Week 6: Theory Solutions

Solution 1

a) The 1-D quantum harmonic oscillator Hamiltonian is given by

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2$$

Normalize the constant A.

$$A = \left(\frac{2\beta}{\pi}\right)^{\frac{1}{4}}$$

We now measure the expectation value of the kinetic and potential energy operators.

$$\left\langle \hat{T} \right\rangle = -\frac{\hbar^2}{2m}|A|^2 \int_{-\infty}^{\infty} e^{-\beta x^2} \frac{d^2}{dx^2}(e^{-\beta x^2})dx = \frac{\hbar^2 \beta}{2m} \tag{1}$$

$$\left\langle \hat{V} \right\rangle = \frac{1}{2}m\omega^2|A|^2 \int_{-\infty}^{\infty} e^{-2\beta x^2} x^2 dx = \frac{m\omega^2}{8\beta} \tag{2}$$

$$\left\langle \hat{H} \right\rangle = \left\langle \hat{T} \right\rangle + \left\langle \hat{V} \right\rangle = \frac{\hbar^2 \beta}{2m} + \frac{m\omega^2}{8\beta} \tag{3}$$

We now differentiate the Hamiltonian operator with respect to the variational parameter to obtain the value of $\beta = \frac{m\omega}{2\hbar}$. Substitute in the Hamiltonian operator to obtain the minimum energy eigenvalue as

$$\left\langle \hat{H} \right\rangle_{min} = \frac{1}{2}\hbar\omega \tag{4}$$

b) Repeat the above process to obtain the $\left\langle \hat{H} \right\rangle_{min} = \frac{3}{2}\hbar\omega$.

We thus find that we luckily choose the correct trial wave functions and got the correct answers for ground state and first excited states respectively.

Solution 2

Maxcut Problem:

$$H_{classical} = \sum_{\mu\nu} x_\mu (1 - x_\nu) \tag{5}$$

where μ, ν are two vertices.

$$H_{quantum} = \sum_{\mu\nu} \frac{1}{4}(1 - Z_\mu + Z_\nu - Z_\mu Z_\nu) \tag{6}$$

Solution 3

Eigenstate	Corresponding Amplitude
$\|000\rangle$	$\cos\frac{\theta_1}{2}\cos\frac{\theta_2}{2}\cos\frac{\theta_3}{2}\cos\frac{\theta_4}{2} - e^{\iota\phi_1}\sin\frac{\theta_1}{2}\sin\frac{\theta_2}{2}\sin\frac{\theta_3}{2}\sin\frac{\theta_4}{2}$
$\|001\rangle$	$e^{\iota\phi_4}(\cos\frac{\theta_1}{2}\cos\frac{\theta_2}{2}\cos\frac{\theta_3}{2}\sin\frac{\theta_4}{2} + e^{\iota\phi_1}\sin\frac{\theta_1}{2}\sin\frac{\theta_2}{2}\sin\frac{\theta_3}{2}\cos\frac{\theta_4}{2})$
$\|010\rangle$	$e^{\iota\phi_3}(\cos\frac{\theta_1}{2}\cos\frac{\theta_2}{2}\sin\frac{\theta_3}{2}\cos\frac{\theta_4}{2} + e^{\iota\phi_1}\sin\frac{\theta_1}{2}\sin\frac{\theta_2}{2}\cos\frac{\theta_3}{2}\sin\frac{\theta_4}{2})$
$\|011\rangle$	$e^{\iota(\phi_3+\phi_4)}(\cos\frac{\theta_1}{2}\cos\frac{\theta_2}{2}\sin\frac{\theta_3}{2}\sin\frac{\theta_4}{2} - e^{\iota\phi_1}\sin\frac{\theta_1}{2}\sin\frac{\theta_2}{2}\cos\frac{\theta_3}{2}\cos\frac{\theta_4}{2})$
$\|100\rangle$	$e^{\iota\phi_2}(\cos\frac{\theta_1}{2}\sin\frac{\theta_2}{2}\cos\frac{\theta_3}{2}\cos\frac{\theta_4}{2} + e^{\iota\phi_1}\sin\frac{\theta_1}{2}\cos\frac{\theta_2}{2}\sin\frac{\theta_3}{2}\sin\frac{\theta_4}{2})$
$\|101\rangle$	$e^{\iota(\phi_2+\phi_4)}(\cos\frac{\theta_1}{2}\sin\frac{\theta_2}{2}\cos\frac{\theta_3}{2}\sin\frac{\theta_4}{2} - e^{\iota\phi_1}\sin\frac{\theta_1}{2}\cos\frac{\theta_2}{2}\sin\frac{\theta_3}{2}\cos\frac{\theta_4}{2})$
$\|110\rangle$	$e^{\iota(\phi_2+\phi_3)}(\cos\frac{\theta_1}{2}\sin\frac{\theta_2}{2}\sin\frac{\theta_3}{2}\cos\frac{\theta_4}{2} - e^{\iota\phi_1}\sin\frac{\theta_1}{2}\cos\frac{\theta_2}{2}\cos\frac{\theta_3}{2}\sin\frac{\theta_4}{2})$
$\|111\rangle$	$e^{\iota(\phi_2+\phi_3+\phi_4)}(\cos\frac{\theta_1}{2}\sin\frac{\theta_2}{2}\sin\frac{\theta_3}{2}\sin\frac{\theta_4}{2} + e^{\iota\phi_1}\sin\frac{\theta_1}{2}\cos\frac{\theta_2}{2}\cos\frac{\theta_3}{2}\cos\frac{\theta_4}{2})$

Solution 4

We use the following exchange-type A gate which respects the particle number symmetry.

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos\theta & e^{\iota\phi}\sin\theta & 0 \\ 0 & e^{-\iota\phi}\sin\theta & -\cos\theta & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

1. On m qubits, apply X gate

2. Put first layer of A gates on all near-neighboring pair of qubits on which in the previous layer $X \otimes I$ or $I \otimes X$ is applied

3. Put second layer of A gates on near-neighboring qubits win such a way that each such pair has one qubit involved in step 2 and one not involved in step 2

4. Repeat this pattern for $2\binom{n}{m}$. For real scenarios, you can put ϕ to be zero in all A gates.

Solution 5

1. Prepare a trial ansatz $U(\theta)$ by selecting ortho-normal input states $\{|\psi_i\rangle\}_{i=0}^{k}$.

2. Minimize $w\left\langle\psi_k|U^\dagger(\theta)HU(\theta)|\psi_k\right\rangle + \sum_{i=0}^{k-1}\left\langle\psi_i|U^\dagger(\theta)HU(\theta)|\psi_i\right\rangle$ using a classical optimizer. The value of w can be anything between 0 and 1.