Brief Reports

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Green's function and propagator for the one-dimensional δ-function potential

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A particle in a one-dimensional δ-function potential possesses both discrete and continuum solutions. The configuration-space Green's function and propagator for this problem are derived by explicit summation over the spectrum of eigenstates. The momentum-space Green's function is also obtained. The propagator does not contain the classical action function in any simple way, in contrast to the usual structure in Feynman's path-integral formalism. Various analogies between the δ-function and Coulomb problems are discussed.

I. INTRODUCTION

A particle moving in an attractive one-dimensional δ-function potential, variously known as a one-dimensional hydrogen atom or a "deltahydrogen" atom, constitutes the simplest quantum-mechanical problem admitting both discrete and continuum solutions. The Schrödinger equation in atomic units ($\hbar=m=e=1$) has the form

$$\left[-\frac{1}{2}\frac{d^2}{dx^2}-Z\delta(x)\right]\psi(x)=E\psi(x) . \tag{1}$$

A δ function scales in the same way as a Coulomb potential, i.e., $V(\lambda x)=\lambda^{-1}V(x)$ for both $\delta(x)$ and $|x|^{-1}$, and has been used as a one-dimensional analog of the Coulomb potential.[1,2] The solutions to Eq. (1) have been discussed by a number of authors.[3–5]

There is but one bound state,

$$\psi_0(x)=Z^{1/2}e^{-Z|x|}, \quad E_0=-Z^2/2 , \tag{2}$$

resembling a hydrogenic 1*s* orbital. To derive the continuum solutions, consider the superposition of a free-particle wave incident from the left, e^{ikx} (or from the right, e^{-ikx}) with a wave scattered by the δ-function potential, $e^{ik|x|}$. These respective solutions can be written

$$\psi_k^{\pm}(x)=\frac{1}{\sqrt{2\pi}}[e^{\pm ikx}+f(k)e^{ik|x|}], \quad k>0 . \tag{3}$$

Substitution into Eq. (1), recalling that $\frac{1}{2}(d^2/dx^2)|x|=\delta(x)$, identifies the scattering amplitude,

$$f(k)=-Z/(Z+ik) , \tag{4}$$

with the energy eigenvalues $E_k=k^2/2$. Note that the pole of the scattering amplitude, at $k=-iZ$, corresponds to the bound state, with the residue proportional to $\psi_0(x)$. Alternative continuum eigenfunctions are the even and odd standing waves,

$$\psi_k^{\text{odd}}(x)=\pi^{-1/2}\sin(kx) ,$$
$$\psi_k^{\text{even}}(x)=[\pi(k^2+Z^2)]^{-1/2}[k\cos(kx)-Z\sin(k|x|)] . \tag{5}$$

The eigenfunctions in the form (3) are δ-function normalized,

$$\langle\psi_{k'}^{\pm}|\psi_k^{\pm}\rangle=\delta(k-k'), \quad \langle\psi_{k'}^{\pm}|\psi_k^{\mp}\rangle=0. \tag{6}$$

For derivation of the Green's functions, we will require the density matrix

$$\rho_0(x,y)=\psi_0(x)\psi_0(y)=Ze^{-ZX}, \quad X\equiv|x|+|y| , \tag{7}$$

and

$$\begin{aligned}\rho_k(x,y)&=\psi_k^+(x)[\psi_k^+(y)]^*+\psi_k^-(x)[\psi_k^-(y)]^*\\&=\psi_k^{\text{odd}}(x)\psi_k^{\text{odd}}(y)+\psi_k^{\text{even}}(x)\psi_k^{\text{even}}(y)\\&=\rho_k^1(x,y)+\rho_k^2(x,y)+\rho_k^3(x,y) ,\end{aligned} \tag{8}$$

with

$$\rho_k^1(x,y)=\frac{1}{\pi}\cos[k(x-y)] , \tag{9}$$

$$\rho_k^2(x,y)=-\frac{1}{\pi}\frac{Z^2}{Z^2+k^2}\cos(kX) , \tag{10}$$

$$\rho_k^3(x,y)=-\frac{1}{\pi}\frac{Zk}{Z^2+k^2}\sin(kX) . \tag{11}$$

The term (9) corresponds to the free particle. One can readily demonstrate the closure property, showing the completeness of the above set of eigenfunctions,[3,6]

$$\rho_0(x,y)+\int_0^\infty \rho_k(x,y)dk=\delta(x-y)\ . \tag{12}$$

II. GREEN'S FUNCTIONS

The configuration-space Green's function can be obtained by explicit summation over eigenstates,

$$G^+(x,y,\lambda)=\frac{\rho_0(x,y)}{\frac{1}{2}\lambda^2+\frac{1}{2}Z^2}+\int_0^\infty \frac{\rho_k(x,y)}{\frac{1}{2}\lambda^2-\frac{1}{2}k^2}dk,\quad \mathrm{Im}\lambda>0\ . \tag{13}$$

The contribution from the terms (9)–(11) are evaluated by contour integration along the real axis closed by an infinite semicircle in the upper half of the complex plane, as follows:

$$\frac{2}{\pi}\int_0^\infty \frac{\cos[k(x-y)]dk}{\lambda^2-k^2}=\frac{1}{\pi}\oint \frac{e^{ik|x-y|}dk}{\lambda^2-k^2}=\frac{e^{i\lambda|x-y|}}{i\lambda}\ , \tag{14}$$

$$-\frac{2Z^2}{\pi}\int_0^\infty \frac{\cos(kX)dk}{(Z^2+k^2)(\lambda^2-k^2)}=-\frac{Z^2}{\pi}\oint \frac{e^{ikX}dk}{(Z^2+k^2)(\lambda^2-k^2)}=-\frac{Ze^{-ZX}}{\lambda^2+Z^2}+\frac{iZ^2}{\lambda}\frac{e^{i\lambda X}}{\lambda^2+Z^2}\ , \tag{15}$$

$$-\frac{2Z}{\pi}\int_0^\infty \frac{k\sin(kX)dk}{(Z^2+k^2)(\lambda^2-k^2)}=\frac{iZ}{\pi}\oint \frac{ke^{ikX}dk}{(Z^2+k^2)(\lambda^2-k^2)}=-\frac{Ze^{-ZX}}{\lambda^2+Z^2}+\frac{Ze^{i\lambda X}}{\lambda^2+Z^2}\ . \tag{16}$$

Adding these together, we find that the contribution of the discrete spectrum is exactly cancelled, just as in the case of the Coulomb Green's function.[7,8] With reversion to k as the wave-number variable, the deltahydrogen Green's function works out to

$$G^+(x,y,k)=\frac{1}{ik}\left[e^{ik|x-y|}-\frac{Z}{Z+ik}e^{ik(|x|+|y|)}\right]\ . \tag{17}$$

This result can alternatively be obtained from Sturm-Liouville theory, whereby the solution to

$$\left[\frac{k^2}{2}+\frac{1}{2}\frac{d^2}{dx^2}+Z\delta(x)\right]G^+(x,y,k)=\delta(x-y) \tag{18}$$

is given by

$$G^+(x,y,k)=\frac{2u(y)v(x)}{u(x)v'(x)-v(x)u'(x)}\ . \tag{19}$$

For the case $x>y>0$, we use

$$v(x)=e^{ikx},\quad u(y)=e^{-iky}+f(k)e^{iky}\ . \tag{20}$$

Thus

$$G^+(x,y,k)=(ik)^{-1}e^{ikx}[e^{-iky}+f(k)e^{iky}]\ , \tag{21}$$

in agreement with (17).

The deltahydrogen and Coulomb Green's functions show remarkable structural analogies. As shown originally by Hostler,[7] the three-dimensional Coulomb Green's function can be represented in the form[8,9]

$$G^+(\mathbf{r}_1,\mathbf{r}_2,k)=-[\pi(x-y)]^{-1}\left[\frac{\partial}{\partial x}-\frac{\partial}{\partial y}\right]g^+(x,y,k)\ , \tag{22}$$

with

$$g^+(x,y,k)=(ik)^{-1}\Gamma(1-i\nu)M_{i\nu}^{1/2}(-iky)\times W_{i\nu}^{1/2}(-ikx)\ , \tag{23}$$

in terms of the variables

$$x\equiv r_1+r_2+r_{12},\quad y\equiv r_1+r_2-r_{12},\quad \nu\equiv Z/k\ . \tag{24}$$

The function $g^+(x,y,k)$ is a solution of the quasi-one-dimensional Coulomb problem

$$\left[\frac{k^2}{4}+\frac{d^2}{dx^2}+\frac{Z}{x}\right]g^+(x,y,k)=\delta(x-y),\quad 0\le y\le x\le\infty\ . \tag{25}$$

Using formulas given by Buchholz,[10] the asymptotic forms of the Whittaker functions M and W as $x,y\to\infty$ imply

$$g^+(x,y,k)\sim(ik)^{-1}\exp(ikx/2+i\nu\ln kx)\times\left[\exp(-iky/2-i\nu\ln ky)-\frac{\Gamma(1-i\nu)}{\Gamma(1+i\nu)}\exp(iky/2+i\nu\ln ky)\right],\quad x,y\to\infty \tag{26}$$

somewhat resembling the deltahydrogen Green's function (21).

The momentum-space Green's function can be obtained by Fourier transformation of (17),

$$G(p,p',E)=\frac{1}{2\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}G(x,y,E)e^{-ipx}e^{ip'y}dx\,dy\ . \tag{27}$$

Noting that $\mathrm{Im}k>0$ in carrying out the integrations, we obtain

$$G(p,p',E)=\frac{\delta(p-p')}{E-T}-\frac{1}{2\pi}\frac{Z}{Z+ik}\frac{ik}{(E-T)(E-T')}\ ,\quad E\equiv k^2/2,\quad T\equiv p^2/2\ . \tag{28}$$

The first term represents the free-particle Green's function while the residue at $k=-iZ$ identifies the ground-state momentum-space eigenfunction,[11]

$$\phi_0(p)=\left[\frac{2}{\pi}\right]^{1/2}\frac{Z^{3/2}}{p^2+Z^2}\ . \tag{29}$$

For comparison with (28) we give a representation of the momentum-space Coulomb Green's function derived by Schwinger,[12]

$$G(p,p',E)=\frac{\delta(p-p')}{E-T}-\frac{Z}{2\pi^2}\frac{I}{(E-T)(E-T')}\ , \quad (30)$$

where I is a complicated definite integral which we need not enumerate.

III. DELTAHYDROGEN PROPAGATOR

Goovaerts *et al.*[4] had earlier considered the δ-function potential in the context of Feynman's path-integral formalism. We will now evaluate the propagator for this problem, again by summation over eigenstates,

$$K(x,y,t)=\rho_0(x,y)e^{iZ^2t/2}+\int_0^\infty \rho_k(x,y)e^{-ik^2t/2}dk\ . \quad (31)$$

This result is equivalent to Fourier transformation of the Green's function using

$$K=\frac{i}{2\pi}\int_{-\infty}^{\infty}(G^+-G^-)e^{-iEt}dE\ . \quad (32)$$

The following integrals are required:[13]

$$\int_0^\infty \frac{\cos(kX)}{Z^2+k^2}e^{-\beta k^2}dk=\frac{\pi}{4Z}e^{\beta Z^2}[2\cosh(ZX)-e^{-ZX}\mathrm{erf}(Z\sqrt{\beta}-X/2\sqrt{\beta})-e^{ZX}\mathrm{erf}(Z\sqrt{\beta}+X/2\sqrt{\beta})] \quad (33)$$

and

$$\int_0^\infty \frac{k\sin(kX)}{Z^2+k^2}e^{-\beta k^2}dk=-\frac{\pi}{4}e^{\beta Z^2}[2\sinh(ZX)+e^{-ZX}\mathrm{erf}(Z/\sqrt{\beta}-X/2\sqrt{\beta})-e^{ZX}\mathrm{erf}(Z\sqrt{\beta}+X/2\sqrt{\beta})]\ . \quad (34)$$

Note that

$$1+\mathrm{erf}(-u)=1-\mathrm{erf}(u)=\mathrm{erfc}(u)\ . \quad (35)$$

Identifying β with $it/2$ and defining

$$u\equiv X/2\sqrt{\beta}-Z\sqrt{\beta}=(|x|+|y|)/\sqrt{2it}-Z\sqrt{it/2}\ , \quad (36)$$

the propagator works out to

$$K(x,y,t)=K^0(x,y,t)+\frac{Z}{2}e^{-ZX}e^{iZ^2t/2}\mathrm{erfc}(u)$$
$$=K^0(x,y,t)+\frac{Z}{2}\exp[i(|x|+|y|)^2/2t]\times e^{u^2}\mathrm{erfc}(u)\ , \quad (37)$$

in which K^0 is the free-particle propagator

$$K^0(x,y,t)=(2\pi it)^{-1/2}\exp[i(x-y)^2/2t]\ . \quad (38)$$

It can be verified that (37) satisfies the time-dependent Schrödinger equation

$$\left[i\frac{\partial}{\partial t}+\frac{1}{2}\frac{\partial^2}{\partial x^2}+Z\delta(x)\right]K(x,y,t)=0\ , \quad (39)$$

with the initial condition $K(x,y,0)=\delta(x-y)$.

The function of u in (37) can alternatively be expressed as follows:[14]

$$e^{u^2}\mathrm{erfc}(u)=-\frac{i}{\pi}\int_{-\infty}^{\infty}\frac{e^{-z^2}dz}{z-iu}=\frac{2u}{\pi}\int_0^\infty\frac{e^{-z^2}dz}{z^2+u^2}$$
$$=\sum_{n=0}^{\infty}\frac{(-u)^n}{\Gamma\left[\frac{n}{2}+1\right]}=\frac{1}{\sqrt{\pi}}U(\tfrac{1}{2},\tfrac{1}{2},u^2)$$
$$\sim\frac{1}{\sqrt{\pi}}u^{-1}\sum_{n=0}^{\infty}(-1)^n(\tfrac{1}{2})_n u^{-2n}\ , \quad (40)$$

where U is a confluent hypergeometric function of the second kind.

Again, we compare (37) with the asymptotic form of the Coulomb propagator:[15]

$$K(x,y,t)\sim(2\pi it)^{-3/2}\exp\left[\frac{i(x-y)^2}{8t}+\frac{2iZt}{x-y}\ln\left[\frac{x}{y}\right]\right]$$
$$-\frac{Z}{\pi^2}\frac{(2\pi it)^{1/2}}{(x+y)xy}\times\exp\left[\frac{i(x+y)^2}{8t}+\frac{2iZt}{x+y}\ln(xy)\right]\ . \quad (41)$$

In contrast to the case when the Hamiltonian is a quadratic form in generalized coordinates and momenta, the deltahydrogen propagator does *not* exhibit the canonical structure in Feynman's path-integral formalism,[16]

$$K(q_1,q_2,t)=F(t)\exp[iS(q_1,q_2,t)]\ . \quad (42)$$

Here S represents the classical action function, a solution of the corresponding Hamilton-Jacobi equation. In other nonquadratic cases which we recently considered,[17] the propagator still contains S in a slightly disguised form. For example, the radial propagator for the two-dimensional harmonic oscillator is given by

$$K_m(\rho_1,\rho_2,t)=(-i)^m\rho_1\rho_2\omega\csc(\omega t)\times\exp[\tfrac{1}{2}i\omega(\rho_1^2+\rho_2^2)\cot(\omega t)]\times J_m[\omega\rho_1\rho_2\csc(\omega t)]\ , \quad (43)$$

whereby the corresponding action is

$$S(\rho_1,\rho_2,t)=\tfrac{1}{2}\omega(\rho_1^2+\rho_2^2)\cot(\omega t)-\omega\rho_1\rho_2\csc(\omega t)\ . \quad (44)$$

In Sec. IV we will derive the action function for deltahydrogen. Evidently, the deltahydrogen propagator does not make use of this function in any direct way. From another point of view, the structure of (37) does suggest a sum containing two alternative classical trajectories, an idea discussed by Crandall.[18]

IV. DELTAHYDROGEN ACTION FUNCTION

In the context of quantum-mechanical propagators, the action function denotes the integral of the Lagrangian over a classically allowed trajectory, viz.,

$$S(x,y,t)=\int_{y,0}^{x,t}L(x',t')dt' \ . \tag{45}$$

This is called Hamilton's principal function in classical dynamics. S is a solution of the Hamilton-Jacobi equation

$$\frac{\partial S}{\partial t}+\frac{1}{2}\left[\frac{\partial S}{\partial x}\right]^2-Z\delta(x)=0 \ . \tag{46}$$

Let us first consider the time-independent analog, Hamilton's characteristic function $W(x,y,k)$, which satisfies the equation

$$\frac{1}{2}\left[\frac{\partial W}{\partial x}\right]^2-Z\delta(x)=\frac{k^2}{2} \ . \tag{47}$$

A solution with the appropriate symmetry between x and y is

$$W(x,y,k)=k(x-y)+\frac{Z}{k}\theta \ , \tag{48}$$

where

$$\theta\equiv\theta(x)-\theta(y),\quad \theta(z)\equiv\begin{cases}1 & \text{if } z>0\\ 0 & \text{if } z<0 \ .\end{cases} \tag{49}$$

The solution (48) fails, however, at the singular points $x=0$ and $y=0$. This is to be expected in any event since a classical δ-function potential behaves as a black hole.

Hamilton's principal function can now be obtained by a Legendre transformation,

$$S(x,y,t)=W(x,y,k)-\tfrac{1}{2}k^2t \ . \tag{50}$$

Thus

$$t=\frac{1}{k}\frac{\partial W}{\partial k}=\frac{x-y}{k}-\frac{Z}{k^2}\theta \ , \tag{51}$$

which gives k as an implicit function of x, y, and t. With $\nu=Z/k$, (51) becomes

$$Z^2t=\nu Z(x-y)-\nu^3\theta \ . \tag{52}$$

It is convenient to introduce the auxilliary variable α such that

$$\frac{(x-y)^{3/2}}{Z^{1/2}t}=\frac{\alpha^{3/2}}{\alpha-\theta} \ . \tag{53}$$

We have accordingly

$$Z(x-y)=\nu^2\alpha,\quad Z^2t=\nu^3(\alpha-\theta) \ . \tag{54}$$

The action function thus works out to

$$S(x,y,t)=\tfrac{1}{2}\nu(\alpha+3\theta) \ . \tag{55}$$

This reduces to the free-particle result $S=(x-y)^2/2t$ when $\theta=0$ ($x,y>0$ or $x,y<0$).

For purposes of comparison, we recount the action function for the Coulomb problem:[19]

$$S(\lambda,\mu,\nu)=\nu[\sinh(\lambda-\mu)\cosh(\lambda+\mu)+3(\lambda-\mu)] \ , \tag{56}$$

in terms of the variables λ,μ,ν determined by the implicit relations

$$Zx=4\nu^2\sinh^2\lambda,\quad Zy=4\nu^2\sinh^2\mu \ ,$$
$$Z^2t=2\nu^3[\sinh(\lambda-\mu)\cosh(\lambda+\mu)-(\lambda-\mu)] \ , \tag{57}$$

where x and y are defined in (24).

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