Some remarks on the evolution of a Schrödinger particle in an attractive $1/r^2$ potential*

Charles Radin

Department of Mathematics, University of Pennsylvania, Philadelphia, Pennsylvania
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Comparing the different solutions of Case and Nelson for the evolution operators of a Schrödinger particle in the potential $V(r) = -1/r^2$, we show that Nelson's nonunitary solution is a simple average, over a physical parameter related to a boundary condition at the singularity, of Case's family of solutions.

1. INTRODUCTION

In two well-known papers, Case[1] and Nelson[2] have used different approaches, and arrived at different conclusions, in calculating the evolution operators for a Schrödinger particle in the presence of the singular, attractive potential $V(r) = -1/r^2$. The most striking difference is that Case finds the operators to be unitary but not unique, whereas Nelson finds them to be unique but not unitary.

As the potential is not physical (see, however, Ref. 3, esp. Secs. V, VI), we do not try to justify one solution or the other on physical grounds. All we attempt to do is clarify the relationship between the two; we show that Nelson's nonunitary solution is a simple (time independent) average over Case's family of unitary solutions.

We choose units so that Planck's constant, $\hbar$, has magnitude 1, and for complex numbers z and w we define

$$z^w \equiv \exp[w(\ln|z| + i \arg z)],$$

where $-\pi \leqslant \arg z < \pi$.

2. THE TWO SOLUTIONS

We consider the Schrödinger equation in three space dimensions:

$$\frac{\partial\psi}{\partial t} = i\left(\frac{1}{2m}\Delta + \frac{1}{r^2}\right)\psi, \quad \psi(\cdot, t) \in L_2(\mathbf{R}^3), \ \forall\, t. \qquad (1)$$

In spherical coordinates the Laplace operator is

$$\Delta = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{J^2}{r^2},$$

where J^2, the square of the angular momentum operator, is

$$J^2 = -\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right].$$

The natural identification of $\mathbf{R}^3$ with $S\times\mathbf{R}^+$, where S is the unit sphere in $\mathbf{R}^3$, induces a Hilbert space isomorphism $L_2(\mathbf{R}^3) \cong L_2(S) \otimes L_2(0,\infty)$. We associate with the formal differential operator J^2, in the standard way, a self-adjoint operator (also denoted J^2) on $L_2(S)$ whose spectrum is purely discrete, with eigenspaces $\mathcal{L}_j$ and eigenvalues $j(j+1)$, where $j = 0, 1, 2, \cdots$. Finally we decompose in the natural manner

$$\mathcal{H} \equiv L_2(\mathbf{R}^3) \cong \bigoplus_{j=0}^{\infty} [\mathcal{L}_j \otimes L_2(0,\infty)] \equiv \bigoplus_{j=0}^{\infty} \mathcal{H}_j.$$

As the potential $V = -1/r^2$ is spherically symmetric, we will only consider solutions U^t for (1) which commute with $J^2 \otimes I_2$ [where I_2 is the identity operator on $L_2(0,\infty)$], so that U^t can be decomposed as $U^t = \oplus U^t(j)$, where $U^t(j)$ is of the form $I_1 \otimes X^t(j)$ with I_1 the identity operator on $\mathcal{L}_j$ and $X^t(j)$ an operator on $L_2(0,\infty)$. [By an abuse of notation we will no longer distinguish $U^t(j)$ and $X^t(j)$]. We will usually be considering evolution operators U^t be means of their "restrictions" $U^t(j)$ to an arbitrary but fixed $\mathcal{H}_j$.

Assume that ψ is a separable solution of (1) in $\mathcal{H}_j$, with radial part ψ_ρ, and let $u(r) = r\psi_\rho(r)$. Then (1) becomes

$$\frac{\partial u}{\partial t} = \frac{1}{2mi}\left(-\frac{\partial^2}{\partial r^2}u + \frac{(\nu^2 - \frac{1}{4})}{r^2}u\right) \equiv \frac{1}{2mi}Hu, \qquad (2)$$

where $\nu^2 = \frac{1}{4} + [j(j+1) - 2m]$ and $u(\cdot, t)$ is in $L_2(0,\infty)$ for each fixed time t. Our problem now is to determine evolution operators $U^t(j)$ on $L_2(0,\infty)$ for (2) whose generator is appropriately related to the formal differential operator $(2mi)^{-1}H$, which we will consider to be an operator on $L_2(0,\infty)$ with domain C_0^∞, the (equivalence classes of) infinitely differentiable functions with compact support in the open interval $(0,\infty)$. We seek a generator which is an extension of $(2mi)^{-1}H$, which is not, itself, a generator.

Nelson in Ref. 2 defines such evolution operators $U_N{}^t(j)$, $t \geqslant 0$, of (2) with Laplace transform

$$Q_N(\lambda)u = \int_0^\infty \exp(-\lambda t)U_N{}^t(j)u\,dt, \quad \mathrm{Re}\lambda > 0,$$

and shows that

$$[Q_N(\lambda)u](x) = \int_0^\infty G_N(x,y;\lambda)u(y)\,dy$$

with

$$G_N(x,y;\lambda) = \begin{cases} x^{1/2}H_\nu^1[(2mi\lambda)^{1/2}x]f(y), & x > y, \\ x^{1/2}J_\nu[(2mi\lambda)^{1/2}x]g(y), & x < y, \end{cases}$$

where J_ν and H_ν^1 are the usual Bessel functions as defined in Ref. 4, f and g are unknown, and $\nu = (\nu^2)^{1/2}$; he also shows that $U_N{}^t(j)$ is not unitary for $\nu^2 < 0$ but is unitary for $\nu^2 \geqslant 0$. Thus his solutions $U_N{}^t$ for (1) are nonunitary if and only if $m > 1/8$, the only range of mass we will consider henceforth. From his definition of $U_N{}^t(j)$ it follows easily that $Q_N(\lambda) = K[Q_N(\lambda)]^*K$ [where K is the complex conjugation operator on $L_2(0,\infty)$ and * denotes operator adjoint] and then that $G_N(x,y;\lambda) = G_N(y,x;\lambda)$ so that

$$G_N(x,y;\lambda)=n(\lambda)$$
$$\times\begin{cases} x^{1/2}H_\nu^1[(2mi\lambda)^{1/2}x](y)^{1/2}J_\nu[(2mi\lambda)^{1/2}y], & x>y,\\ x^{1/2}J_\nu[(2mi\lambda)^{1/2}x](y)^{1/2}H_\nu^1[(2mi\lambda)^{1/2}y], & x<y,\end{cases}\tag{3}$$

where $n(\lambda)$ is independent of x and y but as yet undetermined.

An alternative approach to the problem was put forth by Case in Ref. 1, and consists of determining all possible *unitary* evolution operators $U^t(j)$ for (2) whose generators extend $(2mi)^{-1}H$. Rather than use Case's method of carrying out this approach, we will use the method of von Neumann as described in Ref. 5, which has the advantages of being of very general character, widely known, and most importantly, of leading directly to quantities that we need to calculate. We will discuss separately the cases $\nu^2 \geqslant 0$ and $\nu^2<0$.

For $\nu^2>0$, Nelson's solution is, as he indicates, the commonly accepted one corresponding to a Friedrichs extension of H. The case $\nu=0$ is slightly more complicated, but as we show in Sec. 4 it turns out that for $\nu^2\geqslant 0$ Nelson's solution can be "justified" by a regularization procedure if necessary (except possibly for the $j=0$ restriction). Therefore, the only part of Nelson's solution that can be regarded as unusual is that for $\nu^2<0$, the nonunitary restrictions.

A straightforward application of Theorem 10.20 of Ref. 5, most of which is explicitly exhibited in Ref. 6, shows that for $\nu^2<0$ there is a one-parameter family of unitary solutions $U_\theta{}^t(j)$, $-\infty<t<\infty$, $0\leqslant\theta<2\pi$, whose Laplace transforms $Q_\theta(\lambda)$ have kernels

$$G_\theta(x,y;\lambda)=m\pi/[1-\eta^4(2mi\lambda)^\nu L(\theta)]$$
$$\times\begin{cases} x^{1/2}H_\nu^1[(2mi\lambda)^{1/2}x](y)^{1/2}\{J_\nu[(2mi\lambda)^{1/2}y] \\ \quad -(2mi\lambda)^\nu L(\theta)J_{-\nu}[(2mi\lambda)^{1/2}y]\}, & x>y,\\ x^{1/2}\{J_\nu[(2mi\lambda)^{1/2}x]-(2mi\lambda)^\nu L(\theta) \\ \quad \times J_{-\nu}[(2mi\lambda)^{1/2}x]\}(y)^{1/2}H_\nu^1[(2mi\lambda)^{1/2}y], & x<y,\end{cases}\tag{4}$$

for $\mathrm{Re}\lambda>0$, where $\eta=\exp(-i\nu\pi/4)$ and

$$L(\theta)=\exp(-i\theta)\left(\frac{\exp(i\theta)+\eta^2}{\exp(-i\theta)+\eta^2}\right).$$

We emphasize that this is a complete list of the unitary solutions for $\nu^2<0$ and that the parameter θ is directly related to a boundary condition at the singular point $r=0$; for the relation see Refs. 5 and 7. The parameter s for the corresponding evolution operators $U_s{}^t$ on $\mathcal{H}=\oplus\mathcal{H}_j$ is a variable in $[0,2\pi)^N$; we emphasize that $j\subset\mathrm{N}$ and $\theta\in[0,2\pi)$ are independent parameters, and $U_\theta{}^t(j)\equiv U_N{}^t(j)$ if $\nu\geqslant 0$.

3. COMPARISON OF SOLUTIONS FOR $\nu^2<0$

Since $L(\theta)$, defined above, is of absolute value 1, we can simplify the form of $G_\theta(x,y;\lambda)$ by defining $\chi(\theta)=\arg L(\theta)+\pi$. From

$$\frac{d\chi}{d\theta}=\frac{1-\eta^4}{|\exp(i\theta)+\eta^2|^2}>0$$

we see that $\chi(\theta)$ increases monotonically from 0 to 2π with θ, and has an inverse function $\theta(\chi)$. Defining the average

$$\langle G_\theta(x,y;\lambda)\rangle=\frac{1}{2\pi}\int_0^{2\pi}G_{\theta(\chi)}(x,y;\lambda)\,d\chi$$
$$=\frac{1}{2\pi}\int_0^{2\pi}G_\theta(x,y;\lambda)\,\frac{d\chi}{d\theta}\,d\theta,$$

and replacing $\exp(i\chi)$ by the complex variable z and using Cauchy's integral formula, we find for $\mathrm{Re}\lambda>0$

$$\langle G_\theta(x,y;\lambda)\rangle=m\pi\begin{cases} x^{1/2}H_\nu^1[(2mi\lambda)^{1/2}x](y)^{1/2}J_\nu[(2mi\lambda)^{1/2}y], \\ \qquad x>y,\\ x^{1/2}J_\nu[(2mi\lambda)^{1/2}x](y)^{1/2}H_\nu^1[(2mi\lambda)^{1/2}y], \\ \qquad x<y.\end{cases}\tag{5}$$

From (3) and (4) we see that for $\mathrm{Re}\lambda>0$ the bounded operator $Q_\theta(\lambda)$ is the sum of two bounded operators

$$Q_\theta(\lambda)=h(\theta)Q^1(\lambda)+k(\theta)Q^2(\lambda)$$

with the numerical coefficients h and k carrying all the θ dependence. Clearly $Q_\theta(\lambda)$, as a function of θ, is continuous in the operator norm topology, and the average operator

$$\langle Q_\theta(\lambda)\rangle u\equiv\frac{1}{2\pi}\int_0^{2\pi}Q_{\theta(\chi)}(\lambda)u\,d\chi$$

is an integral operator with kernel $\langle G_\theta(x,y;\lambda)\rangle$.

From Theorem 11.5.2 of Ref. 8,

$$Q_N(\lambda)=2mi(2mi\lambda-H_N)^{-1},\quad Q_\theta(\lambda)=2mi(2mi\lambda-H_\theta)^{-1},$$

where $(2mi)^{-1}H_N$ [resp. $(2mi)^{-1}H_\theta$] is the generator of $U_N{}^t(j)$ [resp. $U_\theta{}^t(j)$]. Let u be a nonzero function in C_0^∞, and therefore in the domain of H, H_N and H_θ. Then $H_Nu=H_\theta u$, and $v\equiv(2mi\lambda-H_N)u=(2mi\lambda-H_\theta)u$ is nonzero since H_θ is self-adjoint. Therefore, $2miu=Q_N(\lambda)v=Q_\theta(\lambda)v=\langle Q_\theta(\lambda)\rangle v$, which implies that $n(\lambda)=m\pi$ in (3), and $Q_N(\lambda)=\langle Q_\theta(\lambda)\rangle$.

From Theorem 11.6.2 of Ref. 8, if $\mathrm{Re}q>0$ we have

$$\frac{1}{2mi}\lim_{s\to\infty}\int_0^s dp\int_{q-ip}^{q+ip}\exp(\lambda t)Q_\theta(\lambda)u\,d\lambda=\begin{cases}U_\theta{}^t(j)u, & t>0,\\ u/2, & t=0,\end{cases}\tag{6}$$

with a similar equation for $U_N{}^t(j)$. Defining

$$\langle U_\theta{}^t(j)\rangle u=\frac{1}{2\pi}\int_0^{2\pi}U_{\theta(\chi)}{}^t(j)u\,d\chi,$$

we note that the limit in (6) is uniform in θ so that for $\mathrm{Re}q>0$,

$$\frac{1}{2\pi i}\lim_{s\to\infty}\int_0^s\,dp\int_{q-ip}^{q+ip}\exp(\lambda t)\langle Q_\theta(\lambda)\rangle\,u\,d\lambda$$

$$= \begin{cases} U_\theta{}^t(j)u, & t>0, \\ u/2, & t=0, \end{cases}$$

which proves that $U_N{}^t(j)=\langle U_\theta{}^t(j)\rangle$ for $t\geq 0$.

4. REGULARIZING THE POTENTIAL

In this section we consider the possibility of regularizing the potential $V=-1/r^2$, that is, altering it in a region of the origin so as to be nonsingular, calculating the associated evolution operators as a function of the region of regularization, and then looking for limits as we allow the region of regularization to become arbitrarily small while keeping all other parameters, in particular t, fixed. (A similar program is carried out in Sec. 5 of Ref. 6, but there even the centrifugal potential term is regularized, which we prefer not to do.)

Thus we consider the differential operator

$$\tilde{H}_R=-\frac{d^2}{dr^2}+\frac{\mu^2-\frac{1}{4}}{r^2}+\tilde{V}_R,$$

where

$$\tilde{V}_R(r)=\begin{cases} -2m/r^2, & r>R, \\ -2m/R^2, & r\leq R, \end{cases}$$

where $R>0$, and $\mu=[\frac{1}{4}+j(j+1)]^{1/2}$. If $j\geq 1$, $\tilde{H}_R$, with domain C_0^∞, is essentially self-adjoint as we see by applying Theorem 10.21 of Ref. 5. We will postpone discussion of the case $j=0$ to the end of the section.

Assuming $j\geq 1$ and denoting by H_R the closure of $\tilde{H}_R$, we wish to study its behavior as R approaches 0. We will discuss separately the cases where ν is, or is not, an integer.

A straightforward calculation using Theorem 10.21 of Ref. 5 shows that if $\mathrm{Re}\lambda>0$ and ν is not an integer, $Q_R(\lambda)$ defined as $2mi(2mi\lambda-H_R)^{-1}$ is a bounded integral operator will kernel

$$G_R(x,y;\lambda)=\begin{cases} w_1(x)w_2(y)/W, & x>y, \\ w_2(x)w_1(y)/W, & x<y, \end{cases}$$

where

$$w_1(x)=\begin{cases} a_R(x)^{1/2}H_\nu^1[(2mi\lambda)^{1/2}x], & x>R, \\ x^{1/2}\{J_\mu[(2mi\lambda+2m/R^2)^{1/2}x] \\ \quad +b_RJ_{-\mu}[(2mi\lambda+2m/R^2)^{1/2}x]\}, & x\leq R, \end{cases}$$

$$w_2(x)=\begin{cases} x^{1/2}\{J_\nu[(2mi\lambda)^{1/2}x]+d_RJ_{-\nu}[(2mi\lambda)^{1/2}x]\}, & x>R, \\ c_R(x)^{1/2}J_\mu[(2mi\lambda+2m/R^2)^{1/2}x], & x\leq R, \end{cases}$$

$$a_R=\frac{J_\mu[(2mi\lambda+2m/R^2)^{1/2}R]+b_RJ_{-\mu}[(2mi\lambda+2m/R^2)^{1/2}R]}{H_\nu^1[(2mi\lambda)^{1/2}R]},$$

$$c_R=\frac{J_\nu[(2mi\lambda)^{1/2}R]+d_RJ_{-\nu}[(2mi\lambda)^{1/2}R]}{J_\mu[(2mi\lambda+2m/R^2)^{1/2}R]},$$

$$\tilde{b}_R=\frac{\Gamma(1-\mu)}{\Gamma(1+\mu)}\left(\frac{2mi\lambda R^2+2m}{4}\right)^\mu$$

$$\times\left(\frac{(-\mu-\nu)[(2mi\lambda)^{1/2}/2]^{-\nu}\Gamma(1+\nu)+R^{2\nu}(\mu-\nu)[(2mi\lambda)^{1/2}/2]^\nu\exp(-\nu\pi i)\Gamma(1-\nu)}{(-\mu+\nu)[(2mi\lambda)^{1/2}/2]^{-\nu}\Gamma(1+\nu)+R^{2\nu}(\mu+\nu)[(2mi\lambda)^{1/2}/2]\exp(-\nu\pi i)\Gamma(1-\nu)}\right).$$

$$\tilde{d}_R=-R^{2\nu}\frac{\Gamma(1-\nu)}{\Gamma(1+\nu)}\left(\frac{2mi\lambda}{4}\right)^\nu\left(\frac{\mu-\nu}{\mu+\nu}\right),$$

$$W=\frac{a_R}{m\pi}(d_R\exp(-\nu\pi i)+1)=-b_Rc_R\frac{\sin(\mu\pi)}{m\pi i},$$

$$b_R=\tilde{b}_R+O(R^2)\quad\text{as } R\to 0,$$
$$d_R=\tilde{d}_R+O(R^2)\quad\text{as } R\to 0.$$

It is easy to see that if $\nu^2<0$ and we let R approach zero along the sequence $\{R^\theta{}_n;\ n=1,2,\cdots\}$, chosen so that $d_{R_n^\theta}=-(2mi\lambda)^\nu L(\theta)$, then for each x,y in $(0,\infty)$

$$G_{R_n^\theta}(x,y;\lambda)\underset{n\to\infty}{\to}G_\theta(x,y;\lambda)$$

and, also, for each θ there exists such a sequence. From simple estimates of $[G_{R_n^\theta}(x,y;\lambda)-G_\theta(x,y;\lambda)]$ in each of the regions of integration corresponding to the possible linear orderings of x,y and R_n^θ, it follows that $Q_{R_n^\theta}(\lambda)$ converges strongly to $Q_\theta(\lambda)$ and therefore from Theorem IX.2.16 of Ref. 9, $U_{R_n^\theta}^t(j)$ converges, in the strong operator topology, to $U_\theta^t(j)$ for each t in $(-\infty,\infty)$. In particular, for $\nu^2<0$ and fixed $t\neq 0$, $U_R^t(j)$ does not converge as R approaches zero, except along special sequences, in contrast with the imaginary mass case in Sec. 2 of Ref. 2. This makes explicit the connection between the radius of regularization in the cutoff model and the associated $U_\theta{}^t$, as discussed in Sec. IV of Ref. 1; the fact that R_n^θ is a function of j could be interpreted as a means by which to select some of the evolution operators U_s^t on $\mathcal{H}=\oplus\mathcal{H}_j$ over others. For $\nu>0$ but not integral, the above analysis shows that $U_R^t(j)$ does converge as R approaches zero, and converges to $U_N^t(j)$. A similar analysis confirms that this latter behavior holds for all $\nu\geq 0$.

There remains the case $j=0$. When the above program is begun for $j=0$, one finds that $\tilde{H}_R$ is not essentially self-adjoint for any ν. That this problem is basically unrelated to the potential is evident from the fact that the same result would emerge for a free particle. The point is that when we have a singular potential, it is reasonable to first restrict the formal Hamiltonian H to a domain of functions with support isolated from the singularity, and then look for extensions. If the potential is not singular, this procedure can lead to unwanted solutions as it does in our problem for $j=0$. [It is important to keep in mind that $r=0$ is only a boundary point for the radial equation (2), not the full Schrödinger equation (1); there is no reason to distinguish $r=0$ from neighboring points for the nonsingular $\tilde{V}$.] Thus the regularization method does not select out particular solutions for $j=0$ as it does for $j \geq 1$. Fortunately ν and j cannot vanish simultaneously for $m > 1/8$, so we can "justify" all the unitary restrictions of Nelson's, either by the Friedrichs extension or regularization.

We summarize our results in the following

Proposition: The nonunitary evolution operators U^t on $L_2(\mathbf{R}^3)$ for

$$\frac{\partial \psi}{\partial t} = i\left(\frac{1}{2m}\Delta + \frac{1}{r^2}\right)\psi$$

defined by Nelson in Ref. 2, i.e., those for $m > 1/8$, are (time independent) averages of unitary evolution operators $U_s{}^t$ obtained by the traditional approach discussed by Case in Ref. 1; in other terms,

$$U^t\psi = \int U_s{}^t \psi \, d\mu(s) \quad \text{for all } \psi \text{ in } L_2(\mathbf{R}^3), \quad t \geq 0,$$

for some (time independent) probability measure μ on $[0, 2\pi)^N$.

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