\right]\Psi_\ell^{(+)}(r) = 0. \tag{2}$$

J-matrix Approach

Operator $\hat{U}$ is replaced by:

$$\hat{U} \to \hat{U}^N = \sum_{m,n=0}^{N-1} \left|\overline{m,\ell}\right\rangle \langle m,\ell| \, \hat{U} \, |n,\ell\rangle \left\langle\overline{n,\ell}\right| \quad (3)$$

In the case of charged particles

$$\begin{aligned} |n,\ell\rangle &= \phi_{n,\ell}(\lambda,r) = N_{n,l}\, e^{-\lambda r}\, (2\lambda r)^{\ell+1} L_n^{2\ell+1}(2\lambda r), \\ \left|\overline{n,\ell}\right\rangle &= \phi_{n,\ell}(\lambda,r)/r \end{aligned} \quad (4)$$

$$N_{n,l} = \sqrt{\frac{n!}{(n+2\ell+1)!}}$$

J-matrix Approach

Potential separable expansion method

Lippman-Schwinger equation

$$\left|\Psi_\ell^{N(+)}\right\rangle = \left|\Psi_\ell^{C}\right\rangle - \hat{G}^{\ell(+)}\hat{U}^N\left|\Psi_\ell^{N(+)}\right\rangle. \tag{5}$$

where:

Ψ_ℓ^C — regular Coulomb solution, show

$\hat{G}^{\ell(+)}$ — the Green's function operator kernel show

J-matrix Approach

Discrete Lippman-Schwinger equation

$$\mathbf{a} = \mathcal{S} - \mathbf{G}\mathbf{U}\mathbf{a}, \tag{6}$$

where:

$$\begin{aligned}
\mathbf{a}: \quad & a_n &=& \left\langle \overline{n,\ell} \middle| \Psi_\ell^{N(+)} \right\rangle \\
\mathcal{S}: \quad & \mathcal{S}_{n,\ell}(k) &=& \left\langle \overline{n,\ell} \middle| \Psi_\ell^{C} \right\rangle \\
\mathbf{U}: \quad & U_{m,n} &\equiv& \left\langle m,\ell \middle| \hat{U} \middle| n,\ell \right\rangle \\
\mathbf{G}: \quad & G_{m,n}^{\ell(+)} &\equiv& \left\langle \overline{m,\ell} \middle| \hat{G}^{\ell(+)} \middle| \overline{n,\ell} \right\rangle.
\end{aligned} \tag{7}$$

J-matrix Approach

$$\mathcal{S}_{n,\ell}(k) = \langle \overline{n,\ell} | \Psi_\ell^C \rangle = \int_0^\infty dr \frac{1}{r} \phi_{n,\ell}(\lambda, r) \Psi_\ell^C(r), \tag{8}$$

$$G_{m,n}^{\ell(\pm)}(k;\lambda) = \int_0^\infty \int_0^\infty dr dr' \frac{1}{r} \phi_{m,\ell}(\lambda, r) G^{\ell(\pm)}(k; r, r') \frac{1}{r'} \phi_{n,\ell}(\lambda, r'), \tag{9}$$

$$G_{m,n}^{\ell(\pm)}(k;\lambda) = \frac{2\mu}{k} \mathcal{S}_{n_<,\ell}(k) \mathcal{C}_{n_>,\ell}^{(\pm)}(k), \tag{10}$$

$\mathcal{S}, \mathcal{C}$ — linear independent J-matrix solutions show

J-matrix Approach

from (6) follows:

$$\mathbf{a} = [\mathbf{I} + \mathbf{GU}]^{-1} \mathcal{S} \tag{11}$$

In this case:

$$\left|\Psi_\ell^{N(+)}\right\rangle = \left|\Psi_\ell^{C}\right\rangle - \sum_{n=0}^{N-1} c_n \hat{G}^{\ell(+)} \left|\overline{n,\ell}\right\rangle, \tag{12}$$

where c_n — components of the vector $\mathbf{c} = \mathbf{Ua}$.

J-matrix Approach

Improving the convergence

Smoothing factors

$$\sigma_n^N = \frac{1-\exp\left\{-[\alpha(n-N)/N]^2\right\}}{1-\exp(-\alpha^2)}, \quad \alpha \approx 6. \tag{13}$$

Replacement:

$$U_{m,n} \to \sigma_m^N U_{m,n} \sigma_n^N. \tag{14}$$

Sturmian functions method

Problem is formulated in form of the inhomogeneous Schrödinger equation

Wave function is expressed as the sum

$$\Psi(k,r) = \Psi_\ell^C(k,r) + \Psi_{sc}^{(+)}(k,r) \tag{15}$$

(15) → (2): **Driven Equation**

$$\left[-\frac{1}{2\mu}\left(\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2}\right) + \frac{Z_1 Z_2}{r} + U(r) - E\right]\Psi_{sc}^{(+)}(k,r) = -U(r)\Psi_\ell^C(k,r) \tag{16}$$

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Sturmian functions method

solution of (16)

$$\Psi_{sc}^{(+)}(r) = \sum_n c_{n,\ell}\, S_{n,\ell}^{(+)}(r) \tag{17}$$

$S_{n,\ell}^{(+)}$ — basis Sturmian functions

In the case of charged particles the basis is generated by equation

$$\left[-\frac{1}{2\mu}\left(\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2}\right) - E\right] S_{n,\ell}^{(+)}(r) = -\beta_n \frac{Z_1 Z_2}{r} S_{n,\ell}^{(+)}(r). \tag{18}$$

Representation of scattering wafefunction

We suggest:

$$\Psi_{sc}^{(+)}(r) = \sum_{n=0}^{N-1} c_{n,\ell}\, Q_{n,\ell}^{(+)}(r), \tag{19}$$

Quasi-Sturmian functions

$$Q_{n,\ell}^{(+)}(r) \equiv \hat{G}^{\ell(+)} \left|\overline{n,\ell}\right\rangle \tag{20}$$

are satisfy the inhomogeneous equation:

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Quasi-Sturmians

Integral representation

Let us use the integral representation of Green's functions: show

$$Q_{n,\ell}^{(\pm)}(r) = N_{n,\ell}\,(2\lambda r)^{\ell+1}\,e^{-\lambda r}\,\frac{2\mu}{(\lambda \mp ik)} \times \int_0^1 dz\,(1-z)^{\ell\pm i\alpha}(1-\omega^{\pm 1}z)^{\ell\mp i\alpha}(1-z-\omega^{\pm 1}z)^n \times \exp\left(z\,[\lambda \pm ik]\,r\right)\,L_n^{2\ell+1}\left(\frac{(1-z)(1-\omega^{\pm 1}z)}{(1-z-\omega^{\pm 1}z)}\,2\lambda r\right) \quad (22)$$

(Variable change: $u = \tanh\left(\frac{y}{2}\right)$ and farther $z = \frac{1-u}{1-\omega u}$)

Quasi-Sturmians

Expansion

From (22) it follows the expansion in powers of r: show

(4),(9), $\langle\overline{n,\ell}| \times$ (20) integrating over r:

$$Q_{n,\ell}^{(\pm)}(r) = \sum_{m=0}^{\infty} \phi_{m,\ell}(\lambda, r) G_{m,\,n}^{\ell(\pm)}(k;\lambda). \qquad (23)$$

Asyptotic behavior

Inserting Green's function represintation (32) into defenition of Quasi-Sturmians (20) and taking limit $r \to \infty$ we find

$$Q_{n,\ell}^{(\pm)}(r) \underset{r\to\infty}{\sim} A_{n,\ell} e^{\pm i\left(kr - \alpha \ln(2kr) - \frac{\pi\ell}{2} + \sigma_\ell\right)},$$
$$A_{n,\ell} = \frac{2\mu}{k} \mathcal{S}_{n,\ell}(k), \tag{24}$$

where $\sigma_\ell = \frac{\Gamma(\ell+1+i\alpha)}{|\Gamma(\ell+1+i\alpha)|}$ — Coulomb phase.

s–wave scattering, Yukawa potential

Input data

s-wave scattering of a particle of mass $\mu = 1$, momentum $k = 1$, Coulomb potential $Z_1 Z_2 = 1$ and Yukawa potential

$$U(r) = b\frac{e^{-ar}}{r}, \quad a = 1.3, b = 1. \tag{25}$$

Matrix elements of potential (25):

$$U_{m,n} \equiv \int_0^\infty dr\, \phi_{m,\ell}(\lambda, r) U(r) \phi_{n,\ell}(\lambda, r). \tag{26}$$

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Asyptotic behavior for Yukawa potential

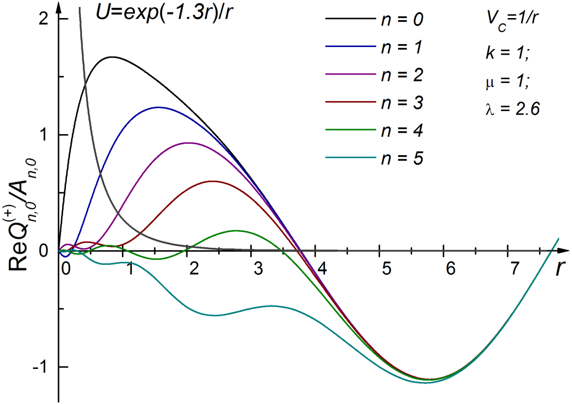


Figure: The real parts of the first six QS functions for the Coulomb potential $V_C = \frac{1}{r}$.

Discrete Drive Equation

equation for the coefficients of wavefunction expansion

$$[\mathbf{I} + \mathcal{U}]\,\mathbf{c} = \mathbf{d}. \qquad (27)$$

$$\begin{aligned} \mathbf{d}: \quad d_m &= -\int_0^\infty dr\, \phi_{m,0}(\lambda, r) U(r) \Psi_0^C(r), \\ \mathcal{U}: \quad \mathcal{U}_{m,n} &= \int_0^\infty dr\, \phi_{m,0}(\lambda, r)\, U(r)\, Q_{n,0}^{(+)}(r) \end{aligned} \qquad (28)$$

from QSF expansion (23) follows:

$$\mathcal{U}_{m,n} = \sum_{n'=0}^{\infty} U_{m,n'}\, G_{n',n}^{\ell(+)}(k;\lambda), \qquad (29)$$

s–wave scattering, Yukawa potential

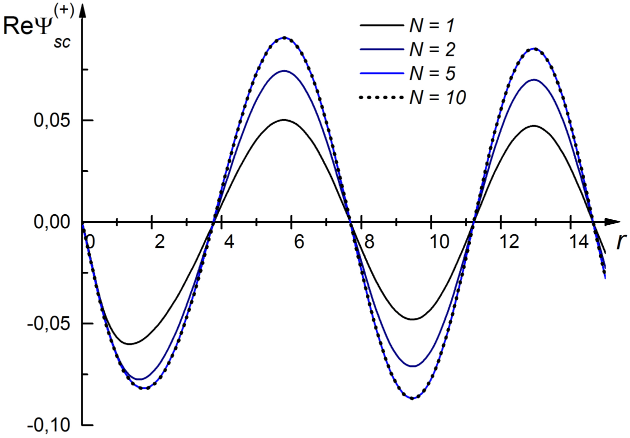


Figure: Convergence for the real part of the scattering wave as N increases.

Amplitude

partial-wave Coulomb-modified scattering amplitude

$$f'_\ell \equiv \frac{1}{2ik}(e^{2i\delta_\ell} - 1) = \frac{2\mu}{k^2}\sum_{n=0}^{N} a_n \mathcal{S}_{n,\ell}(k). \qquad (30)$$

J-matrix method

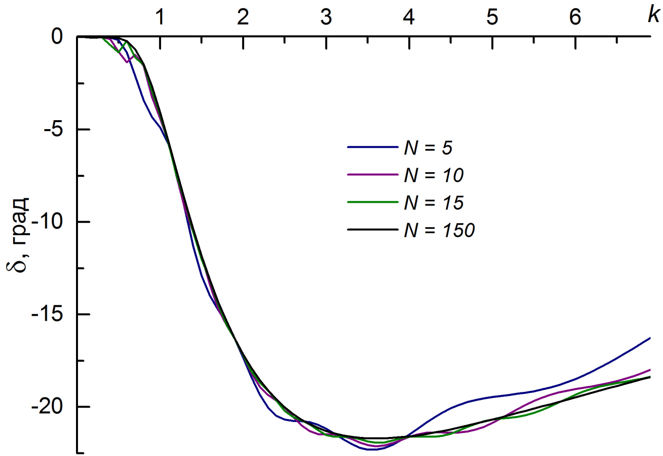
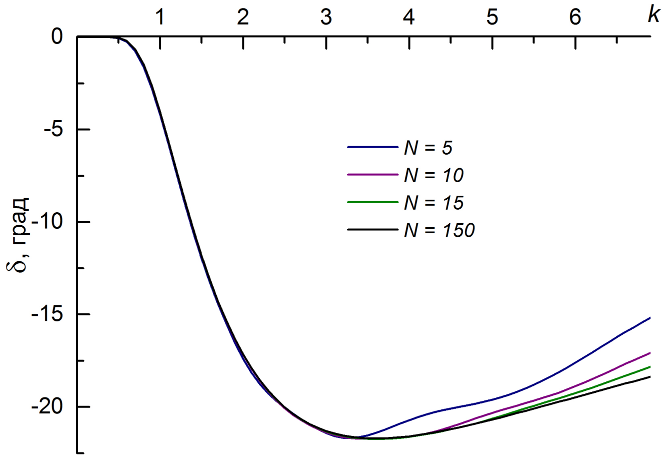


Figure: Convergence of the phase shift as the number N increases

J-matrix method with smoothing



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QS-functions method

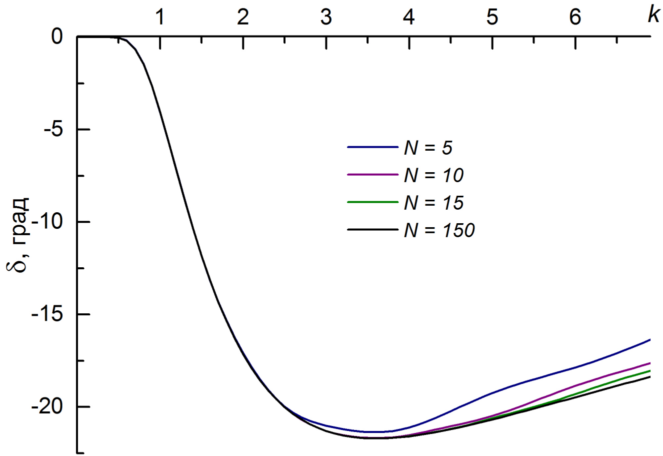

Figure: Convergence of the phase shift as the number N increases

Comparing of approaches for N = 10

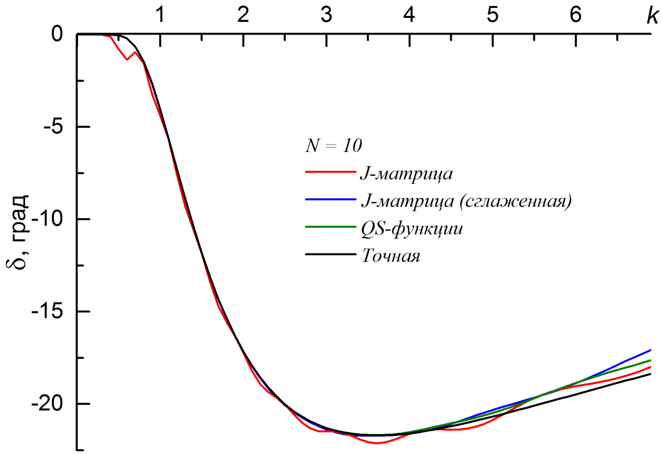

Figure: Comparing of the phase shift as the number N increases

Comparing of approaches

J-matrix approach

- Analytic form of Coulomb Green's function
- Phase shift oscillation

Sturmias approach

- No phase shift oscillation
- generation of the basis poses a problem as difficult as the original scattering problem

Conclusion

Quasi-Sturmians

- Basis set obtained, which can effectively solve the problem of the two-particle scattering in the representation of square integrable functions
- QS function can be represented in the form of well-known special functions

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Thanks for attention!

Coulomb solution

$$\Psi_\ell^C(k,r) = \frac{1}{2}(2kr)^{\ell+1}\, e^{-\pi\alpha/2}\, e^{ikr}\, \frac{|\Gamma(\ell+1+i\alpha)|}{(2\ell+1)!} \times {}_1F_1(\ell+1+i\alpha; 2\ell+2; -2ikr). \tag{31}$$

Here:
$\alpha = \frac{\mu Z_1 Z_2}{k}$ — Sommerfeld parameter;
$E = \frac{k^2}{2\mu}$ — energy.

back

The Green's function operator

$$G^{\ell(\pm)}(k;r,r') = \mp \frac{\mu}{ik} \frac{\Gamma(\ell+1\pm i\alpha)}{(2\ell+1)!} \times \mathcal{M}_{\mp i\alpha;\ell+1/2}(\mp ikr_<)\mathcal{W}_{\mp i\alpha;\ell+1/2}(\mp ikr_>). \tag{32}$$

$\mathcal{M}, \mathcal{W}$ — Whittaker functions

back

The Green's function operator integral representation

Using the integral representation for the Whittaker functions product:

$$G^{\ell(\pm)}(k;r,r') = 2\mu\sqrt{r\,r'}\int_0^\infty dy\, e^{\pm ik(r+r')\cosh(y)} \times \left[\coth\left(\frac{y}{2}\right)\right]^{\mp 2i\alpha} I_{2\ell+1}\left(\mp 2ik\sqrt{r\,r'}\sinh(y)\right). \quad (33)$$

back

Sin-like & Cos-like J-matrix solutions

$$\mathcal{S}_{n,\ell}(k) = \frac{1}{2N_{n,\ell}} (2\sin\zeta)^{\ell+1} e^{-\pi\alpha/2} \omega^{-i\alpha} \frac{|\Gamma(\ell+1+i\alpha)|}{(2\ell+1)!} \times (-\omega)^n {}_2F_1\left(\begin{matrix} -n, \ell+1+i\alpha \\ 2\ell+2 \end{matrix} ; 1-\omega^{-2} \right), \tag{34}$$

$$\mathcal{C}^{(\pm)}_{n,\ell}(k) = -\frac{n!}{N_{n,\ell}} \frac{e^{\pi\alpha/2}\omega^{i\alpha}}{(2\sin\zeta)^{\ell}} \frac{\Gamma(\ell+1\pm i\alpha)}{|\Gamma(\ell+1\pm i\alpha)|} \times \frac{(-\omega)^{\pm(n+1)}}{\Gamma(n+l+2\pm i\alpha)} {}_2F_1\left(\begin{matrix} -\ell \pm i\alpha,\ n+1 \\ n+\ell+2\pm i\alpha \end{matrix} ; \omega^{\pm 2} \right), \tag{35}$$

where

$$\omega \equiv e^{i\zeta} = \frac{\lambda+ik}{\lambda-ik}, \quad \sin\zeta = \frac{2\lambda k}{\lambda^2+k^2}.$$

back

Quasi-Sturmian expansion in powers of r

$$Q_{n,\ell}^{(\pm)}(r) = N_{n,\ell}\,(2\lambda r)^{\ell+1}\,e^{-\lambda r}\,\frac{2\mu}{(\lambda \mp ik)}\sum_{m=0}^{\infty}\frac{\left(r[\lambda \pm ik]\right)^{m}}{m!}$$

$$\times\left[\sum_{q=0}^{n}(-1)^{q}\binom{n}{q}\frac{(2\lambda r)^{q}}{(2l+1+q)!}\right.$$

$$\times\left\{\sum_{p=0}^{n-q}(-1)^{p}\binom{n-q}{p}(1+\omega^{\pm 1})^{p}\,\frac{\Gamma(m+p+1)\,\Gamma(\ell+1\pm i\alpha+q)}{\Gamma(\ell+m+p+q+2\pm i\alpha)}\right.$$

$$\left.\left.\times\ {}_2F_1\left(\begin{matrix}-\ell-q\pm i\alpha,\ m+p+1\\ \ell+m+p+q+2\pm i\alpha\end{matrix};\omega^{\pm 1}\right)\right\}\right]. \quad (36)$$

back