δ' potential arising in exterior complex scaling

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In the method of exterior complex scaling the coordinates of the Hamilton operator are scaled by a constant factor starting at a radius $R \neq 0$. We show that this procedure induces a singularity in the kinetic-energy term which must be interpreted as the derivative of a δ function.

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The method of exterior complex scaling [1] is a technique to analytically continue a self-adjoint Hamiltonian operator of the general form

$$H = -d^2/dr^2 + V,$$
$$D(H) = D(-d^2/dr^2) = \{\Psi \in W_2^2(\mathcal{R}_+), \Psi(0) = 0\} \tag{1}$$

to a family of non-self-adjoint operators $\{H_z\}$. If there are resonances in the physical system described by H, then H_z will have complex eigenvalues whose real and imaginary parts give the positions and half the widths of the resonances, respectively. The family $\{H_z\}$ is constructed such that the point spectra $\sigma_p(H_z)$ have the property

$$\sigma_p(H_{z_1}) \subset \sigma_p(H_{z_2}), \quad 0 < \arg(z_1) \leq \arg(z_2) < \alpha_c, \tag{2}$$

i.e., the eigenvalues are independent of the modulus of z and any eigenvalue of H_z that appeared for z_1 stays constant when one increases $\arg(z)$ up to a certain critical angle α_c. Such continuation techniques are widely used in physics and quantum chemistry to determine, in a nonperturbative way, the widths of resonance states (see reviews in Ref. [2]). We will point out below that for the particular variant of exterior complex scaling the proper choice of the functions on which the Hamiltonian is defined is nontrivial and also of immediate computational relevance. In the case of a discontinuous transition from the unscaled (interior) region of coordinates to the scaled (exterior) region these functions must have a well defined discontinuity. Any attempt to define a discontinuously scaled kinetic energy on smooth functions would encounter similar difficulties as to define the unscaled kinetic energy on discontinuous functions.

The usual procedure to construct $\{H_z\}$ is to define the operator of scaling of the coordinates

$$\Psi \to U_z\Psi : \; (U_z\Psi)(r) = q_z^{1/2}(r)\Psi\left(\int_0^r q_z(r')dr'\right). \tag{3}$$

In Ref. [1] q_z was chosen to be

$$q_z(r) = \begin{cases} 1, & r < R \\ z, & r \geq R. \end{cases} \tag{4}$$

From this one obtains the family of scaled Hamiltonians

$$H_z = U_z H U_z^*, \qquad D(H_z) = U_z D(H). \tag{5}$$

For $0 < z \in \mathcal{R}$ the operator U_z is unitary and therefore $\{H_z\}$ is a family of self-adjoint operators. When the potential V has the property of being "dilation analytic" [3] the continuation of this family to complex values of z has the spectral property Eq. (2).

It is important to notice that for $R > 0$ the domains $D(H_z)$ depend on z in the form

$$\Psi \in D(H_z): \quad \begin{cases} \Psi(R+0) &= z^{1/2}\Psi(R-0) \\ \Psi'(R+0) &= z^{3/2}\Psi'(R-0). \end{cases} \tag{6}$$

Conditions (6) mean that H_z is only defined on functions that are discontinuous at $r = R$, and also the derivatives must be discontinuous. Suppose we have a set of basis functions from the domain of H, say, $r\exp(-\alpha r) \in D(H)$. Then, according to Eq. (5), a set of basis functions for H_z can be obtained in the form

$$U_z[r\exp(-\alpha r)] = \begin{cases} r\exp(-\alpha r), & r < R \\ z^{1/2}[R + z(r-R)]\exp\{-\alpha[R + z(r-R)]\}, & r \geq R. \end{cases} \tag{7}$$

In this Brief Report we want to show that the kinetic-energy term $-d^2/dr^2$ upon scaling produces a zero-range singular potential at the point $R > 0$. This fact as such is not surprising and earlier an attempt was made to take it into account by introducing a Bloch term at R to calculate matrix elements of the kinetic-energy [4]. We will show that the correct form of the scaled kinetic-energy operator contains the derivative of the δ function with support at the point R. For this purpose it will be sufficient to restrict the discussion to the case with $z \in \mathcal{R}$.

We first encounter the problem that the domain of H_z contains functions whose values and derivatives will in

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general be discontinuous at R. In order to define δ' on discontinuous functions, in Ref. [5] the generalized definition of the δ function

$$\int \delta(r-R)\Psi(r)\,dr = \frac{\Psi(R-0)+\Psi(R+0)}{2} \qquad (8)$$

was used. The function values $\Psi(R-0)$ and $\Psi(R+0)$ were chosen to enter symmetrically in order to keep δ an even function: $\delta(r-R)=\delta(R-r)$. For the usual δ' function and a continuously differentiable function $f(x)$ the equation

$$f(x)\delta'(x) = f(0)\delta'(x) - f'(0)\delta(x) \qquad (9)$$

holds. To extend this equation to discontinuous functions, in Ref. [5] the values and derivatives at $x=0$ were replaced by the mean values of the left and right limits to 0, which is implied by the definition (8):

$$f(x)\delta'(x) = \frac{f(-0)+f(+0)}{2}\delta'(x) - \frac{f'(-0)+f'(+0)}{2}\delta(x). \qquad (10)$$

While δ' does not have an interpretation as an operator in the Hilbert space, the operator which is formally defined by

$$A\Psi \equiv \left[-d^2/dr^2 + c\delta'(r-R)\right]\Psi = \chi \qquad (11)$$

can be given meaning by demanding that χ contain no δ-like singularities. This subjects the domain of functions where A is defined to the conditions [5,6]

$$\Psi \in D(A): \begin{cases} \Psi(R+0) &= [(2+c)/(2-c)]\Psi(R-0) \\ \Psi'(R+0) &= [(2-c)/(2+c)]\Psi'(R-0). \end{cases} \qquad (12)$$

The eigenfunctions of this operator can be easily given as

$$\varphi_A(k,r) = \begin{cases} \sin kr, & r<R \\ ue^{-ik(r-R)} + u^* e^{ik(r-R)}, & r\geq R, \end{cases} \qquad (13)$$

where $u = \frac{1}{2}\{[(2+c)/(2-c)]\sin kR + i[(2-c)/(2+c)]\cos kR\}$.

Let us now return to the scaled Hamiltonian H_z and try to write down explicitly the action of scaling on the kinetic-energy operator $-d^2/dr^2$. For $0\leq r<R$ the second derivative remains unchanged, while for $r>R$ a factor of z^{-2} appears due to the multiplication of r by z. Thus everywhere except at the point $r=R$, the scaled kinetic-energy operator acts as follows:

$$-q_z^{-2}d^2/dr^2 = -q_z^{-1}d^2/dr^2 q_z^{-1}, \qquad r\neq R. \qquad (14)$$

Here the second symmetric expression suggests as a natural choice for the domain the functions of the form $q_z\phi,\quad \phi\in D(-d^2/dr^2)$. It is easy to verify that

$$K_z = -q_z^{-1}d^2/dr^2 q_z^{-1},$$
$$D(-q_z^{-1}d^2/dr^2 q_z^{-1}) = q_z D(-d^2/dr^2) \qquad (15)$$

is self-adjoint and therefore a suitable candidate for a kinetic-energy operator. Functions from its domain obey the boundary conditions at R

$$\chi\in D(K_z): \begin{cases} \chi(R+0) &= z\chi(R-0) \\ \chi'(R+0) &= z\chi'(R-0) \end{cases} \qquad (16)$$

and the eigenfunctions of K_z are

$$\varphi_{K_z}(k,r) = \begin{cases} \sin kr, & r<R \\ ve^{-ikz(r-R)} + v^* e^{ikz(r-R)}, & r\geq R \end{cases} \qquad (17)$$

with $v=\frac{1}{2}[z\sin kR + i\cos kR]$. One sees that this naively scaled kinetic-energy operator does not coincide with the one obtained by the scaling Eq. (5). The essential difference is that the logarithmic derivatives of $\chi\in D(K_z)$ are continuous, while, according to Eq. (6),

$$\frac{\Psi'(R+0)}{\Psi(R+0)}\Big/\frac{\Psi'(R-0)}{\Psi(R-0)} = z \quad \text{for} \quad \Psi\in D(H_z). \qquad (18)$$

From Eq. (12) one sees that the constant c in front of δ' parametrizes the discontinuity of the logarithmic derivative. It is easy to verify that the operator

$$A_z = q_z^{-1}\left[-d^2/dr^2 + 2\frac{1-\sqrt{z}}{1+\sqrt{z}}\delta'(r-R)\right]q_z^{-1},$$
$$D(A_z) = q_z D(A) \qquad (19)$$

acts as defined in Eq. (14) and its domain coincides with the domain of the properly scaled Hamiltonian: $D(A_z)=D(H_z)$. The eigenfunctions of the properly scaled kinetic-energy operator A_z have the form

$$\varphi_{A_z}(k,r) = \begin{cases} \sin kr, & r<R \\ we^{-ikz(r-R)} + w^* e^{ikz(r-R)}, & r\geq R \end{cases} \qquad (20)$$

with $w=\frac{1}{2}[z^{1/2}\sin kR + iz^{1/2}\cos kR]$. These functions fulfill the boundary conditions (6).

Thus we have shown that the difference between the naive operator (15) and the correctly scaled operator (5) is the zero-range potential

$$2(1-\sqrt{z})/(1+\sqrt{z})\,q_z^{-1}\delta'(R-r)q_z^{-1}. \qquad (21)$$

For the variational determination of eigenvalues of H_z one needs to calculate matrix elements $\langle\chi|H_z\Psi\rangle$. It is interesting to note that such a matrix element for either operator, A_z or K_z, for $z\in\mathcal{R}$ is given by the integral

$$-\int_0^R \chi^*(r)\Psi''(r)\,dr - z^{-2}\int_R^\infty \chi^*(r)\Psi''(r)\,dr$$
$$= \int_0^R (\chi')^*(r)\Psi'(r)\,dr + z^{-2}\int_R^\infty (\chi')^*(r)\Psi'(r)\,dr. \tag{22}$$

The only difference between the two functionals lies in the domains: Trial functions for K_z have to be chosen according to conditions (16). For example, starting again from trial functions for the unscaled operator of the form $r\exp(-\alpha r)$ one obtains

$$q_z(r) r\exp(-\alpha r) = \begin{cases} r\exp(-\alpha r), & r < R \\ zr\exp(-\alpha r), & r \geq R. \end{cases} \tag{23}$$

The crucial difference between these functions and the functions (7) is that the discontinuity amounts to a factor z here, while it is a factor $z^{1/2}$ in the set (7). [The conditions on the derivatives can actually be omitted if one calculates only matrix elements as in Eq. (22).]

Finally we would like to remark that $\{H_z\}$ is the only self-adjoint family of scaled operators which can be constructed if we do not allow one to connect the boundary values of the functions with the boundary values of their derivatives.

Obviously, any self-adjoint operator S_z needs to fulfill the symmetry condition

$$\langle\chi|S_z\Psi\rangle - \langle S_z\chi|\Psi\rangle = 0. \tag{24}$$

By substituting for S_z the explicit differential form Eq. (14) the symmetry condition reads

$$\int_0^R dr\left[-\chi^*\frac{d^2\Psi}{dr^2} + \frac{d^2\chi^*}{dr^2}\Psi\right]$$
$$+z^{-2}\int_R^\infty dr\left[-\chi^*\frac{d^2\Psi}{dr^2} + \frac{d^2\chi^*}{dr^2}\Psi\right] = 0. \tag{25}$$

Integrating by parts we get the following condition on the values of the function at the point $r = R$:

$$-\chi^*(R-0)\Psi'(R-0) + (\chi')^*(R-0)\Psi(R-0)$$
$$+z^{-2}[\chi^*(R+0)\Psi'(R+0) - (\chi')^*(R+0)\Psi(R+0)] = 0. \tag{26}$$

The operator can be made self-adjoint by choosing as the domain an adequate set of functions obeying this condition.

Consider now boundary conditions of the particular form

$$\Psi'(R+0) = \alpha\Psi'(R-0), \quad \Psi(R+0) = \beta\Psi(R-0). \tag{27}$$

Substitution into the boundary form (26) implies for the constants

$$\alpha\beta^* = z^2, \quad \alpha^*\beta = z^2. \tag{28}$$

This condition can be satisfied for $z^2 \in \mathcal{R}$. One can show that the corresponding operator will be not only symmetric, but also self-adjoint.

On the other hand, scaling the coordinates of a function with continuous derivative by the substitution $r \to R+q_z(r)(r-R)$ will always lead to a jump in the logarithmic derivative of the scaled function as given in Eq. (18). That equation combined with the symmetry requirement uniquely defines the domain $D(H_z)$.

If one gives up the condition that H_z be self-adjoint for real z, then one can readily construct families of operators, which are defined on continuous functions and which have the spectral property (2). For example, when the potential V is local, the operator

$$\tilde{H}_z = q_z^{1/2} H_z q_z^{-1/2}, \qquad D(\tilde{H}_z) = q_z^{1/2} D(H_z) \tag{29}$$

has an eigenfunction $\tilde{\Psi}_{z,E} = q_z^{1/2}\Psi_{z,E}$ with eigenvalue E for each eigenfunction $\Psi_{z,E}$ of H_z at the same eigenvalue E. Now we have otained a domain $D(\tilde{H}_z)$ that contains only continuous functions. (Note that the logarithmic derivatives remain discontinuous.) When one sets up a variational functional such as (22) for this nonsymmetric operator, one has to be careful to choose the left functions from the domain of the adjoint operator $D(\tilde{H}_z^*) = q_z^{-1}D(\tilde{H}_z) \neq D(\tilde{H}_z)$. These functions differ from the functions on the right-hand side of the operator and are discontinous. We see that by this manipulation at best nothing was gained. In practice, it would lead to nonsymmetric matrices, which are harder to handle computationally.

In exterior complex scaling one has $z \in \mathcal{C}$ such that the resulting operator H_z is non-self-adjoint. The reasoning that leads to the identification of the boundary conditions (12) with the δ' function only uses that the right-hand side of Eq. (11) contain no δ-function-like singularities and does not depend on self-adjointness. Therefore Eq. (12) is equally valid for complex z and the difference between the operators defined with the domains Eqs. (6) and (16), respectively, is still given by Eq. (21).

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