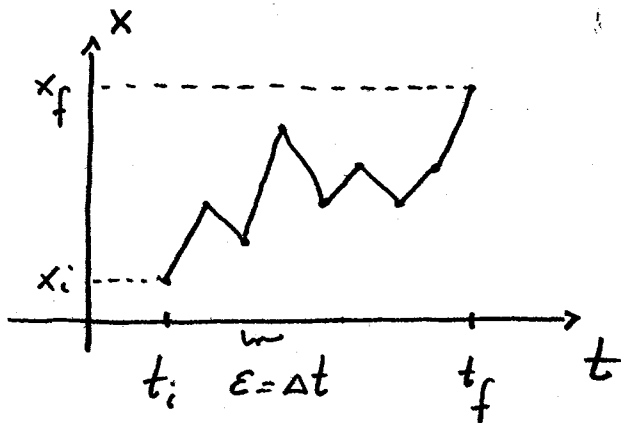


Lecture 2/3

1.

Feynman Path Integral (continued)



$$K(f, i) = \lim_{\epsilon \rightarrow 0} \frac{1}{A} \int \dots \int e^{\frac{i}{\hbar} S[f, i]} \frac{dx_1}{A} \frac{dx_2}{A} \dots \frac{dx_{N-1}}{A}$$

$$A = \sqrt{\frac{2\pi i \hbar \Delta t}{m}}$$

$$S[f, i] = \int_{t_i}^{t_f} L(\dot{x}, x, t) dt$$

$$K(x_f, t_f; x_i, t_i) = \int \mathcal{D}[x(t)] e^{\frac{i}{\hbar} S}$$

Feynman Path Integral

$$S = \sum_{i=1}^N \left[\frac{1}{2} m \frac{(x_i - x_{i-1})^2}{\Delta t} - V\left(\frac{x_i + x_{i-1}}{2}\right) \right]$$

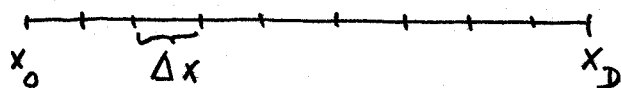
zig-zag

We will approximate integration over zig-zag paths by approximate Riemann sum

$$K_E^{(i,j)} = \frac{1}{A} \exp \left\{ \frac{i \Delta t}{\hbar} \left(\frac{1}{2} m \frac{(x_j - x_i)^2}{\Delta t^2} - V \left(\frac{x_j + x_i}{2} \right) \right) \right\}$$

"infinitesimal" propagation

$$K(T) = (\Delta x)^{N-1} K_E^N(\Delta t) \quad T = N \cdot \Delta t$$



$$x_D = x_0 + N_D \cdot \Delta x$$

$N_D + 1$ dimension of matrix

matrix multiplication problem

$$\text{Tr } K(t) = \sum_n e^{-\frac{i}{\hbar} E_n t}$$

energy levels
by Fourier transformation

$$H |n\rangle = E_n |n\rangle$$

$$\text{Tr } K(t) = \int dx \langle x | e^{-\frac{i}{\hbar} H t} | x \rangle =$$

$$= \sum_n \int dx \langle x | e^{-\frac{i}{\hbar} H t} | n \rangle \langle n | x \rangle = \sum_n e^{-\frac{i}{\hbar} E_n t}$$

Harmonic Oscillator

$$L(x, \dot{x}) = \frac{1}{2} \dot{x}^2 - \frac{1}{2} x^2$$

$$\left. \begin{array}{l} \hbar = 1 \\ m = 1 \end{array} \right\} \text{units}$$

$$T_0 = 2\pi \text{ eigenfrequency}$$

We will perform propagator calculations

in $T = \frac{T_0}{16}$ intervals with 4 time slices

for each $(N=4, \Delta t = \frac{T_0}{64})$

First, we investigate time evolution of real

Gaussian wavefunction $\psi_0(x)$

$$\psi_0(x) = \left(\frac{\alpha}{\pi}\right)^{\frac{1}{4}} e^{-\frac{\alpha}{2} (x - x_{\text{start}})^2}$$

$$\psi(x, t) = \int dx' K(x, t; x', 0) \psi_0(x')$$

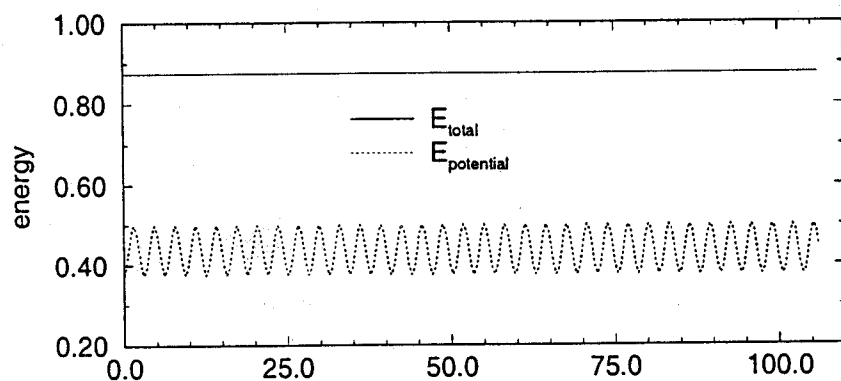
superposition principle for probability amplitudes

Spatial resolution $N_D = 600$

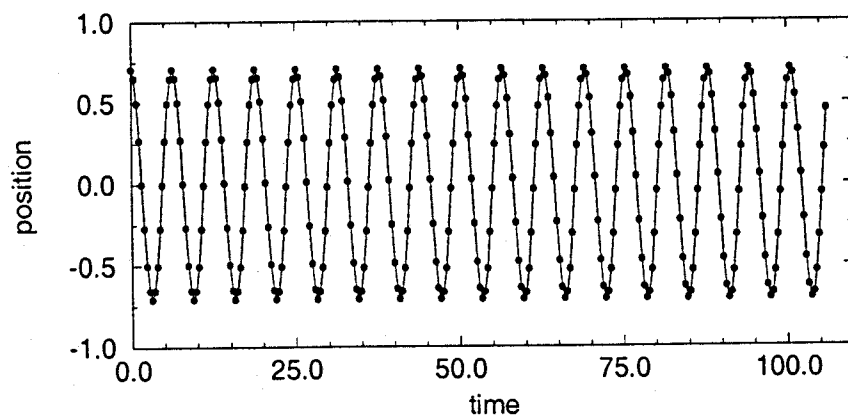
$$X_0 = -4$$

$$X_D = +4$$

time evolution becomes matrix multiplication of the propagator matrix



← energy
virial theorem
is well satisfied ✓



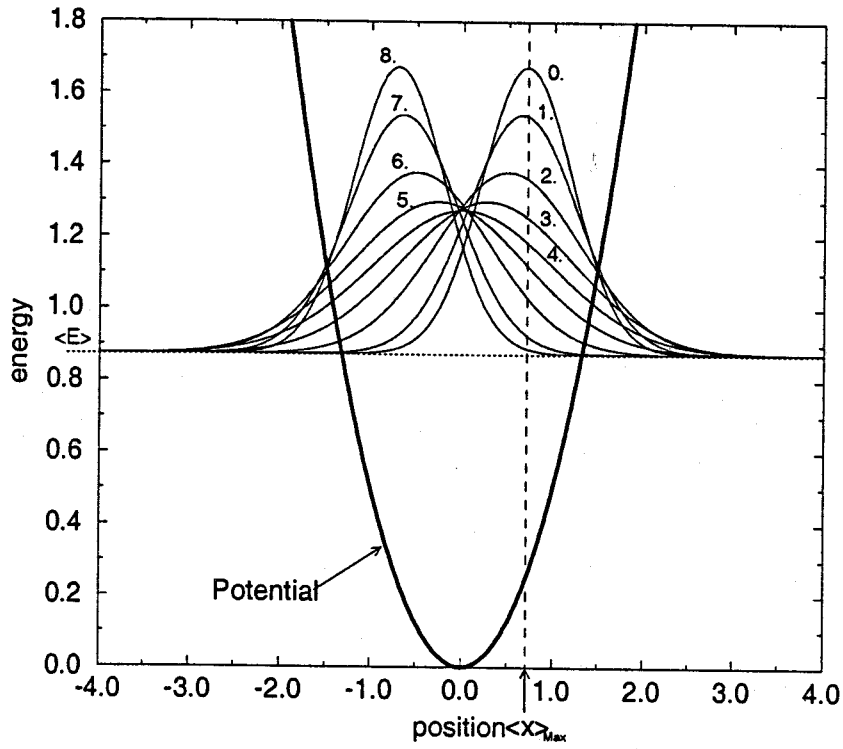
← average
position

16 samples in each period

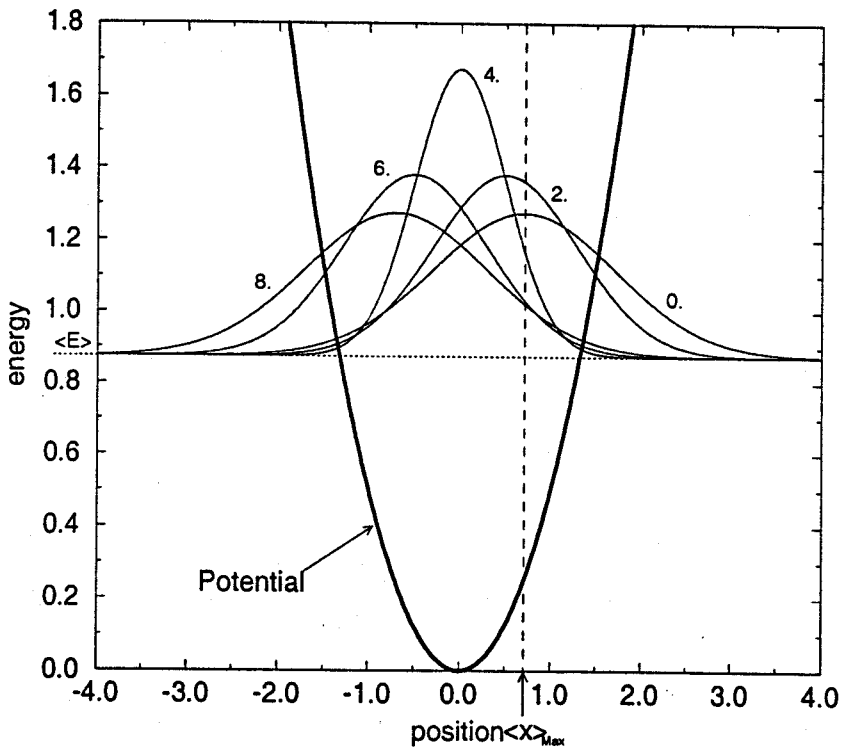
solid line is the analytic result of continuum path integral

Time evolution of wave function:

5.



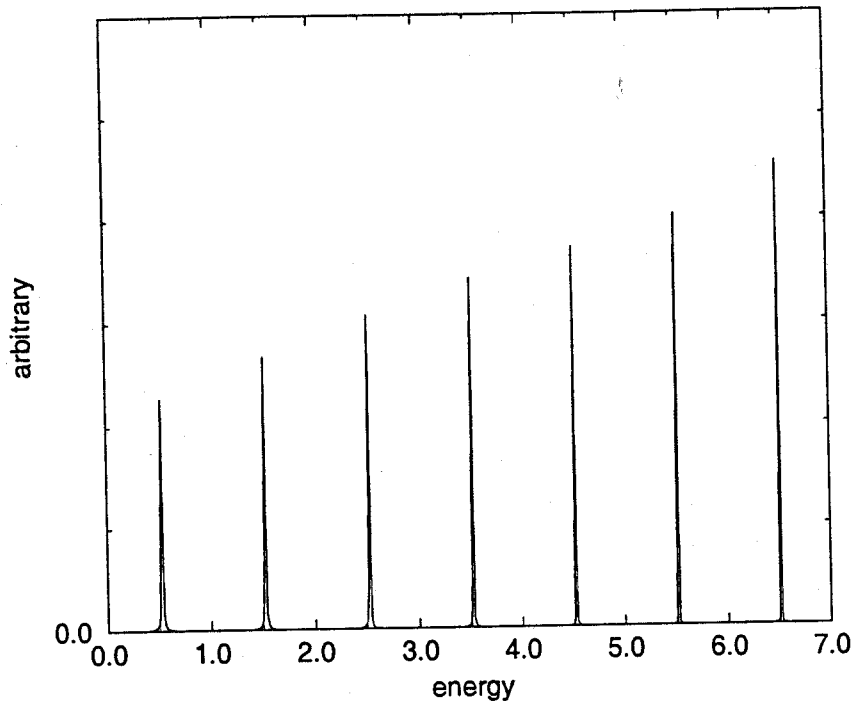
$\alpha = 2$



$\alpha = 0.5$

Energy spectrum (Fourier transformation)

6.



$$E_n = n + \frac{1}{2}$$

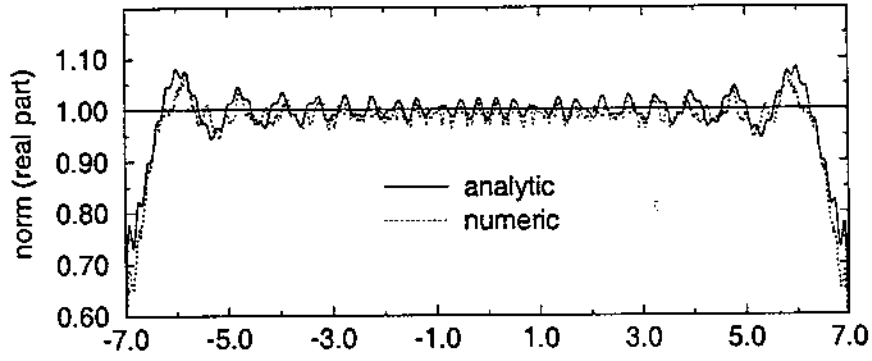
$$n = 0, 1, \dots$$

Error of discretization is checked by
normalization condition on propagator:

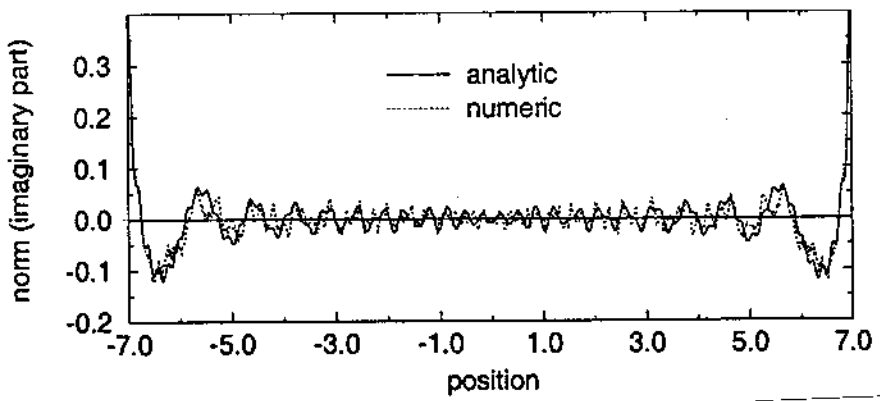
$$1 = \int dx' \langle x' | x \rangle = \int dx' dx'' (\langle x'' | \hat{K} | x' \rangle)^* \langle x'' | \hat{K} | x \rangle$$

$$\sum_{i,j=0}^{N_D} (\Delta x)^2 K_{ij}^*(t) K_{ik}(t) = 1$$

7.



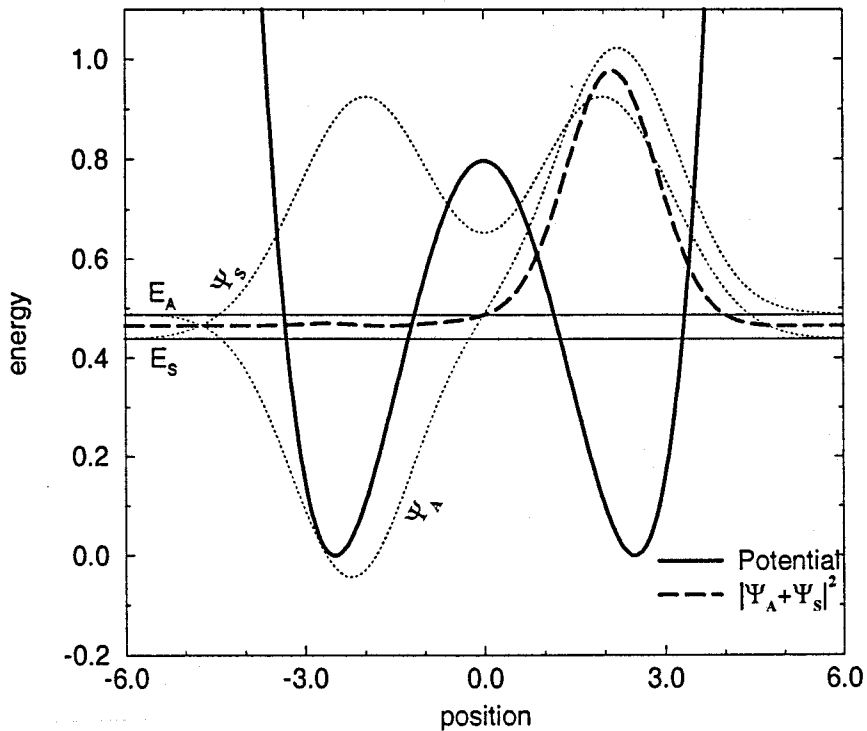
check on error
of spatial resolution



Double Well Potential

$$L(x, \dot{x}) = \frac{1}{2} \dot{x}^2 - d(x - x_{\min})^2 (x + x_{\min})^2$$

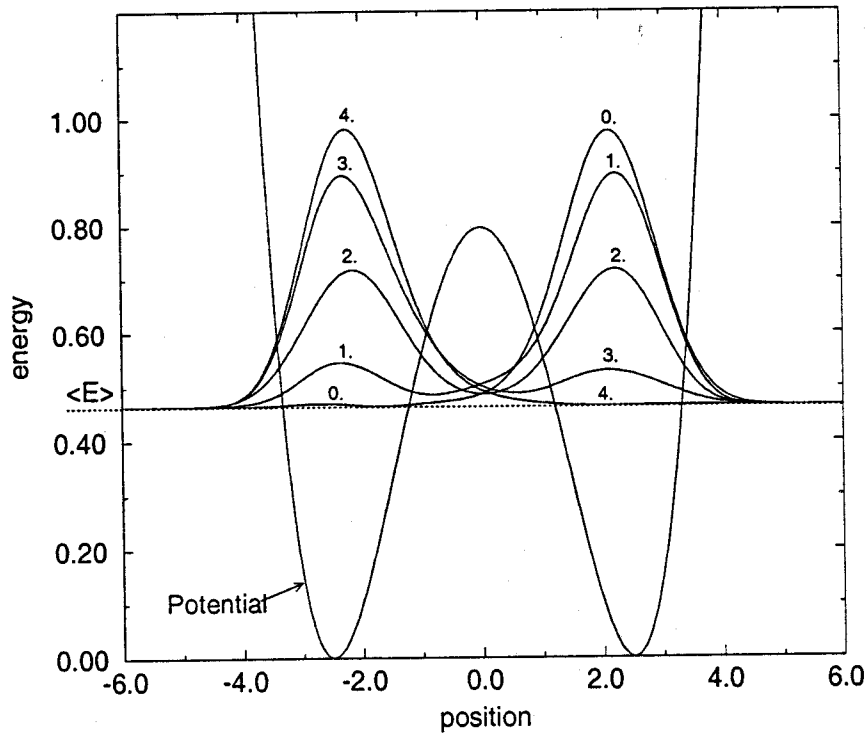
$$\psi_{S/A}(x) = \frac{1}{d\sqrt{2\pi}} \left(e^{-\frac{(x-\beta)^2}{2d^2}} \pm e^{-\frac{(x+\beta)^2}{2d^2}} \right)$$



wavefunctions

Time evolution :

9.

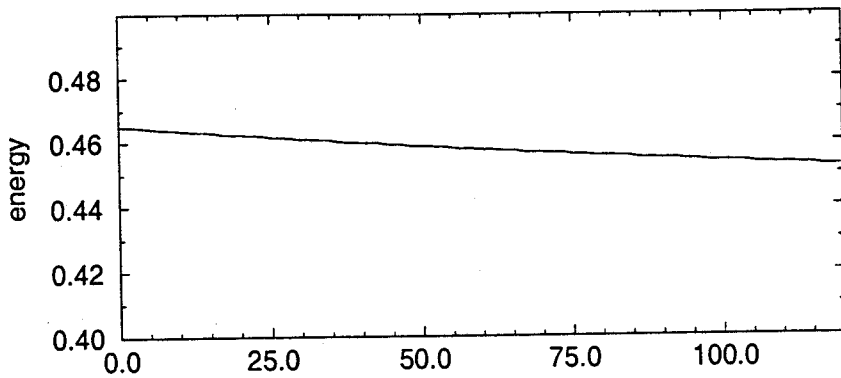


every 55th time
step is plotted

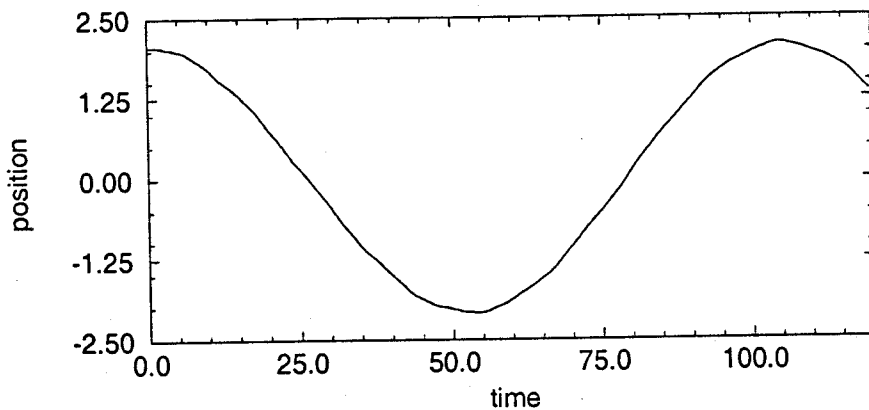
$$\psi_m = K(\pi) \psi_0$$

$$T = 54.4$$

tunneling time

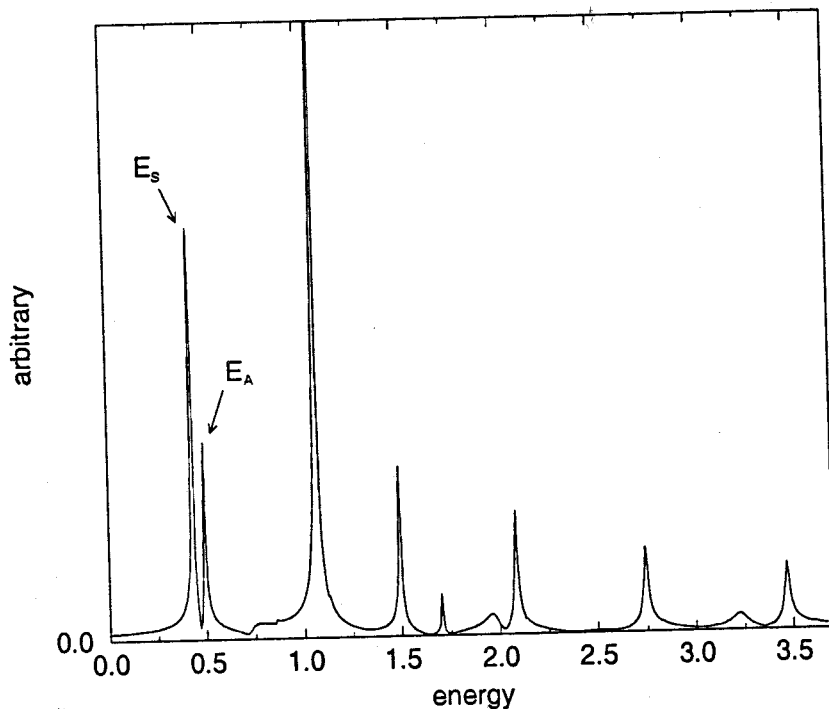


energy



average
position

Energy Spectrum :



↑
peaks occur at

$$E_S = 0.433$$

$$E_A = 0.494$$

$$T_{es} = 51.7$$

5% off from
observed value