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# Extension of the zero-range potential model onto the Hamiltonians with a singularity at the origin

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**Abstract.** We evaluate the short-range asymptotic behavior of the Green function for a Hamiltonian when its potential energy part has an inverse power singularity at the origin. The analytically solvable case of sharply screened Coulomb potential is considered firstly. For this potential the additional logarithmic singular term has been found in the short-range asymptote of the Green function as in the case of the pure Coulomb potential. The case of a short-range potential of an arbitrary form with inverse power singularity is treated on the basis of the integral Lippmann-Schwinger equation. It is shown that, if the singularity is weaker than the Coulomb one, the Green function has only standard singularity. For the case of $r^{-\rho}$ singularity of the potential with $1 \leq \rho < 2$ the additional singularity in the asymptotic behavior of the Green function appears. In the case of $\rho = 1$ the additional logarithmic singularity has the same form as in the case of the pure Coulomb potential. In the case of $1 < \rho < 2$ the additional singularity of the Green function has the form of the polar singularity $r^{-\rho+1}$. These results are applied for extending the zero-range potential formalism on Hamiltonians with singular potentials.

**Keywords:** Green function, sharply screened Coulomb potential, exact solutions, zero-range potential

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## 1. Introduction and formulation of the problem

In this paper we concentrate on those attributes of Green's function $G(z)$ of a Hamiltonian $H$, which are needed for evaluating the short-range asymptotic behavior of the Green function in the configuration space. As an operator $G(z)$ is defined as $G(z) = (H - z)^{-1}$ for $z \in \mathbb{C}$. The Hamiltonian is assumed to have the form

$$H = -\Delta + V(\boldsymbol{r}), \tag{1}$$

where $\Delta$ stands for the Laplacian over $\boldsymbol{r} \in \mathbb{R}^3$. While the three-dimensional configuration space is considered, the case of arbitrary dimension $d > 1$ can be treated by similar methods.

The potential energy term $V(\boldsymbol{r})$ is supposed to represent a short-range potential, i.e. it is a real-valued smooth function for all $r \equiv |\boldsymbol{r}| > 0$ and it vanishes asymptotically as $V(\boldsymbol{r}) \propto r^{-1-\delta}, \quad \delta > 1$ [1] when $r \to \infty$. More precisely, we assume that there exists a constant $C > 0$ such that the inequality

$$|V(\boldsymbol{r})| \le C(1 + r)^{-1-\delta}, \delta > 1 \tag{2}$$

holds for all $\boldsymbol{r}$ except of a small neighborhood of the origin $\boldsymbol{r} = 0$. The specific concern of the paper is the singular short-range behavior of the potential $V(\boldsymbol{r}) \propto r^{-\rho}$, when $r \to 0$. More precisely, we assume that the potential $V(\boldsymbol{r})$ in a neighborhood of the origin $\boldsymbol{r} = 0$ can be represented as

$$V(\boldsymbol{r}) = r^{-\rho} W(\boldsymbol{r}), \tag{3}$$

where $W(\boldsymbol{r})$ is a smooth bounded function with the finite limit

$$\lim_{r\to 0} W(\boldsymbol{r}) = V_0. \tag{4}$$

In what follows this class of potentials will be referred to as $\mathfrak{V}(\rho, \delta)$. For Hermiticity of $H$ it is sufficient to require $\rho < 2$ and therefore it will be assumed throughout the paper that this inequality is fulfilled.

The short-range asymptote of the Green function plays the decisive role in the zero-range potential formalism [1]. In our recent paper [2] by studying the Green function we have shown that the zero-range potential has to be modified from the standard form, if it is constructed for the particles interacting by the Coulomb potential $V^{\mathcal{C}}(r) = V_0 r^{-1}$. This modification is represented in the short-range behavior of the solution $\phi$ of the Schrödinger equation

$$\phi \sim \frac{\alpha}{4\pi}\left[1/r + V_0 \log(r)\right] + \beta, \quad r \to 0 \tag{5}$$

by the logarithmic singularity that is additional to the standard $r^{-1}$ one. The modification appears in fact as the result of the interplay between singularities of the

[1] This condition for $\delta$ can be weakened up to $\delta > 0$. However we will use the stronger condition $\delta > 1$ since it guaranties the absolute convergence of integrals we deal with in the paper below.

Coulomb potential and the zero-range potential. Before treating the general case we will deal with the sharply screened Coulomb potential $V_R^{\mathcal{C}}(r) = V^{\mathcal{C}}(r)\theta(R-r)$, where $R > 0$ is a screening radius and $\theta$-function is defined as $\theta(t) = 1\,(0)$ when $t \geq 0\,(< 0)$. We consider this particular case of the screened Coulomb potential $V_R^{\mathcal{C}}$, which is also analytically solvable [3] as $V^{\mathcal{C}}$, in order to emphasize that only the short-range behavior of the Coulomb potential is responsible for the effect of that interplay and therefore the long-range behavior of the tail of the Coulomb potential does not affect the zero-range potential structure.

One of the approaches for constructing the zero-range potential in the general case of $V \in \mathfrak{V}(\rho,\delta)$ consists in inserting a delta-functional term into the Schrödinger equation [2]

$$\left[-\Delta + V(r) - k^2\right]\phi(\boldsymbol{r},\boldsymbol{k}) + \lambda\delta(\boldsymbol{r})\beta = 0, \tag{6}$$

where $\lambda$ is a coupling constant and $\beta$ is actually a linear functional of $\phi$ [1]. Then the solution of (6) can be given by the Lippmann-Schwinger integral equation

$$\phi(\boldsymbol{r},\boldsymbol{k}) = \phi_0(\boldsymbol{r},\boldsymbol{k}) - \lambda\int \mathrm{d}\boldsymbol{r}'\, G^+(\boldsymbol{r},\boldsymbol{r}',k^2)\delta(\boldsymbol{r}')\beta. \tag{7}$$

Here by $G^+(k^2)$ we denote $\lim_{\epsilon\to 0} G(k^2 + \mathrm{i}\epsilon)$ and this notation will be used systematically throughout the paper. In (7) the function $\phi_0$ is the solution to the equation

$$\left[-\Delta + V(r) - k^2\right]\phi_0(\boldsymbol{r},\boldsymbol{k}) = 0, \tag{8}$$

obeying the asymptotic boundary condition

$$\phi_0(\boldsymbol{r},\boldsymbol{k}) \sim \exp\left(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}\right) + Ar^{-1}\exp\left(\mathrm{i}kr\right) \tag{9}$$

as $r \to \infty$. The dot-product here and further means the scalar product of vectors in $\mathbb{R}^3$.

The integration in (7) is performed easily due to the delta-function which yields

$$\phi(\boldsymbol{r},\boldsymbol{k}) = \phi_0(\boldsymbol{r},\boldsymbol{k}) - \lambda G^+(\boldsymbol{r},0,k^2)\beta. \tag{10}$$

As will be shown below the limit of $\phi_0$ as $r \to 0$ is finite for $V \in \mathfrak{V}(\rho,\delta)$ and therefore the non trivial short-range asymptote of $\phi$ is completely determined by Green's function term in (10). Hence, from (10) it is seen that the principal features of the zero-range potential formalism follow from the short-range behavior in $\boldsymbol{r}$ of the Green function $G^+(\boldsymbol{r},0,k^2)$ as occurs in the case of regular potentials [1]. In consecutive sections we will evaluate the corresponding asymptote of the Green function and as the result the zero-range potential will be constructed.

The paper is organized as follows. In section 2 we derive the closed form representation for the Green function of the Hamiltonian with sharply screened Coulomb potential $V_R^{\mathcal{C}}$ and infer the asymptote from it. As to the best of our knowledge, this representation for $r, r' < R$ has been obtained here for the first time. The section 3 is devoted to studying the general case of potentials from $\mathfrak{V}(\rho,\delta)$. In the section 4 the asymptotes of the Green function are used for evaluating the short-range behavior of the solution of (6) and establishing the zero-range potentials for different values of $\rho$. Also in this section the respective pseudo-potentials are constructed. The section 5 gives concluding remarks.

## 2. Green's function for Screened Coulomb potential

The Green function is defined by the solution to the inhomogeneous equation

$$\left[-\Delta + V_R^{\mathcal{C}}(r) - k^2\right] G_R^{+}(\boldsymbol{r}, \boldsymbol{r'}, k^2) = \delta(\boldsymbol{r} - \boldsymbol{r'}). \tag{11}$$

One of the convenient ways for constructing the Green function for radial potentials is the use of the partial wave decomposition [4]. The Green function is represented then as the series in terms of Legendre polynomials $P_\ell$

$$G_R^{+}(\boldsymbol{r}, \boldsymbol{r'}, k^2) = \frac{1}{4\pi}\sum_{\ell=0}^{\infty}(2\ell+1)\frac{G_{R\ell}(r, r', k^2)}{rr'}P_\ell(\hat{\boldsymbol{r}}\cdot\hat{\boldsymbol{r}}'), \tag{12}$$

where $\hat{\boldsymbol{r}} = \boldsymbol{r}r^{-1}$. The partial Green function $G_{R\ell}$ obviously obeys the one-dimensional equation

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{\ell(\ell+1)}{r^2} + V_R^{\mathcal{C}}(r) - k^2\right] G_{R\ell}(r, r', k^2) = \delta(r - r') \tag{13}$$

with natural boundary condition $G_{R\ell} = 0$ as $r = 0$. The radiation boundary condition as $r \to \infty$ requires the outgoing wave asymptote $G_{R\ell} \propto \exp(\mathrm{i}kr - \mathrm{i}\pi\ell/2)$.

The Green function $G_{R\ell}$ can be constructed following the standard procedure [5]

$$G_{R\ell}(r, r', k^2) = -\frac{u_\ell(r_<)v_\ell(r_>)}{W(u_\ell, v_\ell)}, \tag{14}$$

where $r_> = \max\{r, r'\}$, $r_< = \min\{r, r'\}$ and $W(u_\ell, v_\ell)$ means the Wronskian of solutions to the equation

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{\ell(\ell+1)}{r^2} + V_R(r) - k^2\right] u(r) = 0. \tag{15}$$

The particular solutions $u_\ell$ and $v_\ell$ should be defined by boundary conditions $u_\ell(0) = 0$, and $v_\ell(r) \to \exp\{\mathrm{i}kr - \mathrm{i}\pi\ell/2\}$ as $r \to \infty$. The exact representations for both $u_\ell$ and $v_\ell$ depend on whether the coordinate $r$ is within or outside the interval $0 < r \le R$. These representations can be obtained by the matching technique as in [3]. For $u_\ell$ one gets

$$\begin{aligned} u_\ell(r) &= F_l(\eta, kr), \quad r \le R, \\ u_\ell(r) &= a_1\hat{j}_l(kr) + b_1\hat{n}_l(kr), \quad r > R. \end{aligned} \tag{16}$$

For $v_\ell$ the solution takes the form

$$\begin{aligned} v_\ell(r) = a_2 F_\ell(\eta, kr) + b_2 G_\ell(\eta, kr), \quad r \leq R \\ v_\ell(r) = \hat{h}^+_\ell(kr), \quad r > R. \end{aligned} \tag{17}$$

In these representations the Sommerfeld parameter $\eta$ is defined by the standard expression $\eta = V_0/(2k)$. By $\hat{j}_l$, $\hat{n}_l$ and $\hat{h}^+_\ell$ we denote the Riccati-Bessel, Riccati-Neumann and Riccati-Hankel functions which are related to the respective spherical Bessel functions as for example $\hat{j}_l(z) = z j_l(z)$. For spherical Bessel functions and for the regular $F_\ell$ and irregular $G_\ell$ Coulomb functions we use the normalization of [6]. Coefficients $a_1$, $b_1$, $a_2$ and $b_2$ should be determined in such a way that both functions $u_\ell$, $v_\ell$ and their first derivatives are continuous at $r = R$. This yields

$$\begin{aligned} a_1 = -W_R(F_\ell, \hat{n}_\ell)/k, \quad b_1 = W_R(F_\ell, \hat{j}_\ell)/k, \\ a_2 = -W_R(\hat{h}^+_\ell, G_\ell)/k, \quad b_2 = W_R(\hat{h}^+_\ell, F_\ell)/k, \end{aligned} \tag{18}$$

where $W_R$ is the Wronskian evaluated at $r = R$. Now the Wronskian $W(u_\ell, v_\ell)$ from (14) can easily be computed and takes the form

$$W(u_\ell, v_\ell) = W_R(F_l, \hat{h}^+_\ell). \tag{19}$$

Equations (14) – (19) completely determine the partial Green function $G_{R\ell}$.

For our needs of evaluating the short-range asymptotic behavior of the Green function $G_R$, if $R$ is well separated from zero, the region should be considered where $r < R$ and $r' < R$ . In this case, by inserting into (14) the quantities calculated above we finally represent the partial Green function by the sum of two terms

$$G_\ell(r, r', k^2) = \frac{1}{k} F_\ell(\eta, kr_<) H^+_\ell(\eta, kr_>) + \frac{\chi_{R\ell}(k)}{k} F_\ell(\eta, kr) F_\ell(\eta, kr'), \tag{20}$$

where $\chi_{R\ell}(k)$ is given by

$$\chi_{R\ell}(k) = -W_R(\hat{h}^+_\ell, H^+_\ell)/W_R(\hat{h}^+_\ell, F_\ell). \tag{21}$$

Here the Coulomb outgoing wave $H^+_\ell$ is introduced according to the definition $H^+_\ell = G_\ell + \mathrm{i}F_\ell$.

Now we have all components which are needed for calculating the Green function $G^+_R$ by the formula (12). In view of (20) the representation for $G^+_R$ in the region where $r, r' < R$ is given by the sum of two terms

$$G^+_R(\boldsymbol{r}, \boldsymbol{r'}, k^2) = G_{\mathcal{C}}(\boldsymbol{r}, \boldsymbol{r'}, k^2 + \mathrm{i}0) + Q_R(\boldsymbol{r}, \boldsymbol{r'}, k^2). \tag{22}$$

The first term is the conventional Coulomb Green function which is calculated by the partial wave series [4] as

$$G_{\mathcal{C}}(\boldsymbol{r}, \boldsymbol{r'}, k^2 + \mathrm{i}0) = \frac{1}{4\pi k} \sum_{\ell=0}^{\infty} (2\ell + 1) \frac{F_\ell(\eta, kr_<) H^+_\ell(\eta, kr_>)}{rr'} P_\ell(\hat{\boldsymbol{r}} \cdot \hat{\boldsymbol{r}}'). \tag{23}$$

The second term $Q_R$ reads

$$Q_R(\boldsymbol{r},\boldsymbol{r'},k^2) = \frac{1}{4\pi k}\sum_{\ell=0}^{\infty}(2\ell+1)\chi_{R\ell}(k)\frac{F_\ell(\eta,kr)F_\ell(\eta,kr')}{rr'}P_\ell(\hat{\boldsymbol{r}}\cdot\hat{\boldsymbol{r}}'). \tag{24}$$

The last formula can be rewritten in terms of the Coulomb Green functions taken on the upper and lower rims of the cut along the positive real semi axis of the complex energy plane. This can be made by using the formula $F_\ell = (H^+_\ell - H^-_\ell)/(2\mathrm{i})$ and the method of the paper [3]. The result reads

$$Q_R(\boldsymbol{r},\boldsymbol{r}') = \frac{1}{2\mathrm{i}}\int_{-1}^{1} \mathrm{d}\zeta\, Z_R(\xi,\zeta)[G_{\mathcal{C}}(r,r',\zeta,k^2+\mathrm{i}0) - G_{\mathcal{C}}(r,r',\zeta,k^2-\mathrm{i}0)]. \tag{25}$$

Here the parameter $\xi$ is defined as $\xi = \hat{\boldsymbol{r}}\cdot\hat{\boldsymbol{r'}}$. The kernel $Z_R$ is given by the decomposition in Legendre polynomials

$$Z_R(\xi,\zeta) = \sum_{\ell=0}^{\infty}(\ell+1/2)\chi_{R\ell}(k)P_\ell(\xi)P_\ell(\zeta). \tag{26}$$

As it may be seen from the Hostler representation [7], the Coulomb Green function $G_R(\boldsymbol{r},\boldsymbol{r'},z)$ actually depends on $r$, $r'$ and the angle between vectors $\boldsymbol{r}$ and $\boldsymbol{r'}$ through the expression $\hat{\boldsymbol{r}}\cdot\hat{\boldsymbol{r'}}$. We have reflected this fact in notations in the integrand of (25) where $\zeta$ stands for $\hat{\boldsymbol{r}}\cdot\hat{\boldsymbol{r'}}$. The formulae (20-26) are valid only in that part of configuration space where $r, r' < R$. Nevertheless, this representation of the Green function in that region completely defines the transition operator $T_R(z) = V_R - V_R G_R(z) V_R$ . Indeed, with (22) the operator $T_R$ takes the form

$$T_R(z) = V_R - V_R G_{\mathcal{C}}(z) V_R - V_R Q_R(z) V_R. \tag{27}$$

It is interesting to see what is the consequence of (27) when $R \to \infty$. Evaluating the right hand side of (21) asymptotically when $kR \gg \ell(\ell+1)$ and $kR \gg \ell(\ell+1)+\eta^2$ [8] we come to the expression for $\chi_{R\ell}(k)$

$$\chi_{R\ell}(k) = \mathrm{i}\eta\exp(2\mathrm{i}\theta_\ell)/(kR) + \mathcal{O}(1/R^2), \tag{28}$$

where $\theta_\ell = kR - \eta\log(2kR) - \pi\ell/2 + \sigma_\ell$ and $\sigma_\ell = \arg\Gamma(\ell+1+\mathrm{i}\eta)$ is the Coulomb phase shift. From (26) we have for the $L_2(-1,1)$ norm of the kernel $Z_R$

$$\|Z_R\| = \max_\ell|\chi_{R\ell}(k)| = \eta/(kR) + \mathcal{O}(R^{-2}). \tag{29}$$

Hence, the last term in (27) is negligible when $R \to \infty$ and therefore

$$T_R(z) = V_R - V_R G_{\mathcal{C}}(z) V_R + \mathcal{O}(R^{-1}). \tag{30}$$

This can be used for calculating the limit of $T_R$ when $R \to \infty$ and it will be done in another publication.

In the last part of this section we calculate the asymptote of $G^{+}(\boldsymbol{r},0,k^2)$ when $r\to 0$. We start from the second term in (22). Since [8]

$$F_\ell(\eta,x)=C_\ell(\eta)x^{\ell+1}\left(1+\eta x/(\ell+1)+\mathcal{O}(x^2)\right), \tag{31}$$

as $x\to 0$, the leading order behavior of $Q_R$ reads

$$Q_R(\boldsymbol{r},0,k^2)=C_0(\eta)\chi_{R0}(k)F_0(\eta,kr)/(4\pi r)+\mathcal{O}(kr) \tag{32}$$

as $kr\to 0$. From this it is seen that $Q_R(\boldsymbol{r},0,k^2)$ has the finite limit

$$\lim_{r\to 0}Q_R(\boldsymbol{r},0,k^2)=kC_0^2(\eta)\chi_{R0}(k)/(4\pi), \tag{33}$$

where $C_0^2(\eta)=2\pi\eta(e^{2\pi\eta}-1)^{-1}$. This analysis shows us that the singular behavior of $G_R^{+}(\boldsymbol{r},0,k^2)$ at small $r$ comes exclusively from the first term in (22), i.e. from the Coulomb Green function, which as $r\to 0$ has the asymptote [2]

$$G_{\mathcal{C}}(\boldsymbol{r},0,k^2+\mathrm{i}0)=\frac{1}{4\pi}\left[1/r+V_0\log r\right]+C(k)+\mathcal{O}(r\ln r). \tag{34}$$

Here $C(k)$ is given by

$$C(k)=\frac{\mathrm{i}k}{4\pi}+\frac{V_0}{4\pi}\left[\log(-2\mathrm{i}k)+\psi\left(1+\mathrm{i}\eta\right)+2\gamma_0-1\right], \tag{35}$$

where $\gamma_0$ is the Euler-Mascheroni constant and $\psi(z)$ is the digamma function [8].

Collecting together the expressions obtained above we arrive at the following result on the short-range behavior of the Green function $G_R^{+}$

$$G_R^{+}(\boldsymbol{r},0,k^2)=\frac{1}{4\pi}\left[1/r+V_0\log r\right]+C(k)+\frac{kC_0^2(\eta)\chi_{R0}(k)}{4\pi}+\mathcal{O}(r\ln r). \tag{36}$$

This completes our study of the Green function for the sharply screened Coulomb potential. It is apparent that in this case the zero-range potential will be identical to that of the case of the pure Coulomb potential [2].

## 3. Green's function behavior in the case of $\mathfrak{V}(\rho,\delta)$ class potentials

In this section we study the Green function short-range asymptote for potentials of the $\mathfrak{V}(\rho,\delta)$ class. The Lippmann-Schwinger integral equation

$$G^{+}(\boldsymbol{r},\boldsymbol{r}',k^2)=G_0^{+}(\boldsymbol{r},\boldsymbol{r}',k^2)-\int \mathrm{d}\boldsymbol{q}\, G_0^{+}(\boldsymbol{r},\boldsymbol{q},k^2)V(\boldsymbol{q})G^{+}(\boldsymbol{q},\boldsymbol{r}',k^2) \tag{37}$$

with

$$G_0^{+}(\boldsymbol{r},\boldsymbol{r}',k^2)=\frac{1}{4\pi}\frac{\exp(\mathrm{i}k|\boldsymbol{r}-\boldsymbol{r}'|)}{|\boldsymbol{r}-\boldsymbol{r}'|} \tag{38}$$

in this case has the unique solution [4, 9] which completely defines the Green function $G^+(k^2)$ . For our purpose of evaluating the short-range behavior we set $\boldsymbol{r'}=0$ and iterate (37) one time which results

$$G^+(\boldsymbol{r},0,k^2) = G_0^+(\boldsymbol{r},0,k^2) - \int \mathrm{d}\boldsymbol{q}\, G_0^+(\boldsymbol{r},\boldsymbol{q},k^2)V(\boldsymbol{q})G_0^+(\boldsymbol{q},0,k^2) + \int \mathrm{d}\boldsymbol{q}\, G_0^+(\boldsymbol{r},\boldsymbol{q},k^2)V(\boldsymbol{q}) \int \mathrm{d}\boldsymbol{q'} G_0^+(\boldsymbol{q},\boldsymbol{q'},k^2)V(\boldsymbol{q'})G^+(\boldsymbol{q'},0,k^2). \tag{39}$$

Now we consecutively consider the short-range behavior of right hand side terms. The first term asymptote as $r\to 0$ is obvious

$$G_0^+(\boldsymbol{r},0,k^2) = \frac{1}{4\pi r} + \frac{\mathrm{i}k}{4\pi} + \mathcal{O}(r). \tag{40}$$

For evaluating the second term on the right hand side of (39) it is useful to split the integral into two parts in order to separate the short-range and long-range contributions of the integrand. Let us consider the integrals

$$I_j(\boldsymbol{r}) = \int_{\Omega_j} \mathrm{d}\boldsymbol{q}\, G_0^+(\boldsymbol{r},\boldsymbol{q},k^2)V(\boldsymbol{q})G_0^+(\boldsymbol{q},0,k^2) \tag{41}$$

over domains $\Omega_j \in \mathbb{R}^3$ defined as $\Omega_{1(2)} = \{\boldsymbol{q} : q < (>) r_0\}$. The radius $r_0$ can be chosen as any positive bounded number well separated from zero and will be specified below.

For the integral $I_1(\boldsymbol{r})$ we can expand the Green function factors of the integrand by using the Taylor decomposition up to quadratic terms as

$$G_0^+(\boldsymbol{r},\boldsymbol{q},k^2) = 1/(4\pi|\boldsymbol{r}-\boldsymbol{q}|) + \mathrm{i}k/(4\pi) + \mathcal{O}(|\boldsymbol{r}-\boldsymbol{q}|^2) \tag{42}$$

and similar expression holds for $G_0^+(\boldsymbol{q},0,k^2)$ with $\boldsymbol{r}$ set to 0. For the potential $V(\boldsymbol{q})$ in $\Omega_1$ we assume that $r_0$ is chosen such that the formula (3) can be used and the $W(\boldsymbol{q})$ factor can be given by its Taylor decomposition

$$W(\boldsymbol{q}) = V_0 + \boldsymbol{q}\cdot\nabla W(0) + \mathcal{O}(q^2). \tag{43}$$

Then the most singular term of $I_1(\boldsymbol{r})$ as $r\to 0$ will be generated by introducing in (41) with $j=1$ the leading terms of integrand constituents which are defined by (42) and (43). This will lead us to the integral

$$I_1^s(\boldsymbol{r}) = V_0/(4\pi)^2 \int_{\Omega_1} \mathrm{d}\boldsymbol{q}\, |\boldsymbol{r}-\boldsymbol{q}|^{-1}\, q^{-\rho-1}. \tag{44}$$

Since we need to find the short-range behavior of this integral when $r\to 0$ we can always take $r$ such that $r<r_0$. In this case the evaluation of the integral in (44) is easy to perform with the help of the formula

$$\frac{1}{|\boldsymbol{q}-\boldsymbol{q'}|} = \frac{1}{q_>}\sum_{\ell=0}^{\infty} \frac{q_<^\ell}{q_>^\ell} P_\ell\left(\hat{\boldsymbol{q}}\cdot\hat{\boldsymbol{q}}'\right), \tag{45}$$

where as usual $q_> = \max\{q, q'\}$ and $q_< = \min\{q, q'\}$. The results fall naturally into two cases, i.e. if $\rho \neq 1$ it reads

$$I_1^s(\boldsymbol{r}) = \frac{V_0}{4\pi(2-\rho)(\rho-1)} r^{-\rho+1} + \frac{V_0}{4\pi(1-\rho)} r_0^{-\rho+1} \tag{46}$$

and when $\rho = 1$ the integral $I_1^s$ takes the form

$$I_1^s(\boldsymbol{r}) = -\frac{V_0}{4\pi}\log(r) + \frac{V_0}{4\pi}[1 + \log(r_0)]. \tag{47}$$

From (46) it is seen that if $1 < \rho < 2$ then $I_1^s$ has the polar singularity $r^{-\rho+1}$ whereas if $\rho < 1$ the first term in (46) vanishes as $r \to 0$ and $I_1^s$ is regular and has a finite limit. From this analysis of the integral (44) it becomes clear that taking into account the less singular terms in the expressions for the integrand of the integral $I_1(\boldsymbol{r})$ one will obtain non singular contributions as $r \to 0$.

Let us now consider the integral $I_2(\boldsymbol{r})$. For the modulus of $I_2(\boldsymbol{r})$ we can easily arrive at the inequality

$$|I_2(\boldsymbol{r})| \leq \frac{1}{(4\pi)^2} \int_{\Omega_2} \mathrm{d}\boldsymbol{q}\, \frac{|V(\boldsymbol{q})|}{q\,|\boldsymbol{r}-\boldsymbol{q}|}. \tag{48}$$

Let us now suppose that $r_0$ is chosen such that the inequality (2) can be used for $q > r_0$ then with the help of (45) the right hand side of (48) can be estimated as

$$\int_{\Omega_2} \mathrm{d}\boldsymbol{q}\, \frac{|V(\boldsymbol{r})|}{q\,|\boldsymbol{r}-\boldsymbol{q}|} \leq C \int_{r_0}^{\infty} \mathrm{d}q\, (1+q)^{-1-\delta}. \tag{49}$$

Since the last integral converges, the integral $I_2(\boldsymbol{r})$ is uniformly bounded for all $\boldsymbol{r}$ such that $r < r_0$.

It remains to estimate the last third term in (39). The inner integral over $\boldsymbol{q}'$ by its structure is quite similar to the integrals considered above if $G_0^+(\boldsymbol{q}', 0, k^2)$ replaces $G^+(\boldsymbol{q}', 0, k^2)$. In this case the inner integral as the function of $\boldsymbol{q}$ may have a singularity that is not stronger than $q^{-\rho+1}$ one. As it has been already shown such a singularity in the integrand of the outer integral over $\boldsymbol{q}$ will lead to the nonsingular behavior of the result as the function of $\boldsymbol{r}$ in the vicinity of the point $\boldsymbol{r} = 0$. On using the iterative arguments this result can easily be extended on the case of the actual integrand in the third term of (39) [9]. Thus, the last term in (39) should have a finite limit as $r \to 0$.

Collecting the results obtained in this section we formulate the final statement about the short-range behavior of the function $G^+(\boldsymbol{r}, 0, k^2)$ for the case of $1 < \rho < 2$ as

$$G^+(\boldsymbol{r}, 0, k^2) = \frac{1}{4\pi}\left[1/r + A_0/r^{\rho-1}\right] + B_1 + o(1), \tag{50}$$

for the case of $\rho = 1$ as

$$G^+(\boldsymbol{r}, 0, k^2) = \frac{1}{4\pi}\left[1/r + V_0 \log(r)\right] + B_2 + o(1), \tag{51}$$

and for the case of $\rho < 1$ as

$$G^{+}(\boldsymbol{r},0,k^2) = \frac{1}{4\pi r} + B_3 + o(1). \tag{52}$$

Here the constant $A_0$ is given by

$$A_0 = \frac{V_0}{(2-\rho)(1-\rho)}$$

and all finite contributions from respective integrals are denoted by $B_j$, $j = 1,2,3$.

## 4. Application to zero-range potential formalism

The zero-range potential is introduced by implementation of a special singular boundary condition on the solution of the Schrödinger equation at small inter-particle distances [1]. This boundary condition can be enforced [2] if the delta functional term is inserted into equation (6). In this case the solution is represented by

$$\phi(\boldsymbol{r},\boldsymbol{k}) = \phi_0(\boldsymbol{r},\boldsymbol{k}) - \lambda G^{+}(\boldsymbol{r},0,k^2)\beta. \tag{53}$$

Here $\phi_0$ is defined according to (8, 9). Since the asymptotic behavior of Green's function has been studied in details in preceding section it remains to estimate the short range behavior of $\phi_0$. It can be done on the basis of the Lippmann-Schwinger integral equation

$$\phi_0(\boldsymbol{r},\boldsymbol{k}) = \exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}) - \int \mathrm{d}\boldsymbol{q}\, G_0^{+}(\boldsymbol{r},\boldsymbol{q},k^2)V(\boldsymbol{q})\phi_0(\boldsymbol{q},\boldsymbol{k}). \tag{54}$$

It is easy to see that for a potential $V \in \mathfrak{V}(\rho,\delta)$ with $\rho < 2$, $\delta > 1$ any iteration of (54) is bounded function with a finite limit at $\boldsymbol{r} = 0$ and so is the solution. For completeness let us show this for the first iteration which we represent as the sum of two integrals $J_1$ and $J_2$ defined by

$$J_j(\boldsymbol{r}) = \int_{\Omega_j} \mathrm{d}\boldsymbol{q}\, G_0^{+}(\boldsymbol{r},\boldsymbol{q},k^2)V(\boldsymbol{q})\exp(\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{k}), \quad j = 1,2. \tag{55}$$

As in the previous section, we can obtain the following estimate for the modulus of $J_2(\boldsymbol{r})$ for all $r$ such that $r < r_0$

$$|J_2(\boldsymbol{r})| \le \frac{C}{4\pi}\int_{\Omega_2} \mathrm{d}\boldsymbol{q}\; q^{-1}(1+q)^{-1-\delta}. \tag{56}$$

The integral on the right hand side of (56) converges. Thus, $J_2(\boldsymbol{r})$ is uniformly bounded in the neighborhood of the origin. The integral $J_1(\boldsymbol{r})$ can be treated by similar method which was used in the previous section for the integral $I_1(\boldsymbol{r})$. In particular, if the most singular terms in the integrand are kept then the leading order of the integral $J_1(\boldsymbol{r})$ takes the form

$$J_1(\boldsymbol{r}) \sim \frac{V_0}{(4\pi)^2} \int_{\Omega_1} \mathrm{d}\boldsymbol{q}\, |\boldsymbol{r}-\boldsymbol{q}|^{-1} q^{-\rho}. \tag{57}$$

The integral on the right hand side of this formula coincides with the integral from (44) if there $\rho+1$ is replaced by $\rho$. Then from the analysis made in the previous section it follows that the integral $J_1(\boldsymbol{r})$ is regular as $r \to 0$. As the result we can conclude that for the potentials of the class $\mathfrak{V}(\rho,\delta)$ the short-range asymptote of the wave function $\phi_0(\boldsymbol{r},\boldsymbol{k})$ is regular as $r \to 0$ and therefore $\phi_0(\boldsymbol{r},\boldsymbol{k})$ has a finite limit at the origin.

The singular behavior of the full solution $\phi$ is therefore completely determined by the singularities of the Green function. Accordingly, we have the three following cases of wave function asymptotes depending on the value of $\rho$. If $2 > \rho > 1$ the asymptote is of the form

$$\phi(\boldsymbol{r},\boldsymbol{k}) = \frac{\alpha_1}{4\pi}\left[1/r + A_0/r^{\rho-1}\right] + \beta_1 + o(1). \tag{58}$$

For the case of $\rho = 1$ it is given by

$$\phi(\boldsymbol{r},\boldsymbol{k}) = \frac{\alpha_2}{4\pi}\left[1/r + V_0 \log(r)\right] + \beta_2 + o(1), \tag{59}$$

and for the case of $\rho < 1$ the asymptote reads

$$\phi(\boldsymbol{r},\boldsymbol{k}) = \frac{\alpha_3}{4\pi r} + \beta_3 + o(1). \tag{60}$$

Here the constants are given by following expressions

$$A_0 = \frac{V_0}{(2-\rho)(1-\rho)},$$

$\alpha_j = -\lambda\beta_j$ and $\beta_j = \phi_0(0,\boldsymbol{k}) - \lambda B_j \beta_j$ for $j = 1,2,3$. The case of $\rho = 1$ completely coincides with the case of the zero-range potential for the Coulomb potential [2].

Alternatively, the zero range potential is defined by the pseudo-potential. Following the procedure described in the paper [2] the form of the pseudo-potential is calculated from the asymptotic expansions (58-60). For all three cases the pseudo-potential may be given by the uniform representation

$$\lambda W_j(\boldsymbol{r}) = \lambda\delta(\boldsymbol{r})\frac{\mathrm{d}}{\mathrm{d}\omega_j}\omega_j \tag{61}$$

with variables $\omega_j$ determined by formulae

$$1/\omega_1 = r^{-1} + A_0 r^{-\rho+1}, \tag{62}$$

$$1/\omega_2 = r^{-1} + V_0 \log(r), \tag{63}$$

$$1/\omega_3 = r^{-1}. \tag{64}$$

## 5. Conclusion

We have shown that the Green function of a Hamiltonian with a potential possessing singular behavior $\mathcal{O}(r^{-\rho})$ at small inter-particle distances has an additional singularity $\mathcal{O}(r^{-\rho+1})$ except for the case of $\rho = 1$ when the logarithmic singularity appears. We have considered the class $\mathfrak{V}(\rho, \delta)$ of potentials with $\rho < 2$ and $\delta > 1$. This choice of parameters is not exhaustive especially for $\delta$. With little effort the weaker condition $\delta > 0$ can easily be implemented in the theory by performing more delicate estimations for integrals $I_2$ and $J_2$ treated as not absolutely convergent. We have left out such an analysis in order not to make the paper too long.

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## References

[1] Albeverio S., Gesztesy F., Hoegh-Krohn R., Holden H., *Solvable Models in Quantum Mechanics.* 2005, AMS Chelsea Publishing: Providence, RI

[2] Yakovlev S.L., Gradusov V.A. *Zero-range potential for particles interacting via Coulomb potential.* J. Phys. A 2012, **46**, 035307, 15pp.

[3] Yakovlev S.L., Volkov M.V., Yarevsky E., Elander N. *The impact of sharp screening on the Coulomb scattering problem in three dimensions.* J. Phys. A 2010, **43**, 245302, 14pp.

[4] Newton R.G. *Scattering Theory of Waves and Particles.* 1982, Springer-Verlag: New York

[5] Titchmarsh E.C. *Eigenfunction Expansions Associated with Second-order Differential Equations. Part 1.* 1962, Oxford at the Clarendon Press: London

[6] Messiah A. *Quantum Mechanics. Vol. 1.* 1962, J Willey and Sons, Inc.: New-York

[7] Hostler L. *Coulomb Green's Functions and the Furry Approximation.* J. Math. Phys. 1964, **5**, pp. 591-611

[8] Abramowitz M., Stegun I. *Handbook of Mathematical Functions.* 1964, National Bureau of Standards: Washington, D.C.

[9] Povzner A.Ya. *On the expansion of arbitrary functions in characteristic functions of the operator* $-\Delta u + cu$. Matem. Sbornik 1953, **32(74)**, pp. 109-156