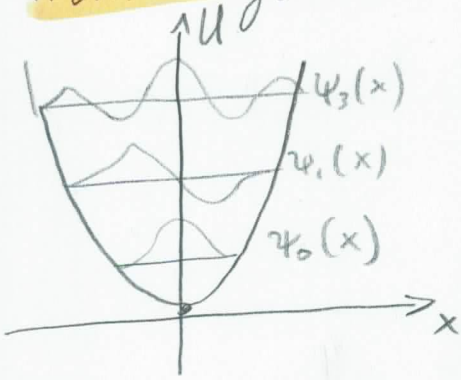
Selection Rules on the example of $\bar{e}$ in harmonic potential

1) Show that the eigenfunctions of the harmonic oscillator are "symmetric" or "antisymmetric" from general principles.



Write down the Hamiltonian:

$$H(x) = -\frac{\hbar^2 d^2}{dx^2} + V(x)$$

and time-independent Schrödinger equation

$$\left(-\hbar^2 \frac{d^2}{dx^2} + V(x)\right)\Psi_n(x) = E_n \Psi_n(x)$$

Note that the Hamiltonian is invariant under: $x \to -x$

$\Rightarrow \quad H(x)\,\Psi_n(x) = E_n \Psi_n(x) \quad \Rightarrow \quad H(-x)\,\Psi_n(-x) = E_n \Psi_n(-x)$

$\Rightarrow \quad H(x)\,\Psi_n(-x) = E_n \Psi_n(-x)$

We see that $\Psi_n(x)$ and $\Psi_n(-x)$ are both eigenfunctions with the same eigenvalue E_n $\Rightarrow$ (if spectrum is not degenerate)

$$\Psi_n(x) = \alpha \underbrace{\Psi(-x)}_{\Psi(-x) = \alpha\Psi(x)} \quad \text{where } \alpha \text{ is a constant}$$

$\Rightarrow$

$$\Psi_n(x) = \alpha^2 \Psi_n(x) \quad \Rightarrow \quad \alpha = \pm 1 \quad \Psi(x) = \pm \Psi(-x)$$

From that it follows that eigenfunctions are symmetric or antisymmetric

From the solution we now that

$\Psi_n(x)$ $\quad n = 0, 2, \dots, 2k, \dots$ are even or symmetric

$\Psi_n(x)$ $\quad n = 1, 3, \dots, 2k+1, \dots$ are odd or antisymmetric

Also functions $\Psi(x) = +\Psi(-x)$ are called to have positive parity and $\Psi(x) = -\Psi(-x)$ have negative parity

2) $\bar{e}$ is interacting with electric oscillating field. What transitions can be excited? (selection rules)

If one has the ext. electric field $\vec{E} = \vec{E}_0 \cos\omega t$ than its interaction with $\bar{e}$ is descibed by Hamiltonian: $\hat{H}_{int} = \vec{d} \cdot \vec{E}$ where $\vec{d} = \vec{r} \cdot e$ - is dipole moment of $\bar{e}$

Transitions are only allowed if $\langle \psi_i | \hat{H}_{int} | \psi_f \rangle \neq 0$ and other way around $\Rightarrow$ selection rules

Consider: $\langle \psi_m | \hat{H}_{int} | \psi_n \rangle = \int dx\, \psi_m^*(x)\, e \cdot x E \psi_n(x) =$

$= e E_0 \cos\omega t \int dx\, \psi_m^*(x)\, x\, \psi_n(x)$

if $\psi_m(x)$ an $\psi_n(x)$ have the same parity than

$\int dx\, \psi_m^*(x) x \psi_n(x) = 0$ $\rightarrow$ transitions are forbiden

↗ from integration rules

So $\bar{e}$ can be excited from ground state to 1st excited state but not to 2d excited state

Can $\bar{e}$ be excited from $n=0$ to $n=3$?

To answer consider more precise form of $\psi_n(x)$

$\hat{x} = \sqrt{2} x_0 (b + b^+)$ with $x_0 = \sqrt{\frac{\hbar}{m\omega}}$

$\Rightarrow \int dx\, \psi_m(x)\, x\, \psi_n(x) \propto \langle \psi_m | b + b^+ | \psi_n \rangle$

One can use properties of b, b^+: $b^+ |\psi_n\rangle = \sqrt{n+1} |\psi_{n+1}\rangle$
$b |\psi_n\rangle = \sqrt{n} |\psi_{n-1}\rangle$
and $\langle \psi_m | \psi_n \rangle = \delta_{mn}$

$\Rightarrow \langle \psi_m | b + b^+ | \psi_n \rangle = \langle \psi_m | \psi_{n-1} \rangle \sqrt{n} +$
$+ \sqrt{n+1} \langle \psi_m | \psi_{n+1} \rangle = \sqrt{n}\, \delta_{m(n-1)} + \sqrt{n+1}\, \delta_{m(n+1)}$

$\Rightarrow$ follows that transitions are allowed only when $m = n \pm 1$. So excitation from $n=0$ to $n=3$ is not allowed

3) Relation to classical physics

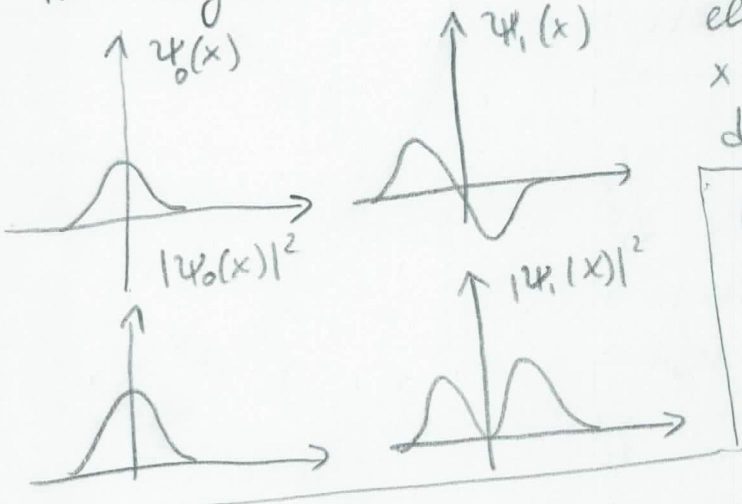
From selection rules we know that $\bar{e}$ can absorb and emitt photons only for allowed transition. How to understand it from the point of view of classical physics.

Consider radiation from $\bar{e}$.

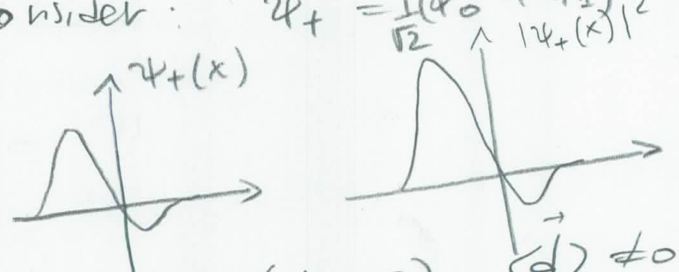
Since $\bar{e}$ has dipole moment $\vec{d}$ it can radiate e/m waves according to electrodynamics (Maxwell equations) ($\vec{d}$ should be time dependent)

Average value of $\vec{d} = \vec{x} \cdot e$: $\propto \langle \psi_n | x | \psi_n \rangle = 0$ for any n.

It can be explained that electron density is symmetric around $x = 0$ for any eigenstate due to symmetry.



Consider: $\psi_+ = \frac{1}{\sqrt{2}}(\psi_0 + \psi_1)$



the electron density is not symmetric $\Rightarrow$ $\langle \vec{d} \rangle \neq 0$

Indeed from QM $\langle \psi_+ | \vec{d} | \psi_+ \rangle = \frac{1}{2} \left(\langle \psi_0 | x | \psi_1 \rangle + c.c. \right)$, $\langle \psi_0 | x | \psi_1 \rangle \neq 0$

What is time-dependence of $\langle \vec{d}(t) \rangle$?

$$\langle \vec{d}(t) \rangle = \langle \psi_+(t) | \vec{d} | \psi_+(t) \rangle = \frac{1}{2} \left(\langle \psi_0 | e^{\frac{iE_0 t}{\hbar}} + \langle \psi_1 | e^{\frac{iE_1 t}{\hbar}} \right) \hat{d} \left(|\psi_0\rangle e^{-i\frac{E_0}{\hbar}t} + |\psi_1\rangle e^{-\frac{iE_1}{\hbar}t} \right) = \frac{1}{2} \left(e \langle \psi_0 | x | \psi_1 \rangle e^{i\omega t} + c.c. \right)$$

Here $\omega = \frac{E_1 - E_0}{\hbar}$

It follows that dipole moment oscillates with the frequency of the allowed transition. According to Maxwell equations $\bar{e}$ will radiate e/m waves with the frequency of transition.