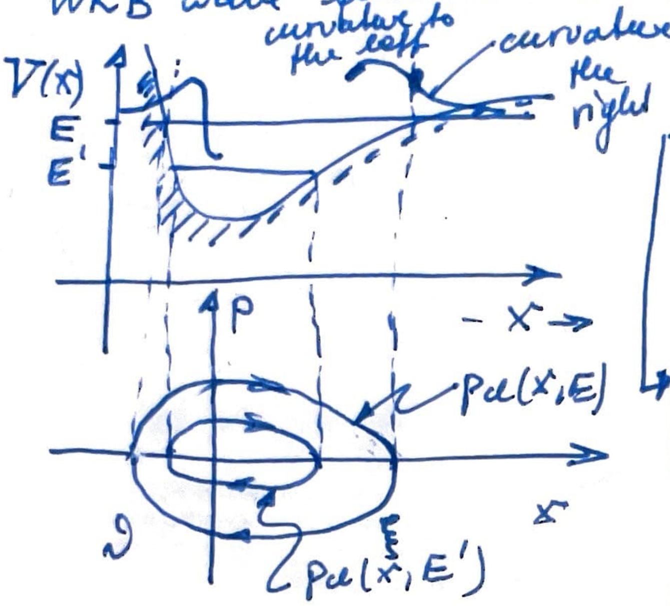
Interference in phase space

WKB wave function in one dimension



classical Hamiltonian: depends on E as paramet

$$H \equiv \frac{p^2}{2M} + V(x) \equiv E$$

$$p(x) = \pm\sqrt{2M[E-V(x)]} \equiv \pm p_{cl}(x,E)$$

multiplication by $u \equiv u(x)$ and replacement of p by $\hat{p} = \frac{\hbar}{i}\frac{d}{dx}$

$$\left[-\frac{\hbar^2}{2M}\frac{d^2}{dx^2} + V(x)\right]u(x) = E\,u(x)$$

$$\frac{d^2}{dx^2}u(x) + \frac{p_{cl}^2(x)}{\hbar^2}u(x) = 0$$

$$u''(x) + k^2(x)u(x) = 0$$

$$k = \frac{p_{cl}}{\hbar}$$

analogous to Newton equation of harmonic oscillator with time dependent frequency;

Schrödinger equation ≡ boundary value problem

Newton equation ≡ initial value problem

at the turning points ξ and ϑ we have $V(\vartheta) = V(\xi) = E$

and thus $p_{cl}(\xi, E) = p_{cl}(\vartheta, E) = 0$; $\Rightarrow u''(\xi) = u''(\vartheta) = 0$

wave function changes the sign of the curvature

classical picture of energy eigenstate: energy is known

but not phase ≡ microcanonical ensemble

if k is constant k_0 $u^{(W)}(x) = N\cos(k_0 x - \alpha) = N\cos\left[\int^{\xi} dx' k_0 - \alpha\right]$

if k is slowly varying $u^{(W)}(x) = N\cos\left[\int_x^{\xi} dx\, k(x) - \alpha\right]$

differential equation for $u^{(W)}$:

$$(u^{(W)})'' + \left\{k^2 - k'\tan\left[\int_x^{\xi} dx'\, k(x') - \alpha\right]\right\} u^{(W)}(x) = 0;$$

Born interpretation: $W(x)dx = |u(x)|^2 dx$

probability density $W(x) = \frac{N}{k(x)}$ $\Rightarrow u^{(P)}(x) = \frac{N}{\sqrt{k(x)}} = N k^{-1/2}(x) = N e^{-\frac{1}{2}\ln k}$

differential equation for $u^{(P)}$: $(u^{(P)})'' + \left[\frac{1}{2}(\ln k)'' - \left(\frac{1}{2}\ln k'\right)^2\right] u^{(P)} = 0$

ansatz : particle + wave

$$u^{(WKB)}(x) = u^{(P)} \cdot u^{(W)} = \frac{N}{\sqrt{k(x)}} \cos\left[\int_x^{\xi} dx' k(x') - \alpha\right]$$

differential equation for $u^{(WKB)}$:

$$\underline{\left(u^{(WKB)}\right)''} + \left[k^2 - \underbrace{\left(k^{-1/2}\right)'' k^{1/2}}_{\approx 0}\right] \underline{u^{(WKB)}} = 0$$

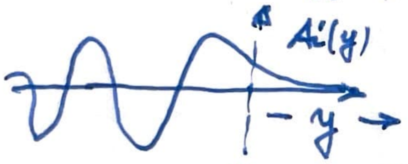
translates into slowly varying potential in first and second derivatives

≈ 0 except at the turning points

determination of α : expand potential around a turning point $V(x) = V(\xi) + V'(\xi)(x-\xi) + \ldots$

$$u'' - \frac{2m}{\hbar^2} V'(\xi)(x-\xi) u = 0$$

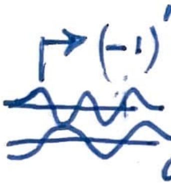
differential equation of Airy function



$$\Rightarrow \underline{\alpha = \frac{\pi}{4}}$$

energy quantization: expand around both turning points ≡ wave function at a given point should be the same

$$(-1)^m \cos\left[\int_{\vartheta}^{x} dx' k(x') - \frac{\pi}{4}\right] = \cos\left[\int_x^{\xi} dx' k(x') - \frac{\pi}{4}\right]$$



$$\cos\left[\int_{\vartheta}^{x} dx' k(x') - \frac{\pi}{4} - m\pi\right] - \cos\left[\int_x^{\xi} dx' k(x') - \frac{\pi}{4}\right] = 0$$

we recall : $\underset{=0}{\cos}\, \gamma - \cos\beta = 2 \sin\left(\frac{\gamma+\beta}{2}\right) \sin\left(\frac{\beta-\gamma}{2}\right)$

$$2 \underbrace{\sin\left\{\frac{1}{2}\left[\int_{\vartheta}^{\xi} dx\, k(x) - m\pi - \frac{\pi}{2}\right]\right\}}_{\text{has to vanish}} \sin\left\{\frac{1}{2}\underbrace{\left[\int_x^{\xi} dx' k(x') - \int_{\vartheta}^{x} dx' k(x')\right]}_{\text{depends on } x}\right\} = 0$$

$$\underline{\int_{\vartheta}^{\xi} dx\, k(x') = \pi\left(m + \frac{1}{2}\right)} \qquad \underline{2\int_{\vartheta}^{\xi} dx\, p_{cl}(x, E) = 2\pi\hbar\left(m + \frac{1}{2}\right)}$$

↓ sum of phase shifts

normalization:

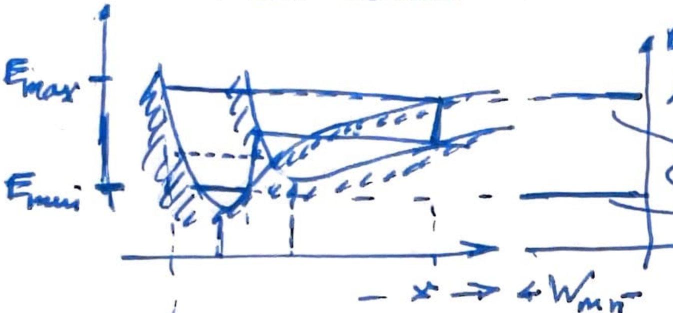
$$W(x) = \left(u^{(WKB)}\right)^2 = \frac{N^2}{k} \cos^2 \int \ldots$$

↓ oscillation never goes away

$$1 = \int_{\vartheta}^{\xi} dx\, W(x) = N^2 \int_{\vartheta}^{\xi} dx \frac{1}{k} \underbrace{\cos^2 \int \ldots}_{1/2} = \hbar N^2 \frac{1}{2} \int_{\vartheta}^{\xi} dx \frac{1}{\hbar k} = \hbar N^2 \frac{1}{2} \int \frac{dx}{p_{cl}}$$

$$= \hbar N^2 \frac{1}{2} \int_{\vartheta}^{\xi} dx \frac{1}{M \frac{dx}{dt}} = \hbar N^2 \frac{1}{M} \frac{1}{4} T \Rightarrow \underline{N = 2\sqrt{\frac{M}{\hbar T}}}$$

scalar product between two shifted potentials ≡
Franck - Condon transitions ≡ sudden approximation



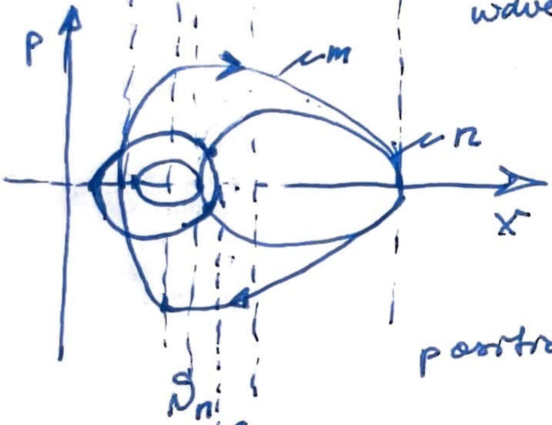
transitions occur at the classical turning points

two maxima in the transition probability

$$W_{mn} \equiv \left| \int_{-\infty}^{\infty} dx\, u_m(x) \cdot v_n(x) \right|^2$$

↑ wave function of right potential

↑ wave function of left potential



phase space trajectories of energy states of different potentials touch each other;
there exist also m states where the trajectory crosses in two symmetrically positions

$$W_{mn} \equiv \int_{-\infty}^{\infty} dx\, u_m(x) \cdot v_n(x) \cong \int_{\vartheta_n}^{\xi_m} dx\, u_m^{(WKB)} \cdot v_n^{(WKB)}$$

$$= \frac{1}{4} N_m N_n \int_{\vartheta_n}^{\xi_m} dx \frac{1}{\sqrt{k_m(x) k_n(x)}} \left(e^{i\Theta_m} + e^{i\Theta_m} \right)\left(e^{i\Theta_n} + e^{-i\Theta_n} \right)$$

$$\underline{\Theta_m(x) \equiv \int_x^{\xi_m} dx' k_m(x') - \frac{\pi}{4}} \qquad \underline{\Theta_n(x) \equiv \int_{\vartheta_n}^{x} dx' k_n(x') - \frac{\pi}{4}}$$

$$W_{mn} = \frac{1}{4} N_m N_n \int_{\vartheta_n}^{\xi_m} dx \frac{1}{\sqrt{k_m(x) k_n(x)}} \left[e^{i(\Theta_m + \Theta_n)} + e^{i(\Theta_m - \Theta_n)} + c.c. \right]$$

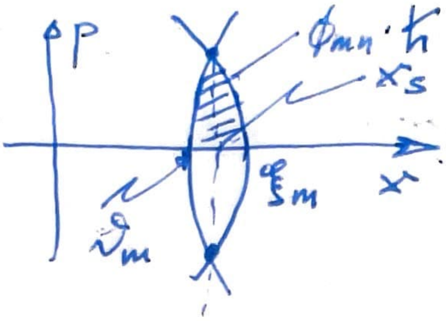
method of stationary phase

$$\Theta_m \pm \Theta_n = (\Theta_m \pm \Theta_n)\big|_{x_s} + (\Theta_m \pm \Theta_n)'\big|_{x_s} + \frac{1}{2}(\Theta_m \pm \Theta_n)''\big|_{x_s} (x - x_s)^2 + \ldots$$

$$(\Theta_m \pm \Theta_n)' = \left[\int_x^{\xi_m} dx' k_m(x') \pm \int_{\vartheta_n}^{x} dx' k_n(x')\right]' = -k_m(x_s) \pm k_n(x_s) = 0$$

only "+" sign satisfies equation. point of stationary phase x_s appears where $k_m(x_s) = k_n(x_s)$, or

$$\underline{\hbar k_m(x_s) = \hbar k_n(x_s)}$$



$$(\theta_m + \theta_n)\Big|_{x_s} = $$

$$\phi_{mn} \equiv \int_{\vartheta_n}^{x_s} dx\, k_n(x) + \int_{x_s}^{\xi_m} dx\, \underset{m}{k}(x)$$

$$= \frac{1}{\hbar}\int_{\vartheta_n}^{x_s} dx\, p_n(x) + \frac{1}{\hbar}\int_{x_s}^{\xi_m} dx\, p_m(x)$$

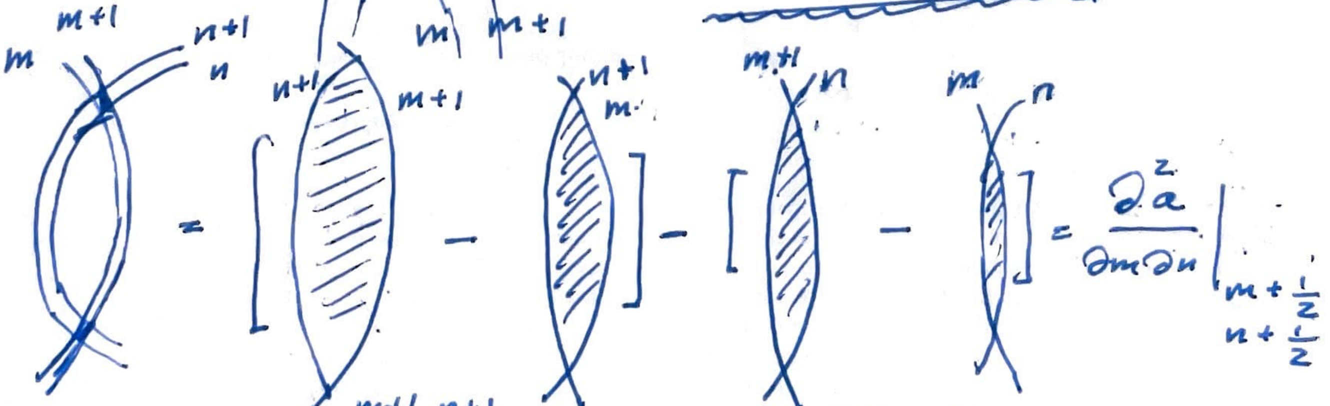
$$w_{mn} \simeq \frac{1}{4}\frac{N_m N_n}{k_m(x_s)} e^{i\phi_{mn}} \underbrace{\int_{\vartheta_n\to-\infty}^{\xi_m\to+\infty} dx\, \exp\left[-i\frac{1}{2}(k_m' - k_n')\Big|_{x_s}(x-x_s)\right]}_{\sqrt{\frac{2\pi}{i(k_m'-k_n')}}} + c.c.$$

$$w_{mn} = a_{mn}\, e^{i(\phi_{mn}-\frac{\pi}{4})} + a_{mn}\, e^{-i\left[\phi_{mn}-\frac{\pi}{4}\right]}$$

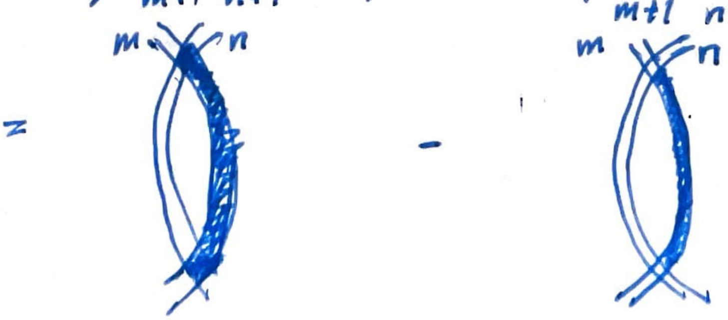
$$a_{mn} \equiv \frac{M}{\sqrt{T_m T_n}} \frac{\sqrt{2\pi\hbar}}{p_m(x_s)} \sqrt{\frac{1}{(p_m' - p_n')\big|_{x_s}}}$$

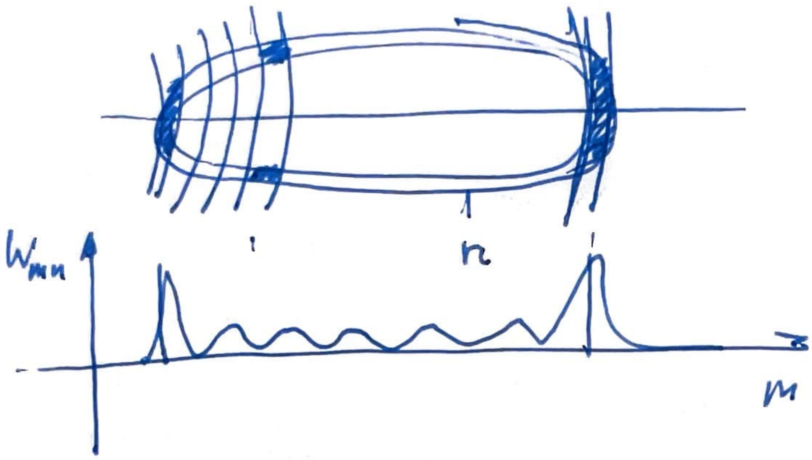
interpretation of Amn as area in phase space

$$\sqrt{\frac{A_{mn}}{2\pi\hbar}} = a_{mn}$$



$$\frac{\partial^2 a}{\partial m\,\partial n}\Big|_{\substack{m+\frac{1}{2}\\ n+\frac{1}{2}}}$$





$$w_{mn} \overset{\sim}{=} \sqrt{\frac{A_{mn}}{2\pi\hbar}}\, e^{i(\phi_{mn}-\frac{\pi}{4})} + \sqrt{\frac{A_{mn}}{2\pi\hbar}}\, e^{-i(\phi_{mn}-\frac{\pi}{4})}.$$

References:

- W.P. Schleich, Quantum Optics in Phase Space, (Wiley-VCH, Weinheim, 2001) Chapters 5, 7, 8 and Appendix I
- W.P. Schleich and J.A. Wheeler, Nature 326, 574-577 1987
- J.P. Dowling, W.P. Schleich and J.A. Wheeler, Ann. Phys. (Leipzig) 48, 423-502 (1991).