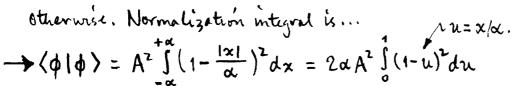
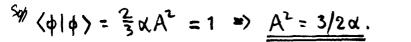


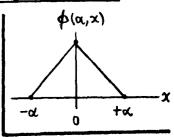
- To approximate the ground state of the simple harmonic oscillator (SHO), use the trial wavefunction:  $\phi(x) = A[1-(|x|/\alpha)]$ , for  $|x| \le \alpha$ , and  $\phi(x) = 0$ , for  $|x| > \alpha$ . Here A =enst and  $\alpha =$ variable (length) parameter. Calculate  $E(\alpha) = \frac{\langle \phi | \mathcal{H}_0(SHO) | \phi \rangle}{\langle \phi | \phi \rangle}$  and for optimum  $\alpha -$  Show that this energy lies less than 10% above the exact value.
- 2 [Davydor Ch. VII # 6, p. 205]. Use the trial wavefunction:  $\frac{\phi(\alpha, r) = Ae^{-\frac{1}{2}\alpha r^2}}{1}$ , to estimate the ground state energy of the hydrogen atom. <u>NOTE</u>: here you are approximating the atom's radial motion by that of an "equivalent" 1D SHO.
- ② In a QM system with Hamiltonian Hb, let the eigenfunctions & eigenenergies be  $\frac{1}{4}$  € En, so: HbH = En. Hr. To approximate the ground state energy Eo, suppose you use the trial function:  $\frac{1}{4}$ =  $\frac{1}{4}$ 0 +  $\frac{1}{4}$ 0,  $\frac{1}{4}$ 9 = actual ground state wavefon,  $\frac{1}{4}$  is a small (real) parameter, and  $\frac{1}{4}$  is an arbitrary for with the expansion  $\frac{1}{4}$ 0 =  $\frac{1}{4}$ 0 Cn. Show that if the approximate (variational) energy: E( $\frac{1}{4}$ 0) =  $\frac{1}{4}$ 1 Hb |  $\frac{1}{4}$ 2 /  $\frac{1}{4}$ 4 |  $\frac{1}{4}$ 3, is expanded in a power series in  $\frac{1}{4}$ 3,  $\frac{1}{4}$ 2. E( $\frac{1}{4}$ 3) = Eo +  $\frac{1}{4}$ 2 Ez +  $\frac{1}{4}$ 3 Ez +  $\frac{1}{4}$ 3 Ez +  $\frac{1}{4}$ 4. Then E1 ≡ O, while Ez is the positive quantity: Ez =  $\frac{1}{4}$ 1 Cn|2 (En Eo). <u>CONCLUSION</u>: for any penturbation on Hb which shifts  $\frac{1}{4}$ 3 →  $\frac{1}{4}$ 4 Ap by a term first order in some small parameter  $\frac{1}{4}$ 3, the ground state energy E3 +  $\frac{1}{4}$ 5 Ez shift is only a second order correction.
- (3) (A) Show lby substitution) that a solution to:  $y''(\xi) + \alpha \xi^n y(\xi) = 0$ , was n = cnsts and  $\xi > 0$ , is given by:  $y(\xi) = AJ\xi J_{\nu}(\zeta)$ , where x = cnst,  $v = \frac{1}{n+2}$ ,  $\zeta = \left(\frac{2J\alpha}{n+2}\right) \xi^{\frac{1}{2}(n+2)}$ .  $J_{\nu}(\zeta)$  is the Bessel for of order  $\nu$ . (B) Assume the asymptotic form:  $y(\xi) \sim \xi^{-k} e^{-a\xi^2}$ , as  $\xi \to \infty$ . By proper choice of the consts  $k, l \notin a$ , show that as  $\xi \to \infty$ , this form satisfies the differential extra:  $y''(\xi) + \alpha \xi^n y(\xi) = \frac{n}{4} \left(\frac{n}{4} + 1\right) \xi^{-2} y(\xi) \to 0$ .
- Bessel's ODE is:  $\frac{y'' + \frac{1}{x}y' + (1 \frac{v^2}{x^2})y = 0}{y''} = 0$ , we real const. Find an approximate solution for the Bessel for  $y \simeq J_v(x)$  by the WKB method. Find an asymptotic form for  $J_v(x)$  as  $x \rightarrow "large"$  (specifically:  $x \gg |v|$ ). You may assume  $|v| \gg \frac{1}{z}$ .

## \$507 Solutions

- Estimate SHO groundstate energy " trial wave for : \$ (x,x) = A [1-(1x1/x)].
- 1. A &  $\alpha$  = consts, and :  $\phi(\alpha_1 x) = A[1-(|x|/\alpha|)]$  for  $|x| \le \alpha$ ;  $\phi = 0$ , otherwise. Normalization integral is ...  $n = x/\alpha$ .







2. The SHO Hamb is; He (SHO) = - th dx2 + 1 mw2 x2, where m= SHO mass and w is its natural freq. Then, with value of A in Eq. (1), the energy for \$\phi\$ is

$$\rightarrow E(\alpha) = \langle \phi | \mathcal{H}(SHO) | \phi \rangle = \frac{3}{2\alpha} \int_{-\infty}^{+\alpha} \left(1 - \frac{|x|}{\alpha}\right) \left[ -\frac{k^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2 \right] \left(1 - \frac{|x|}{\alpha}\right) dx. \quad (2)$$

To evaluate  $E(\alpha)$ , we need to notice that  $\frac{d^2}{dx^2}|x|$  generates a 8-fan. Because...

$$\int_{-\epsilon}^{+\epsilon} \left( \frac{d^2}{dx^2} |x| \right) dx = \int_{-\epsilon}^{+\epsilon} \frac{d}{dx} \left( \frac{d|x|}{dx} \right) dx = \left( \frac{d|x|}{dx} \right) \Big|_{x=+\epsilon} \left( \frac{d|x|}{dx} \right) \Big|_{x=-\epsilon} = (+1) - (-1) = 2,$$

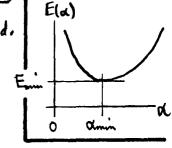
$$\frac{d^2}{dx^2}|x| = 2\delta(x).$$

Use this fact in Eq.(2) to calculate...

3. As a fen of the parameter of, Elal looks like the graph sketched. The minimum is at...

$$\frac{\partial E}{\partial \alpha} = 0 \implies \alpha^2 = \sqrt{30} \left( \frac{\pi}{m\omega} \right) = \alpha^2_{\min};$$

$$\frac{\cos E_{\min}}{E_{\min}} = E(\alpha_{\min}) = \sqrt{\frac{6}{5}} \left( \frac{1}{2} \pi \omega \right) = 1.095 E_0.$$



(6)

(5)

Emin is the best estimate for the groundstate energy Eo = 2 to for this type of trial p.

- (21) Estimate H- atom groundstate energy " trial wavefon:  $\phi(\alpha, \tau) = Ae^{-\frac{1}{2}\alpha \tau^2}$ .
  - 1) Just follow Davydov's Eqs. (51.12) (51.15), where he does the calculation for the trail for  $\phi(\alpha, r) = Ae^{-\beta r} [a lucky gness!]$ . We have...

$$\rightarrow E(\alpha) = \langle \phi | \mathcal{H} | \phi \rangle / \langle \phi | \phi \rangle$$
,  $\mathcal{H} = -\frac{k^2}{2m} \nabla^2 - \frac{e^2}{r}$ , for H atom.

For  $\phi$  with radial variation only:  $\nabla^2 = \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \frac{\partial}{\partial r})$ . Norm integral is:

2) E(a) in Eq. (1) is now... (with: a = t2/me2 = Bohr vadius)...

$$\Rightarrow E(\alpha) = \left(\frac{\alpha}{\pi}\right)^{\frac{3}{2}} \int_{0}^{\infty} 4\pi r^{2} dr \cdot e^{-\frac{1}{2}\alpha r^{2}} \left[-\frac{\hbar^{2}}{2m} \frac{1}{r^{2}} \frac{\partial}{\partial r} (r^{2} \frac{\partial}{\partial r}) - \frac{e^{2}}{r^{2}}\right] e^{-\frac{1}{2}\alpha r^{2}}$$

$$= 4\pi e^{2} \left(\frac{\alpha}{\pi}\right)^{\frac{3}{2}} \int_{0}^{\infty} dr \left[-\frac{a_{0}}{2} e^{-\frac{1}{2}\alpha r^{2}} \frac{\partial}{\partial r} (r^{2} \frac{\partial}{\partial r} e^{-\frac{1}{2}\alpha r^{2}}) - re^{-\alpha r^{2}}\right]$$

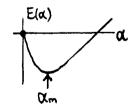
$$= 4\pi e^{2} \left(\frac{\alpha}{\pi}\right)^{\frac{3}{2}} \left\{ \frac{a_{0}\alpha}{2} \int_{0}^{\infty} dr \cdot e^{-\frac{1}{2}\alpha r^{2}} \frac{\partial}{\partial r} (r^{3} e^{-\frac{1}{2}\alpha r^{2}}) - \frac{1}{2\alpha} \right\}$$

 $\left( r^3 e^{-\frac{1}{2}\alpha r^2} \right) = -\int_0^\infty dr \cdot \left( r^3 e^{-\frac{1}{2}\alpha r^2} \right) \frac{\partial}{\partial r} \left( e^{-\frac{1}{2}\alpha r^2} \right) = + \alpha \int_0^\infty r^4 e^{-\alpha r^2} dr$ 

$$E(\alpha) = 4\pi e^{2} \left(\frac{\alpha}{\pi}\right)^{3/2} \left\{ \frac{\Omega_{0}\alpha}{2} \cdot \frac{3\sqrt{\pi}}{8\alpha^{3/2}} - \frac{1}{2\alpha} \right\}$$

$$= \frac{3\sqrt{\pi}}{8}/\alpha^{3/2}$$

$$E(\alpha) = \frac{2e^2}{\sqrt{\pi}} \left\{ \left( \frac{3\sqrt{\pi} a_0}{8} \right) \alpha - \sqrt{\alpha} \right\}, \text{ w.a.t. } \phi = Ae^{-\frac{1}{2}\alpha r^2}, (4)$$



3) Minimize Ela) in Eq.(4)...

$$\rightarrow \partial E/\partial \alpha = 0 \Rightarrow \underline{\alpha = 16/9\pi a_0^2 = \alpha_m}, \text{ and } E(\alpha_m) = -\left(\frac{8}{3\pi}\right)\frac{e^2}{2a_0}. \tag{5}$$

E(am) is the best estimate to E(gnd) =  $-e^2/2a_0$ , with a trial for  $\phi = e^{-\frac{8}{9\pi}(r/a_0)^2}$ . E(am) lies above E(gnd) by:  $\Delta E/E = [E(a_m) - E(gnd)]/[E(gnd)] = 1 - (8/3\pi) = 0.1512$ , i.e. about 15%. So  $\phi(SHO)$  gives a rather poor fit.

(4)

② For ground state ( $\Psi_0, E_0$ ),  $\theta(\lambda)$  perturbation on wavefor  $\Psi_0 \Rightarrow \theta(\lambda^2)$  correction to energy  $E_0$ .

1) Calculation is best done by putting in  $\phi = \sum c_n V_n$  at the very end. Straightforwordly:

 $E(\lambda) = \langle \psi | \mathcal{Y} | \psi \rangle / \langle \psi | \psi \rangle = \langle \psi_{+} \lambda \phi | \mathcal{Y}_{0} | \psi_{0} + \lambda \phi \rangle / \langle \psi_{0} + \lambda \phi | \psi_{0} + \lambda \phi \rangle$ 

$$\frac{\partial y}{\partial y} = \frac{\langle \psi_0 | y_0 | \psi_0 \rangle + \lambda [\langle \psi_0 | y_0 | \psi_0 \rangle + \langle \phi | y_0 | \psi_0 \rangle] + \lambda^2 \langle \phi | y_0 | \phi \rangle}{\langle \psi_0 | \psi_0 \rangle + \lambda [\langle \psi_0 | \phi \rangle + \langle \phi | \psi_0 \rangle] + \lambda^2 \langle \phi | \phi \rangle}.$$

We've used  $\lambda$ =real here. Term  $\mathfrak{D} \equiv E_0$ , and in terms  $\mathfrak{D} \notin \mathfrak{D}$ , use  $\langle \Psi_0 | \mathcal{H}_0 \rangle = E_0 \langle \Psi_0 | \mathcal{H}_0 \rangle = E_0 \langle \Psi_0 | \mathcal{H}_0 \rangle$ , resp. ( $\mathcal{H}_0 = E_0 \langle \Psi_0 | \mathcal{H}_0 \rangle = E_0 \langle \Psi_0 | \mathcal{H}_0 \rangle$ ). Term  $\mathfrak{D} \equiv 1$ , by normalization. With the shorthand notation  $N = \langle \Psi_0 | \Phi \rangle + \langle \Phi | \Psi_0 \rangle$ , Eq. (1) becomes...

$$E(\lambda) = \left[ (1+\lambda N)E_0 + \lambda^2 \langle \phi | \mathcal{H} | \phi \rangle \right] / \left[ (1+\lambda N) + \lambda^2 \langle \phi | \phi \rangle \right]. \tag{2}$$

2) In Eq. (2), 2-> small. If we define the quantity: K = 22/(1+2N), then

The leading term in K is O(22) in smallness. To O(22), E(2) expands as...

 $E(\lambda) \simeq E_o \left[ 1 + \frac{\lambda^2}{E_o} \langle \phi | \mathcal{H} | \phi \rangle \right] \left[ 1 - \lambda^2 \langle \phi | \phi \rangle \right] \simeq E_o + \lambda^2 E_z$ 

$$\frac{1}{2} = \langle \phi | \mathcal{H} | \phi \rangle - E_0 \langle \phi | \phi \rangle.$$

As advertised, the first correction to Eo is O(2), not O(2).

3) Calculate Ez in Eq. (4) by putting in  $\phi = \sum Cn \, \Psi_n$ . Since  $\{\Psi_n\}$  is an orthonormal set:  $\{\Psi_m\} \, \Psi_n\} = S_{mn}$ , we get ...

$$\frac{\mathcal{E}_{z}}{\mathcal{E}_{z}} = \sum_{m,n} c_{m}^{*} c_{n} \left[ \langle \Psi_{m} | \mathcal{H}_{n} \rangle - E_{o} \langle \Psi_{m} | \Psi_{n} \rangle \right] = \sum_{n} |c_{n}|^{2} \left( E_{n} - E_{o} \right), \quad (5)$$

as required. Ez >0, since En-E. >0. So E(2) in Eq. (4) lier above Eo.

(2)

Solution to: y"+αξηy=0 for y=y(ξ). Asymptotic form for ξ→ω.

This problem appears in the WKB turning point problem, for a=-1, n=1 (Airy's ODE).

1) Let:  $x(\xi) = \sqrt{\xi} \int_{V(\xi)}^{\infty}$ ,  $\frac{v}{2} = 1/(n+z) \notin \underline{\xi} = (\frac{2\sqrt{\alpha}}{n+2}) \notin \underline{\xi}^{\frac{1}{2}(n+2)}$ . By direct differentiation...

$$\rightarrow \frac{dx}{d\xi} = \sqrt{\xi} \left( \frac{d\xi}{d\xi} \right) \frac{d}{d\zeta} J_{\nu}(\zeta) + \frac{1}{2} \xi^{-\frac{1}{2}} J_{\nu}(\zeta). \tag{1}$$

But:  $\left(\frac{d\zeta}{d\xi}\right) = \sqrt{\alpha} \xi^{\frac{n}{2}}$ , and  $\left(\frac{d}{d\xi} J_{\nu}(\zeta)\right) = -\frac{\nu}{\zeta} J_{\nu}(\zeta) + J_{\nu-1}(\zeta) \left\{\frac{\text{Mathems } \xi \text{ Walker}}{\text{Eq. (7-54)}}\right\}$ . So,..

 $\frac{\mathrm{d}x}{\mathrm{d}\xi} = \sqrt{\alpha} \xi^{\frac{1}{2}(n+1)} J_{\nu-1}(\xi) .$ 

2) The second derivative is calculated as ...

Use  $\left(\frac{d\xi}{d\xi}\right) = \sqrt{\alpha} \xi^{\frac{N}{2}}$  as above, and:  $\frac{d}{d\xi} J_{\nu-1}(\xi) = \frac{\nu-1}{\xi} J_{\nu-1}(\xi) - J_{\nu}(\xi) \left\{ \frac{M \pm W}{(7-55)} \right\}$ . So...

$$\frac{1}{\sqrt{\alpha}} \frac{d^2 x}{d \xi^2} = \sqrt{\alpha} \xi^{n+\frac{1}{2}} \left[ \left( \frac{v-1}{\zeta} \right) J_{v-1}(\zeta) - J_v(\zeta) \right] + \frac{n+1}{2} \xi^{\frac{1}{2}(n-1)} J_{v-1}(\zeta) \tag{4}$$

$$= -\sqrt{\alpha} \, \xi^{n} \, \chi(\xi) + \left[ \sqrt{\alpha} \, \xi^{n+\frac{1}{2}} \left( \frac{\nu-1}{\zeta} \right) + \frac{n+1}{2} \, \xi^{\frac{1}{2}(n-1)} \right] J_{\nu-1}(\zeta) \tag{5}$$

$$= \sqrt{\alpha} \, \xi^{n+\frac{1}{2}} \frac{\frac{1}{n+2} - 1}{\left( \frac{2\sqrt{\alpha}}{2} \right) \xi^{\frac{n}{2}+1}} = -\left( \frac{n+1}{2} \right) \xi^{\frac{1}{2}(n-1)} \int_{-\infty}^{\infty} \frac{cancels}{s} ds$$

Soly 
$$\frac{1}{\sqrt{\alpha}} \frac{d^2x}{d\xi^2} = -\sqrt{\alpha} \xi^n \chi(\xi) + 3ero, \quad \frac{d^2x}{d\xi^2} + \alpha \xi^n \chi = 0, \quad \frac{fry}{\chi(\xi) = \sqrt{\xi} J_v(\zeta)}.$$

3) We have shown that  $\chi(\xi) = \sqrt{\xi} \int_{V} J_{v}(\xi)$ ,  $v = \frac{1}{n+2} \frac{4}{3} \xi = \left(\frac{2\sqrt{x}}{n+2}\right) \xi^{\frac{1}{2}(n+2)}$ , satisfies the ODE of interest, viz  $\chi'' + \alpha \xi^{n} \chi = 0$ . Then  $y(\xi) = A\chi(\xi)$  is also a soln, for A = cnst. For the Airy problem:  $y'' - \xi y = 0$ , the soln is:  $y(\xi) = A\sqrt{\xi} \int_{1/3} \left(\frac{2i}{3} \xi^{3/2}\right)$ .

## \$ 507 Solutions

(3) (cont'd)

4) Now assume an asymptotic form: X(ξ)~ ξ-k e-aξ², as ξ→∞. Differentiate...

(B) 
$$\rightarrow \frac{dx}{d\xi} = -k \xi^{-(k+1)} e^{-a\xi^{\ell}} + \xi^{-k} [-a \ell \xi^{\ell-1} e^{-a\xi^{\ell}}] = -(k \xi^{-1} + a \ell \xi^{\ell-1}) x;$$
 (7)

$$\rightarrow \frac{d^2x}{d\xi^2} = -\left[-k\xi^{-2} + al(l-1)\xi^{l-2}\right] \times + \left[k\xi^{-1} + al\xi^{l-1}\right]^2 \times$$

... gather terms to get ...

5) The parameters k, l, a are free. We fix them by the following choices ...

Set factor 
$$\mathfrak{D} = -\alpha \xi^n \Rightarrow \begin{cases} 2(l-1) = n, \text{ or } ; \underline{l = \frac{1}{2}(n+2)}; \\ (\alpha l)^2 = -\alpha, \text{ or } : \underline{\alpha} = 2\sqrt{-\alpha}/(n+2). \end{cases}$$

Set factor 
$$@=0 \Rightarrow k = \frac{1}{2}(l-1) = \frac{1}{4}n$$
.

Then fuctor 3: 
$$k(k+1)/(al)^2 = -\frac{1}{\alpha} \frac{n}{4} (\frac{n}{4} + 1)$$
. (9c)

With the choices in Eq. (9), Eq. (8) becomes ...

$$\frac{d^2x}{d\xi^2} = -\alpha \xi^n \left[ 1 - 0 - \frac{1}{\alpha} \frac{n}{4} \left( \frac{n}{4} + 1 \right) \xi^{-(n+2)} \right]. \tag{10}$$

6) We can now state that: 
$$\chi(\xi) = \xi^{-\frac{n}{4}} \exp\left[-\left(\frac{2\sqrt{-\alpha}}{n+2}\right)\xi^{\frac{1}{2}(n+2)}\right]$$
, satisfies the ODE:

$$\frac{d^2\alpha}{d\xi^2} + \alpha \xi^n x = \frac{n}{4} \left( \frac{n}{4} + 1 \right) \xi^{-2} x(\xi) \xrightarrow{1} 0, \text{ is } \xi \to \infty. \tag{11}$$

as required.  $X(\xi)$  is therefore an asymptotic form for  $\sqrt{\xi} \, J_V(\xi)$  of part (A). For the Airy problem:  $X'' - \xi \, x = 0$ , the asymptotic form is as was used in Eq. (39), p. 14 of "Notes on the WKB Method", viz:  $\underline{X(\xi)} \sim \xi^{-\frac{1}{4}} \exp(-\frac{2}{3}\xi^{3/2})$ .

Find an asymptotic form for the Bessel fon Julx), x+ "large", ria TVKB.

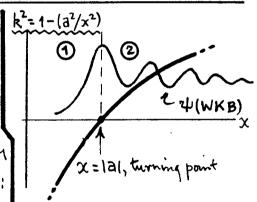
1) Bessel's Egtn: y"+(1/x)y'+[1-(v2/x2)]y=0, converts to WKB form, via:

$$\Rightarrow y(x) = \psi(x) \exp\left(-\frac{1}{2} \int \frac{dx}{x}\right) = \psi(x)/\sqrt{x},$$

$$\Rightarrow \left[\psi'' + k^{2}(x) \psi = 0, \frac{w}{k}(x) = \left[1 - \frac{1}{x^{2}} (v^{2} - \frac{1}{4})\right]^{\frac{1}{2}}\right].$$

This egt is exact. A WKB approxime to U(x) [and three to y= Y/1x] will work at values of x where k is "slowly-varying", i.e.

2) Let  $\underline{\partial} = (\sqrt{2} - \frac{1}{4})^{1/2}$ , so  $k(x) = [1 - (\partial^2/x^2)]^{\frac{1}{2}}$ . x = |a| is a "turning point" for the prob [k(a) = 0], and we want  $\Psi(WKB)$  for x > |a|. To be an acceptable Solution,  $\Psi$  should decrease exponentially in region  $\underline{\partial}$ , and oscillate in region  $\underline{\partial}$ . So we write:



soy since 
$$k \approx 1$$
 as  $x \to \text{"large"}$ , then:  $\frac{\psi(x)}{|a|} \approx A \sin\left(x - \frac{\sqrt{\pi}}{2} + \beta\right)$ . (3)

3) Since  $y = \Psi/\sqrt{x}$ , the WKB solution to Bessel's Egtn, for  $\frac{1}{2} << |v| << x \to \infty$ , is  $y(x) = J_v(x) \simeq \frac{cnst}{\sqrt{x}} \sin(x - \frac{v\pi}{2} + \beta)$  (4) When the phase  $\beta = \pi/4$ , this is a standard result; see NBS Math.

Handbook # (9.2.1). The phase & can be fixed by the WKB Connection Formulas.