University of Kentucky, Physics 520
Homework #8, Rev. A, due Monday, 2015-11-16

1. We will apply the formalism of quantum mechanics to one the simplest nontrivial system: the **ammonia molecule**, ignoring rotations and vibrations. It has two quantum states $|1\rangle$ and $|2\rangle$, corresponding the nitrogen atom above $(+)$ or below $(-)$ the triangle of hydrogen atoms. These would be degenerate ground states of energy E were it not for the small interaction energy $-A$ which couples the two states (tunnelling amplitude between states). The Hamiltonian of this system in the $|1,2\rangle$ basis is $\mathcal{H} = \begin{pmatrix} E_0 & -A \\ -A & E_0 \end{pmatrix}$.

a) Calculate the eigenstates $|I, II\rangle$ and energy spectrum $E_{I,II}$ of $\mathcal{H}$.

b) Given the initial state $|\psi_0\rangle = \begin{pmatrix} a \\ b \end{pmatrix}$ in the $|1,2\rangle$ basis, change components to the $|I, II\rangle$ basis. Calculate the time-dependence $|\psi(t)\rangle$ in both the $|I, II\rangle$ and $|1,2\rangle$ bases.

c) What is the probability of measuring E_I and E_{II} at time t? Calculate $\langle E(t)\rangle$.

d) Let the 'position' X of the nitrogen atom be $+a$ in state $|1\rangle$ and $-a$ in the state $|2\rangle$. Write the matrix of the operator $\hat{X}$ in both the $|1,2\rangle$ and $|I, II\rangle$ bases. Calculate the probability of measuring $X(t) = \pm a$, and $\langle X(t)\rangle$. What is the state after measuring X? Describe the possible results and probabilities of a subsequent measurement of E.

e) Calculate the emission frequency of transitions in this system and compare to $\langle X(t)\rangle$.

2. Minimum uncertainty wave packet.

a) Following the Griffiths requirement for equality in the Heisenberg Uncertainty Principle, that $|g\rangle = ia|f\rangle$, where $|f\rangle = (\hat{x} - x_0)|\psi\rangle$ and $|g\rangle = (\hat{p} - p_0)|\psi\rangle$, show that the general minimum uncertainty wave packet is $\psi(x) = Ae^{-\frac{1}{2}(\frac{x-x_0}{\sigma_x})^2} e^{ip_0x/\hbar}$. Plot this wavefunction in the complex plane as a function of x. Show that $\langle x\rangle = x_0$ and $\langle x^2\rangle - x_0^2 = \sigma_x^2$. What is the relation between a and σ_x? Normalize the wavefunction to obtain the amplitude A up to an arbitrary phase $e^{i\theta}$.

b) Perform the *Fourier transform* $\phi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dx\, e^{-ipx/\hbar}\psi(x)$ to show that the momentum amplitudes $\phi(p) = Be^{-\frac{1}{2}(\frac{p-p_0}{\sigma_p})^2} e^{-ix_0p/\hbar}$ have the same Gaussian distribution. Compare the roles of x and p in these two representations, and explain the new $-$ sign in front of x_0. Plot the complex function $\phi(p)$. Calculate $\langle p\rangle$ and $\langle p^2\rangle$ (you already did the math above!). Verify that $\sigma_x\sigma_p = \hbar/2$, and that $\phi(p)$ is still normalized (the Fourier transform is a *unitary* operator).

c) Perform the *Inverse Fourier transform* $\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dp\, e^{ipx/\hbar}\phi(p)$ to recover the original wave function in x-space. (you already did the math above!)

d) What is the effect on the Fourier transform of multiplying $\psi(x)$ by i) a global phase $e^{i\theta}$, ii) a linear phase e^{ikx}; iii) translating $\psi(x) \to \psi(x-dx)$ (operating by $i\hat{p}dx/\hbar$); iv) scaling $\psi(x) \to \psi(x/b)$ (changing the uncertainty of x)? Repeat for the analogous transforms on $\phi(p)$.

e) **[bonus]** Transform this wavefunction into the basis of energy eigenfunctions $|n\rangle$ of the harmonic oscillator to obtain the coefficients $c_n(x_0, p_0, \sigma_x)$ and compare with Griffiths 2ed problem 3.35. Note the significance of $|g\rangle = ia|f\rangle$; you may want to use the operator algebra method.