

FIGURE 8.3 Left- and right-hand sides of Eq. (8.32) as a function of  $E$  for the model parameters given in the text.

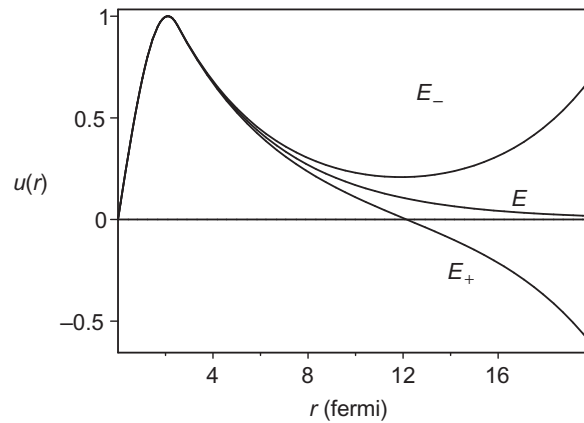


FIGURE 8.4 Wavefunctions for the deuteron problem when the energy is chosen to be less than the eigenvalue  $E$  ( $E_- < E$ ) or greater than  $E$  ( $E_+ > E$ ).

### Exercises

8.3.1 Solve the Legendre equation

$$(1 - x^2)y'' - 2xy' + n(n + 1)y = 0$$

by direct series substitution.

(a) Verify that the indicial equation is

$$s(s - 1) = 0.$$

(b) Using  $s = 0$  and setting the coefficient  $a_1 = 0$ , obtain a series of even powers of  $x$ :

$$y_{\text{even}} = a_0 \left[ 1 - \frac{n(n + 1)}{2!}x^2 + \frac{(n - 2)n(n + 1)(n + 3)}{4!}x^4 + \dots \right],$$

where

$$a_{j+2} = \frac{j(j+1) - n(n+1)}{(j+1)(j+2)} a_j.$$

- (c) Using  $s = 1$  and noting that the coefficient  $a_1$  must be zero, develop a series of odd powers of  $x$ :

$$y_{\text{odd}} = a_0 \left[ x - \frac{(n-1)(n+2)}{3!} x^3 + \frac{(n-3)(n-1)(n+2)(n+4)}{5!} x^5 + \dots \right],$$

where

$$a_{j+2} = \frac{(j+1)(j+2) - n(n+1)}{(j+2)(j+3)} a_j.$$

- (d) Show that both solutions,  $y_{\text{even}}$  and  $y_{\text{odd}}$ , diverge for  $x = \pm 1$  **if the series continue to infinity**. (Compare with Exercise 1.2.5.)  
 (e) Finally, show that by an appropriate choice of  $n$ , one series at a time may be converted into a polynomial, thereby avoiding the divergence catastrophe. In quantum mechanics this restriction of  $n$  to integral values corresponds to **quantization of angular momentum**.

**8.3.2** Show that with the weight factor  $\exp(-x^2)$  and the interval  $-\infty < x < \infty$  for the scalar product, the Hermite ODE eigenvalue problem is Hermitian.

**8.3.3** (a) Develop series solutions for Hermite's differential equation

$$y'' - 2xy' + 2\alpha y = 0.$$

*ANS.*  $s(s-1) = 0$ , indicial equation.

For  $s = 0$ ,

$$a_{j+2} = 2a_j \frac{j - \alpha}{(j+1)(j+2)} \quad (j \text{ even}),$$

$$y_{\text{even}} = a_0 \left[ 1 + \frac{2(-\alpha)x^2}{2!} + \frac{2^2(-\alpha)(2-\alpha)x^4}{4!} + \dots \right].$$

For  $s = 1$ ,

$$a_{j+2} = 2a_j \frac{j+1-\alpha}{(j+2)(j+3)} \quad (j \text{ even}),$$

$$y_{\text{odd}} = a_1 \left[ x + \frac{2(1-\alpha)x^3}{3!} + \frac{2^2(1-\alpha)(3-\alpha)x^5}{5!} + \dots \right].$$

- (b) Show that both series solutions are convergent for all  $x$ , the ratio of successive coefficients behaving, for a large index, like the corresponding ratio in the expansion of  $\exp(x^2)$ .

- (c) Show that by appropriate choice of  $\alpha$ , the series solutions may be cut off and converted to finite polynomials. (These polynomials, properly normalized, become the Hermite polynomials in Section 18.1.)

8.3.4 Laguerre's ODE is

$$xL_n''(x) + (1-x)L_n'(x) + nL_n(x) = 0.$$

Develop a series solution and select the parameter  $n$  to make your series a polynomial.

8.3.5 Solve the Chebyshev equation

$$(1-x^2)T_n'' - xT_n' + n^2T_n = 0,$$

by series substitution. What restrictions are imposed on  $n$  if you demand that the series solution converge for  $x = \pm 1$ ?

*ANS.* The infinite series does converge for  $x = \pm 1$  and no restriction on  $n$  exists (compare with Exercise 1.2.6).

8.3.6 Solve

$$(1-x^2)U_n''(x) - 3xU_n'(x) + n(n+2)U_n(x) = 0,$$

choosing the root of the indicial equation to obtain a series of **odd** powers of  $x$ . Since the series will diverge for  $x = 1$ , choose  $n$  to convert it into a polynomial.

## 8.4 VARIATION METHOD

We saw in Chapter 6 that the expectation value of a Hermitian operator  $H$  for the normalized function  $\psi$  can be written as

$$\langle H \rangle \equiv \langle \psi | H | \psi \rangle,$$

and that the expansion of this quantity in a basis consisting of the orthonormal eigenfunctions of  $H$  had the form given in Eq. (6.30):

$$\langle H \rangle = \sum_{\mu} |a_{\mu}|^2 \lambda_{\mu},$$

where  $a_{\mu}$  is the coefficient of the  $\mu$ th eigenfunction of  $H$  and  $\lambda_i$  is the corresponding eigenvalue. As we noted when we obtained this result, one of its consequences is that  $\langle H \rangle$  is a weighted average of the eigenvalues of  $H$ , and therefore is at least as large as the smallest eigenvalue, and equal to the smallest eigenvalue only if  $\psi$  is actually an eigenfunction to which that eigenvalue corresponds.

The observations of the foregoing paragraph hold true even if we do not actually make an expansion of  $\psi$  and even if we do not actually know or have available the eigenfunctions or eigenvalues of  $H$ . The knowledge that  $\langle H \rangle$  is an upper limit to the smallest eigenvalue of  $H$  is sufficient to enable us to devise a method for approximating that eigenvalue and the associated eigenfunction. This eigenfunction will be the member of the Hilbert space of our problem that yields the smallest expectation value of  $H$ , and a strategy for finding it is to search for the minimum in  $\langle H \rangle$  within our Hilbert space. This is the essential idea