

Physics 741 – Graduate Quantum Mechanics 1
Solutions to Chapter 5

1. [10] The Lennard-Jones 6-12 potential is commonly used as a model to describe the potential of an atom in the neighborhood of another atom. Classically, the energy is given by $E = \frac{1}{2}m\dot{x}^2 + 4\epsilon\left[\left(\frac{\sigma}{x}\right)^{12} - \left(\frac{\sigma}{x}\right)^6\right]$.

- (a) [6] Find the minimum x_{\min} of this potential, and expand the potential to quadratic order in $(x - x_{\min})$.

The potential is minimized when the derivative vanishes, so we have

$$0 = \frac{dV}{dx} = 4\epsilon \frac{d}{dx} \left[\left(\frac{\sigma}{x}\right)^{12} - \left(\frac{\sigma}{x}\right)^6 \right] = 4\epsilon \left[-\frac{12\sigma^{12}}{x^{13}} + \frac{6\sigma^6}{x^7} \right] = \frac{24\epsilon\sigma^6}{x^7} \left(1 - \frac{2\sigma^6}{x^6} \right)$$

The minimum of this potential is therefore $x_{\min} = 2^{1/6}\sigma$. If we expand this potential out to order $(x - x_{\min})^2$, we have

$$\begin{aligned} V(x) &\approx V(x_{\min}) + V'(x_{\min})(x - x_{\min}) + \frac{1}{2}V''(x_{\min})(x - x_{\min})^2 \\ &= 4\epsilon \left[\left(\frac{\sigma}{\sigma 2^{1/6}}\right)^{12} - \left(\frac{\sigma}{\sigma 2^{1/6}}\right)^6 \right] + 0 + \frac{1}{2} \cdot 4\epsilon \left[\frac{156\sigma^{12}}{(\sigma 2^{1/6})^{14}} - \frac{42\sigma^6}{(\sigma 2^{1/6})^8} \right] (x - x_{\min})^2 \\ &= 4\epsilon \left(\frac{1}{4} - \frac{1}{2} \right) + \frac{4\epsilon}{2\sigma^2} \left[156 \cdot 2^{-7/3} - 42 \cdot 2^{-4/3} \right] (x - x_{\min})^2 = -\epsilon + \frac{4\epsilon[39 - 21]}{2\sigma^2 2^{1/3}} (x - x_{\min})^2 \\ &= -\epsilon + 9 \cdot 2^{5/3} \frac{\epsilon}{\sigma^2} (x - x_{\min})^2. \end{aligned}$$

- (b) [4] Determine the classical frequency ω , and calculate the quantum mechanical minimum energy, as a function of the various parameters.

The Harmonic oscillator is normally written as $E = \frac{1}{2}m\dot{x}^2 + \frac{1}{2}kx^2$. Comparing this with our energy expression, we see that the role of the spring constant is played by the combination

$$k = 9 \cdot 2^{8/3} \frac{\epsilon}{\sigma^2}.$$

The angular frequency is given by $\omega = \sqrt{k/m}$, so we have

$$\omega = \sqrt{\frac{9 \cdot 2^{8/3} \epsilon}{m\sigma^2}} = \frac{3 \cdot 2^{4/3}}{\sigma} \sqrt{\frac{\epsilon}{m}}.$$

The ground state energy is normally $E_0 = \frac{1}{2}\hbar\omega$, but the energy has been shifted downwards by an amount $-\varepsilon$, so we have

$$E_0 = -\varepsilon + \frac{1}{2}\hbar\omega = -\varepsilon + 3 \cdot 2^{1/3} \frac{\hbar}{\sigma} \sqrt{\frac{\varepsilon}{m}}.$$

2. [10] At $t = 0$, a single particle is placed in a harmonic oscillator

$H = P^2/2m + \frac{1}{2}m\omega^2 X^2$ in the superposition state $|\Psi(t=0)\rangle = \frac{3}{5}|1\rangle + \frac{4}{5}|2\rangle$, that is, in a superposition of the first and second excited states.

(a) [3] What is the wave function $|\Psi(t)\rangle$ at subsequent times?

The wave function has been written in terms of eigenstates of the Hamiltonian, so this makes it relatively easy. The energy of the state $|n\rangle$ is $\hbar\omega(n + \frac{1}{2})$, and therefore the state will evolve as

$$|\Psi(t)\rangle = \frac{3}{5}|1\rangle e^{-i3\hbar\omega t/2\hbar} + \frac{4}{5}|2\rangle e^{-i5\hbar\omega t/2\hbar} = \frac{3}{5}|1\rangle e^{-i3\omega t/2} + \frac{4}{5}|2\rangle e^{-i5\omega t/2}.$$

(b) [7] What are the expectation values $\langle X \rangle$ and $\langle P \rangle$ at all times?

These are most easily calculated using the raising and lowering operators

$$\begin{aligned} \langle X \rangle &= \sqrt{\frac{\hbar}{2m\omega}} \langle \Psi(t) | (a + a^\dagger) | \Psi(t) \rangle \\ &= \sqrt{\frac{\hbar}{2m\omega}} \left(\frac{3}{5} \langle 1 | e^{i3\omega t/2} + \frac{4}{5} \langle 2 | e^{i5\omega t/2} \right) (a + a^\dagger) \left(\frac{3}{5} |1\rangle e^{-i3\omega t/2} + \frac{4}{5} |2\rangle e^{-i5\omega t/2} \right) \\ &= \sqrt{\frac{\hbar}{2m\omega}} \left(\frac{3}{5} \langle 1 | e^{i3\omega t/2} + \frac{4}{5} \langle 2 | e^{i5\omega t/2} \right) \left[\frac{3}{5} (|0\rangle + \sqrt{2}|2\rangle) + \frac{4}{5} (\sqrt{2}|1\rangle + \sqrt{3}|3\rangle) e^{-i5\omega t/2} \right] \\ &= \sqrt{\frac{\hbar}{2m\omega}} \frac{3}{5} \cdot \frac{4}{5} \sqrt{2} (e^{-i\omega t} + e^{i\omega t}) = \frac{24}{25} \sqrt{\frac{\hbar}{m\omega}} \cos(\omega t), \end{aligned}$$

and

$$\begin{aligned} \langle P \rangle &= i\sqrt{\hbar m\omega/2} \langle \Psi(t) | (a^\dagger - a) | \Psi(t) \rangle \\ &= i\sqrt{\hbar m\omega/2} \left(\frac{3}{5} \langle 1 | e^{i3\omega t/2} + \frac{4}{5} \langle 2 | e^{i5\omega t/2} \right) (a^\dagger - a) \left(\frac{3}{5} |1\rangle e^{-i3\omega t/2} + \frac{4}{5} |2\rangle e^{-i5\omega t/2} \right) \\ &= i\sqrt{\hbar m\omega/2} \left(\frac{3}{5} \langle 1 | e^{i3\omega t/2} + \frac{4}{5} \langle 2 | e^{i5\omega t/2} \right) \left[\frac{3}{5} (\sqrt{2}|2\rangle - |0\rangle) e^{-i3\omega t/2} + \frac{4}{5} (\sqrt{3}|3\rangle - \sqrt{2}|1\rangle) e^{-i5\omega t/2} \right] \\ &= i\sqrt{\hbar m\omega/2} \frac{3}{5} \cdot \frac{4}{5} \sqrt{2} (e^{i\omega t} - e^{-i\omega t}) = -\frac{24}{25} \sqrt{\hbar m\omega} \sin(\omega t). \end{aligned}$$

3. [15] In class we assumed that the coupled harmonic oscillators all had the same mass. Consider now the case where the oscillators have different masses, so that

$$H = \sum_i P_i^2 / 2m_i + \frac{1}{2} \sum_i \sum_j k_{ij} X_i X_j$$

- (a) [5] Rescale the variables P_i and X_i to new variables \hat{P}_i and \hat{X}_i with the usual commutation relations: $[\hat{X}_i, \hat{P}_j] = i\hbar \delta_{ij}$ such that in terms of the new variables, the Hamiltonian is given by $H = \sum_i \hat{P}_i^2 / 2m + \frac{1}{2} \sum_i \sum_j k'_{ij} \hat{X}_i \hat{X}_j$, where m is an arbitrary mass that you can choose.

We want to rescale the momentum operators so that they all have the same coefficient in the kinetic energy term. If we define $P_i = c\hat{P}_i$ for some constant c , then the term that looked like $P_i^2 / 2m_i$ will become $c^2 \hat{P}_i^2 / 2m_i$, which we want to equal $\hat{P}_i^2 / 2m$, so $c^2 / 2m_i = 1/2m$, and we have $c = \sqrt{m_i/m}$, so that $\hat{P}_i = P_i/c = P_i \sqrt{m/m_i}$. To make sure the commutation relations are not messed up, we take the opposite factor for the X 's, so we have

$$\hat{P}_i = P_i \sqrt{\frac{m}{m_i}} \quad \text{and} \quad \hat{X}_i = X_i \sqrt{\frac{m_i}{m}}$$

Then these new variables will have commutation relations

$$[\hat{X}_i, \hat{P}_j] = \sqrt{\frac{m_i}{m}} \sqrt{\frac{m}{m_j}} [X_i, P_j] = i\hbar \delta_{ij} \sqrt{\frac{m_i}{m_j}} = i\hbar \delta_{ij},$$

where, at the final step, we have taken advantage of the fact that the expression is zero unless $i = j$.

Solving for our old variables in terms of the new, we now work out the Hamiltonian in the new variables.

$$\begin{aligned} H &= \sum_i \frac{P_i^2}{2m_i} + \frac{1}{2} \sum_i \sum_j k_{ij} X_i X_j = \sum_i \frac{\hat{P}_i^2}{2m_i} \left(\sqrt{\frac{m_i}{m}} \right)^2 + \frac{1}{2} \sum_i \sum_j k_{ij} \hat{X}_i \hat{X}_j \sqrt{\frac{m}{m_i}} \sqrt{\frac{m}{m_j}} \\ &= \sum_i \frac{\hat{P}_i^2}{2m} + \frac{1}{2} \sum_i \sum_j \frac{k_{ij} m}{\sqrt{m_i m_j}} \hat{X}_i \hat{X}_j. \end{aligned}$$

This is exactly the form requested., if we identify

$$k'_{ij} = \frac{m k_{ij}}{\sqrt{m_i m_j}}.$$

(b) [5] Find an expression for k'_{ij} in terms of the original variables k_{ij} and m_i , and explain in words how to obtain the eigenvalues of the original Hamiltonian.

Comparing the form we have for the Hamiltonian with the form requested, we see that $k'_{ij} = k_{ij} m / \sqrt{m_i m_j}$. The Hamiltonian is now in the same form as found in class. We now treat the constants k'_{ij} as a matrix k' . If we find the eigenvalues of k' , which we will call k'_i , then the normal modes of the harmonic oscillator will have frequencies $\omega_i = \sqrt{k'_i/m}$, and then the energy eigenstates will have energy $E_{n_1 \dots n_N} = \sum_i \hbar \omega_i (n_i + \frac{1}{2})$.

(c) [5] A system of two particles in one dimension has Hamiltonian

$$H = \frac{P_1^2}{2m} + \frac{P_2^2}{2(m/4)} + \frac{1}{2} m \omega^2 (5X_1^2 + 2X_2^2 + 2X_1X_2).$$

Find the eigenvalues E_{ij} of this Hamiltonian.

We will simply use all the formulas we have already derived. The initial coupling has spring constants given by

$$k_{11} = 5m\omega^2, \quad k_{12} = k_{21} = m\omega^2, \quad k_{22} = 2m\omega^2$$

Note that we have split the cross-term in half. Now, the masses are $m_1 = m$ and $m_2 = m/4$. It is therefore straightforward to get the components of the k' matrix:

$$k'_{11} = \frac{mk_{11}}{\sqrt{mm}} = 5m\omega^2, \quad k'_{12} = k'_{21} = \frac{mk_{12}}{\sqrt{mm/4}} = 2m\omega^2, \quad \text{and} \quad k'_{22} = \frac{mk_{22}}{\sqrt{(m/4)^2}} = 8m\omega^2.$$

We put this together into a single matrix

$$k' = m\omega^2 \begin{pmatrix} 5 & 2 \\ 2 & 8 \end{pmatrix}.$$

We need to find the eigenvalues of this matrix. Pulling out the common factors, we need to find the solutions of

$$0 = \det \begin{pmatrix} 5 - \lambda & 2 \\ 2 & 8 - \lambda \end{pmatrix} = \lambda^2 - 13\lambda + 40 - 4 = (\lambda - 9)(\lambda - 4).$$

Reintroducing the common factor, the eigenvalues of k' are $4m\omega^2$ and $9m\omega^2$.

We then find the frequencies $\omega_i = \sqrt{k'_i/m}$, which yields 2ω and 3ω . Thus the energy eigenvalues are

$$E_{ij} = \hbar(2\omega)(i + \frac{1}{2}) + \hbar(3\omega)(j + \frac{1}{2}) = \hbar\omega(2i + 3j + \frac{5}{2}).$$

4. [10] A particle of mass m is in a one-dimensional harmonic oscillator with angular frequency ω . If the particle is in the coherent state $|z\rangle$, find the uncertainties ΔX , ΔP , and check that they satisfy the uncertainty relation $\Delta X \Delta P \geq \frac{1}{2} \hbar$.

Our strategy will be to rewrite all operators in terms of the raising and lowering operators. Then, whenever we see a on the right, we'll rewrite it using $a|z\rangle = z|z\rangle$; whenever we see a^\dagger on the left, we'll rewrite it using $\langle z|a^\dagger = \langle z|z^*$, and whenever we encounter aa^\dagger we'll rewrite it as $aa^\dagger = a^\dagger a + 1$.

$$\begin{aligned}
 (\Delta X)^2 &= \langle X^2 \rangle - \langle X \rangle^2 = \left(\sqrt{\frac{\hbar}{2m\omega}} \right)^2 \langle z|(a+a^\dagger)^2|z\rangle - \left(\sqrt{\frac{\hbar}{2m\omega}} \right)^2 \langle z|(a+a^\dagger)|z\rangle^2 \\
 &= \frac{\hbar}{2m\omega} \left\{ \langle z|(a^2 + aa^\dagger + a^\dagger a + a^{\dagger 2})|z\rangle - \left[\langle z|(z+z^*)|z\rangle \right]^2 \right\} \\
 &= \frac{\hbar}{2m\omega} \left\{ \langle z|(a^2 + 2a^\dagger a + 1 + a^{\dagger 2})|z\rangle - (z+z^*)^2 \right\} \\
 &= \frac{\hbar}{2m\omega} \left\{ \langle z|(z^2 + 2z^*z + 1 + z^{*2})|z\rangle - (z+z^*)^2 \right\} \\
 &= \frac{\hbar}{2m\omega} (z^2 + 2z^*z + 1 + z^{*2} - z^2 - 2z^*z - z^{*2}) = \frac{\hbar}{2m\omega},
 \end{aligned}$$

$$\begin{aligned}
 (\Delta P)^2 &= \langle P^2 \rangle - \langle P \rangle^2 = \left(i\sqrt{\hbar m\omega/2} \right)^2 \langle z|(a^\dagger - a)^2|z\rangle - \left(i\sqrt{\hbar m\omega/2} \right)^2 \langle z|(a^\dagger - a)|z\rangle^2 \\
 &= -\frac{1}{2} \hbar m\omega \left\{ \langle z|(a^{\dagger 2} - aa^\dagger - a^\dagger a + a^2)|z\rangle - \left[\langle z|(z^* - z)|z\rangle \right]^2 \right\} \\
 &= -\frac{1}{2} \hbar m\omega \left\{ \langle z|(a^{\dagger 2} - 2a^\dagger a - 1 + a^2)|z\rangle - (z^* - z)^2 \right\} \\
 &= -\frac{1}{2} \hbar m\omega \left\{ \langle z|(z^{*2} - 2z^*z - 1 + z^2)|z\rangle - (z^* - z)^2 \right\} \\
 &= -\frac{1}{2} \hbar m\omega (z^{*2} - 2z^*z - 1 + z^2 - z^{*2} + 2z^*z - z^2) = \frac{1}{2} \hbar m\omega.
 \end{aligned}$$

To summarize, taking the square root we have

$$\Delta X = \sqrt{\frac{\hbar}{2m\omega}}, \quad \Delta P = \sqrt{\frac{1}{2} \hbar m\omega}, \quad (\Delta X)(\Delta P) = \frac{1}{2} \hbar$$

The state satisfies the inequality by saturating it; that is, making it an equality. These states are commonly called *minimum uncertainty states* for this reason.