(AND SOLUTIONS TO FINAL REVIEW PROBLEMS)

Uncertainty Principle: $\Delta x \Delta p \approx \hbar/2$

Q: Consider a free electron ~~movin~~ initially confined in a region $\Delta X(0) = 1\,\text{Å}$. Compute its initial uncertainty in momentum. Using the result of review problem 2, find the time it would take for its uncertainty to triple.

A: In review problem 2, you will find that

$$\Delta X(t) = \frac{\hbar}{\Delta p}\left[1 + \frac{(\Delta p)^4 t^2}{m^2\hbar^2}\right]^{1/2}$$

This result can be understood by considering two limits. First, for very small times, the second term is negligible + we see $\Delta x \simeq \frac{\hbar}{\Delta p}$, which is just the Heisenberg uncertainty principle. However, for large t, the uncertainty in momentum gives rise to additional uncertainty in position:

$$\Rightarrow \Delta X(t) \underset{t\to\infty}{\approx} \hbar/\Delta p \left(\cancel{1}+(\Delta p)^4 t^2/m^2\hbar^2\right)^{1/2} \approx \cancel{\hbar}/\cancel{\Delta p}\left((\Delta p)^2 t/m\cancel{\hbar}\right)$$
$$\approx \Delta p\, t/m \approx (\hbar/\Delta x)t/m$$

So, we find, for large t:

$$\Delta X(t) = 3\Delta x = \cancel{(3\hbar/\Delta p)}\, \hbar t/m\Delta x$$
$$\Longrightarrow t = 3m(\Delta x)^2/\hbar$$
$$\approx 3(9.11\times10^{-31}\,kg)(10^{-20}\,m)/1\times10^{-34}\,J\cdot s$$
$$\approx 2.7\times10^{-16}\,s$$

V. 1D Problems & Perturbation Theory:

1) Infinite Square Well $V(x) = \begin{cases} 0 & x\in[0,a] \\ \infty & \text{elsewhere}\end{cases}$

$E_n = \frac{\pi^2\hbar^2 n^2}{2ma^2}$ $\quad \psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)$

Q: Review Problem 5: $H' = \alpha\,\delta(x - a/2)$

(a) + (b) To be sufficiently small, we want: $\Delta E_n \ll E_{n+1} - E_n$

Here, this constraint is strongest when $n=1$.

First, let us calculate the first order correction to energies:

$$\Delta E_n = \langle\psi_n | H' | \psi_n\rangle = \int \psi_n^*(H'\psi_n)\,dx$$
$$= \frac{2}{a}\int_0^a dx\,\sin\left(\frac{n\pi x}{a}\right)\alpha\delta(x-a/2)\sin\left(\frac{n\pi x}{a}\right) = \frac{2\alpha}{a}\sin^2\left(\frac{n\pi}{2}\right)$$
$$= \begin{cases} 0 & \text{if } n \text{ is even} \\ \frac{2\alpha}{a} & \text{if } n \text{ is odd}\end{cases}$$

Thus, we require: $\Delta E_n \ll E_{n+1} - E_n \Rightarrow \frac{2\alpha}{a} \ll \frac{3\pi^2\hbar^2}{2ma^2} \Rightarrow \boxed{\alpha \ll \frac{3\pi^2\hbar^2}{2ma}}$

(c) In order to compute the probability that such a bump would cause a transition to the n^{th} excited state, we first review the 1^{st} order expression for the wave function: If $\{\psi_n^0\}$ are the uncorrected ones,

$$\psi_n = \psi_n^0 + \sum_{m \neq n} \frac{\langle \psi_m^0 | H' | \psi_n^0 \rangle}{(E_n^0 - E_m^0)} \psi_m^0$$

where the $\{E_m^0\}$ are the uncorrected energies. Thus, to 1^{st} order, the new eigenfunctions of the problem with a bump in the middle are the ψ_n. We can think of our problem as an initial condition for this <u>new</u> problem. Then, writing ψ_n^0 in terms of the <u>new</u> eigen$F^{\underline{n}}$s:

$$\psi_n^0 \cong \psi_n - \sum_{m \neq n} \frac{\langle \psi_m^0 | H' | \psi_n^0 \rangle}{(E_n^0 - E_m^0)} \psi_m^0$$

Where we use the fact that corrections to ψ_m^0, $m \neq n$ are second order in this expression!
Thus, the prob. of making a transition is just:

$$P(n \to m) = \left| \frac{\langle \psi_m^0 | H' | \psi_n^0 \rangle}{(E_n^0 - E_m^0)} \right|^2$$

So, for us, we have $P(1 \to m)$ is:

$$P(1 \to m) = \frac{\left| \int_0^a \frac{2}{a} dx\, \kappa\, \delta(x - a/2) \sin\left(\frac{m\pi x}{a}\right) \sin\left(\frac{\pi x}{a}\right) \right|^2}{\left| \frac{\pi^2 \hbar^2 (m^2 - 1)}{2ma^2} \right|^2}$$

$$= \begin{cases} \dfrac{\left(\frac{4\kappa^2}{a^2}\right)}{\left(\frac{\pi^2\hbar^2(m^2-1)}{2ma^2}\right)^2} & \text{if } m \text{ is odd} \\ 0 & \text{if } m \text{ is even} \end{cases}$$

2) SHO $\quad V(x) = \frac{1}{2} m\omega^2 x^2$, $\quad H = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2 = \left(a_+ a_- + \frac{\hbar\omega}{2}\right)$

$a_\pm = \frac{1}{\sqrt{2m}}(p \pm im\omega x) \quad E_n = (n + 1/2)\hbar\omega \quad \psi_n = A_n (a_+)^n e^{-\frac{m\omega}{2\hbar}x^2}$

with $A_n = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{n!(\hbar\omega)^n}} \quad \psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-(m\omega/2\hbar)x^2}$

$\psi_1(x) = (iA_1 \omega\sqrt{2m}) x e^{-\frac{m\omega}{2\hbar}x^2} \quad a_+\psi_n = \sqrt{(n+1)\hbar\omega}\, \psi_{n+1} \quad a_-\psi_n = \sqrt{n\hbar\omega}\, \psi_{n-1}$

<u>Q:</u> Review Problem 4: Use the fact that: $p = \sqrt{2m}\,(a_+ + a_-)$

Then $\langle n | p^4 | n \rangle = (2m)^2 \langle n | (a_+ + a_-)^4 | n \rangle$

Now, use the fact that $[a_+, a_-] = a_+a_- - a_-a_+ = \hbar\omega$

$\Rightarrow (a_+ + a_-)^4 = a_+^4 + a_+^3 a_- + a_+^2 a_- a_+ + a_+ a_- a_+^2 + a_- a_+^3 + a_+^2 a_-^2 + a_+ a_- a_+ a_- + a_- a_+^2 a_-$
$+ a_+ a_-^2 a_+ + a_- a_+ a_- a_+ + a_-^2 a_+^2 + a_-^3 a_+ + a_-^2 a_+ a_- + a_- a_+ a_-^2 + a_+ a_-^3 + a_-^4$

However, as only terms with the same # of a_+s as a_-s can contribute (by orthonormality: each $a_\pm$ changes n by ± 1 and to get a nonzero answer we must have no net change), we find: (using: $a_+|n\rangle = \sqrt{(n+1)\hbar\omega}\,|n+1\rangle$ $\quad a_-|n\rangle = \sqrt{n\hbar\omega}\,|n-1\rangle$)

$$\langle n|p^4|n\rangle = \langle n|(2m)^2(a_+^2a_-^2 + a_+a_-a_+a_- + a_-a_+^2a_- + a_+a_-^2a_+ + a_-a_+a_-a_+ + a_-^2a_+^2)|n\rangle$$
$$= (2m\hbar\omega)^2\left[n(n-1) + n^2 + n^{3/2}\sqrt{n+1} + (n+1)^{3/2}\sqrt{n} + (n+1)^2 + (n+1)(n+2)\right]$$
$$= (2m\hbar\omega)^2\left[4n^2 + 4n + 2 + n^{3/2}\sqrt{n+1} + (n+1)^{3/2}\sqrt{n}\right]$$
$$\Rightarrow \Delta E_n = \langle n|\frac{p^4}{8m^3c^2}|n\rangle = \frac{(2m\hbar\omega)^2}{8m^3c^2}\left[4n^2 + 4n + 2 + n^{3/2}\sqrt{n+1} + (n+1)^{3/2}\sqrt{n}\right]$$

Angular Momentum: (see Midterm Review)

Q: Review Problem 3

(a) The relativistic expression for energy is:

$$E_{nj} = \frac{-13.6\,eV}{n^2}\left[1 + \frac{\alpha^2}{n^2}\left(\frac{n}{j+1/2} - \frac{3}{4}\right)\right]$$

Thus, we have $n=2$, $j=3/2$ $\Rightarrow$ $E_{2\,3/2} = \frac{-13.6\,eV}{2^2}\left[1 + \frac{\alpha^2}{2^2}\left(\frac{2}{3/2+1/2} - \frac{3}{4}\right)\right]$

$$\Rightarrow E_{2\,3/2} = \frac{-13.6\,eV}{4}\left[1 + \left(\frac{1}{137}\right)^2\left(\frac{1}{16}\right)\right]$$

(b) We use the fact that $J_\pm = J_x \pm iJ_y$ and that:

$J_\pm|j\,m\rangle = \hbar\sqrt{j(j+1) - m(m\pm 1)}\,|j\,m\pm1\rangle$. Plugging in to this formula, we get

$$\Rightarrow J_+|3/2\,3/2\rangle = 0|3/2\,3/2\rangle + 0|3/2\,1/2\rangle + 0|3/2\,{-1/2}\rangle + 0|3/2\,{-3/2}\rangle$$
$$J_+|3/2\,1/2\rangle = \hbar\sqrt{3}\,|3/2\,3/2\rangle + \quad '' \quad '' \quad ''$$
$$J_+|3/2\,{-1/2}\rangle = 0|3/2\,3/2\rangle + \hbar 2|3/2\,1/2\rangle + \quad '' \quad ''$$
$$J_+|3/2\,{-3/2}\rangle = 0|3/2\,3/2\rangle + 0|3/2\,1/2\rangle + \hbar\sqrt{3}\,|3/2\,{-1/2}\rangle + 0|3/2\,{-3/2}\rangle$$

The matrix for J_+ is easily read off from the above data, as it is just the transpose of the matrix of coefficients above!

$$J_+ = \hbar\begin{pmatrix} 0 & \sqrt{3} & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & \sqrt{3} \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad \text{Similarly, we find} \quad J_- = \hbar\begin{pmatrix} 0 & 0 & 0 & 0 \\ \sqrt{3} & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & \sqrt{3} & 0 \end{pmatrix}$$

Then, as $J_x = \frac{1}{2}(J_+ + J_-)$, $J_y = \frac{1}{2i}(J_+ - J_-)$, we get:

$$J_x = \hbar\begin{pmatrix} 0 & \sqrt{3}/2 & 0 & 0 \\ \sqrt{3}/2 & 0 & 1 & 0 \\ 0 & 1 & 0 & \sqrt{3}/2 \\ 0 & 0 & \sqrt{3}/2 & 0 \end{pmatrix} \qquad J_y = \hbar\begin{pmatrix} 0 & -i\sqrt{3}/2 & 0 & 0 \\ i\sqrt{3}/2 & 0 & -i & 0 \\ 0 & i & 0 & -i\sqrt{3}/2 \\ 0 & 0 & i\sqrt{3}/2 & 0 \end{pmatrix}$$

Since we are using a basis where:

$$|3/2\,3/2\rangle \longleftrightarrow \begin{pmatrix}1\\0\\0\\0\end{pmatrix}, \quad |3/2\,1/2\rangle \longleftrightarrow \begin{pmatrix}0\\1\\0\\0\end{pmatrix}, \quad |3/2\,{-1/2}\rangle \longleftrightarrow \begin{pmatrix}0\\0\\1\\0\end{pmatrix}, \quad |3/2\,{-3/2}\rangle \longleftrightarrow \begin{pmatrix}0\\0\\0\\1\end{pmatrix}$$

$J_z = \hbar\begin{pmatrix} 3/2 & 0 & 0 & 0 \\ 0 & 1/2 & 0 & 0 \\ 0 & 0 & -1/2 & 0 \\ 0 & 0 & 0 & -3/2 \end{pmatrix}$ is the obvious diagonal matrix.

(c) $$\langle J_x\rangle = (0\,1\,0\,0)\begin{pmatrix} 0 & \hbar\sqrt{3}/2 & 0 & 0 \\ \hbar\sqrt{3}/2 & 0 & \hbar & 0 \\ 0 & \hbar & 0 & \hbar\sqrt{3}/2 \\ 0 & 0 & \hbar\sqrt{3}/2 & 0 \end{pmatrix}\begin{pmatrix}0\\1\\0\\0\end{pmatrix} = 0$$

$$\langle J_y\rangle = (0\,1\,0\,0)\begin{pmatrix} 0 & -i\hbar\sqrt{3}/2 & 0 & 0 \\ i\hbar\sqrt{3}/2 & 0 & -i\hbar & 0 \\ 0 & i\hbar & 0 & -i\hbar\sqrt{3}/2 \\ 0 & 0 & i\hbar\sqrt{3}/2 & 0 \end{pmatrix}\begin{pmatrix}0\\1\\0\\0\end{pmatrix} = 0$$

Addendum:

I. Solution to Review Problem 1:

(a) If we consider small k, i.e. $ka \ll 1$, then ~~cos ka ≈ 1+~~ $\cos(ka) \approx 1 - \frac{1}{2}(ka)^2$, and we have:

$$\omega^2 \approx \left(\frac{K+G}{M}\right) \pm \left(\frac{K+G}{M}\right)\sqrt{1 + \frac{2KG}{(K+G)^2}(\cos ka - 1)}$$
$$\approx \left(\frac{K+G}{M}\right) \pm \left(\frac{K+G}{M}\right)\sqrt{1 - \frac{KG}{(K+G)^2}(ka)^2}$$
$$\approx \left(\frac{K+G}{M}\right) \pm \left(\frac{K+G}{M}\right)\left(1 - \frac{1}{2}\frac{KG}{(K+G)^2}(ka)^2\right)$$

Thus, we have

$$+ \quad \omega^2 \approx \frac{2(K+G)}{M} - \frac{1}{2}\frac{KG}{M(K+G)}(ka)^2 \Rightarrow \omega \approx \sqrt{\frac{2(K+G)}{M}} + O((ka)^2)$$
$$- \quad \omega^2 \approx \frac{1}{2}\frac{KG}{M(K+G)}(ka)^2 \Rightarrow \omega \approx \left(\frac{KGa^2}{2M(K+G)}\right)k + O((ka)^2)$$

Clearly, the $-$ sign looks like an acoustic wave with a linear dispersion relation for small k! Thus, the $+$ is the optical wave, which does not have low freq. low wavelength modes!

(b) Generally, $V_g = \frac{\partial \omega}{\partial k}$, so for the acoustic branch for small k, $V_g = \frac{\partial}{\partial k}\left(\left(\frac{KGa^2}{2M(K+G)}\right)k\right) = \frac{KGa^2}{2M(K+G)} =$ speed of sound. Since $\frac{\partial^2 \omega}{\partial k^2} = \frac{\partial V_g}{\partial k} = 0$, they do <u>not</u> disperse!

(c) In the limit $K \gg G$, we have:

$$\omega^2 \approx \frac{K+G}{M} \pm \frac{K}{M}\sqrt{1 + 2\frac{G}{K}\cos(ka) + \cancel{\left(\frac{G}{K}\right)^2}^{\to 0}} \approx \frac{K+G}{M} \pm \frac{K}{M}\left(1 + \frac{G}{K}\cos(ka)\right) + O\big(\big(\tfrac{G}{K}$$

Therefore, for the optical branch, we see that.

$\omega^2 \approx \frac{2K}{M} \Rightarrow \omega = \sqrt{\frac{2K}{M}}$ This corresponds to the oscillation frequency of the diatomic molecule within the unit cell!

(d) From above, we see $\omega^2 \approx \frac{K+G}{M} - \left(\frac{K}{M} + \frac{G}{M}\cos(ka)\right)$

$$\Rightarrow \omega^2 \approx \frac{G}{M}(1 - \cos(ka)) \Rightarrow \omega = \sqrt{\frac{G}{M}}\sqrt{1-\cos(ka)} = \sqrt{\frac{G}{M}}\sqrt{2\sin^2\left(\frac{ka}{2}\right)}$$
$$\cancel{V_g = \frac{\partial \omega}{\partial k}} \Rightarrow \omega = \sqrt{\frac{2G}{M}}\left|\sin\left(\frac{ka}{2}\right)\right| \Rightarrow \frac{\partial \omega}{\partial k} = V_g = \frac{a}{2}\sqrt{\frac{2G}{M}}\left|\cos\left(\frac{ka}{2}\right)\right|$$

$V_p = \frac{\omega}{k} = \sqrt{\frac{2G}{M}}\frac{\left|\sin\left(\frac{ka}{2}\right)\right|}{k}$. Clearly, as $\frac{\partial^2 \omega}{\partial k^2} = \frac{a^2}{4}\sqrt{\frac{2G}{M}}\left|\sin\left(\frac{ka}{2}\right)\right| \neq 0$ generally, we do not expect that these waves will stay together, unless $k \to 0$. That is, they disperse except in the limit of long wavelength, which is what we expect!

II. Solution to Review Problem 2 (a)

$$\Psi(x,t) \propto \int e^{i(px - \frac{p^2}{2m}t)/\hbar} \cdot e^{-\frac{(p-p_0)^2}{2(\Delta p)^2}} dp$$

Thus, we need to "complete the square" in the exponential:

$$-\left[p^2\left(\frac{+it}{m\hbar} + \frac{1}{2(\Delta p)^2}\right) + p\left(-ix/\hbar - \frac{p_0}{(\Delta p)^2}\right) - \frac{p_0^2}{2(\Delta p)^2}\right]$$

We do this to find: (with $v_g = p_0/m$)

$$\Psi(x,t) \propto \exp\left[\frac{ip_0 x/\hbar - (\Delta p/\hbar)^2 x^2/2 + ip_0^2 t/2m\hbar}{1 + i(\Delta p)^2 t/m\hbar}\right]\left(\int e^{-(p+\cdots)^2}\right)$$

all we care about

we can ignore this!

This is just a const. out front

Thus, $P(x,t) = |\Psi(x,t)|^2 \propto \exp\left[-\frac{(\Delta p/\hbar)^2(x - v_g t)^2}{1 + (\Delta p)^4 t^2/m^2\hbar^2}\right]$

This will go to $1/e$ exactly when x differs from $v_g t$ by:

$$\Delta x(t) = \frac{\hbar}{\Delta p}\left[1 + \frac{(\Delta p)^4 t^2}{m^2\hbar^2}\right]^{1/2}$$