Special 221A Lecture Notes
by
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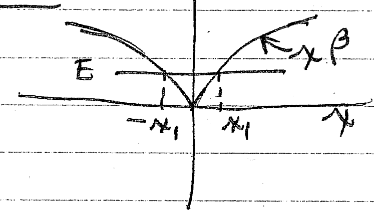
BOHR'S CORRESPONDENCE PRINCIPLE AND SOME WKB SCRAPS

Here are some added goodies about WKB and a topic often neglected, <u>Bohr's Correspondence Principle</u> about energy levels at high excitation and radiative transitions between them.

First, the WKB Scraps.

<u>Example of WKB quantization with a power law potential</u>



Assume $V(x) = V_0|x/a|^\beta$

Rule is $$2\int_0^{x_1}\sqrt{\frac{2mE}{\hbar^2}\left(1-\frac{V_0}{E}|x/a|^\beta\right)}\,dx = (n+\tfrac{1}{2})\pi$$

Put $\frac{V_0}{E}\left|\frac{x}{a}\right|^\beta = t$ $\quad\therefore\quad x = \left(\frac{E}{V_0}\right)^{\frac{1}{\beta}} a\, t^{\frac{1}{\beta}}$

$$dx = \frac{a}{\beta}\left(\frac{E}{V_0}\right)^{\frac{1}{\beta}} t^{\frac{1}{\beta}-1}\,dt$$

Then we have $$I = \frac{2a}{\beta}\left(\frac{E}{V_0}\right)^{\frac{1}{\beta}}\sqrt{\frac{2mE}{\hbar^2}}\int_0^1\sqrt{1-t}\;t^{\frac{1}{\beta}-1}\,dt \longrightarrow \frac{\Gamma\left(\frac{3}{2}\right)\Gamma\left(\frac{1}{\beta}\right)}{\Gamma\left(\frac{1}{\beta}+\frac{3}{2}\right)}$$

$$(n+\tfrac{1}{2})\pi = I = \frac{2}{\beta}\left(\frac{E}{V_0}\right)^{\frac{1}{\beta}+\frac{1}{2}}\sqrt{\frac{2mV_0a^2}{\hbar^2}}\times\left[\frac{1}{2}\frac{\sqrt{\pi}\,\Gamma\left(\frac{1}{\beta}\right)}{\Gamma\left(\frac{1}{\beta}+\frac{3}{2}\right)}\right]$$

We thus see that $$E_n \propto (n+\tfrac{1}{2})^{\frac{2\beta}{\beta+2}}$$

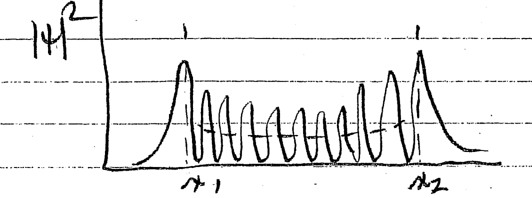
$\beta = 2 \qquad E_n \propto (n+\frac{1}{2}) \qquad$ (SHO)

$\beta = -1 \qquad E_n \propto n^{-2} \qquad$ (Coulomb)

$\lim_{\beta\to\infty} \; E_n \propto n^2 \qquad$ (Particle in a box)

Normalization of WKB Wave Functions

For $n \gg 1$, the probability density looks like



$$\psi_{WKB} = \frac{A_n}{\sqrt{k(x)}} \cos\left(\xi_1 - \frac{\pi}{4}\right) \quad \text{for } x_1 + \delta < x < x_2 - \delta$$

Normalization:

$$\frac{1}{|A_n|^2} = \int_{x_1+\delta}^{x_2-\delta} \frac{\cos^2}{k(x)}\, dx + \text{contributions from near \& beyond classical turning points.}$$

W. H. Furry, "Two Notes on Phase-Integral Methods," Phys. Rev. 71, 360-371 (1947)

Furry showed that (for a single minimum) normalization is given accurately by putting $\cos^2(\ ) = \frac{1}{2}$, integrating from $x_1 \to x_2$, and neglecting the other pieces. i.e.

$$\frac{1}{|A_n|^2} = \frac{1}{2}\int_{x_1}^{x_2} \frac{dx}{k(x)}$$

This has an obvious interpretation: $\displaystyle\int_{x_1}^{x_2} \frac{dx}{k(x)} = \frac{\hbar}{m}\int_{x_1}^{x_2} \frac{dx}{v(x)} = \frac{\hbar\, \tau_{classical}}{2m}$

where $\tau_{classical}$ is the classical period of the motion.

Thus $\quad |A_n|^2 = \dfrac{4m}{\hbar \tau_{cl}} = \dfrac{2m}{\pi\hbar}\, \omega_{classical}$

In the classically allowed region, the average (over $\frac{1}{2}$ wavelength) probability density is

$$\rho_{WKB}(x)\, dx = \frac{1}{2}\frac{|A_n|^2 dx}{k(x)} = \frac{2m}{\hbar k(x)}\frac{dx}{\tau} = \frac{2}{\tau}\, dt$$

This is just the normalized classical probability.

Bohr's Correspondence Principle and Classical Motion

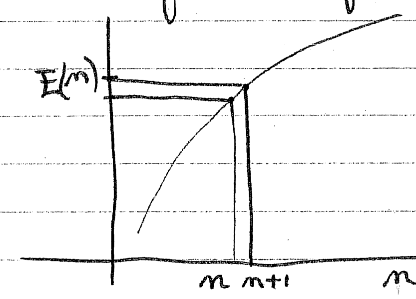
Bohr's correspondence principle states that in some sense the limit of large quantum numbers corresponds to classical physics, and conversely, characteristics that emerge as black & white at the classical level, eg. a symmetry property or special aspect of the motion, will manifest itself as selection rules at the quantum level. The principle is a powerful tool in the understanding of quantum properties.

(1) Energy level spacings and the classical frequency of motion

A key aspect is the behavior of energy levels for large n and the relation to classical motion. The WKB quantization condition is an ideal vehicle for exploring the connection. We have

$$\int_{x_1(E)}^{x_2(E)} \sqrt{\frac{2m}{\hbar^2}\left(E - V(x)\right)}\, dx = \left(n + \tfrac{1}{2}\right)\pi$$

We can think of n as a continuous variable. Then this equation defines $E = E(n)$. Evidently the energy level spacing is given by $E_{n+1} - E_n \cong \frac{dE}{dn}(E_n)$



We can compute $\frac{dE}{dn}$ by differentiating the LHS and RHS above. Since LHS is only a function of E (and m and $\hbar$) we have

$$\frac{d}{dn}(\text{LHS}) = \frac{dE}{dn}\frac{d}{dE}\int_{x_1(E)}^{x_2(E)} \sqrt{\frac{2m}{\hbar^2}(E - V)}\, dx$$

$$= \frac{dE}{dn}\cdot\left\{\frac{2m}{\hbar^2}\times\frac{1}{2}\int_{x_1}^{x_2}\frac{dx}{k(x)} + \underbrace{k(x)\Big|_{x_2}\frac{dx_2}{dE} - k(x)\Big|_{x_1}\frac{dx_1}{dE}}_{=0 \text{ since } k(x_{1,2}) = 0}\right\}$$

But we showed that (on page 2)

$$\int_{x_1}^{x_2}\frac{dx}{k(x)} = \frac{\hbar\tau_{cl}}{2m}$$

Thus

$$\left.\begin{aligned} \frac{d}{dn}(\text{LHS}) &= \frac{\tau_{cl}}{2\hbar}\cdot\frac{dE}{dn} \\ \text{Also } \frac{d}{dn}(\text{RHS}) &= \pi. \end{aligned}\right\}$$

Thus $\boxed{\dfrac{dE}{dn} = \dfrac{2\pi}{\tau_{cl}}\hbar = \hbar\omega_{\text{classical}}}$

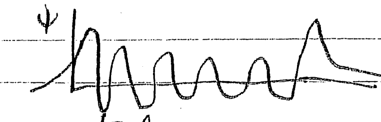
We have thus established the theorem that

In the limit of large quantum numbers, the spacing between adjacent energy levels is equal to $\hbar\omega_{\text{classical}}$, where $\omega_{cl} = 2\pi/\tau_{cl}$ is the classical frequency of the motion at that (average) energy.

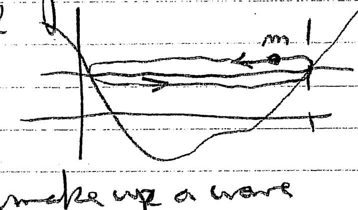
(2) Classical particle motion versus Schrodinger wave function description

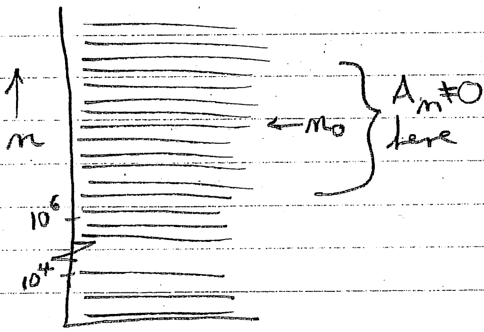
When we speak of energy eigenstates we focus on each state separately and consider

$$\psi_n(x,t) = \psi_n(x)\, e^{-iE_n t/\hbar}$$



It is then not easy to see a connection with a particle oscillating back & forth in a classical potential well.





We choose to make up a wave packet to describe as much as we can the classical particle:

$$\psi(x,t) = \sum_n A_n \psi_n(x)\, e^{-iE_n t/\hbar}$$

We center the expansion on $n = n_0$ and write $n = n_0 + m$

We assume that n_0 is large enough that $1 \ll |m_{max}| \ll n_0$

e.g. $n_0 = 10^6$, $|m_{max}| = 10^3$. (It will work approx. for $n_0 = 10$, $|m|_{max} = 3$)

Then we have $\psi(x,t) = \sum_m A_m \psi_{n_0+m}(x)\, e^{-iE_{n_0+m}t/\hbar}$

Multiply both sides by $e^{iE_{n_0}t/\hbar}$. Then we have

$$e^{iE_{n_0}t/\hbar}\psi(x,t) = \sum_m A_m \psi_{n_0+m}(x)\, e^{-i(E_{n_0+m}-E_{n_0})t/\hbar}.$$

Now we can expand $E_{n_0+m} - E_{n_0} = 0 + \underbrace{\frac{dE}{dn}(E_{n_0})}_{\hbar\omega_{classical}} m + \underbrace{\frac{1}{2}\frac{d^2E}{dn^2} m^2 + \cdots}_{\text{assume these are negligible}}$

Keeping only the first term, we have

$$e^{iE_{n_0}t/\hbar}\psi(x,t) = \sum_m A_m \psi_{n_0+m}(x)\, e^{-im\omega_{cl}t}$$

We pick the A_m to form a localized wave packet at, say $x = x_1$, at $t = 0$. The structure of the wave function shows that

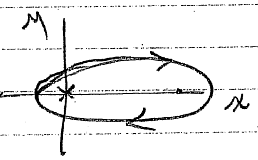
$e^{iE_{n_0}t/\hbar}\psi(x,t)$ is periodic with the classical period τ_{cl}.

It will thus represent the classical motion of a particle oscillating back and forth.

(3) <u>Selection Rules for Radiative Transitions</u>

Classically, an accelerated particle radiates. In the simplest circumstance, when a particle executes <u>sinusoidal</u> periodic motion, it radiates only at the basic frequency of the motion ie $\omega = \omega_{cl}$. The situation is different if (a) the motion is relativistic, or (b) the motion is periodic, but not sinusoidal.

For example, an electron in a classical elliptic orbit has coordinates that can be expanded in Fourier series:



$$x(t) = \sum_m X_m(\epsilon)\, e^{im\omega_{cl} t}$$

$$y(t) = \sum_m Y_m(\epsilon)\, e^{im\omega_{cl} t}$$

where the coefficients depend on the eccentricity of the orbit and the energy. In general, <u>dipole radiation</u> will be emitted at the fundamental frequency ω_{cl} <u>and multiples of ω_{cl}</u>. [See Jackson, Problem 14.22] Only for a circular orbit will there be just the fundamental (because then there is only one $|m|$ value in each series). } See p. 6

Bohr's correspondence principle relates the classical occurrence of radiation to radiative <u>transitions</u> in the quantum system.

Recall (a) Bohr's frequency condition $\hbar\omega_{rad} = E_n - E_{n'}$

(b) At high excitation, level spacing is $\Delta E = \hbar\omega_{cl}$.

$\therefore$ Transitions with $\Delta E = m\hbar\omega_{cl}$ will emit radiation with frequency $m\omega_{cl}$. The correspondence principle states that the intensity of radiation at $\omega = m\omega_{cl}$ in the classical motion will, at high quantum numbers, be equal to the quantum intensity for a transition, $E_n \to E_{n'}$, where $E_n - E_{n'} = m\hbar\omega_{cl}$.

$\Delta l = \pm 1$ selection rule emerges from action-angle description. Circular orbit versus elliptic orbit — see p. 6. Correspondence works down to $n \sim 5$ or less.

For a numerical example, see Jackson, Problem 14.21.

Dipole radiation with multiples of classical frequency:

Larmor's power formula:

$$P = \frac{2}{3}\frac{e^2}{c^3}|\ddot{\vec{x}}|^2$$

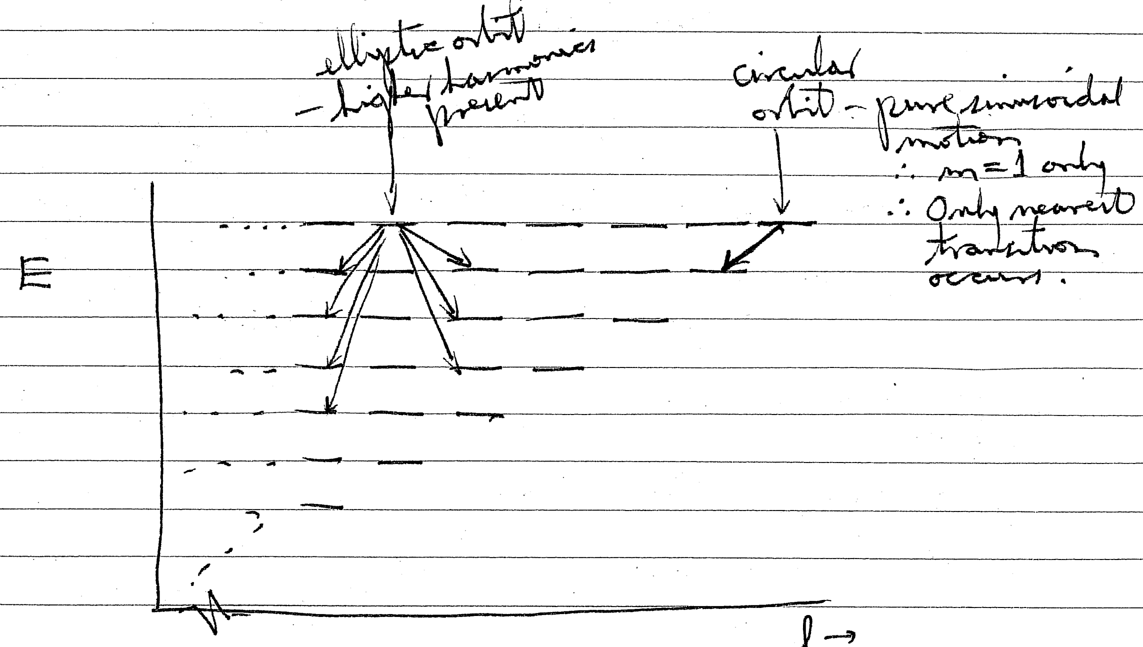
If $x(t) = \sum_m d_m \cos(m\omega_0 t + \alpha_m)$

$$\ddot{x} = \sum_m d_m(-m^2\omega_0^2)\cos(\quad)$$

Time-averaged power is $P = \sum_m P_m$

where $P_m = \frac{1}{3}\frac{e^2}{c^2}(m\omega_0)^4 d_m^2$ (radiation at frequency $\omega = m\omega_0$)

Transitions versus Fourier composition of classical motion — "hydrogen" energy levels



In 1918-1919, H.A. Kramers' Ph.D. thesis (under Niels Bohr) was on the intensities of the Stark effect, using old Bohr-Sommerfeld theory and the correspondence principle. Good agreement with experiment.