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Ladder operators for some spherically symmetric potentials in quantum mechanics

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The energy levels of the free field, Coulomb potential, and the three-dimensional harmonic oscillator are found using the Dirac operator formalism by the construction of suitable ladder operators. The degeneracy of each level is also discussed.

INTRODUCTION

There are three basic methods of solving the simpler problems of quantum mechanics such as the harmonic oscillator; the most widely used is to find a solution of Schrödinger's differential equation using both separation of variables and power series solutions to ordinary differential equations. This method, although adaptable to a wide range of problems, is cumbersome to use. The ladder operator method arises when attempting to find the eigenvalues of an operator within the Dirac operator formalism when we have no other information than a set of commutation relations. It works by induction by assuming that we have one eigenfunction and then finding a (ladder) operator which maps it onto another eigenvector.[1] By examining the relationship between this operator and others we may then construct a difference equation in the eigenvalues. The third technique may be described as "doing the ladder operator method properly"—and this involves a lengthy excursion into the realm of Lie groups.[2]

Of the three, the second method is certainly the simplest and yet in no texts known to the authors is it applied to any of the elementary problems apart from the linear oscillator or the calculation of angular momentum. Here we extend it to deal with the spherically symmetric potentials of the free field, Coulomb potential, and three-dimensional isotropic harmonic oscillator. In order to find the operators we use the "factorization method" of Infield and Hull[3] but whereas they use differential operators, we shall use the Dirac operator notation which does not depend upon any specific realization of the operators but only on their commutation relations.

FACTORIZATION OF THE HAMILTONIAN: GENERAL CONSIDERATIONS

Since we are dealing with spherical problems we introduce the radial operators

$$r = (x^2 + y^2 + z^2)^{1/2},$$

$$p = (x/r)p_x + (y/r)p_y + (z/r)p_z.$$

This choice of p differs from p_r in Dirac[4] by the term $-i\hbar/r$, but this makes it real and self-conjugate. The operators satisfy the commutation relation

$$[r,p] = i\hbar$$

and in the Schrödinger representation are

$$r = r; \quad p = (\hbar/i)\partial/\partial r - i\hbar/r.$$

The Hamiltonian for a spherically symmetric potential is

$$\mathcal{H} = (1/2m)(p_x^2 + p_y^2 + p_z^2) + V(r).$$

A straightforward calculation shows that

$$\begin{aligned} r^2(p_x^2 + p_y^2 + p_z^2) &= r^2p^2 + (xp_y - yp_x)^2 \\ &\quad + (yp_z - zp_y)^2 + (zp_x - xp_z)^2 \\ &= r^2p^2 + \mathbf{L}^2 \end{aligned}$$

so we may rewrite the Hamiltonian as

$$\mathcal{H} = (1/2m)[p^2 + (1/r^2)\mathbf{L}^2] + V(r).$$

We now effect a "separation of variables" by assuming that we have a normalized eigenstate $|nl\rangle$ of the total angular momentum $\mathbf{L}$ (n labels the energy). If we call the resultant radial Hamiltonian $\mathbf{H}_l$ then

$$\mathbf{H}_l = (1/2m)\{p^2 + [l(l+1)/r^2]\hbar^2\} + V(r). \quad (1)$$

The most convenient way of finding an operator $\mathbf{C}_l$ which maps $|nl\rangle$ onto $|n'l+1\rangle$ is to require a factorization of the Hamiltonian:

$$\mathbf{C}_l^\dagger \mathbf{C}_l = 2m\mathbf{H}_l + F_l$$

and (2)

$$\mathbf{C}_l \mathbf{C}_l^\dagger = 2m\mathbf{H}_{l+1} + G_l,$$

where F_l and G_l are scalars.

The vector $\mathbf{C}_l\mathbf{C}_l^\dagger\mathbf{C}_l|nl\rangle$ may be evaluated in two different ways to give

$$\begin{aligned} \mathbf{C}_l\mathbf{C}_l^\dagger\mathbf{C}_l|nl\rangle &= (2mE_l^n + F_l)\mathbf{C}_l|nl\rangle \\ &= (2m\mathbf{H}_{l+1} + \mathbf{G}_l)\mathbf{C}_l|nl\rangle \end{aligned}$$

where E_l^n is the energy of $|nl\rangle$. Rearranging, we find

$$\mathbf{H}_{l+1}(\mathbf{C}_l|nl\rangle) = [E_l^n + (F_l - G_l)/2m](\mathbf{C}_l|nl\rangle)$$

showing that $\mathbf{C}_l|nl\rangle$ is an eigenstate of $\mathbf{H}_{l+1}$ with eigenvalue

$$E_{l+1}^{n'} = E_l^n + (F_l - G_l)/2m. \quad (3)$$

If $F_l = G_l$ the energy is unchanged and $n' = n$. In this case $|nl\rangle$ and $\mathbf{C}_l|nl\rangle$ are states with the same energy and we have a degenerate system.

In a similar manner we may show that $\mathbf{C}_l^\dagger|n'l+1\rangle$ is an eigenstate of $\mathbf{H}_l$. We then get

$$\mathbf{C}_l|nl\rangle = \lambda_l^n|n'l+1\rangle$$

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and

$$\mathbf{C}_l^*|n'l+1\rangle = \mu_l^n|nl\rangle, \tag{4}$$

where λ_l^n and μ_l^n are some constants. The numbers λ_l^n and μ_l^n are complex conjugates as may be verified from

$$\lambda_l^n = \langle n'l+1|\mathbf{C}_l|nl\rangle = \langle nl|\mathbf{C}_l^*|n'l+1\rangle^* = \mu_l^{n*}.$$

We now have the simple relationships from Eq. (2)

$$|\lambda_l^n|^2 = 2mE_l^n + F_l = 2mE_{l+1}^{n'} + G_l \tag{5}$$

which yield the recursion formula

$$|\lambda_l^n|^2 - |\lambda_{l-1}^{n'}|^2 = F_l - G_{l-1}. \tag{6}$$

If this series terminates at some stage with $\mathbf{C}_l|nl\rangle = 0$ the energy is

$$E_l^n = -F_l/2m. \tag{7}$$

No simple rule exists as to whether the series terminates or not. This must be determined by consideration of the potential in each case.

FACTORIZATION OF THE HAMILTONIAN: SPECIFIC CALCULATIONS

The momentum only appears quadratically in the Hamiltonian (1). Since we wish to write the Hamiltonian as a product of the operators $\mathbf{C}_l$ and $\mathbf{C}_l^*$ plus a scalar, we search for operators linear in momentum.

$$\mathbf{C}_l = p + f(r). \tag{8}$$

Recalling[4] that $[f(r),p] = i\hbar\, df/dr$ we find

$$\mathbf{C}_l^*\mathbf{C}_l = p^2 + p(f+f^*) + i\hbar\, df^*/dr + ff^*$$

and

$$\mathbf{C}_l\mathbf{C}_l^* = p^2 + p(f+f^*) + i\hbar\, df/dr + ff^*.$$

Since $\mathbf{H}_l$ contains no term linear in p, $f+f^* = 0$. This, along with Eqs. (1) and (2), gives

$$-i\hbar\, df/dr - f^2 = l(l+1)\hbar^2/r^2 + 2mV + F_l$$

and

$$i\hbar\, df/dr - f^2 = (l+1)(l+2)\hbar^2/r^2 + 2mV + G_l.$$

The equations are readily solved:

$$f(r) = i\hbar(l+1)/r + (i/2\hbar)(F_l - G_l)r + A$$

and

$$2mV(r) = (F_l - G_l)^2r^2/4\hbar^2 - (iA/\hbar)(F_l - G_l)r + (l+1)(F_l - G_l) - (F_l + G_l)/2 - A^2 - 2i\hbar(l+1)A/r, \tag{9}$$

where A is some imaginary constant of integration. The potential has to be independent of l. Thus the coefficients of r^2, r, 1, and r^{-1} must all be independent of l. This restricts the possible values of $(F_l - G_l)$ and A in the following manner: From the term in $1/r$ we have that A is either zero or inversely proportioned to $(l+1)$, and from the term in r^2 that $(F_l - G_l)$ is a constant. The coefficient of r, which contains the *product* of A and $(F_l - G_l)$ must now be zero showing that one of A and $(F_l - G_l)$ or both is zero. We examine each of these three cases separately.

Case 1: Free field

If we set $A = (F_l - G_l) = 0$ we have

$$V(r) = -(F_l + G_l)/4m = -F_l/2m$$

and

$$\mathbf{C}_l = p + i\hbar(l+1)/r.$$

Since F_l is independent of r and V of l they must be constant, which is the potential for the free field.

The Hamiltonian $\mathbf{H}_l$ is now

$$\mathbf{H}_l = (1/2m)p^2 + l(l+1)/r^2 - F_l/2m$$

and the energy is

$$E_l^n = \langle nl|\mathbf{H}_l|nl\rangle = (1/2m)\langle nl|p^2|nl\rangle + l(l+1)\langle nl|1/r^2|nl\rangle - F_l/2m.$$

As p^2 and r^{-2} both have positive eigenvalues and are not simultaneously diagonalizable, the terms $\langle nl|p^2|nl\rangle$ and $\langle nl|1/r^2|nl\rangle$ must both be greater than or equal to zero, and cannot be simultaneously zero. Thus apart from the case when $l = 0$ and $p^2|nl\rangle = 0$ the energy is strictly greater than $V = -F_l/2m$. For the special case when $l = 0$ and $p^2|nl\rangle = 0$ Eq. (5) shows that we only have one state as $\mathbf{C}_l|n0\rangle = 0$, but otherwise from Eq. (7) we see that the series λ_l^n, λ_{l+1}^n, . . . can never terminate and we have infinitely degenerate levels. From Eq. (5) we find the energy as

$$E_l^n = (1/2m)(|\lambda_l^n|^2 + F_l)$$

but since we cannot find an expression for λ_l^n these equations allow a continuous distribution of energy levels.

Case 2: Coulomb potential

If we set $F_l = G_l$ but $A \neq 0$ we have the potential

$$2mV(r) = -F_l - A^2 - 2i\hbar(l+1)A/r.$$

For this to be real and independent of l, we must have

$$A = -iB/(l+1) \quad \text{and} \quad F_l = D + B^2/(l+1)^2$$

with B and D real, giving

$$V(r) = -D/2m - B\hbar/mr.$$

Since the constant $-D/2m$ reflects the choice of zero point for the potential, we follow the usual practice and set it equal to zero so that

$$V(r) = -B\hbar/mr,$$
$$F_l = G_l = B^2/(l+1)^2, \tag{10}$$
$$\mathbf{C}_l = p + i\hbar(l+1)/r - iB/(l+1).$$

As $F_l = G_l$ the operator $\mathbf{C}_l$ leaves the energy unchanged and we may take n' of Eqs. (3), (4), and (6) equal to n. In particular, Eq. (6) becomes

$$|\lambda_l^n|^2 - |\lambda_{l-1}^n|^2 = B^2/(l+1)^2 - B^2/l^2$$

with solution

$$|\lambda_l^n| = \frac{B}{l+1}[1 + K(l+1)]^{1/2}, \tag{11}$$

where K is some real constant. Substitution into Eq. (5) makes the energy equal to $KB^2/2m$.

To proceed further we must examine the possible sign of the energy. The Hamiltonian is

$$\mathbf{H}_l = (1/2m)[p^2 + l(l+1)\hbar^2/r^2] - B\hbar/mr.$$

Now p^2, r^{-2}, and r^{-1} all have positive eigenvalues (r is the *positive* square root of $x^2 + y^2 + z^2$). If B is negative—that is, a repulsive potential—the energy must be positive, whereas if we have an attractive potential we may have either positive or negative energy.

If the energy is positive, then so is K, and in Eq. (11) λ_l^n can never be zero and we have infinite degeneracy. Conversely, if the energy is negative the square root must vanish when $K(l_{\max}+1) = -1$ which provides an upper bound to l. If we identify n with $(l_{\max}+1)$ we have the familiar result

$$E_l^n = -B^2/2mn^2$$

with

$$\mathbf{C}_l|nl\rangle = \frac{B[(n+l+1)(n-l-1)]^{1/2}}{n(l+1)}|n\,l+1\rangle$$

where $l = 0, 1, 2, \ldots (n-1)$. To summarize, for a repulsive potential we have infinitely degenerate positive energy levels, whereas for an attractive potential we have either infinitely degenerate positive energy, or finitely degenerate negative energy.

Case 3: Isotropic harmonic oscillator

The last case to consider is when $A = 0$ but $F_l \neq G_l$. With the usual choice of zero potential and the requirement that V be independent of l we find

$$V(r) = B^2r^2/2m\hbar^2$$

$$F_l = (2l+3)B,$$

$$G_l = (2l+1)B,$$

$$\mathbf{C}_l = p + i\hbar(l+1)/r + iBr/\hbar,$$

where B is some real constant. We note that it appears quadratically in the potential and hence has undetermined sign. This gives two inequivalent operators

$$\mathbf{C}_l = p + i\hbar(l+1)/r - iD^2r/\hbar$$

and

$$\mathbf{D}_l = p + i\hbar(l+1)/r + iD^2r/\hbar$$

with

$$\mathbf{C}_l|nl\rangle = \lambda_l^n|n'l+1\rangle$$

and

$$\mathbf{D}_l|nl\rangle = \mu_l^n|n''l+1\rangle.$$

Since $F_l \neq G_l$, none of n, n', or n'' are equal—the operators are mapping from one energy level to another.

We first consider the equations arising from the operators $\mathbf{C}_l$. Equation (3) becomes

$$\mathbf{E}_{l+1}^{n'} = E_l^n - D^2/m \quad \text{unless } \mathbf{C}_l|nl\rangle = 0 \qquad (12)$$

which may be extended to

$$E_{l+2}^{n''} = E_l^n - 2D^2/m \quad \text{unless } \mathbf{C}_{l+1}|n'l+1\rangle = 0;$$

$$E_{l+3}^{n'''} = E_l^n - 3D^2/m \quad \text{unless } \mathbf{C}_{l+2}|n''l+1\rangle = 0, \text{ etc.}$$

The energy is clearly decreasing, but it can never be negative as all terms in the Hamiltonian have positive eigenvalues. Thus the series must terminate at some stage and

$$E_l^n = -F_l/2m = (n+3/2)D^2,$$

where we have identified the maximum l value with the energy label n. Substituting this into Eq. (12) gives

$$E_{l+1}^{n'} = \{(n-1)+3/2\}D^2$$

showing that $n' = n-1$ or

$$\mathbf{C}_l|nl\rangle = \lambda_l^n|n-1\;\; l+1\rangle.$$

We are now able to solve the recursion formula

$$|\lambda_l^n|^2 - |\lambda_{-1}^{n+1}|^2 = -4B^2$$

with $\lambda_n^n = 0$. The solution is (to within phase)

$$\lambda_l^n = B[2(n-l)]^{1/2}.$$

The degeneracy of the energy level E_l^n is easily established by looking at the chain $|nn\rangle$, $\mathbf{C}_{n-2}^*|n-1\;n-1\rangle$, $\mathbf{C}_{n-4}^*\mathbf{C}_{n-3}^*|n-2\;n-2\rangle, \ldots$ or $|nn\rangle$, $|n\,n-2\rangle$, $|n\,n-4\rangle$, ... so l may take the values n, $n-2$, $n-4$, ... to 0 or 1.

If next we turn to the operator $\mathbf{D}_l$ we may readily establish that

$$\mathbf{D}_l|nl\rangle = \mu_l^n|n+1\;l+1\rangle$$

but this series does not terminate, which means that we can perform no useful calculations with this operator.

CONCLUSION

We have shown that the ladder operator technique may be used to solve three important problems in quantum mechanics. The method is simple and direct, avoiding messy manipulation of differential equations on the one hand and sophisticated group theoretic methods on the other. We have tried to show which cases are soluble, but if it were desired to solve say just the Coulomb potential problem, rather than use the form (8) it would be easier to take $\mathbf{C}_l$ as

$$\mathbf{C}_l = p + A/r$$

with a corresponding simplification in the working. This should bring the material within the reach of an average student and could well supplement the angular momentum and linear oscillator problems.

[1]We do not prove the existence of this first eigenfunction, and so it is possible to gain more solutions than actually exist. This happens with the orbital angular momentum problem, where the ladder operator method gives the inadmissable half-odd integer solutions as well as the integral ones. This existence problem is more difficult [see H. A. Buchdall, Am. J. Phys. **30,** 829 (1962)] and will not be dealt with here.

[2]See, for example, W. Miller, Am. Math. Soc. Memoir No. 50 (1964), or R. Hermann, *Lie Groups for Physicists* (Benjamin, New York, 1966).

[3]L. Infield and T. E. Hull, Rev. Mod. Phys. **23,** 21 (1951).

[4]P. A. M. Dirac, *Principles of Quantum Mechanics* (Clarendon, Oxford, 1958).