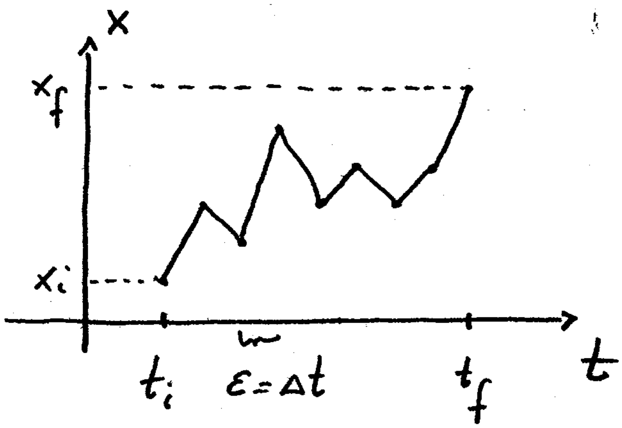
Lecture 2/3

Feynman Path Integral (continued)



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

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

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

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

Feynman Path Integral

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

delta t

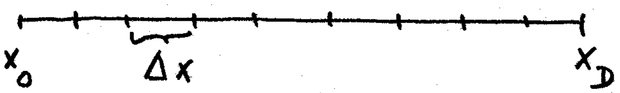
zig-zag

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

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

"infinitesimal" propagation

$$K(T) = (\Delta x)^{N-1} K_\varepsilon^N (\Delta t) \qquad T = N \cdot \Delta t$$



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

$N_D + 1$ dimension of matrix

matrix multiplication problem

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

energy levels by Fourier transformation

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

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

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

Harmonic Oscillator

$$L(x, \dot{x}) = \frac{1}{2}\dot{x}^2 - \frac{1}{2}x^2 \qquad \left.\begin{matrix} \hbar = 1 \\ m = 1 \end{matrix}\right\} \text{units}$$

$T_0 = 2\pi$ eigenfrequency

We will perform propagator calculations in $T = \frac{T_0}{16}$ intervals with 4 time slices for each $\left(N = 4, \ \Delta t = \frac{T_0}{64} \right)$

First, we investigate time evolution of real Gaussian wavefunction $\psi_0(x)$

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

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

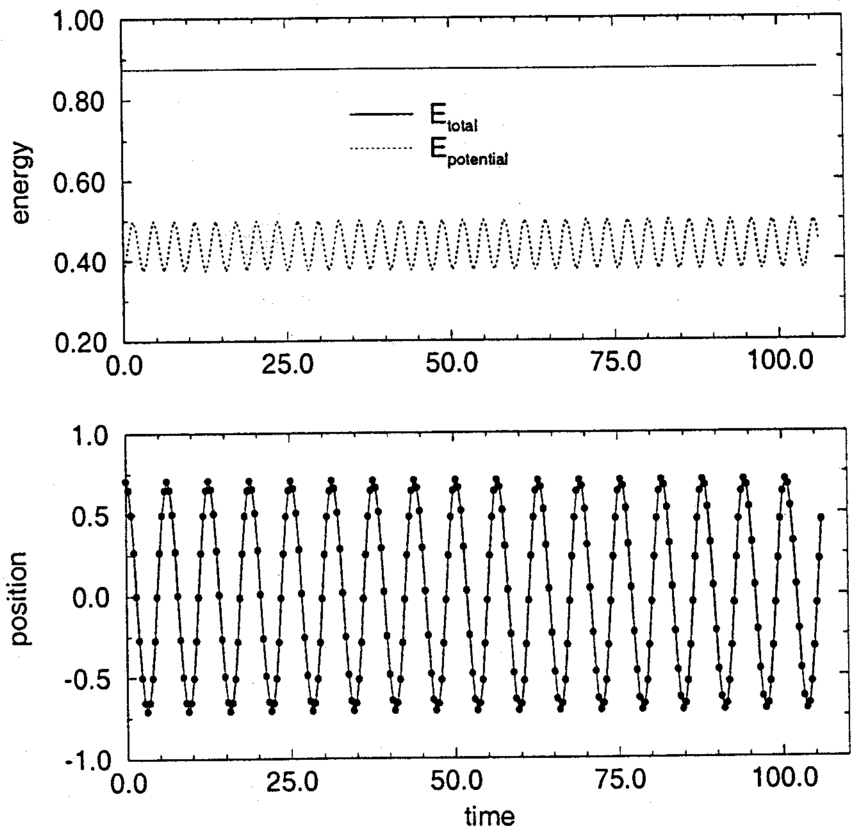
superposition principle for probability amplitudes

Spatial resolution $N_D = 600$

$x_0 = -4$

$x_D = +4$

time evolution becomes matrix multiplication of the propagator matrix



← energy

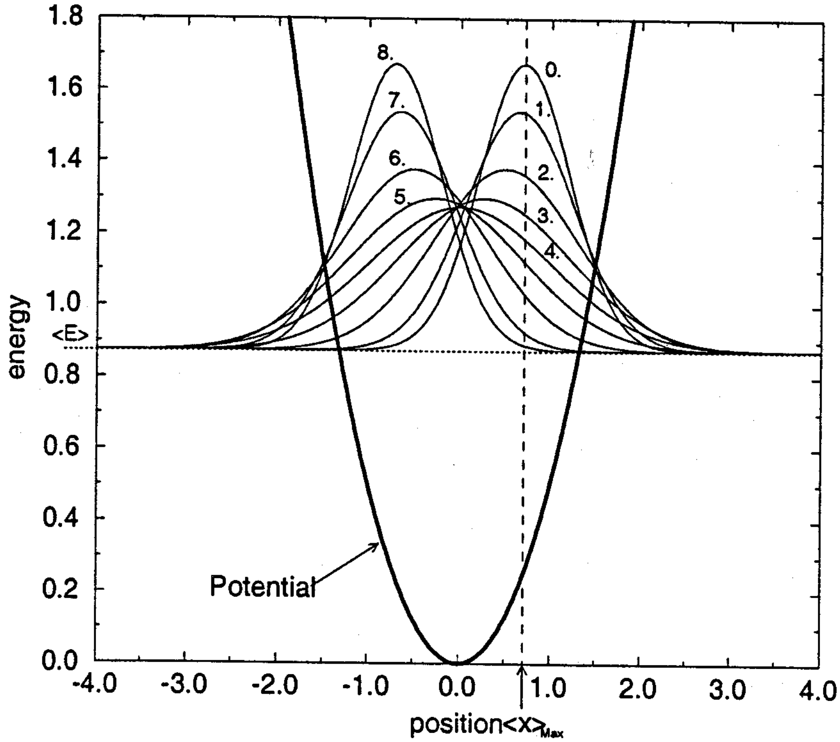
virial theorem is well satisfied

← average position

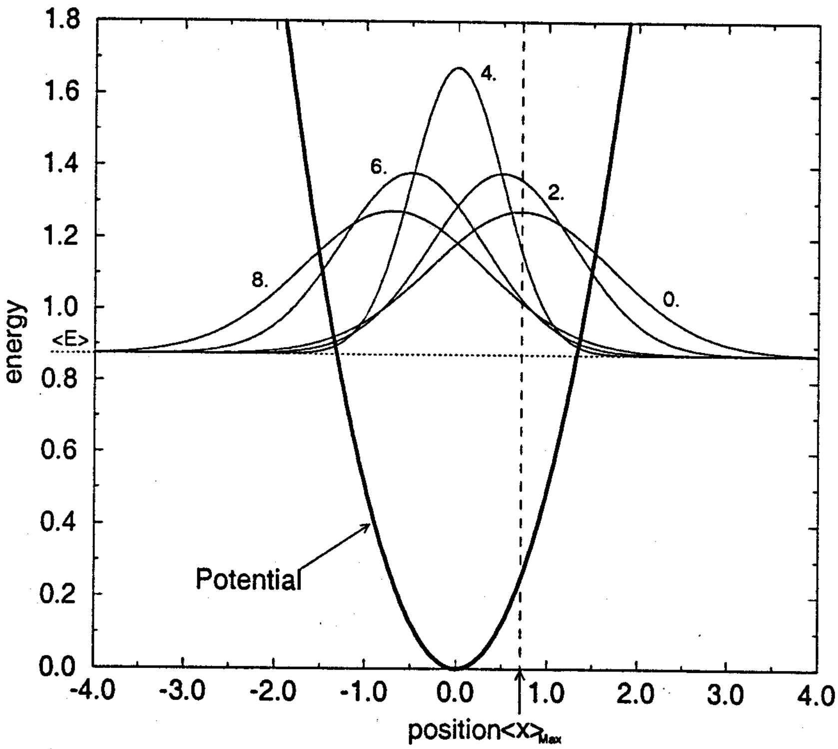
16 samples in each period

solid line is the analytic result of continuum path integral

Time evolution of wave function:

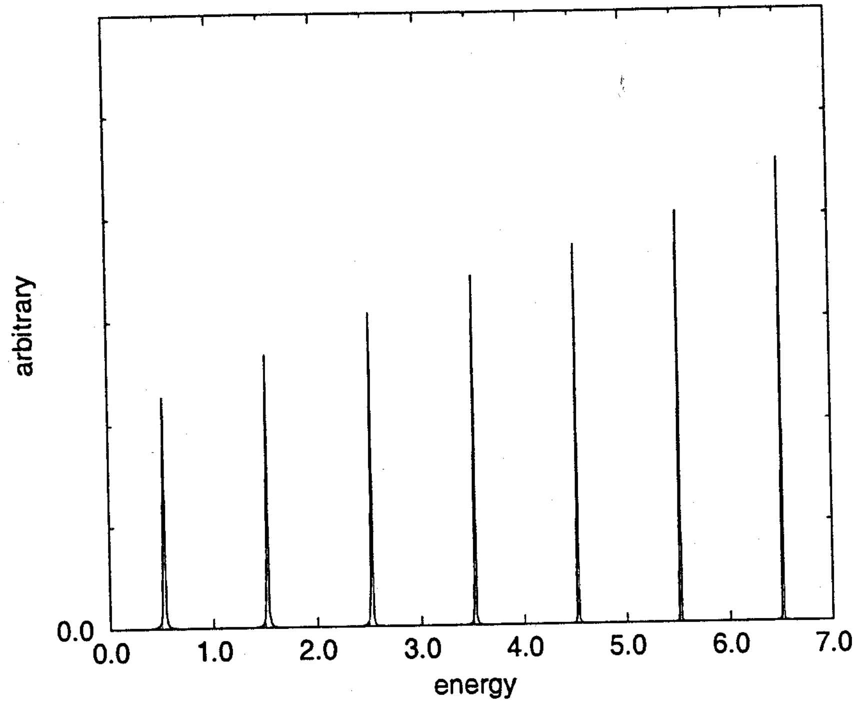


$\alpha = 2$



$\alpha = 0.5$

Energy spectrum (Fourier transformation)



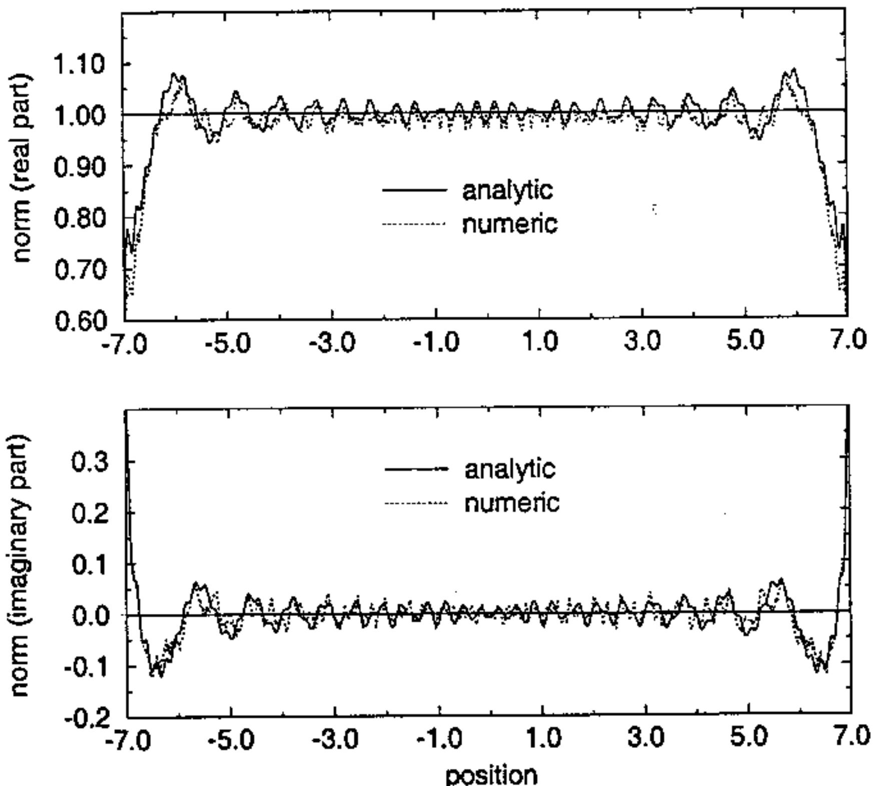
$E_n = n + \frac{1}{2}$

$n = 0, 1, \dots,$

Error of discretization is checked by normalization condition on propagator:

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

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

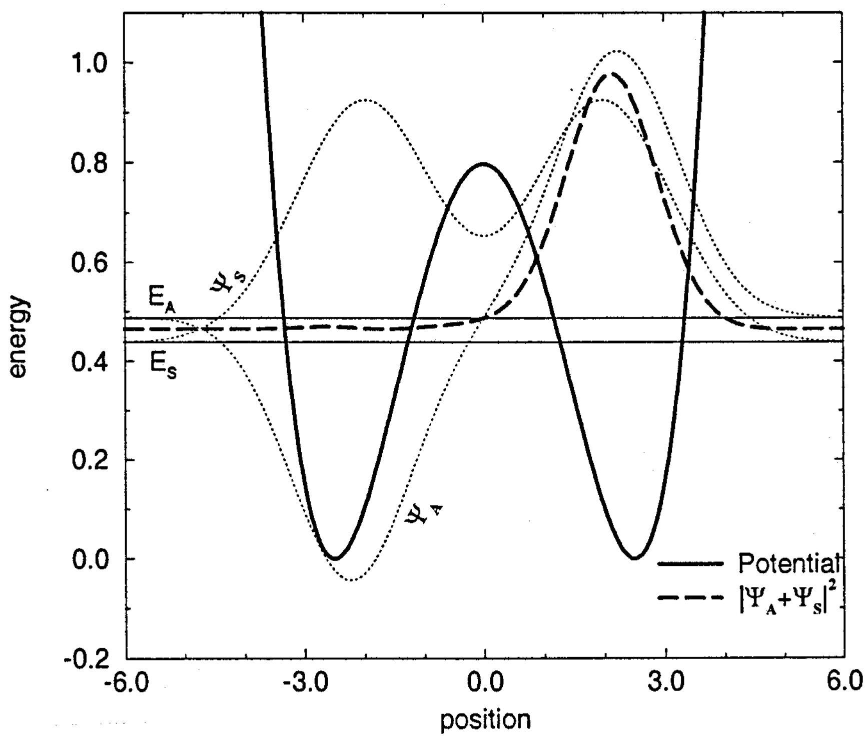


check on error
of spatial resolution

Double Well Potential

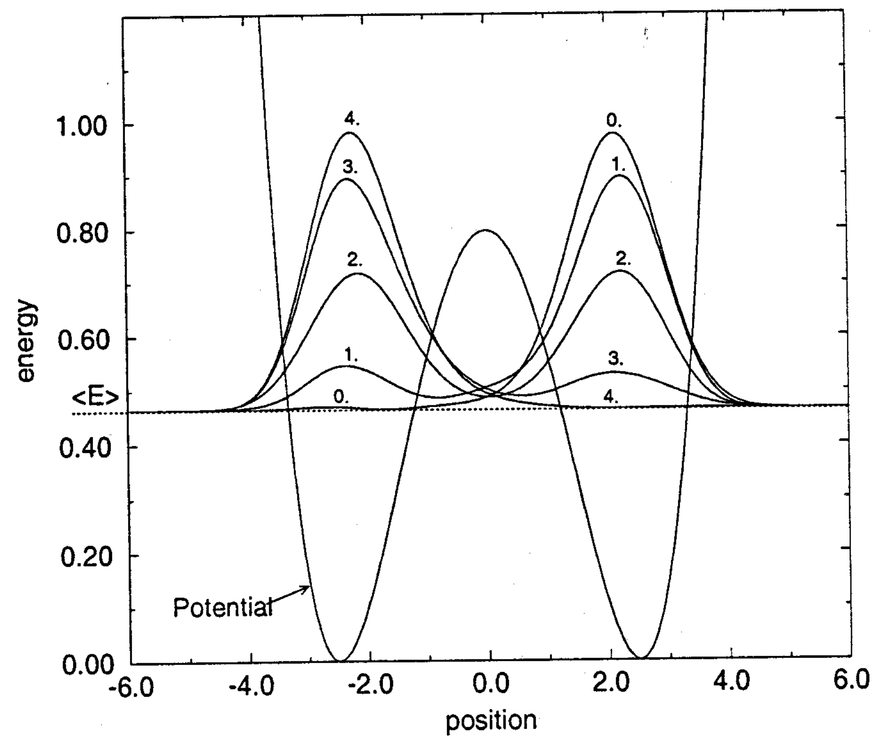
$$L(x, \dot{x}) = \frac{1}{2}\dot{x}^2 - \alpha\left(x - x_{min}\right)^2\left(x + x_{min}\right)^2$$

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



wavefunctions

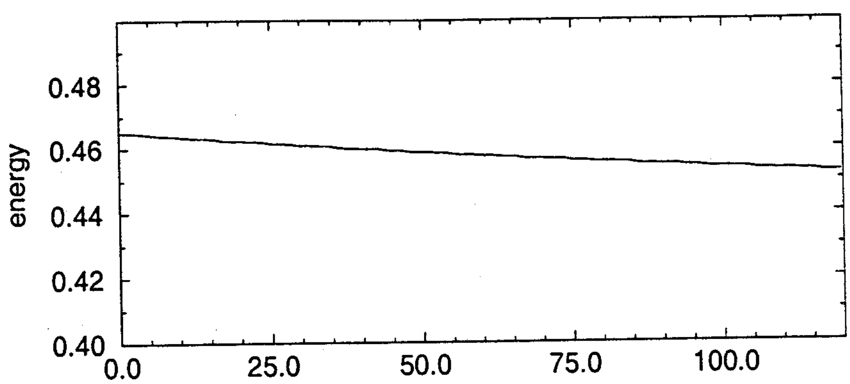
Time evolution :



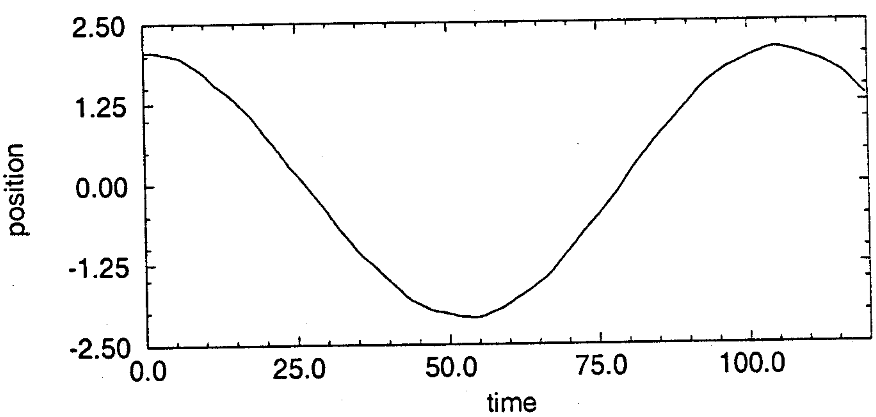
every 55th time step is plotted

$\psi_n = \hat{K}^{55}(\tau)\,\psi_0$

$T = 54.4$ tunneling time

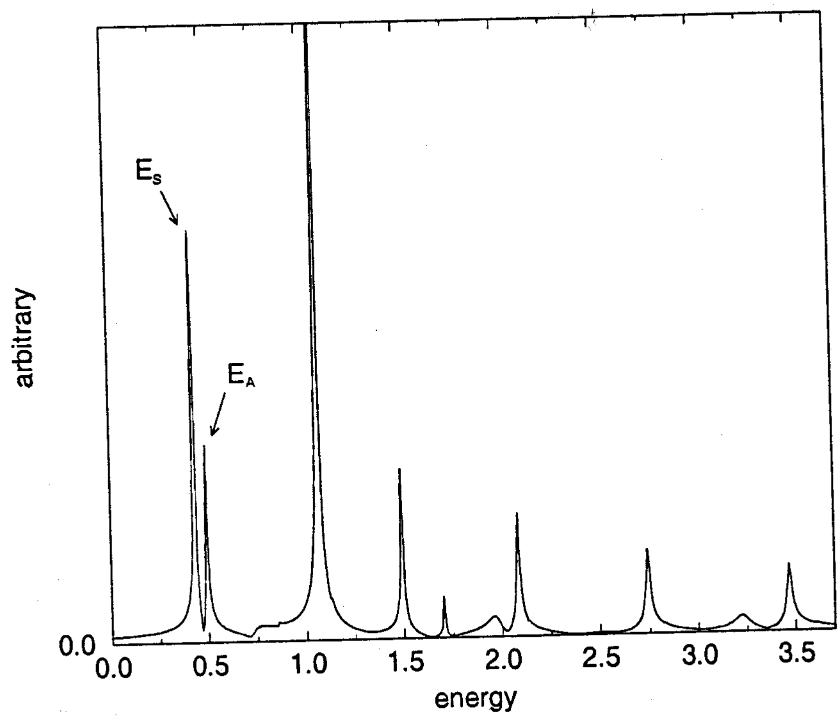


energy



average position

Energy Spectrum :



peaks occur at

$E_S = 0.433$

$E_A = 0.494$

$T_{es} = 51.7$ 5% off from observed value