University of California at San Diego – Department of Physics – TA: Shauna Kravec

Quantum Mechanics A (Physics 212A) Fall 2018
Worksheet 9 – Solutions

Problems

1. **Variational Method**

   Consider the special case of $\dim \mathcal{H} = 2$, with Hamiltonian

   $$\mathbf{H} = \begin{pmatrix} a+c & b \\ b & a-c \end{pmatrix}$$

   with a, b, c real. Parametrizing the variational state as

   $$|\varphi(\alpha)\rangle = \begin{pmatrix} \cos\alpha/2 \\ \sin\alpha/2 \end{pmatrix},$$

   find the values of $\alpha = \alpha_0$ which extremize the expectation value of the Hamiltonian. Show that this reproduces the eigenstates:

   $$|\chi_+\rangle = \begin{pmatrix} \cos\theta/2 \\ \sin\theta/2 \end{pmatrix}, \quad |\chi_-\rangle = \begin{pmatrix} -\sin\theta/2 \\ \cos\theta/2 \end{pmatrix}.$$

   where $\tan\theta = b/c$.

   Note that $\hat{H} = a\mathbb{1} + bX + cZ$ so $\hat{H}|\alpha\rangle = \begin{pmatrix} (a+c)\cos\frac{\alpha}{2} + b\sin\frac{\alpha}{2} \\ (a-c)\sin\frac{\alpha}{2} + b\cos\frac{\alpha}{2} \end{pmatrix}$

   $\langle\hat{H}\rangle_\alpha = a + b\sin(\alpha) + c\cos(\alpha)$ which has extremum at $\tan(\alpha) = \frac{b}{c}$

   This is the answer we get from exact diagonalization as well.

2. **The Feynman-Hellmann theorem.**

   Suppose the Hamiltonian depends on a parameter s, $\mathbf{H} = \mathbf{H}(s)$. Suppose $E(s)$ is a non-degenerate eigenvalue with normalized eigenvector $|\phi(s)\rangle$. Show that

   $$\partial_s E(s) = \langle\phi(s)|\partial_s \mathbf{H}(s)|\phi(s)\rangle.$$

   First we note that $E(s) = \langle\phi(s)|\hat{H}(s)|\phi(s)\rangle$ and $1 = \langle\phi(s)|\phi(s)\rangle$

   Using the chain rule: $\partial_s E(s) = \langle\phi(s)|\partial_s\hat{H}(s)|\phi(s)\rangle + E(s)[\langle\partial_s\phi(s)|\phi(s)\rangle + \langle\phi(s)|\partial_s\phi(s)\rangle]$

   But by normalization and the chain rule:$[\langle\partial_s\phi(s)|\phi(s)\rangle + \langle\phi(s)|\partial_s\phi(s)\rangle] = \partial_s 1 = 0$

   This proves the theorem.