

MA100Y 507
Solutions to PS 7

PS7-1

9.4.2. $\nabla^2 \psi + k^2 \psi = 0$ (r, ϕ, z)

$$\nabla^2 = \frac{1}{r} \frac{\partial}{\partial r} r \frac{\partial}{\partial r} + \frac{1}{r^2} \frac{\partial^2}{\partial \phi^2} + \frac{\partial^2}{\partial z^2}$$

(*) Separable in these coordinates. Now consider the operator: $\nabla^2 + f(r) + \frac{1}{r^2} g(\phi) + h(z) + k^2$

Show this is separable: let $\psi(r, \phi, z) = R(r) \Phi(\phi) Z(z)$

Substitute:

$$\left(\frac{1}{r} \frac{\partial}{\partial r} r \frac{\partial}{\partial r} R \right) (\Phi Z) + \left(\frac{1}{r^2} \Phi'' \right) R Z + R \Phi Z''$$

$$+ (f(r) R) \Phi Z + \frac{1}{r^2} (g(\phi) \Phi) R Z + R \Phi (h(z) Z)$$

$$+ k^2 R \Phi Z = 0.$$

Divide by $R \Phi Z$:

$$\frac{1}{R r} \frac{\partial}{\partial r} r \frac{\partial}{\partial r} R + \frac{1}{r^2} \left(\frac{\Phi''}{\Phi} + g(\phi) \right) + \left(h(z) + \frac{Z''}{Z} \right) = -k^2$$

so

$$\frac{1}{r^2} \left[\left(k^2 r^2 + \frac{r}{R} \frac{\partial}{\partial r} r \frac{\partial}{\partial r} R \right) + \left(\frac{\Phi''}{\Phi} + g(\phi) \right) \right] = - \left(h(z) + \frac{Z''}{Z} \right)$$

Introduce a separation constant β^2 :

$$(1) \quad Z'' + h(z) Z + \beta^2 Z = 0$$

P57-2

and:

$$\oint_R \partial_\mu \rho \partial_\mu R + (k^2 - \beta^2) \rho^2 = - \left(\Phi'' + g(\phi) \Phi \right) \frac{1}{\Phi}$$

and a second separation const. γ^2 to get

$$(2) \quad \rho^2 R'' + \rho R' + ((k^2 - \beta^2) \rho^2 - \gamma^2) R = 0$$

$$(3) \quad \Phi'' + g(\phi) \Phi + \gamma^2 \Phi = 0.$$

(1)-(2)-(3) are 3 ODEs in ρ, ϕ, τ respectively.

(P57-3)

9.4.5 $-\alpha \Delta \psi = E \psi$ $\alpha = \hbar^2/2m$ in cube
 Rectangular symmetry $[0, a] \times [0, b] \times [0, c]$

• Dirichlet boundary conditions

$$\Delta = \partial_x^2 + \partial_y^2 + \partial_z^2 \quad \text{let } \psi(x, y, z) = X(x)Y(y)Z(z)$$

$$-\alpha \{ YZ \partial_x^2 X + XZ \partial_y^2 Y + XY \partial_z^2 Z \} = E XYZ$$

$$(x) \quad \frac{1}{X} \partial_x^2 X + \frac{1}{Y} \partial_y^2 Y + \frac{1}{Z} \partial_z^2 Z = -\frac{E}{\alpha}$$

Separation variables: $\frac{1}{X} \partial_x^2 X = -k_1^2$ $X(0) = X(a) = 0$

$$\partial_x^2 X + k_1^2 X = 0 \quad X(x) = A_1 \cos k_1 x + B_1 \sin k_1 x$$

DBC $X(0) = A_1 = 0$

$$X(a) = B_1 \sin k_1 a = 0 \Rightarrow k_1 a = n_1 \pi \quad \text{so } \boxed{k_1 = \frac{n_1 \pi}{a}}$$

$n_1 \in \mathbb{I}, 2, 3, 4, \dots$

Return to PDE (x)

$$\frac{1}{Y} \partial_y^2 Y + \frac{1}{Z} \partial_z^2 Z = -\frac{E}{\alpha} + \left(\frac{n_1 \pi}{a}\right)^2$$

Set $\frac{1}{Y} \partial_y^2 Y = -k_2^2$. The same calculation shows $Y(y) = \sin\left(\frac{n_2 \pi y}{b}\right)$ & $\boxed{k_2 = \frac{n_2 \pi}{b}}$

Finally: $\frac{1}{Z} \partial_z^2 Z = -\frac{E}{\alpha} + \left(\frac{n_1 \pi}{a}\right)^2 + \left(\frac{n_2 \pi}{b}\right)^2$

set $\frac{1}{Z} \partial_z^2 Z = -k_3^2$ so $Z(z) = \sin\left(\frac{n_3 \pi z}{c}\right)$ & $\boxed{k_3 = \frac{n_3 \pi}{c}}$

Whence $E = \frac{(\hbar^2)}{2m} \left[\left(\frac{n_1}{a}\right)^2 + \left(\frac{n_2}{b}\right)^2 + \left(\frac{n_3}{c}\right)^2 \right]$

The ground state has $n_1 = n_2 = n_3 = 1$.

(ps 7-4)

9.4.7

$$-\alpha \psi'' + \frac{1}{2} k x^2 \psi = E \psi \quad \text{harmonic oscillator}$$

$$\alpha = \hbar^2 / 2m$$

$$\psi'' + \frac{E}{\alpha} \psi - \frac{k x^2}{2\alpha} \psi = 0 \quad \text{or} \quad \psi'' + \frac{2mE}{\hbar^2} \psi - \frac{mk}{\hbar^2} x^2 \psi = 0$$

$$\text{Set } a = \left(\frac{mk}{\hbar^2} \right)^{\frac{1}{4}} \quad \text{and} \quad \lambda = \frac{2E}{\hbar} \sqrt{\frac{m}{k}} \quad \text{and} \quad \xi = ax$$

$$\text{Then } \phi(\xi) = \psi(x/a), \quad \frac{d\phi}{d\xi} = \frac{1}{a} \psi'(x) \quad \text{or} \quad \psi'(x) = a \frac{d\phi}{d\xi}$$

so

$$a^2 \frac{d^2 \phi(\xi)}{d\xi^2} + \left[\lambda a^2 - a^4 \left(\frac{\xi}{a} \right)^2 \right] \phi(\xi) = 0$$

$$\text{so} \quad \frac{d^2 \phi}{d\xi^2} + (\lambda - \xi^2) \phi(\xi) = 0 \quad (*)$$

$$\text{since} \quad \frac{2mE}{\hbar^2} = \frac{2E}{\hbar} \sqrt{\frac{m}{k}} \left(\frac{mk}{\hbar^2} \right)^{\frac{1}{4}} = \lambda a^2$$

$$\text{and} \quad \frac{mk}{\hbar^2} = a^4$$

$$\text{To reduce this ODE set } \phi(\xi) = y(\xi) e^{-\xi^2/2}$$

$$\phi'(\xi) = [y'(\xi) - \xi y(\xi)] e^{-\xi^2/2}$$

$$\begin{aligned} \phi''(\xi) &= [y''(\xi) - y(\xi) - \xi y'(\xi)] e^{-\xi^2/2} + [y'(\xi) - \xi y(\xi)] (-\xi e^{-\xi^2/2}) \\ &= [y''(\xi) - 2\xi y'(\xi) - (1 - \xi^2) y(\xi)] e^{-\xi^2/2} \end{aligned}$$

(*) becomes
Hermite eqn.

$$\boxed{y''(\xi) - 2\xi y'(\xi) + (\lambda - 1) y(\xi) = 0}$$