Lecture $\boxed{12}$ (Sep. 28, Mon.)

Outline for today / this week

Solutions to Schroedinger's wave equation:

(1). Free particle in 3D: density of states

(2). SHO (again): analytic method (more complicated)

(3). Linear potential (no analog of operator/algebraic for SHO): useful for WKB approximation

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(1). Free particle in $\boxed{3}$D in Cartesian coordinates (vs. spherical, related to angular momentum later):

$$\boxed{\nabla^2 u_E(\bar{x}) = -\frac{2mE}{\hbar^2} u_E(\bar{x})}$$

cf. in 1D: $\frac{d^2}{dx^2} u_E(x) = -\frac{2mE}{\hbar^2} u_E(x)$ solved by plane wave: $u_E(x) \sim \exp(ikx)$, with $\boxed{E = \frac{\hbar^2 k^2}{2m}}$

– Use separation of variables (and above):

$$\boxed{u_E(x) = C \exp\left[i(k_x x + k_y y + k_z z)\right]},$$ with

$E = \hbar^2 |\bar{k}|^2/(2m)$, $|\bar{k}|^2 = k_x^2 + k_y^2 + k_z^2$

— **Normalization** : space is cube of length $L (\to \infty)$

periodic boundary condition (BC): $u_x(x+L) = u_x(x)$

$$\boxed{k_x L = 2\pi n_x} \Leftarrow$$

$$\int [u_E(x)]^2 = 1 \ldots \Rightarrow \boxed{u_E(x) = \frac{1}{L^{3/2}} \exp(i\bar{k}\cdot\bar{x})}$$

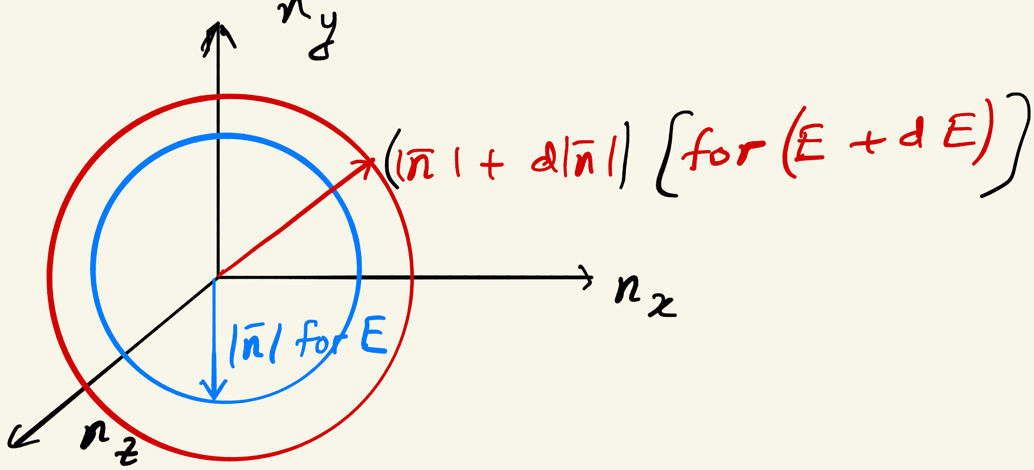
$$\boxed{E = \frac{\hbar^2}{2m}\left(\frac{2\pi}{L}\right)^2 (n_x^2 + n_y^2 + n_z^2)} \quad (n_{x,y,z} \lessgtr 0)$$

$$\boxed{|\bar{n}|^2 = n_x^2 + n_y^2 + n_z^2}$$

— Lot of degeneracy ...

Density of states in 3D (HW 5.2: compare to 1D, 2D)

For large L, fixed $E \Rightarrow |\bar{n}|$ large ... treat $\boxed{n_{x,y,z}}$ as continuous variables



— each point in "n" space is a state $\Rightarrow$ number of states is volume in n-space

— sphere of radius $|\bar{n}| = \sqrt{E \; 2mL^2 / (4\pi^2\hbar^2)}$ is E (states inside it have energy $\leq E$)

... that of $(|\bar{n}| + d|\bar{n}|)$ is $(E + dE)$: $\quad |d\bar{n}| \, 2|\bar{n}| \frac{\hbar^2}{2m} \frac{4\pi^2}{L^2} = dE$

$\Rightarrow$ dN (number of states with energy $\boxed{\text{between}}$ $\boxed{E}$ & $\boxed{E + dE}$) = volume of (thin) spherical $\boxed{\text{shell}}$ of radius $|\bar{n}|$ and thickness $d|\bar{n}|$

$= 4\pi |\bar{n}|^2 d|\bar{n}|$

$= \sqrt{E}\, dE\, L^3\, m^{3/2} / (\pi^2 \sqrt{2}\, \hbar^3)$

$$\boxed{dN/dE = \sqrt{E}\; L^3\; m^{3/2} / (\pi^2 \sqrt{2}\, \hbar^3)}$$

— $dN/dE \times \underbrace{\text{probability density}}_{|u_E|^2} \propto L^3 \times \frac{1}{L^3}$

... $\boxed{L \to \infty \text{ smooth}}$

(2). SHO : solve 2nd order (ordinary in 1D) DE (vs. 1st order used earlier) to get energy eigenfunctions:

$$\boxed{-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}u_E(x) + \frac{1}{2}m\omega^2 x^2 u_E(x) = E\,u_E(x)}$$

– Use dimensionless position, $\boxed{y \equiv x/x_0}$, where $x_0 = \sqrt{\hbar/(m\omega)}$, and energy $\boxed{\varepsilon = 2E/\hbar\omega = E/E_0}$ (where $\frac{1}{2}\hbar\omega$ is ground-state energy, E_0):

$$\boxed{d^2/dy^2\, u(y) + (\varepsilon - y^2)\, u(y) = 0}$$

– Try $\boxed{\varepsilon = \pm 1}$: $d^2u/dy^2 + (\pm 1 - y^2)u = 0 \Rightarrow$

$$u = \exp(\mp y^2/2)$$

[want $u_E(x) \to 0$ as $x \to \infty$]

$\varepsilon = -1$ is $\boxed{\text{not}}$ normalizable

$\varepsilon = +1$ is ground state

– So, for excited states, $\boxed{u_E(y) \equiv e^{-y^2/2}\, h(y)}$

$$\boxed{d^2h/dy^2 - 2y\, dh/dy + (\varepsilon - 1)\, h = 0}$$

– Try series solution for h ... must terminate for normalizable $\Rightarrow$ $\boxed{(\varepsilon - 1) = 2n \;\; (n = 0, 1, 2 \ldots)}$

$$\Rightarrow \boxed{d^2h/dy^2 - 2y\, dh/dy + 2n\, h = 0}$$

— Hermite polynomials satisfy above DE:

$$H_n(y) = (-1)^n e^{y^2} d^n/dy^n \left(e^{-y^2}\right); \quad H_0 = 1, \; H_1 = 2y \ldots$$

with $\int e^{-y^2} H_n(y)\, H_m(y) = \begin{cases} 0 & \text{for } n \neq m \\ \sqrt{\pi}\, 2^n n! & \text{for } n = m \end{cases}$

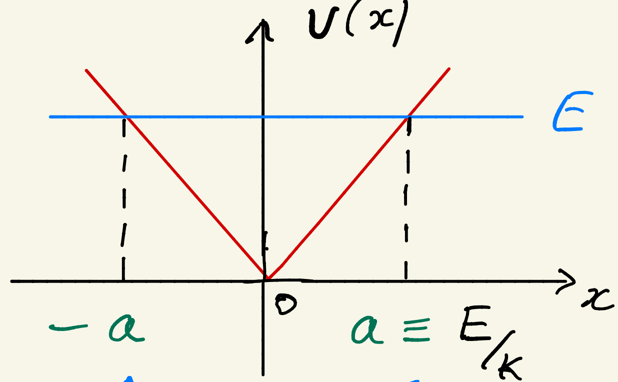
— $\boxed{u_n(y) = e^{-y^2/2} H_n(y)\, 1/N_n}$

get N_n from $\int dx\, u_E^2(x) = 1$ (and above)

— $\boxed{\text{check}}$ $u_{0,1}(x)$ agree $\boxed{\langle x' | 0, 1\rangle}$ of operator approach

(3). Linear potential: motivation: (i) quarkonium (quark-antiquark bound state); (ii) bouncing ball (neutron experiment); (iii) used in obtaining WKB approximation (next topic)

$$V(x) = K\,|x|$$



classical turning points ($E - V =$ kinetic energy)

— Solve :

$$\boxed{-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}u_E + K|x|u_E(x) = E\,u_E(x)}$$

— $\boxed{BC}$ (1) $u_E(x) \to 0$ as $x \to \infty$

or $\int [u_E(x)]^2 = 1$ (normalizable)

(2). $V(x) = V(-x) \Rightarrow u_E(x) = \pm u_E(-x)$ (even/odd parity)

$\boxed{\text{even}}$: $\boxed{u'_E(0) = 0}$: use $\lim_{\delta \to 0} \left\{ \frac{[u_E(\delta) - u_E(-\delta)]}{\delta} \right\} = \lim_{\delta \to 0} \frac{(0)}{\delta}$

$\boxed{\text{odd}}$: $\boxed{u_E(0) = 0}$ use continuity of u_E (u'_E "automatically" continuous)

— dimensionless quantities : $x_0 = (\hbar^2/mK)^{1/3}$;

$E_0 = K x_0 = \left(\frac{\hbar^2 K^2}{m}\right)^{1/3}$

& $y = x/x_0$; $\varepsilon = E/E_0$

$$\boxed{d^2u_E/dy^2 - 2(y - \varepsilon)\,u_E(y) = 0}$$

$\rightarrow$ $\boxed{z \equiv 2^{1/3}(y - \varepsilon)}$: (a). $\boxed{z = 0}$ $(y = \varepsilon)$ is turning point ($z > 0$ classically forbidden)

(b). $\boxed{z \to \infty}$ is $y, x \to \infty$

(c). $\boxed{z \leq 0}$ $(y \leq \varepsilon)$: classically allowed, but

(d). "need" to go till $\boxed{z = 2^{1/3}(-\varepsilon)}$ $(y = 0)$ only, since

$y < 0$ is "reflection" of $y > 0$

$\rightarrow u_E(z)$ satisfies : $\boxed{\frac{d^2}{dz^2} u_E(z) - z\, u_E(z) = 0}$,

with "no" ε [cf. DE for $h(y)$ in SHO] :

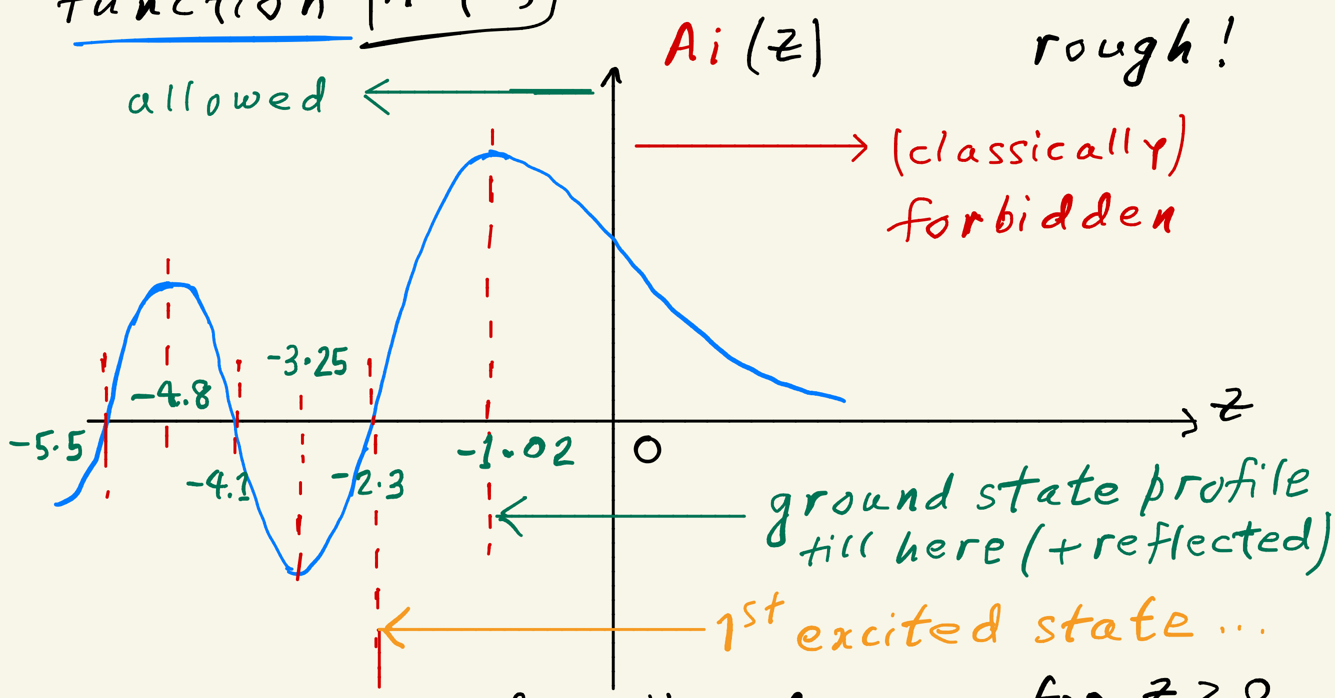
wavefunction "shape" independent of energy...

... just "sampling" it only till $z = 2^{1/3}(-\varepsilon)$

[energy-dependence comes in]

— Airy equation : 2 solutions ; $Bi(z)$ not normalizable

— Airy function $\boxed{Ai(z)}$



... as expected : wavefunction decays for $z > 0$

$(y > \varepsilon$: forbidden classically) : 2^{st} BC satisfied [$u_E(x \to \infty) \to 0$]

vs. oscillatory in allowed $(z < 0 : y < \varepsilon)$ ...

... but "stop" at $\boxed{z = 2^{1/3}(-\varepsilon)}$ $(y = 0)$; then

reflect to get wavefunction for $\boxed{y < 0}$ ...

$\boxed{\text{what determines allowed } \mathcal{E} \text{ ?}}$ 2^{nd} BC

(a) $\boxed{\text{odd}}$ $u_E(x)$: $u_E(x=0) = 0 \Rightarrow \boxed{Ai}\left[2^{1/3}(0-\mathcal{E})\right] = 0$

$u_E(z)$; y

(b) even $u_E(x)$: $u_E'(x=0) = 0 \Rightarrow Ai'\left[2^{1/3}(0-\mathcal{E})\right] = 0$

$$\Rightarrow \boxed{\mathcal{E} = -\frac{1}{2^{1/3}}\left[\text{zeroes of } Ai \ldots \text{or of } Ai'\right]}$$

$-2.3, -4.1 \ldots$; $-1.02, -3.2 \ldots$

1st zero of Ai'

$\boxed{\text{ground state}}$ energy $= \left(\frac{\hbar^2 k^2}{m}\right)^{1/3} \frac{1.02}{2^{1/3}}$

... profile till $z = -1.02$

& 1st excited till $z = -2.3$ (1st zero of Ai)