11

Shape-Invariant Potentials: Soluble One-Dimensional Potential Problems

Having seen and used a number of examples, let us now look at the factorization method in a more general way. For the factorization method to work, we must have

$$[O_+(m)O_-(m) + \mathcal{L}(m)]u_{\lambda m} = \lambda u_{\lambda m}, \tag{1}$$

$$\left(\left[-\frac{d}{dx} + k(x,m)\right]\left[\frac{d}{dx} + k(x,m)\right] + \mathcal{L}(m)\right)u_{\lambda m} = \lambda u_{\lambda m}, \tag{2}$$

$$\begin{aligned}&\left(-\frac{d^2}{dx^2} + [k^2(x,m) - k'(x,m) + \mathcal{L}(m)]\right)u_{\lambda m} = \\ &\left(-\frac{d^2}{dx^2} + V(x,m)\right)u_{\lambda m} = \lambda u_{\lambda m},\end{aligned} \tag{3}$$

where the potential function $V(x, m)$ is expressed in terms of $k(x, m)$ and its first derivative is expressed by a prime. We must also have

$$[O_-(m+1)O_+(m+1) + \mathcal{L}(m+1)]u_{\lambda m} = \lambda u_{\lambda m}. \tag{4}$$

Eqs. (1) and (4) are the two conditions, I and II, of eq. (17) of Chapter 7, which must be satisfied for the factorization method to work. Now, shifting the index m to $(m-1)$ in eq. (4)

$$\begin{aligned}&[O_-(m)O_+(m) + \mathcal{L}(m)]u_{\lambda(m-1)} = \lambda u_{\lambda(m-1)} \\ &= \left(\left[\frac{d}{dx} + k(x,m)\right]\left[-\frac{d}{dx} + k(x,m)\right] + \mathcal{L}(m)\right)u_{\lambda(m-1)} = \lambda u_{\lambda(m-1)}\end{aligned} \tag{5}$$

$$\left(-\frac{d^2}{dx^2} + [k^2(x,m) + k'(x,m) + \mathcal{L}(m)]\right)u_{\lambda(m-1)}$$
$$= \left(-\frac{d^2}{dx^2} + V(x, m-1)\right)u_{\lambda(m-1)} = \lambda u_{\lambda(m-1)}, \tag{6}$$

where

$$V(x,m) = k^2(x,m) - k'(x,m) + \mathcal{L}(m), \tag{7}$$

$$V(x,m-1) = k^2(x,m) + k'(x,m) + \mathcal{L}(m), \tag{8}$$

or

$$V(x,m) - V(x,m-1) = -2k'(x,m). \tag{9}$$

In general, of course, this equation will not be satisfied for arbitrary $k(x, m)$. The factorization method works only if this condition is satisfied. Iterating this equation for $m-1, m-2, \ldots$, down to $m = 1$, we are lead to the relation

$$V(x,m) - V(x,0) = [k^2(x,m) - k'(x,m) + \mathcal{L}(m) - k^2(x,0)$$
$$+ k'(x,0) - \mathcal{L}(0)] = -2\sum_{n=1}^{n=m} k'(x,n). \tag{10}$$

Infeld and Hull studied the question: What kind of $k(x, m)$ can satisfy this equation? Trying first a Taylor series in m

$$k(x,m) = k_0(x) + k_1(x)m + \cdots, \tag{11}$$

they found the potential collapses to a constant independent of x (hence, a trivial unimportant case), if terms quadratic in m or higher powers of m are included. Nevertheless, the possible functions $k_0(x)$ and $k_1(x)$ lead to a number of interesting equations. Similarly, trying Laurent series in m

$$k(x,m) = \cdots + \frac{k_{-1}(x)}{m} + k_0(x) + k_1(x)m + \cdots, \tag{12}$$

they again found inverse quadratic and higher inverse powers of m lead to potentials independent of x and, hence, trivial. With the inverse first power in m, however, they found a number of new interesting cases.

It would of course be much nicer if we could immediately answer the question: Given a potential, $V(x, m)$, can we find solutions for the Schrödinger equation by the factorization method, or, what is equivalent: Can we find expressions for its eigenfunctions and eigenvalues in simple analytic form? Because this question has no simple general answer, we shall be content to follow the backward approach of Infeld and Hull, and starting with a set of possible $k(x, m)$ discover quite a number of soluble problems. Recall again that the factorization method involves nothing more mathematically challenging than the integration of a first-order differential equation and the taking of first derivatives in the laddering process.

A Shape-Invariant Potentials

If the potentials $V(x, m)$ and $V(x, m-1)$ are related as of eq. (9), the following is true.

1. The factorization method works.

2. The spectrum of allowed eigenvalues, λ, for the potential $V(x, m-1)$ is the same as that for $V(x, m)$, except the eigenvalue, $\lambda = \mathcal{L}(m_{\text{min}})$, does not exist in the spectrum for $V(x, m-1)$, because $u_{\lambda m_{\text{min}}-1}$ does not exist, assuming for now we are dealing with a case for which $\mathcal{L}(m)$ is a decreasing function of m. This follows because the eigenvalue λ does not change when we shift m to $m-1$ in equation (II).

3. The potentials $V(x, m)$ and $V(x, m-1)$ are said to have the same shape, because the dependence on x is the same, and only the value of m is replaced by $m-1$ ("Shape invariance" of the potential).

Now, had we written equation (I) of the factorized form with m replaced by $m-1$, and then shifted $m-1$ to $m-2$ in equation (II), we see the equation for $V(x, m-2)$ has the same spectrum as that for $V(x, m-1)$, except the eigenvalue $\lambda = \mathcal{L}(m_{\text{min}} - 1)$ is now missing. Thus, we can have a whole set of potentials with the same shape, all with the same spectrum, except the lowest eigenvalue of $V(x, m)$ is missing in $V(x, m-1)$, the lowest eigenvalue of $V(x, m-1)$, and hence the two lowest eigenvalues of $V(x, m)$ are missing for $V(x, m-2)$, and so on. Thus, the spectrum for $V(x, m-n)$ is the same as that for $V(x, m)$, except the lowest n eigenvalues of $V(x, m)$ are missing in the spectrum for $V(x, m-n)$, provided the factorization is such that the eigenvalues are given by $\lambda = \mathcal{L}(m_{\text{min}})$, that is, cases for which $\mathcal{L}(m)$ is a decreasing function of m. Similar arguments can be made for the other case, i.e., if $\mathcal{L}(m)$ is an increasing function of m. In that case, setting $m \to m+1$ in eqs. (3) and (6), we see $V(x, m+1)$ has the same spectrum of λ values, now with $\lambda = \mathcal{L}(m_{\text{max.}} + 1)$, except $\lambda = \mathcal{L}(m_{\text{max.}} + 1)$, which exists in the spectrum for $V(x, m)$ with eigenfunction $u_{\lambda, m_{\text{max}}}$, does not exist in the spectrum for $V(x, m+1)$, because $u_{\lambda, m_{\text{max}}+1}$ does not exist. Similarly, in the spectrum for $V(x, m+n)$, the eigenvalues $\lambda = \mathcal{L}(m_{\text{max.}} + 1), \mathcal{L}(m_{\text{max.}} + 2), \ldots, \mathcal{L}(m_{\text{max.}} + n)$ do not exist. The lowest eigenvalue for $V(x, m+n)$ is $\lambda = \mathcal{L}(m_{\text{max.}} + n + 1)$, which is also the n^{th} eigenvalue for $V(x, m)$.

B A Specific Example

As a very specific example, consider a 1-D Schrödinger equation for a particle moving in the domain $0 \leq x \leq a$ under the potential

$$
\begin{aligned}
V(x) &= \frac{\mathcal{V}_0}{\sin^2(\frac{\pi x}{a})}, \qquad 0 \leq x \leq a, \\
&= \infty, \qquad x \leq 0, \qquad x \geq a,
\end{aligned} \tag{13}
$$

$$-\frac{\hbar}{2m}\frac{d^2}{dx^2}u(x) + \frac{\mathcal{V}_0}{\sin^2(\frac{\pi x}{a})}u(x) = Eu(x), \tag{14}$$

or, with

$$\frac{\pi x}{a} = \theta, \qquad E = \epsilon\left(\frac{\hbar^2\pi^2}{2ma^2}\right), \qquad \mathcal{V}_0 = V_0\left(\frac{\hbar^2\pi^2}{2ma^2}\right), \tag{15}$$

$$-\frac{d^2u}{d\theta^2} + \frac{V_0}{\sin^2\theta}u = \epsilon u(\theta), \tag{16}$$

to be compared with our factorizable equation

$$-\frac{d^2u}{d\theta^2} + \frac{[m_0^2 - \frac{1}{4}]}{\sin^2\theta}u = \lambda u = \epsilon u. \tag{17}$$

Now, we let

$$V_0(\theta, m_0) = \frac{[m_0^2 - \frac{1}{4}]}{\sin^2\theta}, \qquad \text{with} \quad V_0 + \frac{1}{4} = m_0^2. \tag{18}$$

In order to work in the m region near $m_{\min}$, we shall choose the negative root for m_0

$$m_0 = -\sqrt{V_0 + \frac{1}{4}} = -|m_0|. \tag{19}$$

(We will subsequently investigate the region of m values near the positive root to show these give the same result.) For the above θ equation, we found $\mathcal{L}(m) = (m - \frac{1}{2})^2$, and with $m_{\min} = m_0 = -|m_0|$, we get the lowest eigenvalue, $\lambda_0 = \epsilon_0$,

$$\lambda_0 = \mathcal{L}(m_0) = (m_0 - \frac{1}{2})^2 = (|m_0| + \frac{1}{2})^2 = (\sqrt{V_0 + \frac{1}{4}} + \frac{1}{2})^2. \tag{20}$$

The eigenfunction for the ground state of V_0 is obtained from

$$O_-(m_0)u_{\lambda_0 m_0} = \frac{du}{d\theta} + (m_0 - \frac{1}{2})\cot\theta u(\theta) = 0, \tag{21}$$

with the solution

$$u_{\lambda_0 m_0} = N\big(\sin(\theta)\big)^{\frac{1}{2} - m_0}. \tag{22}$$

This is a square-integrable function, with $m_0 = -|m_0|$. The companion potential $V(\theta, m_0 - 1) = V(\theta, (-|m_0| - 1))$ has ground-state eigenvalue $\lambda = (-|m_0| - 1 - \frac{1}{2})^2 = (|m_0| + 1 + \frac{1}{2})^2$. Let us name this potential V_1, its ground state eigenvalue λ_1, and note that this is the first excited state, λ_1, for the potential V_0. Similarly, the n^{th}-companion potential $V(\theta, m_0 - n) = V(\theta, (-|m_0| - n))$ has lowest eigenvalue λ_n, where we name this potential V_n:

$$\lambda_n = (m_0 - n - \frac{1}{2})^2 = (|m_0| + n + \frac{1}{2})^2. \tag{23}$$

This is the ground state for the potential V_n and the n^{th} excited state for V_0. The ground state wave function for the potential V_n is

$$u_{\lambda_n(m_0-n)} = \sqrt{\frac{\pi}{a}\frac{\Gamma(|m_0|+n+\frac{3}{2})}{\Gamma(\frac{1}{2})\Gamma(|m_0|+n+1)}}\sin^{(|m_0|+n+\frac{1}{2})}(\theta) = N_n \sin^{(|m_0|+n+\frac{1}{2})}(\theta), \tag{24}$$

where we have now included the normalization factor explicitly. Recall

$$\int_0^\pi d\theta \sin^{2\alpha}\theta = B(\tfrac{1}{2},\alpha+\tfrac{1}{2}) = \frac{\Gamma(\frac{1}{2})\Gamma(\alpha+\frac{1}{2})}{\Gamma(\alpha+1)},$$

where B is the Beta function expressed in terms of Γ functions. To get the eigenfunction for the first excited state of the potential V_{n-1}, with this energy λ_n, we need to act with the normalized step-up operator $\mathcal{O}_+(m_0-n+1)$,

$$u_{\lambda_n(m_0-n+1)} = \frac{\mathcal{O}_+(-|m_0|-n+1)}{\sqrt{[\lambda_n-\mathcal{L}(m_0-n+1)]}}u_{\lambda_n(m_0-n)}, \tag{25}$$

with

$$\lambda_n = (|m_0|+n+\frac{1}{2})^2, \qquad \mathcal{L}(m_0-n+1) = (|m_0|+n-\tfrac{1}{2})^2. \tag{26}$$

Finally, to get the eigenfunction for the n^{th} excited state with this energy λ_n in the potential V_0, we need to act n-times with such step-up operators (laddering along the horizontal λ_n-line in Fig. 11.1):

$$\begin{aligned} u_{\lambda_n m_0}(\theta) &= \mathcal{O}_+(-|m_0|)\cdots\mathcal{O}_+((-|m_0|-n+2)\mathcal{O}_+(-|m_0|-n+1) \\ &\quad\times N_n\sin^{(|m_0|+n+\frac{1}{2})}(\theta) \\ &= \frac{\left(-\frac{d}{d\theta}-(|m_0|+\frac{1}{2})\cot\theta\right)}{\sqrt{[\lambda_n-(|m_0|+\frac{1}{2})^2]}}\cdots\frac{\left(-\frac{d}{d\theta}-(|m_0|+n-\frac{3}{2})\cot\theta\right)}{\sqrt{[\lambda_n-(|m_0|+n-\frac{3}{2})^2]}} \\ &\quad\times\frac{\left(-\frac{d}{d\theta}-(|m_0|+n-\frac{1}{2})\cot\theta\right)}{\sqrt{[\lambda_n-(|m_0|+n-\frac{1}{2})^2]}}N_n\sin^{(|m_0|+n+\frac{1}{2})}(\theta). \end{aligned} \tag{27}$$

In Fig. 11.1, a family of shape-invariant potentials of this $(1/\sin^2\theta)$ shape are shown, where we have chosen $m_0=-1.1$, so the strength of V_0 is $(-1.1)^2-\frac{1}{4}=0.96$, leading to potentials V_1, V_2, V_3, V_4 with strengths of 4.16, 9.36, 16.56, 25.76, respectively. The energies given by eq. (23) are shown in the figure.

In particular, if we had tried to continue the laddering process of eq. (27) one more time from $m_0=-1.1$ to an $m_0=-0.1$, we would be led to a potential of strength $(-0.1)^2-\frac{1}{4}=-0.24$, of the opposite sign from the potentials shown, i.e., a repulsive potential, with no bound states. Therefore, the process has to stop at V_0. No connection can exist from the problem with negative m values to the branch with positive m values, as for the θ equation for the spherical harmonics. The negative and positive m values are connected only in two special cases: if m_0

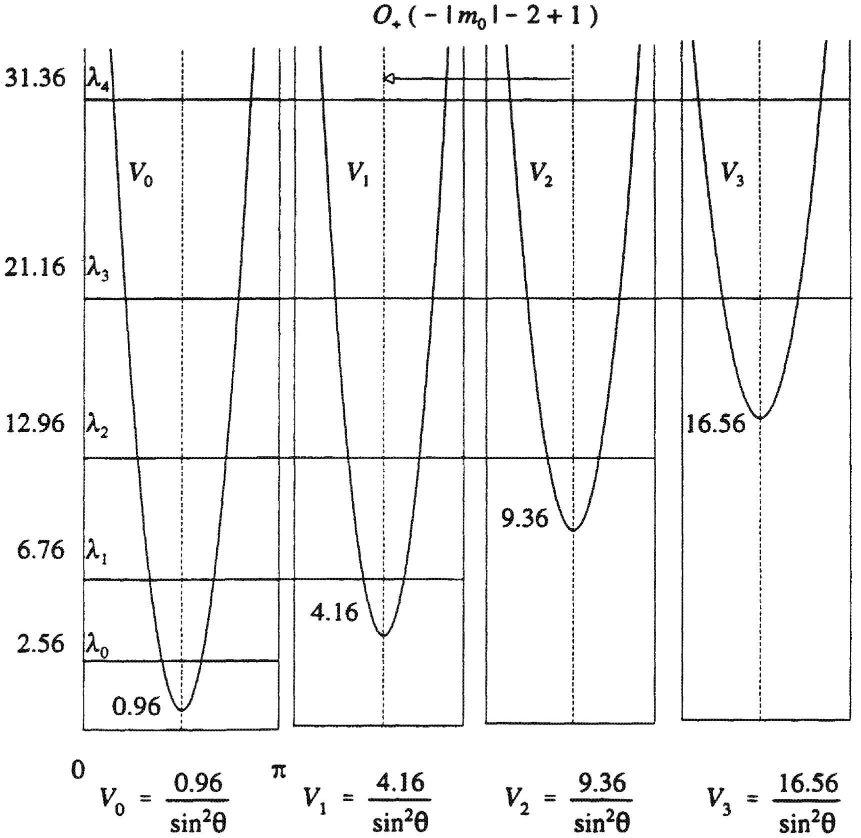

FIGURE 11.1. The family of shape-invariant $1/\sin^2\theta$ potentials, with $m_0 = -1.1$; $m = m_{\text{min.}\to+\infty}$.

is integer or $\frac{1}{2}$-integer. For an arbitrary value of V_0, it remains to be shown that the positive root, $m_0 = +\sqrt{V_0 + \frac{1}{4}}$, gives the same spectrum of eigenvalues and eigenfunctions. In the region of positive m values, $\mathcal{L}(m) = (m - \frac{1}{2})^2$ is an increasing function of m and $\lambda = \mathcal{L}(m_{\text{max.}} + 1)$. The shape-invariant partner potentials are $V_0(\theta, m_0)$, $V_1(\theta, m_0 + 1), \ldots, V_n(\theta, m_0 + n)$, with $m_{\text{max.}} = m_0 = +\sqrt{V_0 + \frac{1}{4}}$ for V_0 and $m_{\text{max.}} = m_0 + n$ for V_n, so λ_n, which is the ground-state eigenvalue for V_n and the n^{th} excited state for V_0, is given by

$$\lambda_n = (m_0 + n + \tfrac{1}{2})^2 \qquad \text{with} \quad m_0 > 0, \tag{28}$$

in agreement with eq. (23). Now the ground-state eigenfunction for V_n is given by

$$O_+(m_0 + n + 1)u_{\lambda_n, m_0+n} = \left(-\frac{d}{d\theta} + (m_0 + n + \tfrac{1}{2})\cot\theta\right)u_{\lambda_n, m_0+n} = 0, \tag{29}$$

leading again to

$$u_{\lambda_n,m_0+n} = N_n \sin^{(m_0+n+\frac{1}{2})}(\theta), \tag{30}$$

and the n^{th} excited state for V_0 is given by

$$\begin{aligned} u_{\lambda_n m_0} &= \mathcal{O}_-(m_0+1)\cdots\mathcal{O}_-(m_0+n-1)\mathcal{O}_-(m_0+n)u_{\lambda_n(m_0+n)} \\ &= \frac{\left(\frac{d}{d\theta}+(m_0+\frac{1}{2})\cot\theta\right)}{\sqrt{[\lambda_n-(m_0+\frac{1}{2})^2]}}\cdots\frac{\left(\frac{d}{d\theta}+(m_0+n-\frac{3}{2})\cot\theta\right)}{\sqrt{[\lambda_n-(m_0+n-\frac{3}{2})^2]}} \\ &\times\frac{\left(\frac{d}{d\theta}+(m_0+n-\frac{1}{2})\cot\theta\right)}{\sqrt{[\lambda_n-(m_0+n-\frac{1}{2})^2]}}u_{\lambda_n(m_0+n)}. \end{aligned} \tag{31}$$

Except for an overall phase factor $(-1)^n$, this function agrees with eq. (27), so the positive branch of m values gives exactly the same results as the negative branch and does not lead to anything new.

C Soluble One-Dimensional Potential Problems

1. The Pöschl–Teller Potential.

All of the factorizable equations we have met so far lead to soluble 1-D potential problems. One of these potentials is the so-called Pöschl–Teller potential, which leads to the 1-D Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2u(x)}{dx^2} - \frac{\mathcal{V}}{\cosh^2(x/a)}u(x) = Eu(x), \tag{32}$$

or introducing dimensionless quantities

$$z = \frac{x}{a}, \qquad V = \mathcal{V}\frac{2ma^2}{\hbar^2}, \qquad \epsilon = E\frac{2ma^2}{\hbar^2},$$

$$-\frac{d^2u(z)}{dz^2} - \frac{V}{\cosh^2 z}u(z) = \epsilon u(z) = \lambda u(z), \tag{33}$$

where the case $V > 0$ leads to an attractive potential. With

$$V = l(l+1), \quad \text{or} \quad l = -\tfrac{1}{2} \pm \sqrt{V + \tfrac{1}{4}},$$

Chapter 9 tells us

$$O_\pm = \mp\frac{d}{dz} + l\tanh z, \qquad \text{with} \quad \mathcal{L}(l) = -l^2. \tag{34}$$

This equation corresponds to an $\mathcal{L}(l)$ of case 4 of Chapter 7 with allowed negative values of $\epsilon = \lambda$ only for positive values of $l = l_{\text{min.}}, (l_{\text{min.}}+1), \ldots, (l_{\text{min.}}+n), \ldots,$

and for negative values of $l = l_{\rm max.}, (l_{\rm max.} - 1), \ldots, (l_{\rm max.} - n), \ldots$. If we choose the positive branch, with $l = -\frac{1}{2} + \sqrt{V + \frac{1}{4}}$,

$$l = l_{\rm min.} + n = -\tfrac{1}{2} + \sqrt{V + \tfrac{1}{4}}, \quad \text{so with} \quad \epsilon = \mathcal{L}(l_{\rm min.}),$$

we have

$$\epsilon_n = \lambda_n = \mathcal{L}(l_{\rm min.}) = -(l - n)^2 = -\Big(\sqrt{V + \tfrac{1}{4}} - (n + \tfrac{1}{2})\Big)^2, \qquad (35)$$

with shape-invariant potential partners $V_0(z, l_0), V_1(z, l_0 - 1), \ldots, V_n(z, l_0 - n)$, where now $l_0 = -\frac{1}{2} + \sqrt{V + \frac{1}{4}}$. Now a maximum possible value of $n = n_{\rm max.}$ exists, however, for which $(l_0 - n_{\rm max.})$ is such that

$$(l_0 - n_{\rm max.})(l_0 - n_{\rm max.} + 1) > 0; \quad \text{but } 0 < (l_0 - n_{\rm max.}) < 1.$$

In that case,

$$\Big(l_0 - (n_{\rm max.} + 1)\Big)\Big(l_0 - (n_{\rm max.} + 1) + 1\Big) < 0,$$

and this implies the potential $V(z, l_0 - (n_{\rm max.} + 1))$ is repulsive and therefore has no bound states. The condition $0 \leq (l_0 - n_{\rm max.}) \leq 1$ determines $n_{\rm max.}$ through

$$n_{\rm max.} + \tfrac{1}{2} \leq \sqrt{V + \tfrac{1}{4}} \leq n_{\rm max.} + \tfrac{3}{2}, \qquad \text{or}$$

$$n_{\rm max.}(n_{\rm max.} + 1) \leq V \leq (n_{\rm max.} + 1)(n_{\rm max.} + 2).$$

For $0 \leq V \leq 2$, $n_{\rm max.} = 0$, and therefore only a single bound state with $\epsilon_0 = -(-\frac{1}{2} + \sqrt{V + \frac{1}{4}})^2$ exists, but always at least this one bound state exists, even as $V \to 0$. Note the similarity in this regard between the Pöschl–Teller potential and the square well potential with $V = -V_0$ for $|z| \leq a$, and $V = 0$ for $|z| > a$ (see section B of Chapter 4).

Finally, $u_{\lambda_n, l_{\rm min.} = (l_0 - n)}$ is determined from

$$\frac{d}{dz} u_{\lambda_n (l_0 - n)} = -[(l_0 - n) \tanh z] u_{\lambda_n (l_0 - n)} = 0, \qquad \text{so}$$

$$u_{\lambda_n (l_0 - n)} = \frac{N_n}{(\cosh z)^{l_0 - n}} = \sqrt{\frac{\Gamma(l_0 - n + 1)}{a\Gamma(\frac{1}{2})\Gamma(l_0 - n)}} \frac{1}{(\cosh z)^{l_0 - n}}, \qquad (36)$$

where this is the ground-state eigenfunction for the potential, $V_n(z, l_0 - n)$, with $\epsilon_n = -(\sqrt{V + \frac{1}{4}} - (n + \frac{1}{2}))^2$, which is also the energy of the $n^{\rm th}$ excited state for the potential, $V_0 = -V/(\cosh^2 z)$. The normalized eigenfunction for this $n^{\rm th}$ excited state of V_0 is again given by

$$u_{\lambda_n l_0} = \frac{O_+(l_0)}{\sqrt{[-(l_0 - n)^2 + l_0^2]}} \cdots \frac{O_+(l_0 - n + 2)}{\sqrt{[(-(l_0 - n)^2 + (l_0 - n + 2)^2]}}$$
$$\times \frac{O_+(l_0 - n + 1)}{\sqrt{[-(l_0 - n)^2 + (l_0 - n + 1)^2]}} u_{\lambda_n (l_0 - n)}. \qquad (37)$$

Finally, the negative branch of allowed l values, with $l = -\frac{1}{2} - \sqrt{V + \frac{1}{4}}$, i.e., with $l < 0$, gives no additional eigenvalues or eigenvectors. In this case, $l = l_{\text{max.}} - n$, and $\lambda = \mathcal{L}(l_{\text{max.}} + 1) = -(l + n + 1)^2 = -(-\sqrt{V + \frac{1}{4}} + n + \frac{1}{2})^2$, in agreement with the result of eq. (35) for the positive branch of allowed l values. Except for a possible overall phase factor, the eigenfunctions again agree with those of the other branch. We could again show this explicitly as in the previous example, but also we note: Because we are dealing with a 1-D eigenvalue problem, we do not expect degeneracies for the general ϵ_n.

The inverse $\sin^2\theta$ potential, $V/(\sin^2\theta)$, and the Pöschl–Teller potential, $-V/(\cosh^2 z)$, are special cases of the general factorizable case, for which the 1-D Schrödinger equation can be written as

$$\left(-\frac{d^2}{dz^2} + V(z, m)\right)u(z) = \lambda u(z), \qquad \text{with}$$
$$V(z, m) = \frac{b^2(m + c)(m + c + 1) + d^2 + 2bd(m + c + \frac{1}{2})\cos b(z + p)}{\sin^2 b(z + p)} \tag{38}$$

and with

$$O_\pm(m) = \mp\frac{d}{dz} + (m + c)b\cot b(z + p) + \frac{d}{\sin b(z + p)},$$
$$\mathcal{L}(m) = b^2(m + c)^2, \tag{39}$$

where b, c, d, and p are arbitrary constants. For example, the Pöschl–Teller potential is obtained by setting $b = -i, c = 0, d = 0, p = (i\pi)/2$. Other specializations of this general case are listed by Infeld and Hull; see also problem 16, which treats the θ equation for the symmetric rigid rotator.

2. One-Dimensionalized Hydrogenic Potential.

The factorization of the radial equation for the hydrogen atom leads to a factorizable Schrödinger equation for a 1-D hydrogen-like potential

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dx^2} + V(x)u(x) = Eu(x), \quad \text{with} \quad V(x) = -\frac{A}{x} + \frac{B}{x^2} \quad \text{for } |x| \geq 0, \tag{40}$$

where we set $V = \infty$ for $x < 0$ and $V(x)$ has a minimum for positive values of $x = 2B/A$ if both $A > 0$, $B > 0$. With dimensionless quantities

$$z = \frac{x}{(\hbar^2/mA)}, \quad \epsilon = E\left(\frac{\hbar^2}{mA^2}\right), \quad l(l + 1) = \frac{2m}{\hbar^2}B,$$

the Schrödinger equation becomes

$$\left(-\frac{d^2}{dz^2} - \frac{2}{z} + \frac{l(l + 1)}{z^2}\right)u(z) = 2\epsilon u(z) = \lambda u(z), \qquad \text{with} \tag{41}$$

$$l = -\frac{1}{2} \pm \sqrt{\frac{2mB}{\hbar^2} + \frac{1}{4}}. \tag{42}$$

The results of Chapter 10 tell us

$$O_{\pm}(l) = \mp\frac{d}{dz} + \Big(\frac{l}{z} - \frac{1}{l}\Big), \qquad \text{with } \mathcal{L}(l) = -\frac{1}{l^2}. \tag{43}$$

From Chapter 10, we also know this equation will have bound states with $\lambda = 2\epsilon < 0$. For the branch of $\mathcal{L}(l)$, which is an increasing function of l, i.e., the positive branch with $l_0 = -\frac{1}{2} + \sqrt{(2mB)/\hbar^2 + \frac{1}{4}}$, the allowed l values range from $l_{\text{max.}}$, $(l_{\text{max.}} - 1), \dots, (l_{\text{max.}} - n), \dots$, and $\lambda = \mathcal{L}(l_{\text{max.}} + 1)$, so, with $\lambda_n = 2\epsilon_n$,

$$2\epsilon_n = -\frac{1}{(l_{\text{max.}} + 1)^2} = -\frac{1}{(l + n + 1)^2} = -\frac{1}{\Big[\sqrt{\frac{2mB}{\hbar^2} + \frac{1}{4}} + (n + \frac{1}{2})\Big]^2}. \tag{44}$$

The shape-invariant partner potentials are $V_0(z, l_0)$, $V_1(l_0 + 1), \dots, V_n(z, l_0 + n)$. The ground-state eigenfunction of $V_n(z, l_0 + n)$, with eigenvalue ϵ_n, is given by

$$O_+(l_0 + n + 1)u_{\lambda_n(l_0+n)} = \Big(-\frac{d}{dz} + \frac{(l_0 + n + 1)}{z} - \frac{1}{(l_0 + n + 1)}\Big)u_{\lambda_n(l_0+n)} = 0 \tag{45}$$

leading to a normalized

$$u_{\lambda_n(l_0+n)} = \sqrt{\Big[\frac{2}{(l_0 + n + 1)}\Big]^{(2l_0+n+3)} \frac{1}{\Gamma(2l_0 + 2n + 3)}}\, z^{l_0+n+1} e^{-\frac{z}{(l_0+n+1)}}. \tag{46}$$

The ground-state eigenfunction of $V_0(z, l_0)$ is obtained from this equation by setting $n = 0$. The eigenfunction of the n^{th} excited state of V_0, with ϵ_n, is again given by

$$u_{\lambda_n l_0} = \frac{O_-(l_0 + 1)}{\sqrt{[\lambda_n - \mathcal{L}(l_0 + 1)]}} \cdots \frac{O_-(l_0 + n - 1)}{\sqrt{[\lambda_n - \mathcal{L}(l_0 + n - 1)]}} \times \frac{O_-(l_0 + n)}{\sqrt{[\lambda_n - \mathcal{L}((l_0 + n)]}} u_{\lambda_n(l_0+n)}. \tag{47}$$

For an arbitrary value of l_0, not equal to an integer or $\frac{1}{2}$-integer, and a fixed $l_{\text{max.}}$, an n value will exist such that $l(l + 1) = (l_{\text{max.}} - n)(l_{\text{max.}} - n + 1)$ becomes a negative quantity. Because the generalized hydrogenic potential remains attractive even for this case, the value of the integer, n, can go to arbitrarily high values, and an infinite number of bound states exist. The values for $(l_0 + n)$ are positive for all positive integers n in the shape-invariant partner potentials, $V_n(z, l_0 + n)$. The action of the n stepdown operators, O_-, on $u_{\lambda_n(l_0+n)}$ produce an eigenfunction of the form, $z^{l_0+1}\mathcal{P}_n(z)e^{-\frac{z}{(l_0+n+1)}}$, where $\mathcal{P}_n(z)$ is a polynomial of degree n. This function is square-integrable over the interval, $0 \le z \le \infty$, for all positive integers, n. Because a second branch of allowed $\mathcal{L}(l)$ values for negative values of l exists, with $l = -\frac{1}{2} - \sqrt{2mB/\hbar^2 + \frac{1}{4}} = -(l_0 + 1)$ and $l = l_{\text{min.}}$, $(l_{\text{min.}} + 1), \dots, (l_{\text{min.}} + n), \dots$, we again need to examine the possibility this branch would lead to new eigenvalues. For $l < 0$, $\mathcal{L}(l)$ is a decreasing function of l. Therefore, now, with $\lambda_n = 2\epsilon_n$,

$$2\epsilon_n = \mathcal{L}(l_{\text{min.}}) = -\frac{1}{l_{\text{min.}}^2} = -\frac{1}{(l - n)^2} = -\frac{1}{\Big[-\frac{1}{2} - \sqrt{2mB/\hbar^2 + \frac{1}{4}} - n\Big]^2}, \tag{48}$$

exactly the same result as that already obtained for the positive l branch. Both the eigenvalues and eigenfunctions obtained from this negative l branch, thus, do not give anything new.

3. The Morse Potential.

Another 1-D potential leading to a factorizable Schrödinger equation is the Morse potential (see Fig. 11.2),

$$V(x) = D(e^{-2(x/a)} - 2e^{-(x/a)}), \tag{49}$$

$$\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dx^2} + D(e^{-2(x/a)} - 2e^{-(x/a)})\right]u(x) = Eu(x). \tag{50}$$

D gives the classical ionization or dissociation energy. The potential has a minimum value, $V_{\text{min.}} = -D$, at $x = 0$. For $E \geq 0$, a continuous spectrum exists. The particle can proceed to $x \to +\infty$. With the introduction of dimensionless quantities,

$$z = \frac{x}{a}, \quad \epsilon = E\frac{2\mu a^2}{\hbar^2}, \quad \delta^2 = D\frac{2\mu a^2}{\hbar^2}, \quad \text{this function leads to}$$

$$-\frac{d^2u}{dz^2} + (\delta^2 e^{-2z} + 2\delta(m+\frac{1}{2})e^{-z})u(z) = \epsilon u(z) = \lambda u(z), \tag{51}$$

where the parameter, m, with

$$\frac{(m+\frac{1}{2})}{\delta} = -1, \tag{52}$$

has been introduced to put the equation into factorizable form, with

$$O_\pm(m) = \mp\frac{d}{dz} + (\delta e^{-z} + m), \qquad \text{and} \quad \mathcal{L}(m) = -m^2. \tag{53}$$

Note, $-\delta - \frac{1}{2} = -\sqrt{(2\mu a^2 D/\hbar^2)} - \frac{1}{2}$, and hence, m, is a patently negative quantity. For $m < 0$, the above $\mathcal{L}(m)$ is an increasing function of m. For bound states, with $\lambda < 0$, a maximum possible value of $m = m_{\text{max.}}$ exists. The allowed m values are $m = m_{\text{max.}}, (m_{\text{max.}} - 1), \dots, (m_{\text{max.}} - n), \dots$, with

$$\begin{aligned}\lambda_n = \epsilon_n = \mathcal{L}(m_{\text{max.}} + 1) &= -(m+n+1)^2 = -(-\delta + n + \tfrac{1}{2})^2 \\ &= -\delta^2 + 2\delta(n+\tfrac{1}{2}) - (n+\tfrac{1}{2})^2,\end{aligned} \tag{54}$$

so

$$E_n = -D + 2\sqrt{\frac{\hbar^2 D}{2\mu a^2}}(n+\frac{1}{2}) - \frac{\hbar^2}{2\mu a^2}(n+\frac{1}{2})^2. \tag{55}$$

For the case $\delta \gg 1$, the last term, quadratic in $(n+\frac{1}{2})$, will be much smaller than the linear term, and the excitation energy is that of a slightly anharmonic oscillator, with

$$E_n + D \approx \hbar\omega(n+\tfrac{1}{2}), \qquad \text{with } \hbar\omega = 2\sqrt{\frac{\hbar^2 D}{2\mu a^2}}. \tag{56}$$

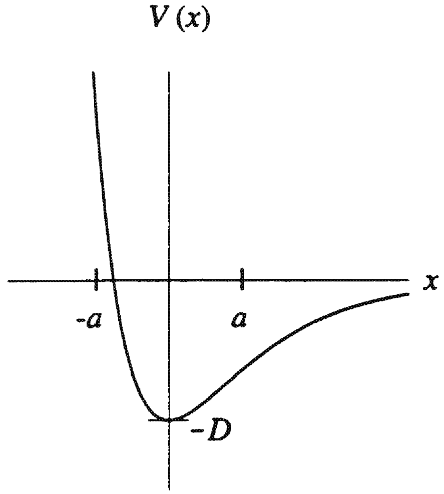

FIGURE 11.2. The Morse potential.

The shape-invariant partner potentials are $V_0(z, m_0)$, $V_1(z, m_0+1), \ldots, V_n(z, m_0+n)$, with $m_0 = -(\delta + \frac{1}{2})$, so

$$V_n(z, m_0 + n) = ((\delta^2 e^{-2z} + 2\delta(-\delta + n)e^{-z}). \tag{57}$$

This potential has the form shown in Fig. 11.2, with an attractive minimum, only for $n < \delta$; and the number of vibrational states is therefore limited. A maximum possible n value, $n_{\text{max.}}$ exists.

The ground-state eigenfunction of V_n is given by

$$O_+(m_0 + n + 1)u_{\lambda_n(m_0+n)} = \left[-\frac{d}{dz} + \left(\delta e^{-z} + (n - \delta + \tfrac{1}{2})\right)\right]u_{\lambda_n(m_0+n)} = 0, \tag{58}$$

$$u_{\lambda_n(m_0+n)} = N_n e^{-[(\delta - n - \frac{1}{2})z + \delta e^{-z}]}. \tag{59}$$

Successive action with the normalized step-down operators, $\mathcal{O}_-(m)$, with $m = (m_0 + n), (m_0 + n - 1), \ldots, (m_0 + 1)$ yields the needed n^{th} excited-state eigenfunction of V_0. These $u_{\lambda_n,m}$ are normalized in the interval $-\infty \leq z \leq +\infty$. Also, the $u_{\lambda_n,m}$ are normalizable only for integers n such that $n < (\delta - \frac{1}{2})$, which determines, $n_{\text{max.}}$.

In the actual applications, the Morse potential is used for the relative motion of the two atoms in a diatomic molecule, i.e., for the radial function of this two-body problem. In that case, therefore, μ is the reduced mass of the diatomic molecule, and $x = (r - r_e)$, where, r_e is the equilibrium value of the interatomic distance, r. Thus, the eigenfunctions *should* apply to the interval, $-(r_e/a) \leq z \leq +\infty$. For realistic parameters for most diatomic molecules, however, the Morse potential has such a large positive value at $z = -(r_e/a)$ that the Morse eigenfunctions are effectively zero for $z < -(r_e/a)$. The 1-D solutions found above for the full z-space

Molecule	$D_{\text{obs.}}\frac{1}{hc}$	$(\hbar^2/2\mu a^2)_{\text{obs.}}\frac{1}{hc}$	δ	$n_{\text{max.}}$	$(\hbar\omega)_{\text{obs.}}\frac{1}{hc}$
H_2	38,276 cm^{-1}	118 cm^{-1}	18.0	17	4395 cm^{-1}
HCl	37,257 cm^{-1}	52.05 cm^{-1}	26.7	26	2990 cm^{-1}
O_2	41,758 cm^{-1}	12.07 cm^{-1}	58.8	58	1580 cm^{-1}

are therefore a good approximation for most diatomic molecules. The parameters D, $(\hbar^2/2\mu a^2)$, and δ are shown for a few molecules in the table provided here. The $D_{\text{obs.}}$ and $(\hbar^2/2\mu a^2)_{\text{obs.}}$ have been extracted from the observed vibrational spectra, [G. Herzberg; *Molecular Spectra and Molecular Structure*. I. *Spectra of Diatomic Molecules*, D. van Nostrand (1950)]. The $\hbar\omega$ predicted by the Morse-potential energy relation, eq. (55), has the values 4128 cm^{-1} for H_2, 2728 cm^{-1} for HCl, and 1407 cm^{-1} for O_2 in reasonable agreement with the values extracted from the observed spectra. (Molecular spectroscopists in general give (energy/hc) in wavenumbers, cm^{-1}.)

4. The Rosen–Morse Potential.

A similar potential is the Rosen–Morse potential, which leads to the 1-D Schrödinger equation

$$-\frac{\hbar^2}{2\mu}\frac{d^2u}{dx^2} + \Big(-\frac{V_1}{\cosh^2(x/a)} + 2V_2\tanh\Big(\frac{x}{a}\Big)\Big)u(x) = Eu(x). \tag{60}$$

With dimensionless quantities,

$$z = \frac{x}{a}, \qquad \epsilon = E\frac{2\mu a^2}{\hbar^2}, \quad m(m+1) = V_1\frac{2\mu a^2}{\hbar^2}, \quad q = V_2\frac{2\mu a^2}{\hbar^2},$$

this equation leads to

$$-\frac{d^2u}{dz^2} + \Big(-\frac{m(m+1)}{\cosh^2 z} + 2q\tanh z\Big)u(z) = \epsilon u(z). \tag{61}$$

This potential has an attractive well with a minimum at z_0, given by

$$\tanh z_0 = -\frac{V_2}{V_1} = -\frac{q}{m(m+1)}, \tag{62}$$

which has a solution only for

$$|q/m(m+1)| < 1. \tag{63}$$

The equation is factorizable, with

$$O_{\pm}(m) = \Big(\mp\frac{d}{dz} + m\tanh z + \frac{q}{m}\Big), \qquad \text{and} \quad \mathcal{L}(m) = -m^2 - \frac{q^2}{m^2}. \tag{64}$$

Choosing the branch of $\mathcal{L}(m)$ with positive values of m, this $\mathcal{L}(m)$ belongs to case 4. The maximum of the function $\mathcal{L}(m)$ occurs at $m = \sqrt{|q|}$, where $\mathcal{L}(m)$ has the value $-2|q|$, which is also the ionization or dissociation value of $V(z)$. Thus, bound states will exist if $\epsilon < -2|q|$, and the requirement $[\lambda - \mathcal{L}(m)] \geq 0$, together with the requirement of eq. (63) leads to an allowed branch of m values with $m > \sqrt{|q|}$, where $\mathcal{L}(m)$ is a decreasing function of m, so $m = m_{\text{min.}}, (m_{\text{min.}}+1), \dots, (m_{\text{min.}}+$

$n), \ldots,$ with

$$\epsilon_n = \lambda_n = \mathcal{L}(m_{\text{min.}}) = -(m-n)^2 - \frac{q^2}{(m-n)^2}$$
$$= -\Big(\sqrt{\frac{2\mu a^2 V_1}{\hbar^2} + \tfrac{1}{4}} - (n+\tfrac{1}{2})\Big)^2 - \frac{q^2}{\Big(\sqrt{\frac{2\mu a^2 V_1}{\hbar^2} + \frac{1}{4}} - (n+\frac{1}{2})\Big)^2}. \quad (65)$$

The shape-invariant partner potentials are $V_0(z, m_0)$, $V_1(z, m_0 - 1), \ldots, V_n(z, m_0 - n)$, with $m_0 = -\frac{1}{2} + \sqrt{(2\mu a^2 V_1/\hbar^2) + \frac{1}{4}}$. The ground-state eigenfunction of $V(z, m_0 - n)$ is determined by

$$\Big(\frac{d}{dz} + (m_0 - n)\tanh z + \frac{q}{(m_0 - n)}\Big) u_{\lambda_n(m_0-n)} = 0,$$
$$u_{\lambda_n(m_0-n)} = N_n \frac{1}{(\cosh z)^{(m_0-n)}} e^{-\frac{q}{(m_0-n)}z}, \quad (66)$$

and the eigenfunction of the n^{th} excited state of V_0 is obtained from this function by the action of n operators $O_+(m)$ with m running from $(m_0 - n + 1)$ to m_0. Again, a maximum n value exists beyond which the potential $V(z, m_0 - n)$ ceases to have an attractive minimum with bound states and square-integrable bound-state eigenfunctions, so V_0 again has only a finite number of bound states.

5. The one-dimensional harmonic oscillator revisited.

The 1-D harmonic oscillator Schrödinger equation

$$\Big(-\frac{d^2}{dx^2} + x^2\Big) u(x) = 2\epsilon u(x), \quad (67)$$

with dimensionless, x and ϵ, is factorizable, with

$$O_\pm = \Big(\mp\frac{d}{dx} + x\Big). \quad (68)$$

The only parameter, however, is the energy, ϵ, itself, and the factors, $O_\pm$, are not functions of ϵ. Now,

$$\begin{aligned} &\text{I} \quad O_+O_-u(x) = (2\epsilon - 1)u(x) = [-1 + 2\epsilon]u(x), \\ &\text{II} \quad O_-O_+u(x) = (2\epsilon + 1)u(x) = [-1 + 2(\epsilon + 1)]u(x), \end{aligned} \quad (69)$$

are to be compared with

$$\begin{aligned} &\text{I} \quad O_+O_-u_{\lambda m} = [\lambda - \mathcal{L}(m)]u_{\lambda m}, \\ &\text{II} \quad O_-O_+u_{\lambda m} = [\lambda - \mathcal{L}(m+1)]u_{\lambda m}. \end{aligned} \quad (70)$$

Therefore, λ has the single-fixed eigenvalue, $\lambda = -1$, and the parameter, m, is replaced by ϵ, with $\mathcal{L}(\epsilon) = -2\epsilon$. Because $\mathcal{L}(\epsilon)$ is a decreasing function of ϵ, an $\epsilon_{\text{min.}}$ exists, with

$$\lambda = -1 = \mathcal{L}(\epsilon_{\text{min.}}) = -2\epsilon_{\text{min.}}, \qquad \text{so } \epsilon_{\text{min.}} = \tfrac{1}{2}. \quad (71)$$

The allowed values of ϵ are $\epsilon = \epsilon_{\text{min.}}, (\epsilon_{\text{min.}} + 1), \dots, (\epsilon_{\text{min.}} + n) = (\frac{1}{2} + n), \dots$. Therefore, $\epsilon_n = (n + \frac{1}{2})$. The starting eigenfunction is obtained from

$$O_- u_{-1,\epsilon_{\min}} = \Big(\frac{d}{dx} + x\Big) u_{-1,\epsilon_{\min.}} = 0,$$
$$u_{-1,\epsilon_{\min}} = \frac{1}{\pi^{\frac{1}{4}}} e^{-\frac{1}{2}x^2}. \qquad (72)$$

The excited-state eigenfunctions are obtained with the normalized step-up operators

$$O_+(n+1) = \frac{(-\frac{d}{dx} + x)}{\sqrt{[-1 + 2\epsilon_{(n+1)}]}} = \frac{(-\frac{d}{dx} + x)}{\sqrt{2(n+1)}},$$

so

$$u_{-1,\epsilon_n}(x) = \frac{1}{\sqrt{2^n n! \sqrt{\pi}}} \Big(-\frac{d}{dx} + x\Big)^n e^{-\frac{1}{2}x^2}. \qquad (73)$$

Using the identities

$$\Big(-\frac{d}{dx} + x\Big) = e^{\frac{1}{2}x^2}\Big[e^{-\frac{1}{2}x^2}\Big(-\frac{d}{dx} + x\Big)e^{\frac{1}{2}x^2}\Big]e^{-\frac{1}{2}x^2} = e^{\frac{1}{2}x^2}\Big[-\frac{d}{dx}\Big]e^{-\frac{1}{2}x^2}, \qquad (74)$$

the normalized n^{th} eigenfunction becomes

$$u_{-1,\epsilon_n}(x) = \frac{1}{\sqrt{2^n n! \sqrt{\pi}}} e^{\frac{1}{2}x^2}\Big(-\frac{d}{dx}\Big)^n e^{-\frac{1}{2}x^2} e^{-\frac{1}{2}x^2}$$
$$= \frac{e^{-\frac{1}{2}x^2}}{\sqrt{2^n n! \sqrt{\pi}}}\Big[e^{x^2}\Big(-\frac{d}{dx}\Big)^n e^{-x^2}\Big] = \frac{e^{-\frac{1}{2}x^2} H_n(x)}{\sqrt{2^n n! \sqrt{\pi}}}, \qquad (75)$$

where we have used the Rodriguez-type definition of the Hermite polynomial, $H_n(x)$, [see eq. (75) of Chapter 4].

Finally, the radial equation for the 3-D harmonic oscillator can also be solved by the factorization method. For details, see problem 15.

Altogether, Infeld and Hull list 31 generalizations or specializations of the Pöschl–Teller, hydrogenic, Morse, Rosen–Morse, 1-D harmonic oscillator, or 3-D harmonic oschillator Schrödinger equations, which lead to eigenvalues and eigenfunctions in analytic form, where the eigenfunctions correspond to many of the well-known functions of classical analysis. The question now arises: Do additional potentials exist for which the 1-D Schrödinger problem can be solved exactly? This question will be partially answered in the next chapter.

Problems

14. (a) Find the eigenvalues, ϵ_n, and the normalized eigenfunctions for all of the bound states of a Pöschl–Teller potential with dimensionless

$$V(z) = -\frac{V_0}{\cosh^2 z}, \qquad \text{with } V_0 = 7.2.$$

(b) A particle of mass μ moves in one dimension subject to the Schrödinger equation

$$-\frac{\hbar^2}{2\mu a^2}\Big(-\frac{d^2}{dz^2}+\frac{m(m+1)}{\sinh^2 z}-2\nu\coth z\Big)u(z)=Eu(z),$$

where z is a dimensionless variable, restricted to $z \geq 0$, and m and ν are dimensionless potential constants. Find the conditions that must be satisfied by these constants, so the potential has an attractive minimum for $z > 0$, and find an expression for the eigenvalues, E_n, as a function of n. Does a maximum possible value of n exist?

15. The 3-D harmonic oscillator. With $u(r) = rR(r)$, and $r = \sqrt{\hbar/m\omega_0}\rho$, $E = \hbar\omega_0\epsilon$, the radial wave equation for the 3-D harmonic oscillator (with $l = 0, 1, 2, \ldots$) takes the form

$$-\frac{d^2u}{d\rho^2}+\left[\frac{l(l+1)}{\rho^2}+\rho^2\right]u(\rho)=2\epsilon u(\rho).$$

Show that this equation is factorizable via

$$O_{\pm}(l)=-\Big(\mp\frac{d}{d\rho}+(\frac{l}{\rho}-\rho)\Big),$$

but the standard λ must be interpreted as $\lambda = 2\epsilon + 2l$; so $O_{\pm}(l)$ steps both l and ϵ. Show that this equation is also factorizable via

$$\bar{O}_{\pm}(l)=\Big(\mp\frac{d}{d\rho}+(\frac{l}{\rho}+\rho)\Big),$$

but now with $\lambda = 2\epsilon - 2l$.

Use these results to show that

$$E=\hbar\omega_0(N+\tfrac{3}{2}), \quad \text{with } N=0,1,2,\ldots$$

and that the allowed l values for a particular, N, are

$$l=N, N-2, N-4, \ldots, 0(\text{or } 1), \quad \text{for } N = \text{even (odd)}.$$

Find the normalized eigenfunctions for the special states with $l = N$. Construct the four normalized step operators, which convert normalized u_{Nl} into normalized $u_{N+1,l-1}$, $u_{N-1,l+1}$, $u_{N+1,l+1}$, and $u_{N-1,l-1}$. Construct all normalized radial eigenfunctions for $N \leq 3$

Find relations giving ρu_{Nl} as a linear combination of (i) $u_{N+1,l+1}$ and $u_{N-1,l+1}$, and as a linear combination of (ii) $u_{N+1,l-1}$ and $u_{N-1,l-1}$. Use these relations to find matrix elements of the operators, $\rho\cos\theta$ and $\rho\sin\theta e^{\pm i\phi}$ in the complete 3-D oscillator basis, ψ_{Nlm}. (The u_{Nl} and $u_{N'l'}$, with $l' \neq l$, are not orthogonal to each other in ρ-space, but the full energy eigenfunctions, $u_{Nl}(\rho)Y_{lm}(\theta,\phi)$ form a complete orthogonal set.)

Find all nonzero matrix elements of the operator, ρ^2.

Note: The above matrix elements of $\rho\cos\theta$ and $\rho\sin\theta e^{\pm i\phi}$ give the matrix elements of the dimensionless z and $(x \pm iy)$. The corresponding matrix elements of the dimensionless p_z and $(p_x \pm ip_y)$ can be obtained by utilizing the commutator relations

$$p_z = i[H, z], \qquad (p_x \pm ip_y) = i[H, (x \pm iy)],$$

together with the known matrix elements of the dimensionless H and z, $(x \pm iy)$. Use this technique to find the expressions for the nonzero matrix elements of p_z.

Solution for Problem 15

With

$$O_{\pm}(l) = -\Big(\mp\frac{d}{d\rho} + (\frac{l}{\rho} - \rho)\Big),$$

(where the extra overall minus sign in this definition is added merely for convenience to gain phases for the final matrix elements in best agreement with the "standard" phases for the 3-D oscillator), we have the two basic equations

$$O_+(l)O_-(l) = -\frac{d^2}{d\rho^2} + \frac{l(l+1)}{\rho^2} + \rho^2 - (2l-1),$$
$$O_-(l+1)O_+(l+1) = -\frac{d^2}{d\rho^2} + \frac{l(l+1)}{\rho^2} + \rho^2 - (2l+3), \qquad (1)$$

and

$$O_+(l)O_-(l)u_{\lambda l} = [2\epsilon - (2l-1)]u_{\lambda l} = [\lambda - \mathcal{L}(l)]u_{\lambda l},$$
$$O_-(l+1)O_+(l+1)u_{\lambda l} = [2\epsilon - (2l+3)]u_{\lambda l} = [\lambda - \mathcal{L}(l+1)]u_{\lambda l}. \qquad (2)$$

These two equations are satisfied only if $\mathcal{L}(l+1) - \mathcal{L}(l) = 4$, and have a proper solution only if

$$\mathcal{L}(l) = 4l + c, \qquad \lambda = 2\epsilon + 2l + c + 1, \qquad c = \text{a constant}. \qquad (3)$$

We will find it convenient to choose, $c = -1$ (this choice is quite arbitrary and will not affect final results). With this choice,

$$\mathcal{L}(l) = (4l - 1), \qquad \lambda = 2\epsilon + 2l. \qquad (4)$$

Because our $l \geq 0$, this $\mathcal{L}(l)$ is an increasing function of l. Thus, an $l_{\text{max.}}$ exists (to be named N), $l_{\text{max.}} = N$, with $\lambda = \mathcal{L}(l_{\text{max.}} + 1) = (4l_{\text{max.}} + 3) = (4N + 3)$, and therefore

$$2\epsilon = (2N + 3), \qquad E_N = \hbar\omega_0(N + \tfrac{3}{2}). \qquad (5)$$

The starting functions of $u_{\lambda l_{\text{max.}}}$ are given by

$$O_+(l_{\text{max.}} + 1)u_{\lambda l_{\text{max.}}}(\rho) = 0, \qquad \Big(\frac{d}{d\rho} - \frac{N+1}{\rho} + \rho\Big)u_{\lambda N}(\rho) = 0, \qquad (6)$$

where this first-order differential equation has the solution

$$u_{\lambda, l=N}(\rho) = \mathcal{N}\rho^{N+1}e^{-\frac{1}{2}\rho^2}, \qquad (7)$$

with $|\mathcal{N}|^2 \int_0^\infty d\rho \rho^{2N+2} e^{-\rho^2} = \frac{1}{2}|\mathcal{N}|^2 \int_0^\infty d\eta \eta^{N+\frac{1}{2}} e^{-\eta} = \frac{1}{2}|\mathcal{N}|^2 \Gamma(N+\frac{3}{2}) = 1.$

$$\left[\text{Note,}\ \tfrac{1}{2}\Gamma(N+\tfrac{3}{2}) = \tfrac{1}{2}(N+\tfrac{1}{2})(N-\tfrac{1}{2})\cdots\tfrac{3}{2}\tfrac{1}{2}\sqrt{\pi} = \frac{(2N+1)!!}{2^{N+2}}\sqrt{\pi}\right].$$

$O_-(l)$ changes $l \to (l-1)$, but because it keeps λ invariant, and $\lambda = 2\epsilon + 2l$, it must simultaneously raise ϵ by one unit, and hence, shifts $N \to (N+1)$. Similarly, $O_+(l+1)$ simultaneously changes $l \to (l+1)$, $N \to (N-1)$. To obtain the possible l values for a fixed N, we first examine the action of the operators

$$\bar{O}_\pm(l) = \left(\mp\frac{d}{d\rho} + (\frac{l}{\rho} + \rho)\right),$$

with

$$\begin{aligned}
\bar{O}_+(l)\bar{O}_-(l)u_{\bar{\lambda}l} &= \left(-\frac{d^2}{d\rho^2} + \frac{l(l+1)}{\rho^2} + \rho^2 + (2l-1)\right)u_{\bar{\lambda}l} \\
&= (2\epsilon + 2l - 1)u_{\bar{\lambda}l} = [\bar{\lambda} - \bar{\mathcal{L}}(l)]u_{\bar{\lambda}l} \\
\bar{O}_-(l+1)\bar{O}_+(l+1)u_{\bar{\lambda}l} &= \left(-\frac{d^2}{d\rho^2} + \frac{l(l+1)}{\rho^2} + \rho^2 + (2l+3)\right)u_{\bar{\lambda}l} \\
&= (2\epsilon + 2l + 3)u_{\bar{\lambda}l} = [\bar{\lambda} - \bar{\mathcal{L}}(l+1)]u_{\bar{\lambda}l}, \qquad (8)
\end{aligned}$$

which can be satisfied by

$$\bar{\mathcal{L}}(l) = -(4l-1), \qquad \bar{\lambda} = (2\epsilon - 2l). \qquad (9)$$

$\bar{\lambda} - \bar{\mathcal{L}}(l)$ remains positive for all possible values of l, even as l is increased indefinitely. No new limits are set on l by the operators $\bar{O}_\pm$. Also,

$\bar{O}_-(l)$ changes $l \to (l-1)$ and simultaneously $N \to (N-1)$, and

$\bar{O}_+(l+1)$ changes $l \to (l+1)$ and simultaneously $N \to (N+1)$.

Starting with the maximum l value for a particular N, $l_{\text{max.}} = N$, successive action with $O_-(l)$ followed by $\bar{O}_-(l-1)$, or equally well $\bar{O}_-(l)$ followed by $O_-(l-1)$, will change a state with quantum numbers, N, l to a state with quantum numbers $N, (l-2)$, skipping states with $N, (l-1)$. The four operators, $O_\pm$, $\bar{O}_\pm$, do not change the parity of $(N+l)$. For a fixed energy (fixed N), the possible l values are

$$l = N, (N-2), (N-4), \cdots, 0\ (\text{or}\ 1), \qquad \text{for}\ N = \text{even}\ (\text{or odd}).$$

It will now be convenient to define the four step operators preserving the normalization of the u_{Nl}, which will be denoted by $\mathcal{O}$. [Also, we will characterize the radial eigenfunctions by the quantum numbers, N, l; that is, we will replace the λ (or $\bar{\lambda}$) with the quantum number N, which gives the energy eigenvalue, ϵ.]

$$\mathcal{O}_-(l) = \frac{O_-(l)}{\sqrt{[\lambda - \mathcal{L}(l)]}}, \qquad \mathcal{O}_+(l+1) = \frac{O_+(l+1)}{\sqrt{[\lambda - \mathcal{L}(l+1)]}},$$

$$\text{with}\ [\lambda - \mathcal{L}(l)] = (2\epsilon + 2l) - (4l-1) = (2N + 3 - 2l + 1).$$

$$\bar{\mathcal{O}}_-(l) = \frac{\bar{O}_-(l)}{\sqrt{[\bar{\lambda} - \bar{\mathcal{L}}(l)]}}, \quad \bar{\mathcal{O}}_+(l+1) = \frac{\bar{O}_+(l+1)}{\sqrt{[\bar{\lambda} - \bar{\mathcal{L}}(l+1)]}},$$

with $= [\bar{\lambda} - \bar{\mathcal{L}}(l)] = (2\epsilon - 2l) + (4l - 1) = (2N + 3 + 2l - 1).$

Thus,

$$u_{(N+1)(l-1)} = \mathcal{O}_-(l)u_{Nl} = \frac{1}{\sqrt{2(N+2-l)}}\left(-\frac{d}{d\rho} - \frac{l}{\rho} + \rho\right)u_{Nl},$$

$$u_{(N-1)(l+1)} = \mathcal{O}_+(l+1)u_{Nl} = \frac{1}{\sqrt{2(N-l)}}\left(\frac{d}{d\rho} - \frac{(l+1)}{\rho} + \rho\right)u_{Nl},$$

$$u_{(N-1)(l-1)} = \bar{\mathcal{O}}_-(l)u_{Nl} = \frac{1}{\sqrt{2(N+1+l)}}\left(\frac{d}{d\rho} + \frac{l}{\rho} + \rho\right)u_{Nl},$$

$$u_{(N+1)(l+1)} = \bar{\mathcal{O}}_+(l+1)u_{Nl} = \frac{1}{\sqrt{2(N+3+l)}}\left(-\frac{d}{d\rho} + \frac{(l+1)}{\rho} + \rho\right)u_{Nl}.$$

Combining the first and third of these relations, we get

$$\rho u_{Nl} = \sqrt{\frac{(N+2-l)}{2}}u_{(N+1)(l-1)} + \sqrt{\frac{(N+1+l)}{2}}u_{(N-1)(l-1)}. \tag{10}$$

Similarly, combining the second and fourth relation, we get

$$\rho u_{Nl} = \sqrt{\frac{(N-l)}{2}}u_{(N-1)(l+1)} + \sqrt{\frac{(N+3+l)}{2}}u_{(N+1)(l+1)}. \tag{11}$$

If we left-multiply the first of these equations with $u^*_{(N+1)(l-1)}$ and integrate over ρ, and use the orthonormality of the u_{Nl} with the *same* l value, we get

$$\int_0^\infty d\rho u^*_{(N+1)(l-1)}\rho u_{Nl} = \int_0^\infty d\rho\rho^2 R^*_{(N+1)(l-1)}\rho R_{Nl} = \sqrt{\frac{(N+2-l)}{2}},$$

where we have used

$$\int_0^\infty d\rho u^*_{(N+1)(l-1)}u_{(N-1)(l-1)} = 0.$$

Both functions have the same l value, viz., $(l-1)$, and where we recall that the 1-D $u_{NL}(\rho)$ is related to the radial function, $R_{Nl}(\rho)$, via $u_{Nl}(\rho) = \rho R_{Nl}(\rho)$, where we also recall ρ is the dimensionless radial coordinate $\rho = r_{\text{phys.}}/\sqrt{\hbar/m\omega_0}$. Finally, if we combine the dimensionless ρ with the angular functions, we get the components of the (dimensionless) vector $\vec{r}$: $z = \rho\cos\theta$; $(x \pm iy) = \rho\sin\theta e^{\pm i\phi}$. With the matrix elements of the angular functions given through eqs. (42)–(44) of Chapter 9, we have, e.g.,

$$\langle\psi_{(N+1)(l-1)m}, \rho\cos\theta\psi_{Nlm}\rangle = \sqrt{\frac{(N+2-l)}{2}}\sqrt{\frac{(l^2-m^2)}{(2l+1)(2l-1)}},$$

$$\langle\psi_{(N-1)(l-1)m}, \rho\cos\theta\psi_{Nlm}\rangle = \sqrt{\frac{(N+1+l)}{2}}\sqrt{\frac{(l^2-m^2)}{(2l+1)(2l-1)}},$$
$$\langle\psi_{(N+1)(l+1)m}, \rho\cos\theta\psi_{Nlm}\rangle = \sqrt{\frac{(N+3+l)}{2}}\sqrt{\frac{[(l+1)^2-m^2]}{(2l+1)(2l+3)}},$$
$$\langle\psi_{(N-1)(l+1)m}, \rho\cos\theta\psi_{Nlm}\rangle = \sqrt{\frac{(N-l)}{2}}\sqrt{\frac{[(l+1)^2-m^2]}{(2l+1)(2l+3)}}, \qquad (12)$$

where the similar matrix elements of $\rho\sin\theta e^{\pm i\phi}$ differ only in the l, m dependent square root factors coming from the angular parts [which now also change m to $(m \pm 1)$].

To get the matrix elements of ρ^2, we can combine eqs. (10) and (11)

$$\rho^2 u_{Nl} = \sqrt{\frac{(N+2-l)}{2}}\left(\sqrt{\frac{(N+2-l)}{2}}u_{Nl} + \sqrt{\frac{(N+3+l)}{2}}u_{(N+2)l}\right)$$
$$+ \sqrt{\frac{(N+1+l)}{2}}\left(\sqrt{\frac{(N-l)}{2}}u_{(N-2)l} + \sqrt{\frac{(N+1+l)}{2}}u_{Nl}\right). \qquad (13)$$

This equation leads to the matrix elements

$$\langle\psi_{Nlm}, \rho^2\psi_{Nlm}\rangle = (N + \tfrac{3}{2}),$$
$$\langle\psi_{(N+2)lm}, \rho^2\psi_{Nlm}\rangle = \tfrac{1}{2}\sqrt{(N+2-l)(N+l+3)},$$
$$\langle\psi_{(N-2)lm}, \rho^2\psi_{Nlm}\rangle = \tfrac{1}{2}\sqrt{(N-l)(N+l+1)}. \qquad (14)$$

Finally, to obtain matrix elements of p_z and $(p_x \pm ip_y)$, we can use the commutator relations

$$p_z = i[H, z], \qquad (p_x \pm ip_y) = i[H, (x \pm iy)],$$

so, e.g.,

$$\langle\psi_{N'l'm}, p_z\psi_{Nlm}\rangle = i[(N' + \tfrac{3}{2}) - (N + \tfrac{3}{2})]\langle\psi_{N'l'm}, z\psi_{Nlm}\rangle, \qquad (15)$$

giving

$$\langle\psi_{(N+1)(l-1)m}, p_z\psi_{Nlm}\rangle = i\sqrt{\frac{(N+2-l)}{2}}\sqrt{\frac{(l^2-m^2)}{(2l+1)(2l-1)}},$$
$$\langle\psi_{(N-1)(l-1)m}, p_z\psi_{Nlm}\rangle = -i\sqrt{\frac{(N+1+l)}{2}}\sqrt{\frac{(l^2-m^2)}{(2l+1)(2l-1)}},$$
$$\langle\psi_{(N+1)(l+1)m}, p_z\psi_{Nlm}\rangle = i\sqrt{\frac{(N+3+l)}{2}}\sqrt{\frac{[(l+1)^2-m^2]}{(2l+1)(2l+3)}},$$
$$\langle\psi_{(N-1)(l+1)m}, p_z\psi_{Nlm}\rangle = -i\sqrt{\frac{(N-l)}{2}}\sqrt{\frac{[(l+1)^2-m^2]}{(2l+1)(2l+3)}}. \qquad (16)$$

As our last result, we shall obtain explicit expressions for the normalized radial eigenfunctions for $N \leq 3$. The functions with $l = l_{\text{max.}} = N$ are given through eq. (7). Functions with lower l values can be obtained with actions of $\mathcal{O}_-$ or $\bar{\mathcal{O}}_-$:

$$u_{N=3,l=3} = \sqrt{\frac{2}{\Gamma(\frac{9}{2})}}\rho^4 e^{-\frac{1}{2}\rho^2} = \sqrt{\frac{2^5}{105\sqrt{\pi}}}\rho^4 e^{-\frac{1}{2}\rho^2},$$

$$u_{N=2,l=2} = \sqrt{\frac{2}{\Gamma(\frac{7}{2})}}\rho^3 e^{-\frac{1}{2}\rho^2} = \sqrt{\frac{2^4}{15\sqrt{\pi}}}\rho^3 e^{-\frac{1}{2}\rho^2},$$

$$u_{N=1,l=1} = \sqrt{\frac{2}{\Gamma(\frac{5}{2})}}\rho^2 e^{-\frac{1}{2}\rho^2} = \sqrt{\frac{2^3}{3\sqrt{\pi}}}\rho^2 e^{-\frac{1}{2}\rho^2},$$

$$u_{N=0,l=0} = \sqrt{\frac{2}{\Gamma(\frac{3}{2})}}\rho e^{-\frac{1}{2}\rho^2} = \sqrt{\frac{2^2}{\sqrt{\pi}}}\rho e^{-\frac{1}{2}\rho^2},$$

$$u_{N=3,l=1} = \mathcal{O}_-(2)u_{N=2,l=2} = \frac{1}{2}\Big(-\frac{d}{d\rho} - \frac{2}{\rho} + \rho\Big)u_{N=2,l=2},$$

$$= \sqrt{\frac{2^2}{15\sqrt{\pi}}}(2\rho^4 - 5\rho^2)e^{-\frac{1}{2}\rho^2},$$

$$u_{N=2,l=0} = \mathcal{O}_-(1)u_{N=1,l=1} = \frac{1}{2}\Big(-\frac{d}{d\rho} - \frac{1}{\rho} + \rho\Big)u_{N=1,l=1},$$

$$= \sqrt{\frac{2}{3\sqrt{\pi}}}(2\rho^3 - 3\rho)e^{-\frac{1}{2}\rho^2}.$$

16. The symmetric top rigid rotator. In problem 5, the Schrödinger equation for the symmetric top rigid rotator, with $A = B \neq C$, led to the θ equation via the assumed form of the solution

$$\psi_{JMK}(\phi, \theta, \chi) = \frac{e^{iM\phi}}{\sqrt{2\pi}}\frac{e^{iK\chi}}{\sqrt{2\pi}}\Theta_{JMK}(\theta).$$

This θ equation is one-dimensionalized via

$$u_{JMK}(\theta) = \sqrt{\sin\theta}\,\Theta_{JMK}(\theta)$$

to give

$$\left(-\frac{d^2}{d\theta^2} + \frac{M^2 + K^2 - 2MK\cos\theta}{\sin^2\theta}\right)u_{\lambda MK}(\theta) = \lambda u_{\lambda MK}(\theta),$$

where

$$E = \frac{\hbar^2}{2A}(\lambda - \tfrac{1}{4} - K^2) + \frac{\hbar^2}{2C}K^2.$$

Show that this equation can be factorized in two ways, via

$$O_{\pm}(M) = \left(\mp \frac{d}{d\theta} + (M - \tfrac{1}{2}) \cot\theta - \frac{K}{\sin\theta} \right)$$

or

$$O_{\pm}(K) = \left(\mp \frac{d}{d\theta} + (K - \tfrac{1}{2}) \cot\theta - \frac{M}{\sin\theta} \right)$$

where $\lambda = (J + \frac{1}{2})^2$, with $J = M_{\text{max.}} = K_{\text{max.}}$. Assume M and K can only be integers, so J is an integer.

Convert the above to normalized M step- and K step-operators, which preserve the normalization

$$\int_0^{\pi} d\theta \sin\theta |\Theta_{JMK}(\theta)|^2 = 1.$$

Find the normalized $\Theta_{JJK}(\theta)$ with $M = J$, but arbitrary allowed K, and $\Theta_{JMJ}(\theta)$ with $K = J$ but arbitrary allowed M.

Find the normalized J step-operators that step $J \to (J \pm 1)$, but keep M and K fixed. These operators will require new normalization factor ratios, c_{J+1MK}/c_{JMK}, as for the corresponding spherical harmonic problem. Prove these ratios are independent of K and, hence, can be taken over from the known case with $K = 0$.

Find all nonzero matrix elements of $\cos\theta$ and $\sin\theta e^{\pm i\phi}$, $\sin\theta e^{\pm i\chi}$:

$$\langle \psi_{J'M'K'}, \cos\theta \psi_{JMK} \rangle,$$

$$\langle \psi_{J'M'K'}, \sin\theta e^{\pm i\phi} \psi_{JMK} \rangle,$$

$$\langle \psi_{J'M'K'}, \sin\theta e^{\pm i\chi} \psi_{JMK} \rangle.$$