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LETTER TO THE EDITOR

Connection between Coulomb and oscillator problems

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Abstract. A connection between the energy eigenvalues of the Coulomb and three-dimensional oscillator potentials is shown both semiclassically and quantum mechanically. The transformation between the corresponding wavefunctions is obtained and is used to give a new derivation of the transmission factor for a one-dimensional parabolic barrier.

It has long been known (e.g. Kemble 1937) that the WKB eigenvalues for the Coulomb and three-dimensional oscillator potentials share the distinction of being exact for all values of the angular momentum l and the radial quantum number n (the number of nodes in the radial wavefunction). The semiclassical quantisation condition for the energy $E=E(n, l)$ of a particle of mass m bound in a potential $V(r)$ is given by the Bohr–Sommerfeld integral (Kemble 1937)

$$\int_{r_1}^{r_2} p_{\mathrm{eff}}(r)\,\mathrm{d}r=(2m)^{1/2}\int_{r_1}^{r_2}[E(n, l)-V(r)-(l+\tfrac{1}{2})^2/2mr^2]^{1/2}\,\mathrm{d}r=(n+\tfrac{1}{2})\pi \tag{1}$$

where we are using units such that $\hbar=1$. Note that the Langer transformation $l(l+1)\rightarrow(l+\frac{1}{2})^2$ which has been applied to the centrifugal term in equation (1) is not a 'classical' approximation but a necessary prerequisite for the application of the WKB method to the radial Schrödinger equation defined in the region $r\geqslant 0$ (Berry and Mount 1972).

The limits of integration $r_{1,2}$ in equation (1) are just the bounds of the classical motion, i.e. the points where the 'effective' radial momentum $p_{\mathrm{eff}}(r)$ vanishes. It is essentially the fact that the two problems we are considering possess no other real or complex solutions to $p_{\mathrm{eff}}(r)=0$ (except at $-r_{1,2}$ for the oscillator) which renders equation (1) exact in these cases (Kemble 1937). The object of this letter is to further illuminate the similarity between these problems.

For the oscillator potential $\frac{1}{2}m\omega^2r^2$ equation (1) becomes

$$(2m)^{1/2}\int_{r_1}^{r_2}[E(n, l)-\tfrac{1}{2}m\omega^2r^2-(l+\tfrac{1}{2})^2/2mr^2]^{1/2}\,\mathrm{d}r=(n+\tfrac{1}{2})\pi \tag{2}$$

and a direct evaluation of this expression exactly yields the correct eigenvalues

$$E(n, l)=(2n+l+\tfrac{3}{2})\omega. \tag{3}$$

Consider now the change of variables $r^2=x$ in the above integral. We readily obtain

$$(2m)^{1/2}\int_{x_1}^{x_2}[-\tfrac{1}{8}m\omega^2+\tfrac{1}{4}E/x-(\tfrac{1}{2}l+\tfrac{1}{4})^2/2mx^2]^{1/2}\,\mathrm{d}x=(n+\tfrac{1}{2})\pi \tag{4}$$

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where $x_{1,2}=r_{1,2}^2$. This equation now has exactly the same form as the quantisation condition for a particle of mass m with energy E' and angular momentum l' bound in a Coulomb potential z/x, i.e.

$$(2m)^{1/2}\int_{x_1}^{x_2}[E'-z/x-(l'+\tfrac{1}{2})^2/2mx^2]^{1/2}\,\mathrm{d}x=(n+\tfrac{1}{2})\pi \tag{5}$$

if we make the transformations

$$-\tfrac{1}{8}m\omega^2=E'=E'(n,l'),\qquad -\tfrac{1}{4}E=z\qquad\text{and}\qquad \tfrac{1}{2}l-\tfrac{1}{4}=l'. \tag{6a,b,c}$$

We do not, therefore, need to solve the Coulomb energy level problem separately, for inserting these expressions into equation (3) immediately gives

$$-4z=(2n+2l'+2)(-8E'/m)^{1/2}\qquad\text{or}\qquad E'(n,l')=-mz^2/2(n+l'+1)^2 \tag{7}$$

which is the correct expression for the bound states of the attractive Coulomb potential. (Ncte that the condition $E>0$ in equation (3) automatically gives $z<0$ from equation (6*b*).)

The transformations (6) may also be obtained from the exact radial Schrödinger equation. If we write the full wavefunction $\psi_{lnm}(r,\theta,\phi)=(\chi(r)/r)Y_l^m(\theta,\phi)$, with the usual notation, then for the oscillator χ satisfies the equation

$$-\ddot{\chi}^{\text{osc}}(r)=2m[E-\tfrac{1}{2}m\omega^2r^2-l(l+1)/2mr^2]\chi^{\text{osc}}(r) \tag{8}$$

where dots denote differentiation with respect to r. We again wish to make the substitution $r^2=x$, but since this will introduce first derivatives on the left of equation (8) we also make the transformation $\chi^{\text{osc}}(r)=g(x)\chi(x)$ and choose $g(x)$ so that there is no term in χ' in the new equation (primes denote differentiation with respect to x). We obtain

$$\ddot{\chi}^{\text{osc}}=2(g\chi'+g'\chi)+4x(g\chi''+2g'\chi'+g''\chi)$$

and choosing $g=x^{-1/4}$ this becomes

$$\ddot{\chi}^{\text{osc}}=4x^{3/4}(\chi''+\tfrac{3}{16}\chi/x^2).$$

Inserting this expression and $r^2=x$ into equation (8) yields

$$-\chi''(x)=2m[-\tfrac{1}{8}m\omega^2+\tfrac{1}{4}E/x-l'(l'+1)/2mx^2]\chi(x) \tag{9}$$

where we again have $l'=\tfrac{1}{2}l-\tfrac{1}{4}$. If we also make the other transformations (6*a*,*b*) we obtain the radial Schrödinger equation for the Coulomb problem (i.e. χ is just the Coulomb radial wavefunction χ^{C}), and we again obtain the Coulomb energy levels of equation (7) from equation (3) without direct evaluation. However, we now also have the transformation between the oscillator and Coulomb bound state wavefunctions

$$\chi_{nl'}^{\text{C}}(x)=Nx^{1/4}\chi_{nl}^{\text{osc}}(\sqrt{x})\qquad\text{or}\qquad \chi_{nl}^{\text{osc}}(r)=r^{-1/2}\chi_{nl'}^{\text{C}}(r^2)/N \tag{10}$$

where for both functions $\chi_{nL}(y)\to y^{L+1}$ as $y\to 0$ and where N is chosen so that if one function is normalised then so is the other. Note that the above transformation preserves the number of nodes in the wavefunction, and so (as in the semiclassical problem) n is the same in the oscillator and Coulomb cases. However, we are again mapping from l to $l'=\tfrac{1}{2}l-\tfrac{1}{4}$, so if l is integral then l' is not. This, though, does not present a problem, since it is not necessary for l to be integral to solve equation (8) or for l' to be integral to solve equation (9). We may therefore regard these equations as defining radial wavefunctions for continuous l and $l'(l, l' > -1)$ which are related by equation (10).

To return to the problem of the normalisation of the wavefunctions we require

$$\int_0^\infty (\chi_{nl'}^{\mathrm{C}}(x))^2\,\mathrm{d}x = \int_0^\infty (\chi_{nl}^{\mathrm{osc}}(r))^2\,\mathrm{d}r = 1 \tag{11}$$

and inserting the expressions (10) we obtain $2N^2 = 1/\langle r^2\rangle_{nl}^{\mathrm{osc}} = \langle x^{-1}\rangle_{nl}^{\mathrm{C}}$. This is a special case of the result $\langle f(x)\rangle_{nl'}^{\mathrm{C}} = 2N^2\langle r^2 f(r^2)\rangle_{nl}^{\mathrm{osc}}$. The normalised oscillator radial wavefunction may be written

$$\chi_{nl}^{\mathrm{osc}}(r) = \left(\frac{2n!\beta^{1/2}}{(\Gamma(n+l+\frac{3}{2}))^3}\right)^{1/2} (\beta r^2)^{l/2+1/2} \exp(-\tfrac{1}{2}\beta r^2) L_n^{l+1/2}(\beta r^2)$$

where $L_n^{l+1/2}$ are the associated Laguerre polynomials and $\beta = m\omega$. Under the transformations (6a,b) β becomes $2(-2mE')^{1/2} = 2K$, and we readily obtain $N^2 = \beta/2(2n+l+\frac{3}{2})$ which becomes $K/2(n+l'+1)$. Equation (10) then immediately gives the correctly normalised radial Coulomb wavefunction

$$\chi_{nl'}^{\mathrm{C}}(x) = \left(\frac{Kn!}{(n+l'+1)(\Gamma(n+2l'+2))^3}\right)^{1/2} (2Kx)^{l'+1} \exp(-Kx) L_n^{2l'+1}(2Kx)$$

where for integral l' we may replace the Γ function by the more usual expression $(n+2l'+1)!$ (Schiff 1955).

The above mapping of the Schrödinger equations is also valid in the scattering problem. We obtain Rutherford scattering from the Coulomb potential for $E' > 0$ and any z, whence equations (6a,b) give the obvious result that for scattering from an oscillator we can have any E but must have $\omega^2 < 0$. While Rutherford scattering is an extremely important physical phenomenon, the scattering from an inverted three-dimensional oscillator is perhaps not so interesting. However, many physical processes are strongly influenced by barrier penetration, and the parabolic approximation is often made for penetration near the top of a barrier. The result for the transmission coefficient is well known (e.g. Ford *et al* 1959), but it is interesting here to see how this result may be related to the Coulomb scattering matrix for non-integral angular momenta.

For Coulomb scattering the two relevant physical quantities are the wavenumber $k = +(2mE')^{1/2}$ (we now have $E' > 0$) and the Coulomb parameter $\eta = mz/k$ which transform, according to equations (6a,b), to $k = \frac{1}{2}m\gamma$ and $\eta = -E/2\gamma$ with $\gamma = +(-\omega^2)^{1/2}$($\omega^2 < 0$ for the scattering problem). Since we want to map the Coulomb wavefunctions on to those of the problem of scattering from a one-dimensional parabolic barrier we must take $l' = -\frac{1}{4}$ (to obtain $l = 0$ from equation (6c)) and we must admit the irregular Coulomb wavefunction for $l' = -\frac{1}{4}$ in order to relax the boundary condition $\chi^{\mathrm{osc}}(0) = 0$. However, the irregular Coulomb wavefunction for $l' = -\frac{1}{4}$ behaves at the origin as $x^{1/4}$ (i.e. x^{L+1} with $L = -\frac{3}{4}$) and is therefore just the regular function for $l' = -\frac{3}{4}$.

For large x the asymptotic form of the Coulomb wavefunction may be written (Landau and Lifshitz 1977)

$$\chi_{l'}^{\mathrm{C}} \propto \exp\{-\mathrm{i}[kx - \eta\ln(2kx)]\} - S_{l'}^{\mathrm{C}} \exp(-\mathrm{i}\pi l') \exp\{\mathrm{i}[kx - \eta\ln(2kx)]\}$$

with $S_{l'}^{\mathrm{C}} = \Gamma(l'+1+\mathrm{i}\eta)/\Gamma(l'+1-\mathrm{i}\eta)$. Consider then the linear combination comprising equal amplitudes of $\chi_{-1/4}^{\mathrm{C}}$ and $\chi_{-3/4}^{\mathrm{C}}$ for which the incident waves are exactly in phase.

We obtain the asymptotic form of the wavefunction

$$\psi \sim \exp\{-\mathrm{i}[kx-\eta\ \ln(2kx)]\}+S\ \exp\{\mathrm{i}[kx-\eta\ \ln(2kx)]\},$$

with $S=-\frac{1}{2}(S^{\mathrm{C}}_{-1/4}+\mathrm{i}S^{\mathrm{C}}_{-3/4})\exp(\frac{1}{4}\mathrm{i}\pi)$. (Note that the incident and outgoing Coulomb waves in the above expression are just plane waves except for the logarithmic terms in the phase, and that for large x the waves still correspond to a particle flux which is independent of x.) Besides containing non-integral values of l' the function ψ does not represent a physical scattering solution because unitarity is violated, i.e. $|S|^2\neq 1$.

The above scattering solutions can no longer be normalised according to equation (11), but we may still use equation (10) in the form $\chi^{\mathrm{osc}}(r)\sim r^{-1/2}\chi^{\mathrm{C}}(r^2)$. We thus obtain an incident 'oscillator' wave

$$\exp\{-\mathrm{i}[\tfrac{1}{2}m\gamma r^2+(E/2\gamma)\ln(m\gamma r^2)]\}r^{-1/2}$$

and an outgoing wave

$$S\ \exp\{\mathrm{i}[\tfrac{1}{2}m\gamma r^2+(E/2\gamma)\ln(m\gamma r^2)]\}r^{-1/2}.$$

These waves still represent constant particle flux, for although the particle density falls off as r^{-1} the asymptotic local momentum is just $m\gamma r$. The function $r^{-1/2}\chi^{\mathrm{C}}_{-3/4}(r^2)$ now tends to a constant value as $r\to 0$ and $r^{-1/2}\chi^{\mathrm{C}}_{-1/4}(r^2)$ behaves as r. For negative r we may take the solutions $\chi^{\mathrm{osc}}(-r)\sim|r|^{-1/2}\chi^{\mathrm{C}}(r^2)$ and in order to match the wavefunctions across $r=0$ we must reverse the sign of the regular component. Thus for large negative r we obtain no component of

$$\exp\{-\mathrm{i}[\tfrac{1}{2}m\gamma r^2+(E/2\gamma)\ln(m\gamma r^2)]\}|r|^{-1/2}$$

but only the term

$$\bar{S}\ \exp\{\mathrm{i}[\tfrac{1}{2}m\gamma r^2+(E/2\gamma)\ln(m\gamma r^2)]\}|r|^{-1/2}$$

with $\bar{S}=\frac{1}{2}(S^{\mathrm{C}}_{-1/4}-\mathrm{i}S^{\mathrm{C}}_{-3/4})\exp(\frac{1}{4}\mathrm{i}\pi)$. Note that this component *again* represents an outgoing wave, since the asymptotic local momentum $m\gamma r$ is negative for negative r. We also see that if we consider the outgoing flux on both sides of the origin we satisfy unitarity, i.e. $|S|^2+|\bar{S}|^2=1$, and we have therefore constructed the physical solution for scattering from a one-dimensional parabolic barrier. This being the case, our 'scattering matrix' S must contain the bound states of the one-dimensional oscillator as poles (de Alfaro and Regge 1965). Writing S explicitly we have

$$S=-\frac{1}{2}\left(\frac{\Gamma(\frac{3}{4}-\frac{1}{2}\mathrm{i}E/\gamma)}{\Gamma(\frac{3}{4}+\frac{1}{2}\mathrm{i}E/\gamma)}+\mathrm{i}\frac{\Gamma(\frac{1}{4}-\frac{1}{2}\mathrm{i}E/\gamma)}{\Gamma(\frac{1}{4}+\frac{1}{2}\mathrm{i}E/\gamma)}\right)\exp(\tfrac{1}{4}\mathrm{i}\pi).$$

The Γ function in the first numerator has poles at $E=-\mathrm{i}\gamma(2m+\frac{3}{2})$, and in the second at $E=-\mathrm{i}\gamma(2m+\frac{1}{2})$ with $m=0,\ 1,\ \ldots$. For a bound state the outgoing waves must be exponentially damped, and we must therefore take $\gamma=\mathrm{i}\omega$ (with ω real and positive). We thus obtain bound states at $E=(2m+1+\frac{1}{2})\omega$ and $E=(2m+\frac{1}{2})\omega$, or combining these equations $E=(m+\frac{1}{2})\omega$. Thus all the correct poles are indeed contained in S (i.e. in the Coulomb S matrix for $l'=-\frac{1}{4},\ -\frac{3}{4}$).

The barrier transmission factor T is readily obtained from $T=|\bar{S}|^2=1-|S|^2$, and we find after a little manipulation of the Γ functions (Abramowitz and Stegun 1965) the well known expression $T=[1+\exp(-2\pi E/\gamma)]^{-1}$. The phase of the reflected wave is also easily shown to be

$$\arg S=2\ \arg\Gamma(\tfrac{3}{4}-\tfrac{1}{2}\mathrm{i}E/\gamma)-\tan^{-1}\{[1-\exp(\pi E/\gamma)]/[1+\exp(\pi E/\gamma)]\}-\tfrac{1}{2}\pi.$$

The above results show an intimate connection between the two best known soluble problems in nonrelativistic quantum mechanics.

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