Non-VQE

$$a_\pm = \frac{1}{\sqrt{2\hbar m\omega}}\left(\mp i\hat{p} + m\omega x\right)$$

$$a_- a_+ = \frac{1}{2\hbar m\omega}\left[\hat{p}^2 + (m\omega x)^2\right] - \frac{i}{2\hbar}[x, p]$$

$$= \frac{1}{\hbar\omega}\hat{H} + 1/2$$

$$\hat{H} = K + V$$

$$= \frac{p^2}{2m} + \frac{1}{2}m\omega x^2 = \frac{1}{2m}\left[\hat{p}^2 + (m\omega x)^2\right]$$

$\frac{1}{2}mv^2$; $\frac{1}{2}kx^2$

$$\rightarrow = \hbar\omega\left(a_- a_+ - 1/2\right)$$

Similarily, $a_+ a_- = \frac{1}{\hbar\omega}\hat{H} - 1/2$ and

$$\hat{H} = \hbar\omega\left(a_+ a_- + 1/2\right) \rightarrow H = \hbar\omega\left(a_\pm a_\mp \pm 1/2\right)$$

TIS Schrodinger: $H\psi = E\psi$

$$\rightarrow \hbar\omega\left(a_\pm a_\mp \pm 1/2\right)\psi = E\psi$$

$$a_-\psi_0 = 0$$

$$\rightarrow \frac{1}{\sqrt{2\hbar m\omega}}\left(\hbar\frac{d}{dx} + m\omega x\right)\psi_0 = 0$$

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2}$$

By plugging into schrodinger, we find $E_0 = \frac{1}{2}\hbar\omega$

and $E_n = (n + 1/2)\hbar\omega$

Typical QM representation for energy levels of an infinite potential well

VQE $E_{gs} = \frac{\hbar\omega}{2}$

Guess: Gaussian (we know this is answer)

$\psi(x) = Ae^{-bx^2}$

$1 = |A|^2 \int_{-\infty}^{\infty} e^{-2bx^2} dx = |A|^2 \sqrt{\frac{\pi}{2b}} \rightarrow |A|^2 = \sqrt{\frac{2b}{\pi}}$

$\langle H \rangle = \langle K \rangle + \langle V \rangle$ $\qquad A = \left(\frac{2b}{\pi}\right)^{1/4}$

$\langle K \rangle = \frac{\hat{p}^2}{2m} \qquad \langle V \rangle = \frac{1}{2} m\omega x^2 \qquad \hat{p} = -i\hbar \partial/\partial x$

$\langle K \rangle = \int_{-\infty}^{\infty} \psi^* K \psi = \frac{-\hbar^2}{2m} \cdot A^2 \int_{-\infty}^{\infty} e^{-bx^2} \frac{\partial^2}{\partial x^2} e^{-bx^2} dx$

$= -\frac{\hbar^2}{2m} A^2 \int_{-\infty}^{\infty} e^{-bx^2} (-2bx)^2 e^{-bx^2} = -\frac{\hbar^2}{2m} \sqrt{\frac{2b}{\pi}} \cdot 4b^2 \int_{-\infty}^{\infty} e^{-2bx^2} x^2 dx$

$= -\frac{\hbar^2}{2m}[-b] = \frac{\hbar^2 b}{2m}$

$\langle V \rangle = \frac{1}{2} m\omega |A|^2 \int_{-\infty}^{\infty} e^{-2bx^2} x^2 dx$

$\hookrightarrow = \frac{m\omega^2}{8b}$

$\langle H \rangle = \frac{\hbar^2 b}{2m} + \frac{m\omega^2}{8b}$

minimization

$\frac{d}{db}\langle H \rangle = \frac{\hbar^2}{2m} - \frac{m\omega^2}{8b^2} = 0 \qquad \frac{\hbar^2}{2m} = \frac{m\omega^2}{8b^2} \qquad 8b^2\hbar^2 = 2m^2\omega^2$

$b^2 = \frac{2m^2\omega^2}{8\hbar^2}$

$b = \frac{m\omega}{2\hbar}$

$\min(\langle H \rangle) = \frac{\hbar^{\cancel{2}}}{2\cancel{m}} \cdot \frac{\cancel{m}\omega}{2\cancel{\hbar}} + \frac{\cancel{m}\omega^{\cancel{2}}}{8} \cdot \frac{2\hbar}{\cancel{m\omega}}$

$= \frac{\hbar\omega}{4} + \frac{\hbar\omega}{4} = \frac{\hbar\omega}{2} < \boxed{E_0}$

A variational guess for the infinite potential well and a minimization to find E_0

Questions

(ansatz)
→ Pauli gates are complete set

How does normalized wavefunction translate to quantum circuits?

Why does the result go below the line? Doesn't that violate variational principle

↳ how do optimizers relate to each "run"?