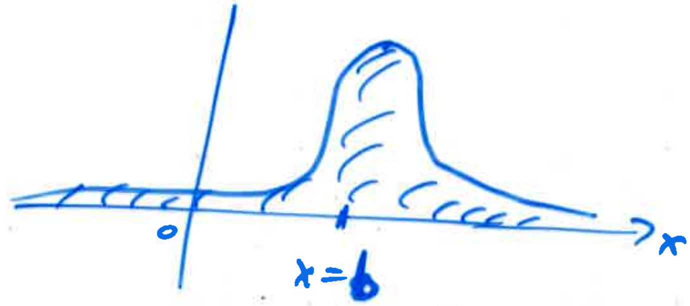
Gaussian Integrals

integrand $A e^{-(x-b)^2}$



Bell curve, Normal distribution

$$I = \int_{x=-\infty}^{\infty} e^{-x^2} dx = ?$$

$$I^2 = \left(\int_{x=-\infty}^{\infty} e^{-x^2} dx \right) \left(\int_{y=-\infty}^{\infty} e^{-y^2} dy \right)$$

x and y are dummy variables of integration

$$= \int_{x=-\infty}^{\infty} \int_{y=-\infty}^{\infty} e^{-x^2} \cdot e^{-y^2} dx\,dy = \int_{x=-\infty}^{\infty} \int_{y=-\infty}^{\infty} e^{-(x^2+y^2)} \underbrace{dx\,dy}_{dA}$$

Reinterpret as an area integral in the x-y plane.
Switch from Cartesian (x, y) coordinates to Polar (r, φ)

$$I^2 = \int_{r=0}^{\infty} \int_{\varphi=0}^{2\pi} e^{-r^2} r\,dr\,d\varphi = \underbrace{\left(\int_{\varphi=0}^{2\pi} d\varphi \right)}_{2\pi} \left(\int_{r=0}^{\infty} r e^{-r^2} dr \right)$$

Notice $\frac{d}{dr}\left(e^{-r^2}\right) = -2r e^{-r^2}$

$$I^2 = 2\pi\left(-\frac{1}{2}\right)\int_{r=0}^{\infty} d\left(e^{-r^2}\right) = -\pi \left. e^{-r^2}\right|_{r=0}^{\infty}$$

$$= -\pi\left[0-1\right] = \pi$$

$$\boxed{I = \sqrt{\pi} = \int_{x=-\infty}^{\infty} e^{-x^2}\,dx}$$

change variables $x = \sqrt{a}\,z$, $dx = \sqrt{a}\,dz$

$x \to \pm\infty \Rightarrow z = \pm\infty$

$$I = \sqrt{\pi} = \int_{z=-\infty}^{\infty} e^{-az^2}\sqrt{a}\,dz$$

$$\int_{z=-\infty}^{+\infty} e^{-az^2}\,dz = \sqrt{\frac{\pi}{a}}$$

differentiate both sides with respect to a.

$$\frac{d}{da}\int_{z=-\infty}^{\infty} e^{-az^2}\,dz = \frac{d}{da}\sqrt{\frac{\pi}{a}}$$

$$= \int_{z=-\infty}^{\infty} (-z^2)\,e^{-az^2}\,dz = \sqrt{\pi}\,\frac{d}{da}a^{-1/2} = \frac{-\sqrt{\pi}}{2a^{3/2}}$$

↑ z is a dummy – rename to x

$$\int_{x=-\infty}^{\infty} x^2 e^{-ax^2}\,dx = \frac{1}{2}\sqrt{\frac{\pi}{a^3}}$$

$\vdots$

$$\int_{x=-\infty}^{\infty} x^{2n} e^{-ax^2}\,dx = \;?$$

$n = 0, 1, 2, 3, \ldots$

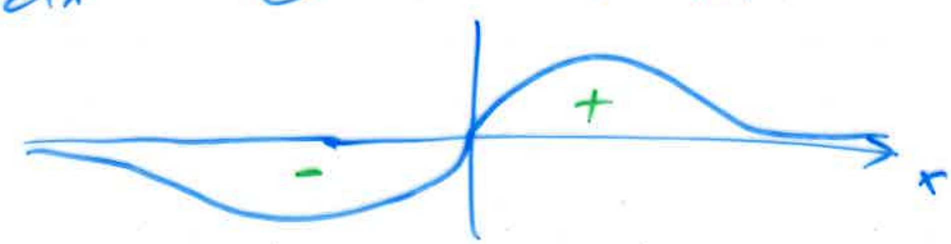
---

odd n?

integrand is odd in x

$f(-x) = -f(x)$ e.g. sine

$$\int_{x=-\infty}^{\infty} \underbrace{x^{2n+1} e^{-ax^2}}_{f(x)}\,dx = 0 \quad \forall n$$



Schrödinger Equation

$$i\hbar \frac{\partial}{\partial t} \Psi_{(x,t)} = \frac{-\hbar}{2m} \frac{\partial^2}{\partial x^2} \Psi_{(x,t)} + V_{(x)} \Psi_{(x,t)}$$

$\Psi_{(x,y,z,t)}$ in general

∇^2 in general $= \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$

could also depend on t.

Separation of Variables

Technique for converting 1 PDE → 2 ODEs

$\psi_{(x)} \cdot \varphi_{(t)}$

Ansatz (Guess): $\Psi_{(x,t)} = f_{(x)} \cdot g(t)$

S.E.: $i\hbar f_{(x)} \frac{dg(t)}{dt} = \frac{-\hbar^2}{2m} \left[\frac{d^2 f_{(x)}}{dx^2} \right] g(t) + V_{(x)} f_{(x)} g(t)$

Divide by $f_{(x)} \cdot g(t) = \Psi_{(x,t)}$

$\frac{dg}{dt}$ Leibniz

$\dot{g}(t)$, $f'_{(x)}$

$$i\hbar \frac{\frac{dg(t)}{dt}}{g(t)} = \frac{-\hbar^2}{2m} \frac{\frac{d^2 f_{(x)}}{dx^2}}{f_{(x)}} + V_{(x)}$$

$$\underbrace{i\hbar\frac{\dot{g}(t)}{g(t)}}_{\substack{\text{some other}\\ \text{function of}\\ \text{time } q(t)}} = \underbrace{-\frac{\hbar^2}{2m}\frac{f''(x)}{f(x)} + V(x)}_{\substack{\text{some other}\\ \text{function of } x\\ r(x)}}$$

$$q(t) = r(x) \quad \forall\, x, t$$
$$= \text{constant} \equiv E$$

L.H.S. $i\hbar\dfrac{\dot{g}(t)}{g(t)} = E$ ← first-order Ordinary Diff. Eq. $\quad \frac{1}{i} = -i$

$$\dot{g}(t) = \frac{E}{i\hbar}g(t) \Rightarrow \frac{dg(t)}{dt} = \frac{-iE}{\hbar}g(t)$$

$$\Rightarrow \int\frac{dg}{g} = \int\frac{-iE}{\hbar}dt$$

$$\ln\left(\frac{g}{g_0}\right) = \frac{-iEt}{\hbar}$$

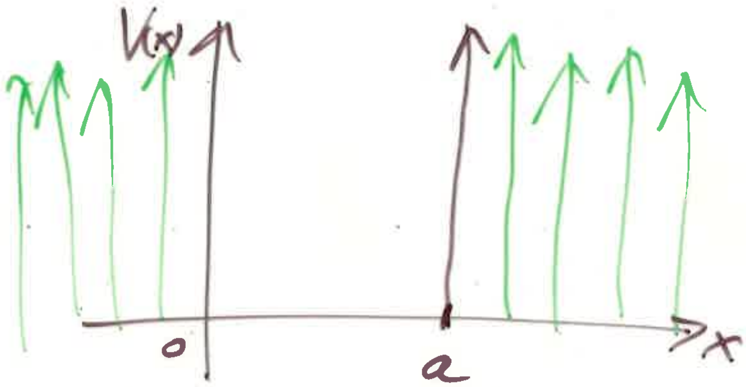
$-\ln(g_0)$ = constant of integration

$$\frac{g(t)}{g_0} = e^{\frac{-iEt}{\hbar}} \Rightarrow \boxed{g(t) = g_0\, e^{\frac{-iEt}{\hbar}}}$$

Space part: $E = -\frac{\hbar^2}{2m}\frac{f''(x)}{f(x)} + V(x)$ 2nd-order O.D.E.

Specific example of $V(x)$

① Infinite Square Well Potential Energy



$$V(x) = \begin{cases} 0, & 0<x<a \\ \infty, & x>a \\ & x<0 \end{cases}$$

where $V(x) = \infty$, $f(x) = 0 \Rightarrow \Psi(x,t) = 0$

cf. Griffiths Problem 2.2

when $E < V$ (negative kinetic energy), Ψ can not be normalized $\rightarrow$ unphysical.

$$E = -\frac{\hbar^2}{2m}\frac{f''(x)}{f(x)} \Rightarrow f''(x) = -\frac{2mE}{\hbar^2} f(x)$$

$$\Rightarrow \frac{d^2 f(x)}{dx^2} = -\underbrace{\left(\frac{2mE}{\hbar^2}\right)}_{\text{positive constant} = k^2} f(x)$$

$$\frac{d^2 f(x)}{dx^2} = -k^2 f(x)$$

$$f(x) = A\sin(kx) + B\cos(kx)$$

$$f'(x) = \frac{df}{dx} = kA\cos(kx) - kB\sin(kx)$$

$$f''(x) = \frac{d^2 f}{dx^2} = -k^2 A\sin(kx) - k^2 B\cos(kx)$$

$$= -k^2\left[A\sin(kx) + B\cos(kx)\right] = -k^2 f(x)$$