PHYS 5002: Homework #3

1 Schroedinger Factorization Method

a.) In the factorization method, we had

$$|\psi_j\rangle = \hat{A}_0^\dagger \hat{A}_1^\dagger \cdots \hat{A}_{j-1}^\dagger |\phi_j\rangle$$

with $\hat{A}_j |\phi_j\rangle = 0$ and $\hat{H}_j = \hat{A}_j^\dagger \hat{A}_j + E_j = \hat{A}_{j-1}\hat{A}_{j-1}^\dagger + E_{j-1}$.

Show that $\langle\psi_j|\psi_{j'}\rangle = 0$ for $j \neq j'$. Feel free to assume $j > j'$ without loss of generality.

b.) Here we show that $E_j > E_{j-1}$.

Compute $\langle\phi_j|H_j|\phi_j\rangle$ using the two expressions for $\hat{H}_j$ to show $E_j > E_{j-1}$ unless $\hat{A}_{j-1}^\dagger |\phi_j\rangle = 0$. Verify that if $\hat{A}_{j-1}^\dagger |\phi_j\rangle = 0$ then $|\psi_j\rangle = 0$ hence, there is no $|\psi_j\rangle$ state (this says the factorization method terminates). Conclude then for all bound states $E_j > E_{j-1}$.

This allows us to use the rule, if there is any ambiguity in choosing E_j, pick $E_j > E_{j-1}$.

2 Position & Momentum are Vector Operators

A *vector operator* $\hat{\mathbf{v}}$ is defined to satisfy

$$[\hat{v}_i, \hat{L}_j] = i\hbar\varepsilon_{ijk}\hat{v}_k$$

Using $\hat{\mathbf{L}} = \hat{\mathbf{r}} \times \hat{\mathbf{p}}$, verify that $\hat{\mathbf{r}}$ and $\hat{\mathbf{p}}$ are both vector operators. Show as well for any vector operator that we have

$$[\hat{\mathbf{v}} \cdot \hat{\mathbf{v}}, \hat{\mathbf{L}}] = [\hat{v}^2, \hat{\mathbf{L}}] = 0$$

Hence we have immediately that $[\hat{r}^2, \hat{\mathbf{L}}] = [\hat{p}^2, \hat{\mathbf{L}}] = [\hat{L}^2, \hat{\mathbf{L}}] = 0$.

3 More Exponential Disentangling

Use the exact result for the 3×3 angular momentum matrices with $l = 1$ (from **Homework #1**) to show that

$$e^{i\theta M_y} = e^{-\tan\left(\frac{\theta}{2}\right)M_-} e^{\ln\left(\cos^2\frac{\theta}{2}\right)M_z} e^{\tan\left(\frac{\theta}{2}\right)M_+}$$

where $M_\pm = M_x \pm iM_y$.

Hint: Compute $e^{i\theta M_y}$ directly, then compute each of the factors on the RHS and multiply them together.

4 Angular Momentum must be Integral

(Following Ballentine) Note that nearly all quantum textbooks incorrectly state that the wavefunction must be periodic when $\phi \to \phi + 2\pi$. It needn't. The only condition is that $|\psi|^2$ be periodic, so ψ can change sign as $\phi \to \phi + 2\pi$. But orbital angular momentum always requires l be an integer. Here is the reason why:

We will find the eigenvalues of $\hat{L}_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x$. Recall that

$$[\hat{x}, \hat{y}] = [\hat{p}_x, \hat{p}_y] = 0$$
$$[\hat{x}, \hat{p}_x] = [\hat{y}, \hat{p}_y] = i\hbar$$

For this problem, we work in units where $\hbar = 1$. Define

$$\hat{q}_1 = \frac{\hat{x} + \hat{p}_y}{\sqrt{2}}$$
$$\hat{q}_2 = \frac{\hat{x} - \hat{p}_y}{\sqrt{2}}$$
$$\hat{p}_1 = \frac{\hat{p}_x - \hat{y}}{\sqrt{2}}$$
$$\hat{p}_2 = \frac{\hat{p}_x + \hat{y}}{\sqrt{2}}$$

Verify that $[\hat{q}_1, \hat{q}_2] = 0,\ [\hat{p}_1, \hat{p}_2] = 0$, and $[\hat{q}_\alpha, \hat{p}_\beta] = i\delta_{\alpha\beta}$.

Show that

$$\hat{L}_z = \frac{1}{2}(\hat{p}_1^2 + \hat{q}_1^2) - \frac{1}{2}(\hat{p}_2^2 + \hat{q}_2^2)$$

Hence, we verify that $\hat{L}_z$ is the difference of two simple harmonic oscillators with mass m and frequency ω_0 both equal to 1. The eigenvalues of each are $n_1 + \frac{1}{2}$ and $n_2 + \frac{1}{2}$ respectively. Because the operators of the two simple harmonic oscillator's commute, they can be diagonalized at the same time. This means the eigenvalues of $\hat{L}_z$ must be

$$\left(n_1 + \frac{1}{2}\right) - \left(n_2 + \frac{1}{2}\right) = n_1 - n_2 = \text{an integer}$$

Therefore, l is an integer for orbital angular momentum!

5 Angular Operators Cannot Exist

a.) Suppose we could define an angle operator $\hat{\theta}$ conjugate to $\hat{L}_z$ such that $[\hat{\theta}, \hat{L}_z] = i\hbar$. We can immediately show such an operator is ill-behaved. Take an eigenstate of $\hat{L}^2$ and $\hat{L}_z$ given by $|lm\rangle$.

Form $e^{-i\alpha\hat{\theta}} |lm\rangle$.

Use Hadamard to compute

$$\hat{L}_z \left(e^{-i\alpha\hat{\theta}} |lm\rangle\right)$$

and verify it is an eigenvector of $\hat{L}_z$ with eigenvalue $(m + \alpha)\hbar$. But we know the eigenvalues of $\hat{L}_z$ are only integers times $\hbar$. Therefore, only $e^{i\hat{\theta}}$ is well-defined, not $\hat{\theta}$ alone.

b.) Using the Hadamard lemma, verify that

$$e^{i\hat{\phi}} |\theta, \phi\rangle = e^{i\phi} |\theta, \phi\rangle$$

and

$$e^{i\hat{\theta}} |\theta, \phi\rangle = e^{i\theta} |\theta, \phi\rangle$$

where $|\theta, \phi\rangle = e^{-i\phi\frac{\hat{L}_z}{\hbar}} e^{-i\theta\frac{\hat{L}_y}{\hbar}} |\theta{=}0, \phi{=}0\rangle$.

Hint: Use

$$e^{i\hat{\theta}} = \frac{\hat{z} + i\sqrt{\hat{x}^2 + \hat{y}^2}}{\hat{r}}$$
$$e^{i\hat{\phi}} = \frac{\hat{x} + i\hat{y}}{\sqrt{\hat{x}^2 + \hat{y}^2}}$$

and recall that $\hat{r}$ commutes with $\hat{\mathbf{L}}$ and $\sqrt{\hat{x}^2+\hat{y}^2}$ commutes with $\hat{L}_z$. Also $\hat{x}\,|\theta{=}0,\phi{=}0\rangle = 0$ and $\hat{y}\,|\theta{=}0,\phi{=}0\rangle = 0$. Recall we worked out $e^{-i\alpha\frac{\hat{L}_y}{\hbar}}(\hat{x} \text{ or } \hat{z})e^{i\alpha\frac{\hat{L}_y}{\hbar}}$ in class.

6 Oscillating Diatomic Molecules

Diatomic molecules are linear molecules shaped like a dumbbell. If they are composed of two different atoms, like chlorine and hydrogen, then as they rotate they vary and because one side has a different charge than the other, this looks like an oscillating charge.

Oscillating charges couple to light, so we can absorb or emit light and change the rotation. In this problem, we work in the "body frame".

$$\hat{H} = \frac{1}{2I}(\hat{L}_x^2 + \hat{L}_y^2) + \frac{1}{2I_z}\hat{L}_z^2$$

a.) Show that if I_z is very small, then we must have $\Delta m = 0$ for absorption by low energy light. (For diatomics $I_z \to 0$)

b.) If $\Delta m = 0$ and $\Delta l = \pm 1$ only, find the change in the energy level between two absorption lines as a function of the angular momentum l.

c.) Compute the moment of inertia as follows:

1. Find $r_{cm} = \frac{M_{Cl} r}{M_H + M_{Cl}} = \alpha r$
2. Compute $I = r_{cm}^2 M_H + (r - r_{cm})^2 M_{Cl}$ in terms of α, r, and the masses.
3. Show $I = \mu r^2 = \frac{M_{Cl} M_H}{M_{Cl} + M_H} r^2$
4. Express $\frac{\hbar^2}{2I}$ as an energy in eV$/r^2$ with r in Å and as a "frequency" f in cm^{-1} via $hcf = \frac{\hbar^2}{2I}$. ($hc = 12400$ eV Å)
5. Use the rotational line spacing of the HCl molecule rotational spectra, given by 21.18cm^{-1} to determine the molecule bond length in Å.