Unexpected Quantum Bound States In Open Potentials

Variational Tests and Classical Periodic Paths

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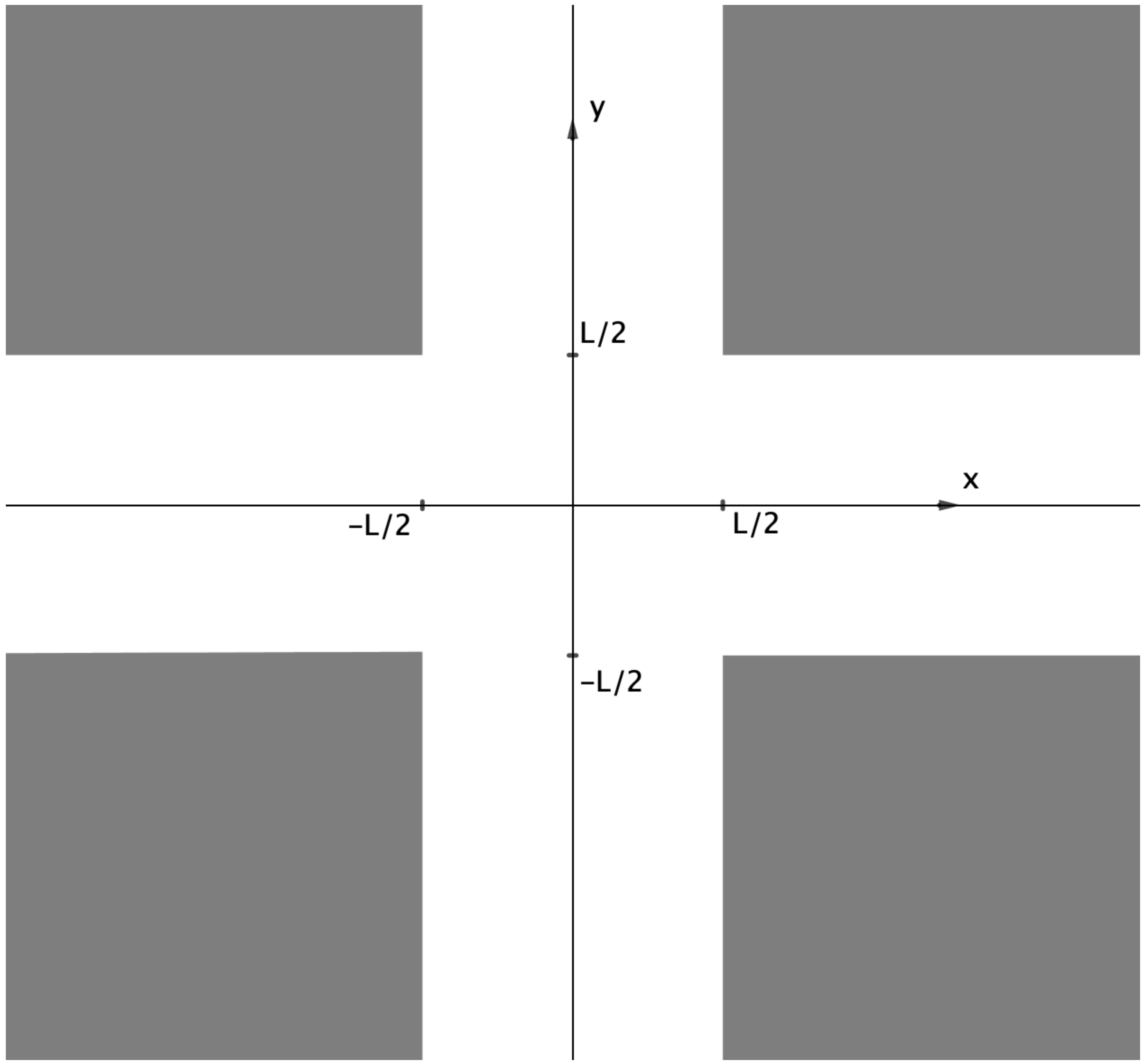
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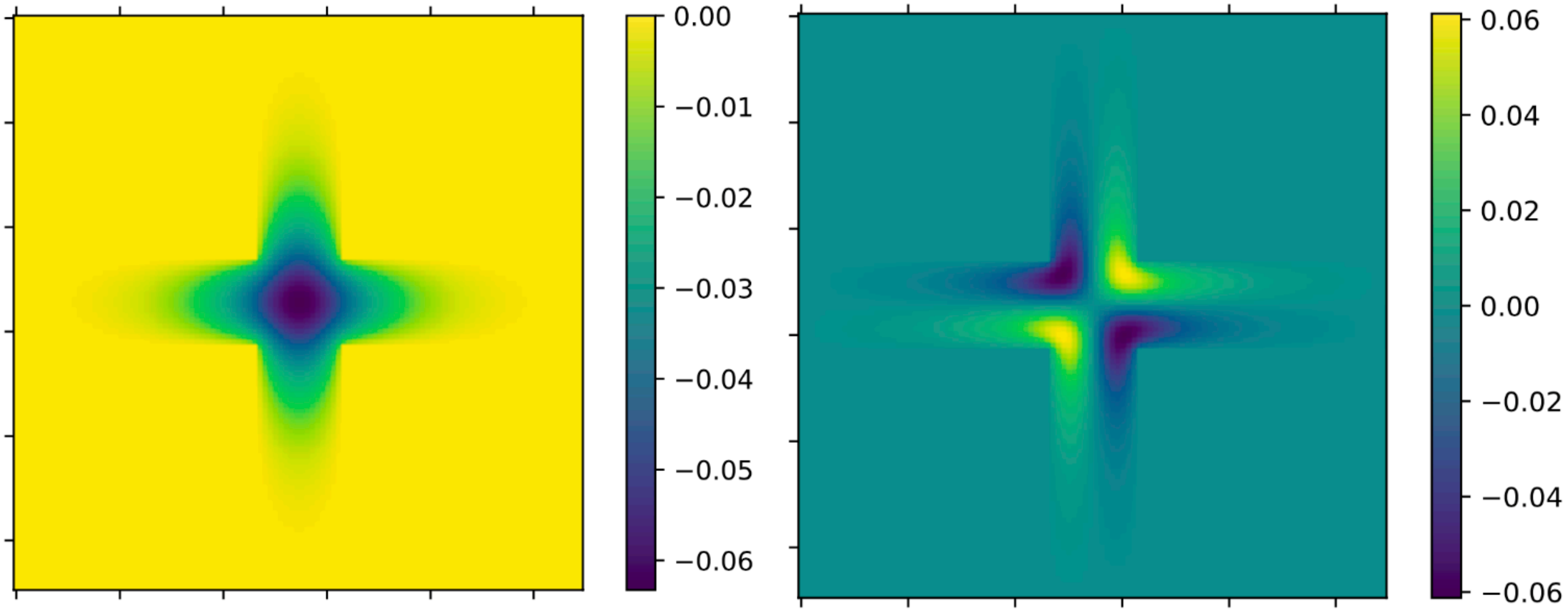


- The two bound states in the cross well potential obtained by solving the 2D TISE numerically on a computer. Plotted are the wavefunctions.

- Possible arguments made by Schult:
  - 1. The potential has sharp corners
  - 2. The potential has bounded classical trajectories

Threshold energy

The potential at infinity in one of the arms is separable as

$$V(x,y) = V_x(x) + V_y(y)$$

where

$$V_x(x) = 0, \quad V_y(y) = \begin{cases} 0, & |y| < L/2 \\ \infty, & \text{else} \end{cases}$$

$$E = \frac{\hbar^2}{2m}\left(k_x^2 + \frac{n^2\pi^2}{L^2}\right), \quad n = 1, 2, 3, \ldots$$

So even threshold is n=1, odd threshold is n=2

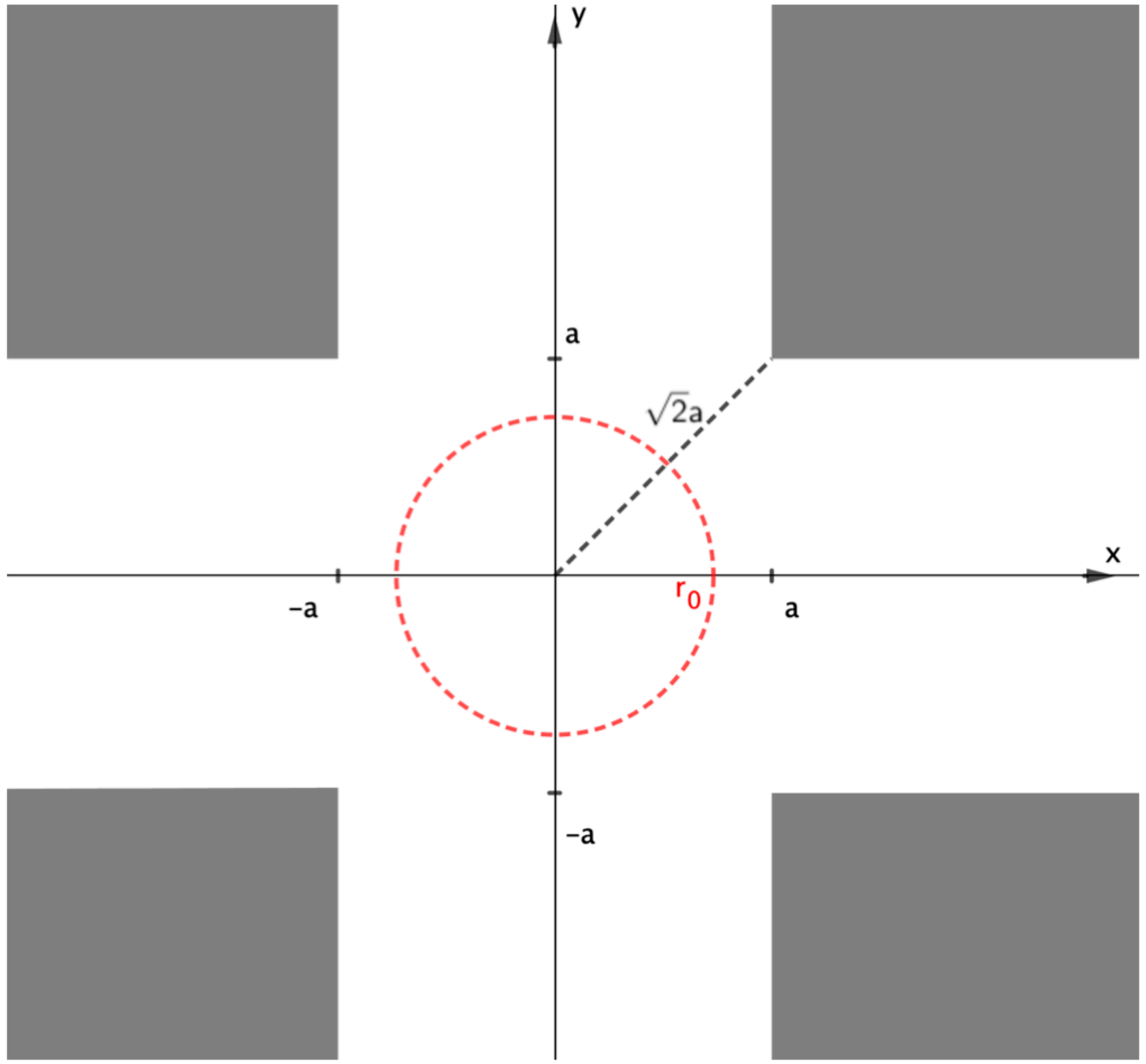
$$E_{\text{t, even}} = \frac{\hbar^2}{2m}\frac{\pi^2}{L^2} \qquad E_{\text{t, odd}} = \frac{\hbar^2}{2m}\frac{4\pi^2}{L^2}$$

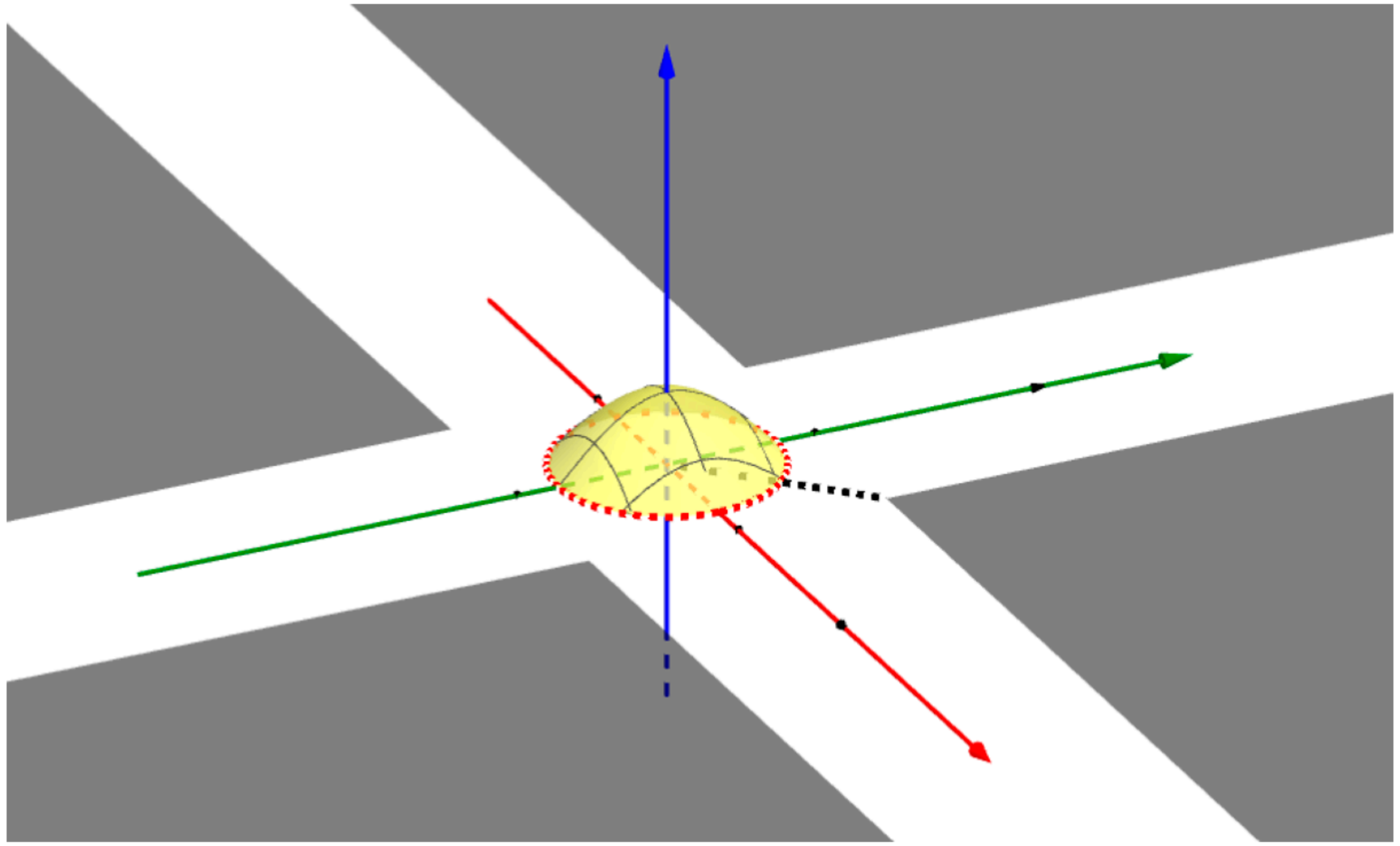
Sharp Corners: Variational Principle

Variational Principle

- For any Hamiltonian, the energy expectation of an arbitrary normalized trail wavefunction is larger than the ground state energy

$$\Psi(r,\phi) = N\cos\left(\frac{\pi}{2r_0}r\right)u(-r+r_0)$$



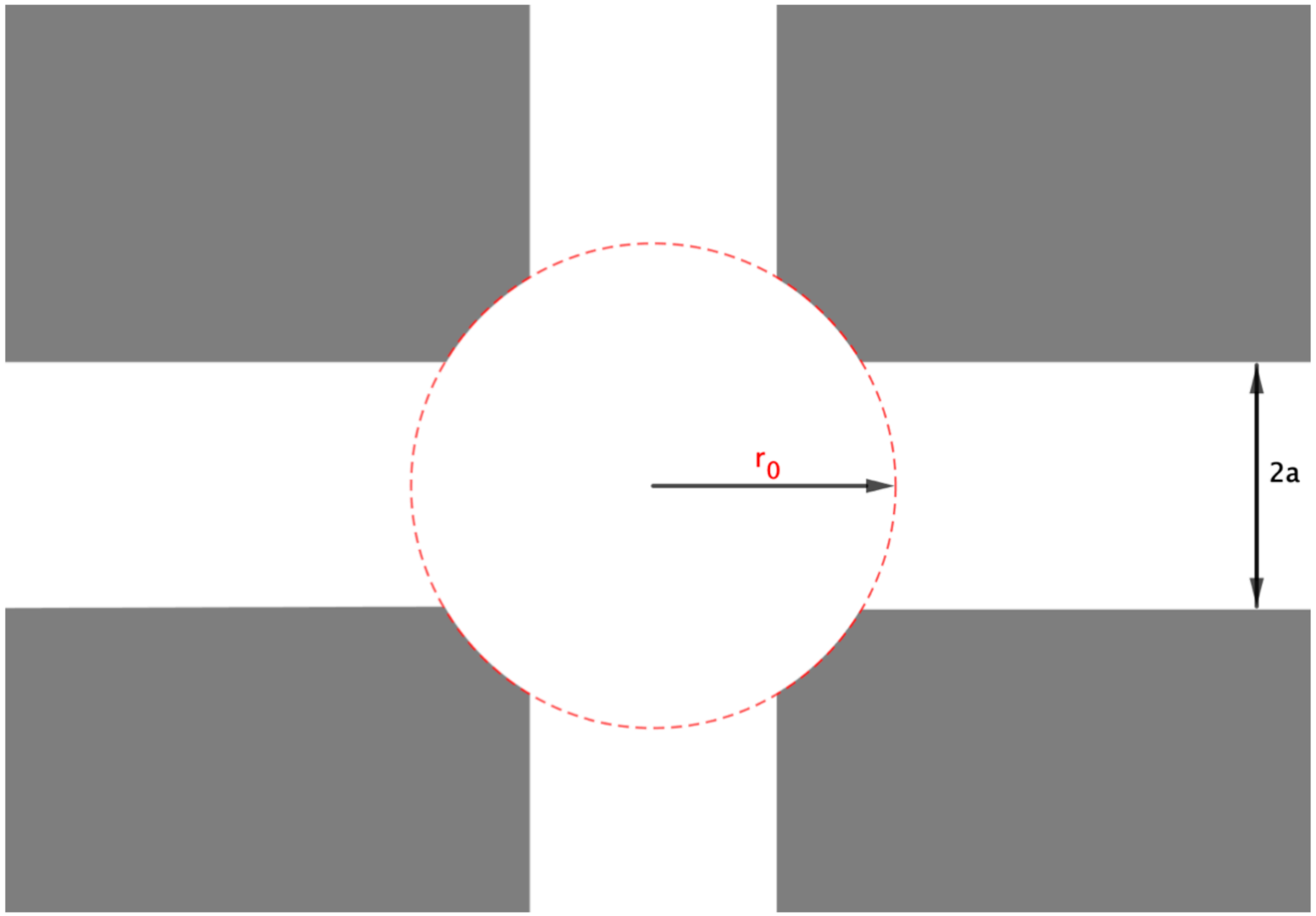


Even threshold: $\dfrac{\hbar^2\pi^2}{8ma^2}$

Normalization: $\int_0^\infty dr \int_0^{2\pi} d\phi \ r|\Psi|^2 = 1$ $\quad N = \sqrt{\frac{2\pi}{(\pi^2-4)\, r_0^2}}$

$$\langle\Psi|\hat{H}|\Psi\rangle$$
$$= \int_0^\infty rdr \int_0^{2\pi} d\phi \left(N\cos\left(\frac{\pi}{2r_0}r\right)u(-r+r_0)\right)\left[-\frac{\hbar^2}{2\mu}N\left(\frac{\partial^2}{\partial r^2}+\frac{1}{r}\frac{\partial}{\partial r}\right)\cos\left(\frac{\pi}{2r_0}r\right)u(-r+r_0)\right]$$
$$= \frac{\hbar^2}{\mu r_0^2}\frac{\pi^2(\pi^2+4)}{8(\pi^2-4)} \approx 2.9152\frac{\hbar^2}{\mu r_0^2} \geq E_{gs}$$

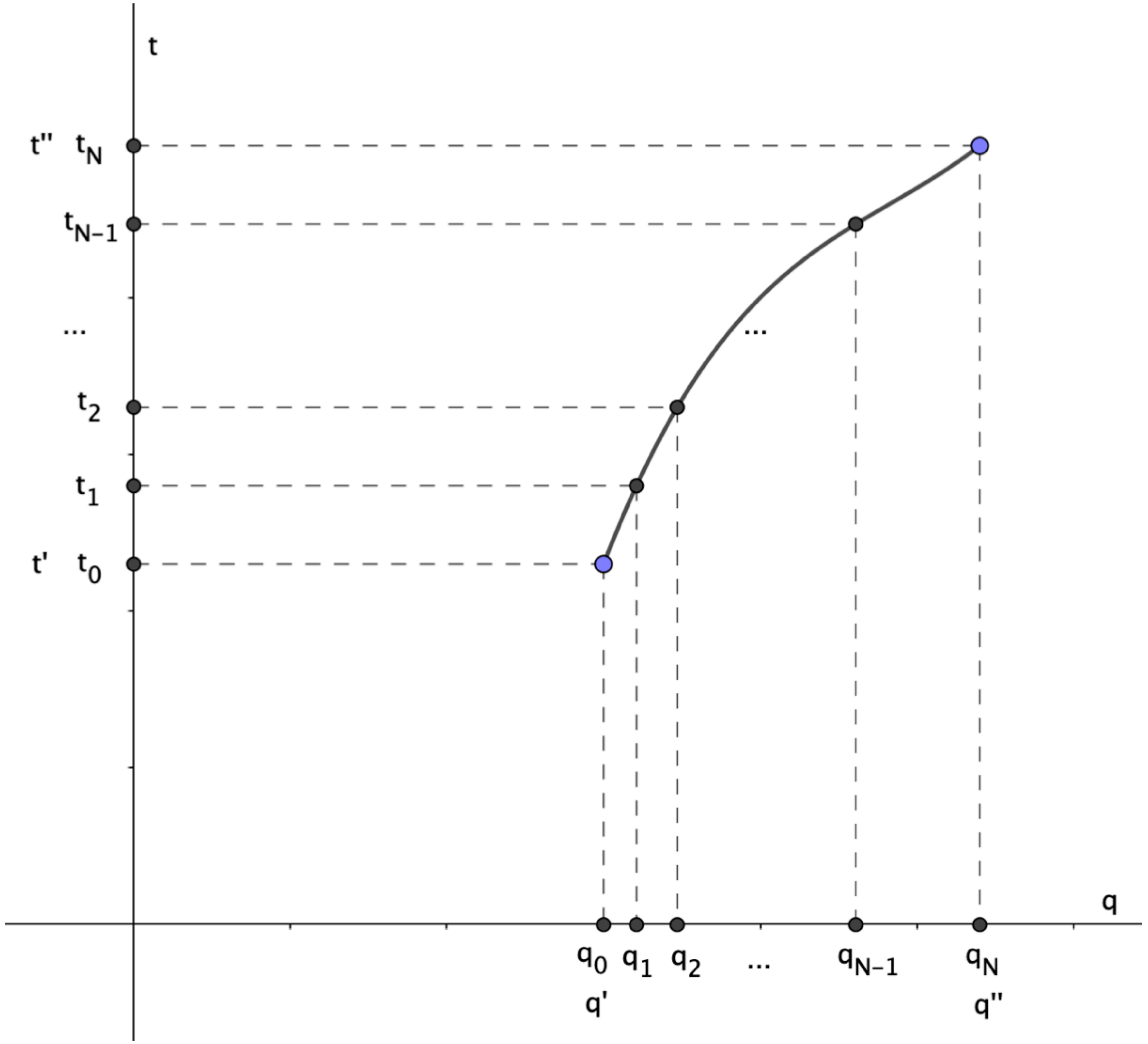
Condition for ground state to be bound: $\frac{\hbar^2}{\mu r_0^2}\frac{\pi^2(\pi^2+4)}{8(\pi^2-4)} < \frac{\hbar^2\pi^2}{8\mu a^2}$ $\quad r_0 > \sqrt{\frac{\pi^2+4}{\pi^2-4}}\,a \approx 1.5372a$



The cross well but the corners are rounded by a central circle of radius r_0. The ground state of this potential is bound if $r_0 > 1.5372a$.

Bounded Classical Trajectories: Gutzwiller Approximation

- Gutzwiller approximation: a method to extract energy levels from the classical periodic trajectories in a potential



$$R = \int \mathcal{L}\, dt$$

$$K(q''t''q't') = \lim_{N\to\infty} \left(\frac{m}{2\pi i\hbar\epsilon}\right)^{\frac{nN}{2}} \int d^n q_1 \int d^n q_2 ... \int d^n q_{N-1} \, \exp\left(i\frac{R(q_1, q_2, .., q_{N-1})}{\hbar}\right)$$

Green's Function

$$G(q'', q', E) = \frac{1}{i\hbar} \int_0^\infty dt K(q''t, q'0) \exp\left(\frac{iEt}{\hbar}\right)$$

$$\int dq\, G(qqE) = \sum_n \frac{1}{E - E_n}$$

The poles are the energy levels!

- Propagator approximation: only integrate over paths sufficiently close to the true classical paths

$$
\begin{aligned}
R(q_1, q_2, .., q_{N-1}) &= R(\bar{q_1} + \delta q_1, ..., \bar{q_{N-1}} + \delta q_{N-1}) \\
&= R(\bar{q_1}, .., \bar{q_{N-1}}) + \left[\delta q_1 \frac{\partial R}{\partial q_1} + ... + \delta q_{N-1} \frac{\partial R}{\partial q_{N-1}}\right] \\
&\quad + \frac{1}{2}\left[(\delta q_1)^2 \frac{\partial^2 R}{\partial q_1^2} + ... + (\delta q_{N-1})^2 \frac{\partial^2 R}{\partial q_{N-1}^2} + 2\delta q_1 \delta q_2 \frac{\partial^2 R}{\partial q_1 \partial q_2} + ...\right] + \mathcal{O}(\delta q^3) \\
&\approx \bar{R} + \frac{1}{2}\sum_{jl} R_{jl}\delta q_j \delta q_l
\end{aligned}
$$

$$
K(q''t''q't') \approx \sum_{\substack{\text{classical}\\ \text{paths}}} \left(\frac{1}{2\pi i\hbar}\right)^{\frac{n}{2}} \sqrt{(-1)^n \det\left(\frac{\partial^2 R}{\partial q'' \partial q'}\right)}\, e^{i\left(\frac{\bar{R}}{\hbar} - M\frac{\pi}{2}\right)}
$$

where $\quad \dfrac{\partial^2 R}{\partial q'' \partial q'} \equiv \begin{pmatrix} \dfrac{\partial^2 R}{\partial q''_x \partial q'_x} & \dfrac{\partial^2 R}{\partial q''_x \partial q'_y} & \\ \dfrac{\partial^2 R}{\partial q''_y \partial q'_x} & \dfrac{\partial^2 R}{\partial q''_y \partial q'_y} & \cdots \\ \vdots & & \ddots \end{pmatrix}$

M, the number of negative eigenvalues of $R_{jl} = \dfrac{\partial^2 R}{\partial q_j \partial q_l}$, is known as the **Maslov index** of the trajectory.

Maslov index for free particle is M=0, since free particle action is always minimum with respect to any path variation and so the Hessian has no negative eigenvalues

$$K(q''t''q't') \approx \sum_{\substack{\text{classical}\\ \text{paths}}} \left(\frac{1}{2\pi i\hbar}\right)^{\frac{n}{2}} \sqrt{(-1)^n \det\left(\frac{\partial^2 R}{\partial q'' \partial q'}\right)}\, e^{i\frac{\bar{R}}{\hbar}}$$

- Plug propagator approximation in Green's function definition for Green's func approx

$$G(q'',q',E) = \frac{1}{i\hbar}\int_0^\infty dt K(q''t,q'0)\exp\left(\frac{iEt}{\hbar}\right)$$

$$\approx \sum_{\substack{\text{classical}\\ \text{paths}}} \frac{1}{i\hbar}\left(\frac{1}{2\pi i\hbar}\right)^{\frac{n}{2}} \int_0^\infty dt \sqrt{(-1)^n \det\left(\frac{\partial^2 R}{\partial q''\partial q'}\right)}\, e^{i\frac{\bar{R}+Et}{\hbar}}$$

This integral can be evaluated with the stationary phase integral approximation

$$\boxed{G(q'',q',E) \approx \sum_{\substack{\text{classical}\\ \text{paths}}} \frac{1}{i\hbar(2\pi i\hbar)^{\frac{n-1}{2}}} \left|\det\begin{pmatrix} \frac{\partial^2 S}{\partial q''\partial q'} & \frac{\partial^2 S}{\partial q''\partial E} \\ \frac{\partial^2 S}{\partial E\partial q'} & \frac{\partial^2 S}{\partial E^2}\end{pmatrix}\right|^{\frac{1}{2}} e^{\frac{i}{\hbar}S(q'',q',E)}}$$

$$S(q'',q',E) = \int_{q'}^{q''} p dq$$

We can calculate the Green's function from only the classical paths and their actions!

Taking q''=q' and integrating over all points give the approximated energy levels.

- e.g. 1D free particle on a torus of size L

$$S(q'', q', E) = \int_{q'}^{q''} p\, dq = \sqrt{2mE}\, |q'' - q'|$$

path length

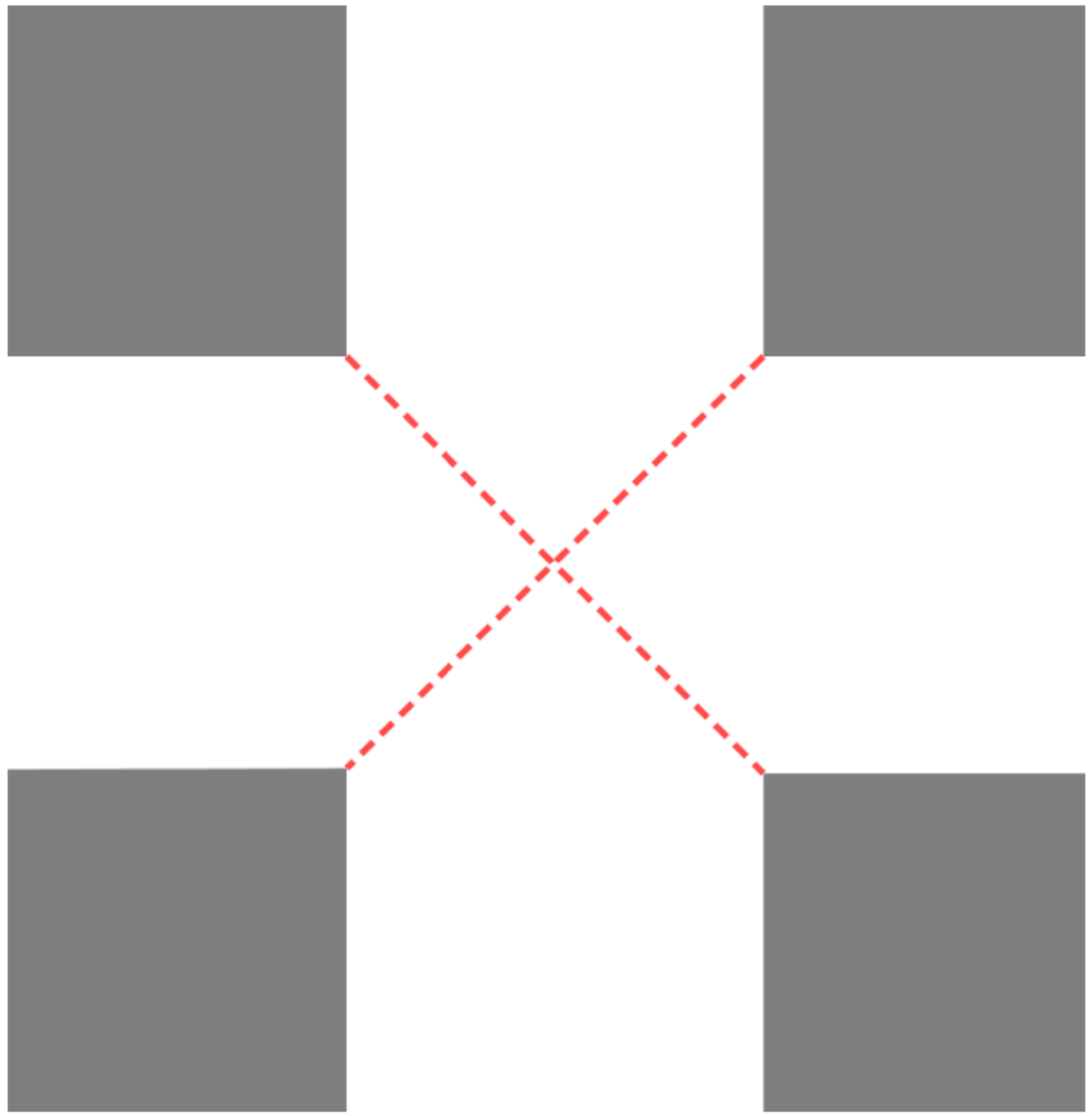
$$G(q'', q', E) \approx \sum_{\substack{\text{classical}\\ \text{paths}}} \frac{1}{i\hbar}\sqrt{\frac{m}{2E}}\, e^{\frac{i}{\hbar}S(q'', q', E)}$$

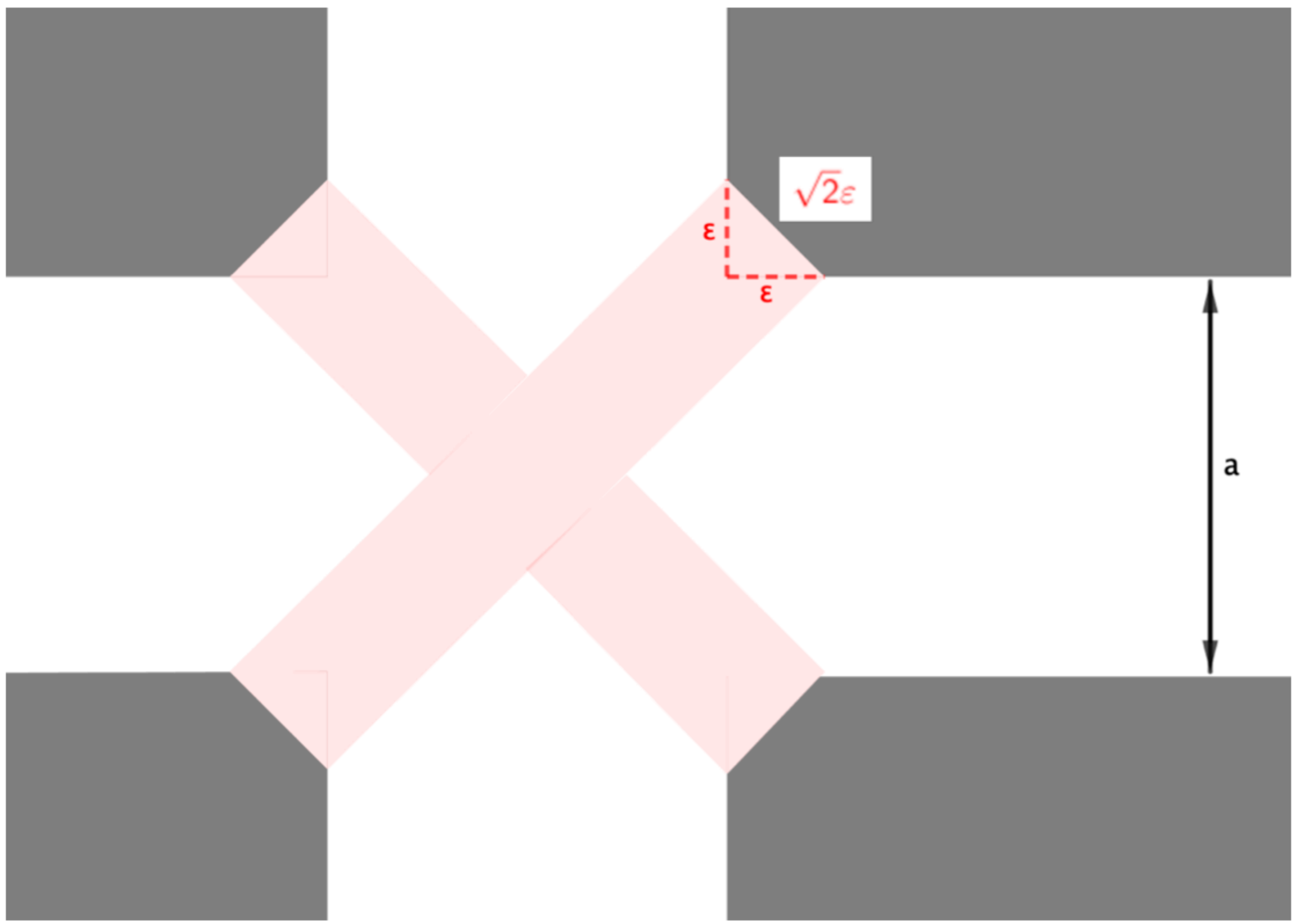
q'' = q' means we need to look at periodic classical paths: $|q'' - q'| = |\nu| L$, ν integer

$$G(q, q, E) \approx \sum_{\nu=-\infty}^{\infty} \frac{1}{i\hbar}\sqrt{\frac{m}{2E}}\, e^{\frac{i}{\hbar}\sqrt{2mE}|\nu| L}$$

We can sum using geometric series

$$\int_0^L dq\, G(qqE) \approx \sum_{\nu=-\infty}^{\infty} \frac{1}{E - \frac{\hbar^2}{2m}\frac{4\pi^2\nu^2}{L^2}}$$





Periodic classical paths are the ones that bounce between the opposite corners:

$$|q'' - q'| = 2\sqrt{2}(a + \epsilon)$$

$$E_{\text{t, even}} = \frac{\hbar^2}{2m}\frac{\pi^2}{a^2}$$

$$E_{\text{t, odd}} = \frac{\hbar^2}{2m}\frac{4\pi^2}{a^2}$$

$$\int d^2q\, G(qqE) \approx -\frac{e^{i\frac{\pi}{4}}}{\sqrt{2\pi}} \frac{m}{\hbar^2}(4a\epsilon + 2\epsilon^2) \sum_\nu \sqrt{\frac{\hbar}{\sqrt{2mE}\nu 2\sqrt{2}(a+\epsilon)}}\, e^{\frac{i}{\hbar}\sqrt{2mE}\nu 2\sqrt{2}(a+\epsilon)}$$

- Diverges when the phases line up in the series, i.e. when we go to the next term of the series, the phase changes by an integer multiple of 2π

$$\frac{\partial}{\partial \nu} \frac{\sqrt{2mE}}{\hbar} \nu 2\sqrt{2}(a+\epsilon) = 2\pi n$$

$$E = \lim_{\epsilon \to 0} \frac{\hbar^2}{2m} \frac{\pi^2 n^2}{2(a+\epsilon)^2} = \frac{\hbar^2}{2m} \frac{\pi^2 n^2}{2a^2}$$

$$E_0 = \frac{\hbar^2}{2m}\frac{\pi^2}{2a^2}, \quad E_1 = \frac{\hbar^2}{2m}\frac{4\pi^2}{2a^2}, \quad E_2 = \frac{\hbar^2}{2m}\frac{9\pi^2}{2a^2}$$

$$E_0 < E_{\text{t, even}} < E_1 < E_{\text{t, odd}} < E_2 < E_3 < \ldots$$

$$E_{\text{t, even}} = \frac{\hbar^2}{2m}\frac{\pi^2}{a^2}$$

$$E_{\text{t, odd}} = \frac{\hbar^2}{2m}\frac{4\pi^2}{a^2}$$