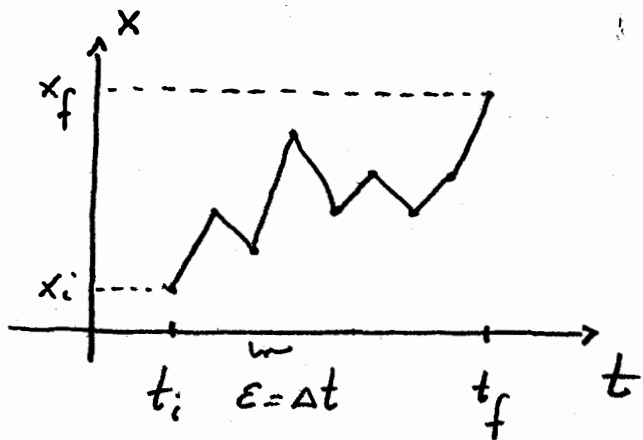


Lectures 3/4/5/6

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

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

Free particle, harmonic oscillator, Schrodinger equation

Free Particle

$$L = \frac{1}{2} m \dot{x}^2 \quad \text{Lagrangian}$$

$$i \leftrightarrow a$$

$$f \leftrightarrow b$$

$$K(b, a) = \lim_{\epsilon \rightarrow 0} \int \dots \int dx_1 \dots dx_{N-1} \left(\frac{2\pi i \hbar \epsilon}{m} \right)^{-\frac{N}{2}} \exp \left[\frac{im}{2\hbar \epsilon} \sum_{i=1}^N (x_i - x_{i-1})^2 \right]$$

Gaussian integrals $\int e^{-ax^2} dx$ or $\int e^{-ax^2+bx} dx$

Integral of a gaussian is a gaussian. Integration can be done variable after variable

$$K(b, a) = \sqrt{\frac{m}{2\pi i \hbar (t_b - t_a)}} \exp \left[\frac{im (x_b - x_a)^2}{2\hbar (t_b - t_a)} \right]$$

final result

Calculation is carried out as follows. Notice first

$$\int_{-\infty}^{+\infty} \left(\frac{m}{2\pi i \hbar \epsilon} \right)^{\frac{1}{2}} \exp \left\{ \frac{i m}{2 \hbar \epsilon} \left[(x_2 - x_1)^2 + (x_1 - x_0)^2 \right] \right\} dx_1$$

$$= \sqrt{\frac{m}{2\pi i \hbar \cdot 2\epsilon}} \exp \left[i \frac{m}{2 \hbar (2\epsilon)} (x_2 - x_0)^2 \right]$$

Next we multiply this result by

$$x_0 = x_a, \quad t_a = t_0$$

$$x_N = x_b, \quad t_b = t_N$$

$$\frac{\sqrt{m}}{\sqrt{2\pi i \hbar \epsilon}} \exp \left[\frac{i m}{2 \hbar \epsilon} (x_3 - x_2)^2 \right]$$

and integrate now over x_2 to get:

$$\left(\frac{m}{2\pi i \hbar 3\epsilon} \right)^{\frac{1}{2}} \exp \left[i \frac{m}{2 \hbar \cdot 3\epsilon} (x_3 - x_0)^2 \right]$$

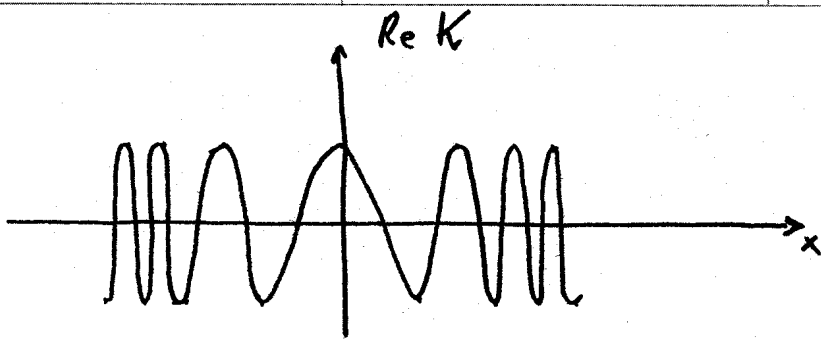
This established a recursion which, after $n-1$ steps, gives

$$\left(\frac{m}{2\pi i \hbar n \cdot \epsilon} \right)^{\frac{1}{2}} \exp \left[i \frac{m}{2 \hbar n \cdot \epsilon} (x_n - x_0)^2 \right]$$

which is identical to the announced result

$$\int_{-\infty}^{+\infty} e^{-\alpha x^2 + \beta x} dx = e^{\frac{\beta^2}{4\alpha}} \left(\frac{\pi}{\alpha} \right)^{1/2} \quad \text{Gaussian}$$

even if α and β are complex
 $\text{Re } \alpha > 0$ guarantees convergence



$$a = (0, 0)$$

$$b = (x, t)$$

$$K(x, t; 0, 0) = \left(\frac{m}{2\pi i \hbar t} \right)^{\frac{1}{2}} e^{\frac{imx^2}{2\hbar t}}$$

For large x , rapidly oscillating real and imaginary parts (90° out of phase) when looked at for fixed t .

wavelength of oscillation:

$$2\pi = \frac{m(x+\lambda)^2}{2\hbar t} - \frac{mx^2}{2\hbar t} = \frac{mx\lambda}{\hbar t} + \frac{m\lambda^2}{2\hbar t}$$

$$\lambda = \frac{2\pi \hbar}{m \left(\frac{x}{t} \right)} \quad x \gg \lambda \quad \uparrow \text{negligible}$$

From classical viewpoint a particle which moves from origin to x in time t has velocity $\frac{x}{t}$ and momentum $m \frac{x}{t}$.

From QM viewpoint, if motion can be adequately described by classical momentum $p = m \frac{x}{t}$, then amplitude varies in space with wavelength $\lambda = \frac{h}{p}$ (de Broglie)

More generally:

$$K \sim \exp \left[\frac{i}{\hbar} S_{cl}(b, a) \right] \quad \begin{array}{l} \text{amplitude of particle to} \\ \text{arrive at point } b \end{array}$$

we want to show that amplitude varies rapidly in space with wavelength $\lambda = \frac{h}{p}$

if $S_{cl} \gg \hbar$, phase varies rapidly as a function of end point b

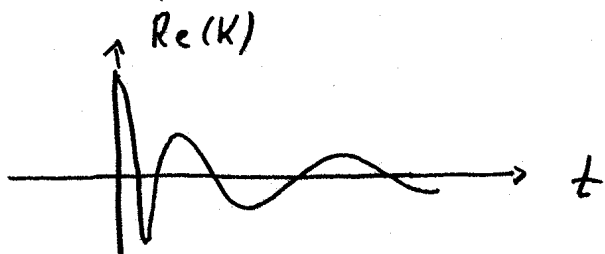
$$k = \frac{1}{\hbar} \frac{\partial S_{cl}}{\partial x_b} \quad \begin{array}{l} \text{change in phase per unit displacement} \\ \text{(wave number)} \end{array} \rightarrow p = \hbar k$$

$$p = \frac{\partial L}{\partial \dot{x}} \quad \left. \frac{\partial L}{\partial \dot{x}} \right|_{x=x_b} = \frac{\partial S_{cl}}{\partial x_b} \quad k = \frac{2\pi}{\lambda}$$

$$\delta S = \int_{t_a}^{t_b} \delta x \left[\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{x}} \right) - \frac{\partial L}{\partial x} \right] dt$$

$$p = \frac{h}{\lambda} \quad \text{de Broglie}$$

Next, we look at time dependence of K :



both frequency and amplitude change

For large t

$$2\pi = \frac{m x^2}{2\hbar t} - \frac{m x^2}{2\hbar (t+T)} = \frac{m x^2}{2\hbar t^2} \left(\frac{T}{1 + \frac{T}{t}} \right)$$

T period of oscillation

$$\omega = \frac{2\pi}{T}$$

$$\omega \approx \frac{m}{2\hbar} \left(\frac{x}{t} \right)^2$$

↓

$$\text{Energy} = \hbar \omega$$

more generally:

$$\omega = \frac{1}{\hbar} \frac{\partial S_{cl}}{\partial t} \rightarrow \omega = \frac{E}{\hbar}$$

$$E = L - \dot{x} p$$

$$L(x_b) - \dot{x}_b \left(\frac{\partial L}{\partial \dot{x}} \right)_{x=x_b} = \frac{\partial S_{cl}}{\partial t_b}$$

(1) If the amplitude K varies as e^{ikx} , we say particle has momentum $\hbar k$

(2) If amplitude K has a definite frequency $e^{-i\omega t}$ we say energy is $\hbar \omega$

By substitution for free particle:

$$-\frac{\hbar}{i} \frac{\partial K(b,a)}{\partial t_b} = -\frac{\hbar^2}{2m} \frac{\partial^2 K(b,a)}{\partial x_b^2}$$

required to show
in hw 2

$$t_b > t_a$$

wave function:

$$\psi(x'_1, t') = \int_{-\infty}^{+\infty} K(x'_1, t'; x, t) \psi(x, t) dx$$

Using the equation for K ,

$$-\frac{\hbar}{i} \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2}$$

Schrödinger Eq.!

required to show
in hw2

Harmonic Oscillator

$$L = \frac{1}{2} m \dot{x}^2 - \frac{1}{2} m \omega^2 x^2$$

$$K_{L(b,a)} = \left(\frac{m\omega}{2\pi i \hbar \sin \omega T} \right)^{\frac{1}{2}} \exp \left\{ \frac{i m \omega}{2 \hbar \sin \omega T} \left[(x_a^2 + x_b^2) \cos \omega T - 2 x_a x_b \right] \right\}$$

$$T = t_b - t_a$$

the exponent has the form $e^{\frac{i}{\hbar} S_{cl}}$

$$S_{cl} = \frac{m\omega}{2 \sin \omega T} \left[(x_a^2 + x_b^2) \cos \omega T - 2x_a x_b \right]$$

required to show in hw 2

Proof comes from recursive integration

Schrödinger Equation

$$\psi(x, t+\epsilon) = \int_{-\infty}^{+\infty} \frac{1}{A} \left\{ \exp \left[\frac{i}{\hbar} \frac{m(x-y)^2}{2\epsilon} \right] \right\} \cdot$$

rapidly oscillates for large $y-x$

$$\times \left\{ \exp \left[-\frac{i}{\hbar} \epsilon V \left(\frac{x+y}{2}, \epsilon t \right) \right] \right\} \psi(y, t) dy$$

$y = x + \eta$ substitution, expect large contribution for small η only

$$\psi(x, t+\epsilon) = \int_{-\infty}^{+\infty} \frac{1}{A} e^{\frac{im\eta^2}{2\hbar\epsilon}} e^{-\frac{i\epsilon}{\hbar} V \left[\frac{x+\eta}{2}, t \right]} \psi(x+\eta, t) d\eta$$

integral contributes in $0 \leq |\eta| \leq \sqrt{\frac{\hbar\epsilon}{m}}$ range

$$\psi(x,t) + \epsilon \frac{\partial \psi}{\partial t} = \int_{-\infty}^{+\infty} \frac{1}{A} e^{\frac{im\eta^2}{2\hbar\epsilon}} \left[1 - \frac{i\epsilon}{\hbar} V(x,t) \right]$$

power series $\times \left[\psi(x,t) + \eta \frac{\partial \psi}{\partial x} + \frac{1}{2} \eta^2 \frac{\partial^2 \psi}{\partial x^2} \right] d\eta$

$$\frac{1}{A} \int_{-\infty}^{+\infty} e^{\frac{im\eta^2}{2\hbar\epsilon}} d\eta = \frac{1}{A} \left(\frac{2\pi i \hbar \epsilon}{m} \right)^{\frac{1}{2}}$$

$$A = \left(\frac{2\pi i \hbar \epsilon}{m} \right)^{\frac{1}{2}} \text{ was chosen before !}$$

$$\int_{-\infty}^{+\infty} \frac{1}{A} e^{\frac{im\eta^2}{2\hbar\epsilon}} \cdot \eta d\eta = 0$$

$$\int_{-\infty}^{+\infty} \frac{1}{A} e^{\frac{im\eta^2}{2\hbar\epsilon}} \cdot \eta^2 d\eta = \frac{i\hbar\epsilon}{m}$$

Therefore $\psi + \epsilon \frac{\partial \psi}{\partial t} = \psi - \frac{i\epsilon}{\hbar} V\psi - \frac{\hbar\epsilon}{2im} \frac{\partial^2 \psi}{\partial x^2}$

$$\boxed{-\frac{\hbar}{i} \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V(x,t) \psi(x,t)}$$

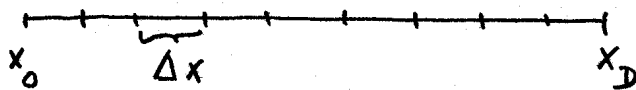
Schrödinger Eq. !

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

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

"infinitesimal" propagation

$$K(\tau) = (\Delta x)^{N-1} K_{\epsilon}^N(\Delta t) \quad \tau = N \cdot \Delta t$$



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

$N_D + 1$ 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 $\psi_0(x)$

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

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

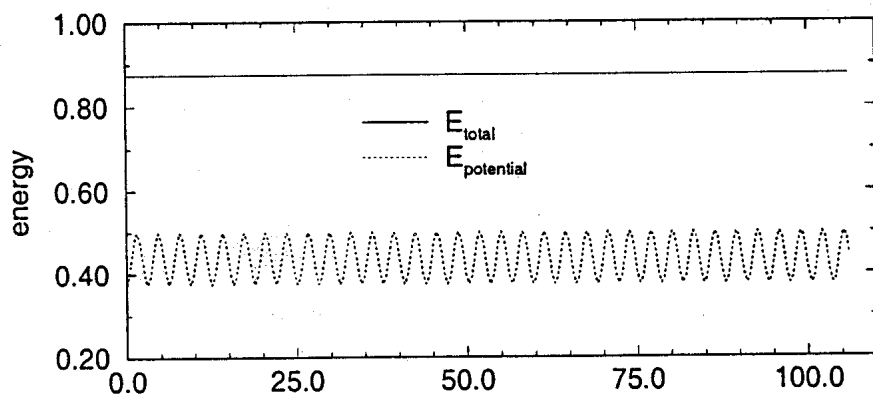
superposition principle for probability amplitudes

Spatial resolution $N_D = 600$

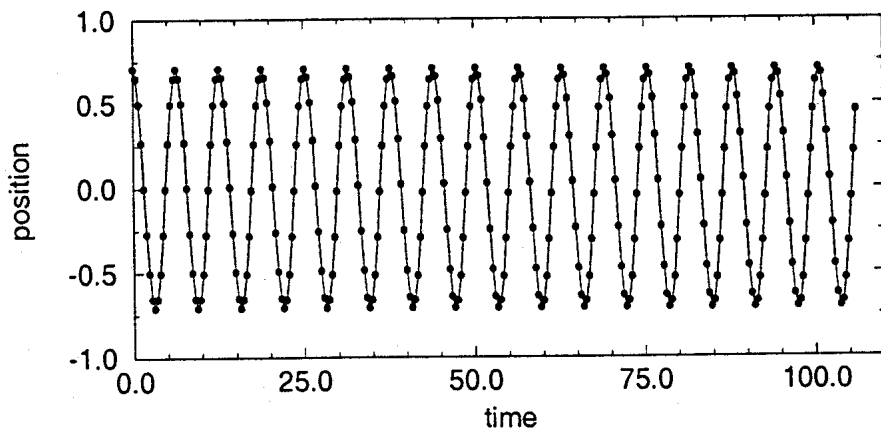
$$x_0 = -4$$

$$x_D = +4$$

time evolution becomes matrix multiplication of the propagator matrix



← energy
virial theorem
is well satisfied ✓

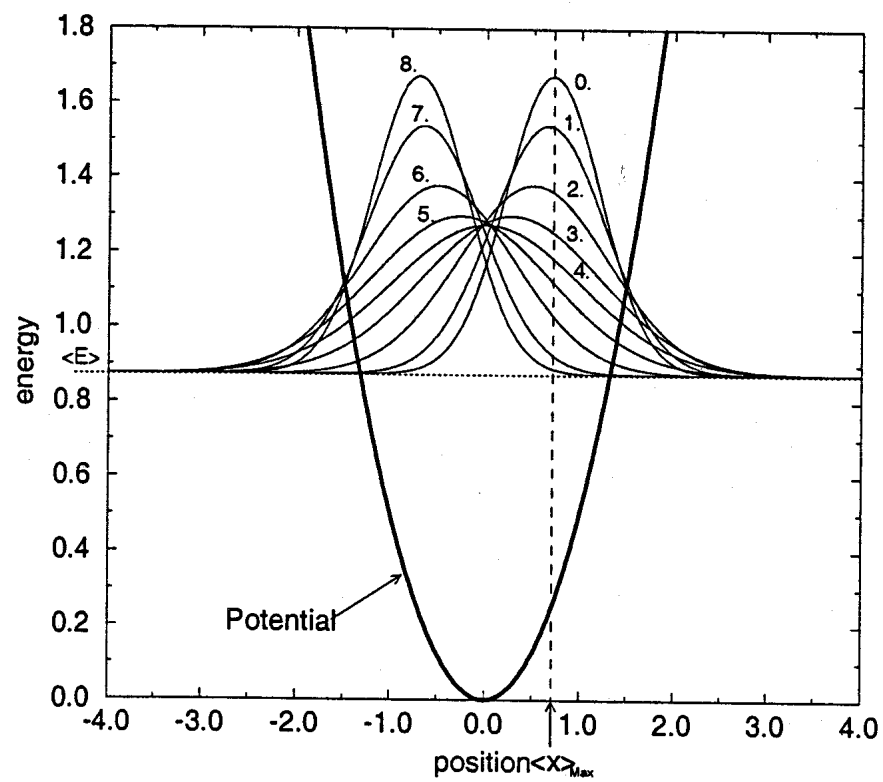


← average
position

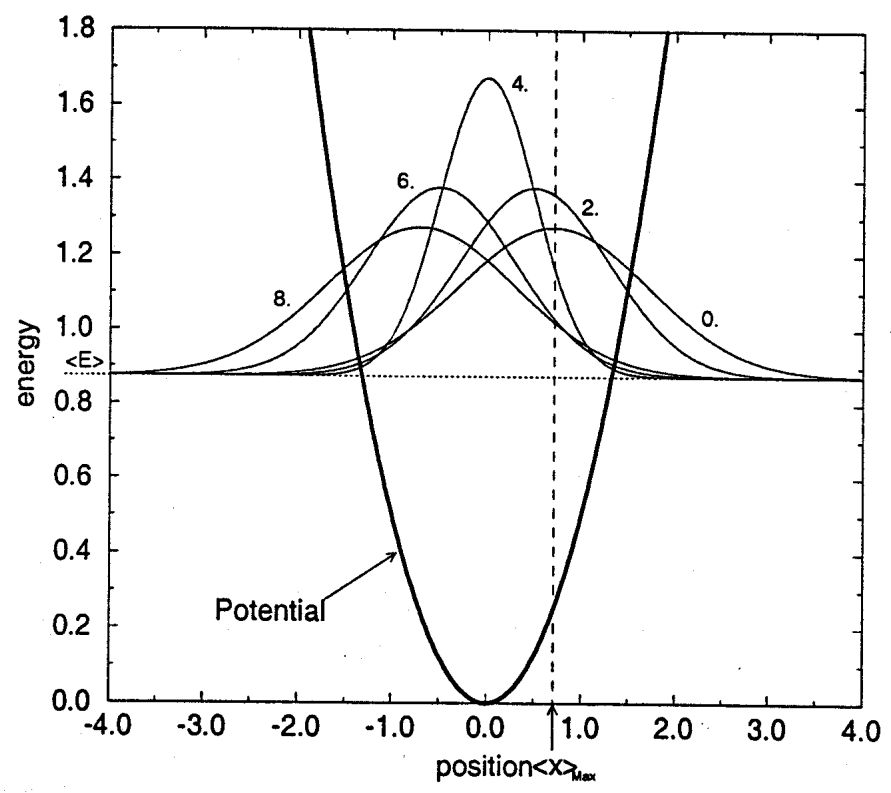
16 samples in each period

solid line is the analytic result of continuous path integral

Time evolution of wave function:



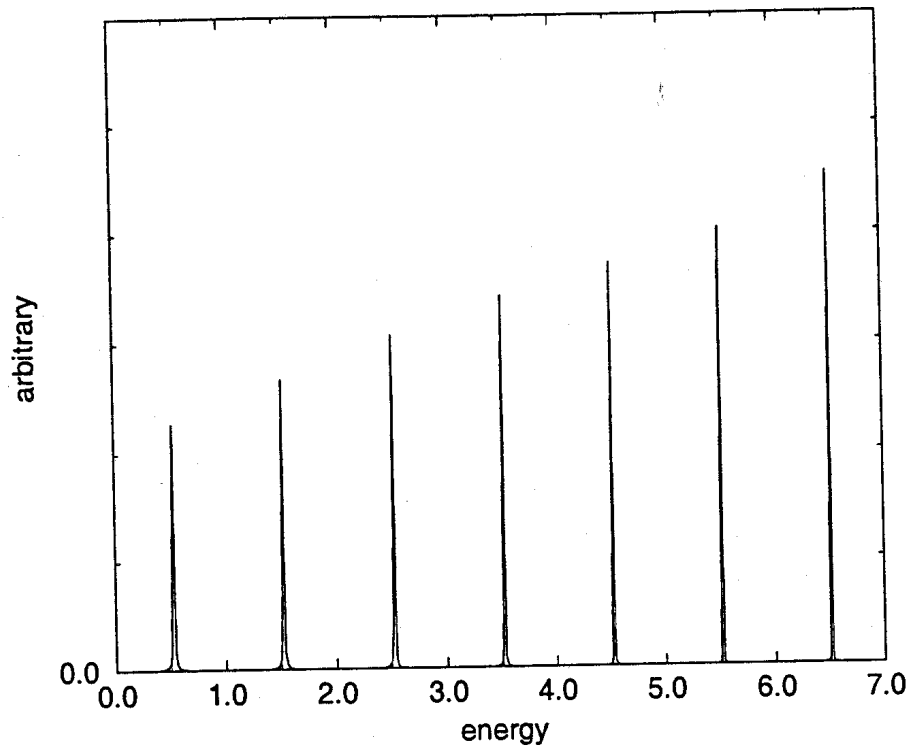
$\alpha = 2$



$\alpha = 0.5$

Energy spectrum (Fourier transformation)

13.



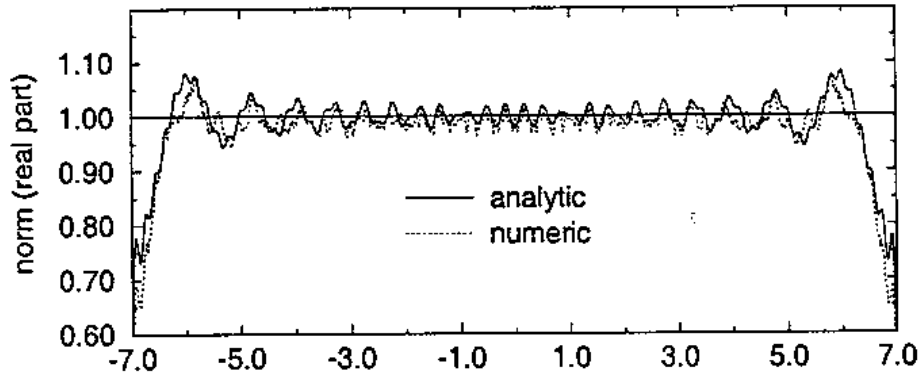
$$E_n = n + \frac{1}{2}$$

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

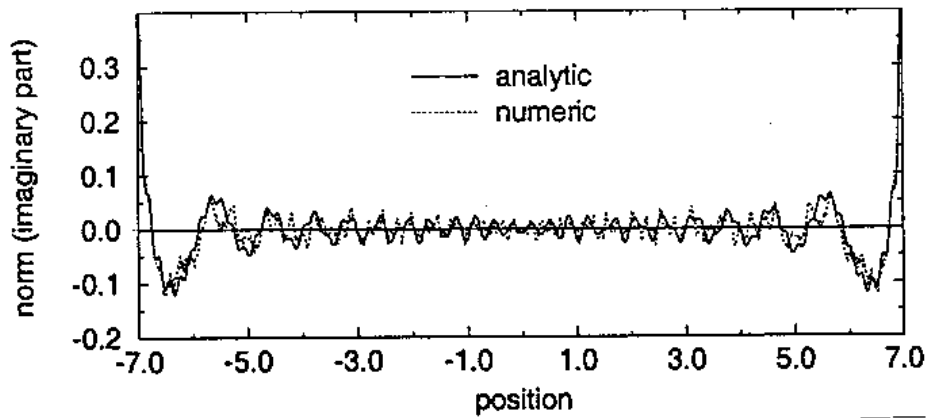
Error of discretization is checked by normalization condition on propagator:

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

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



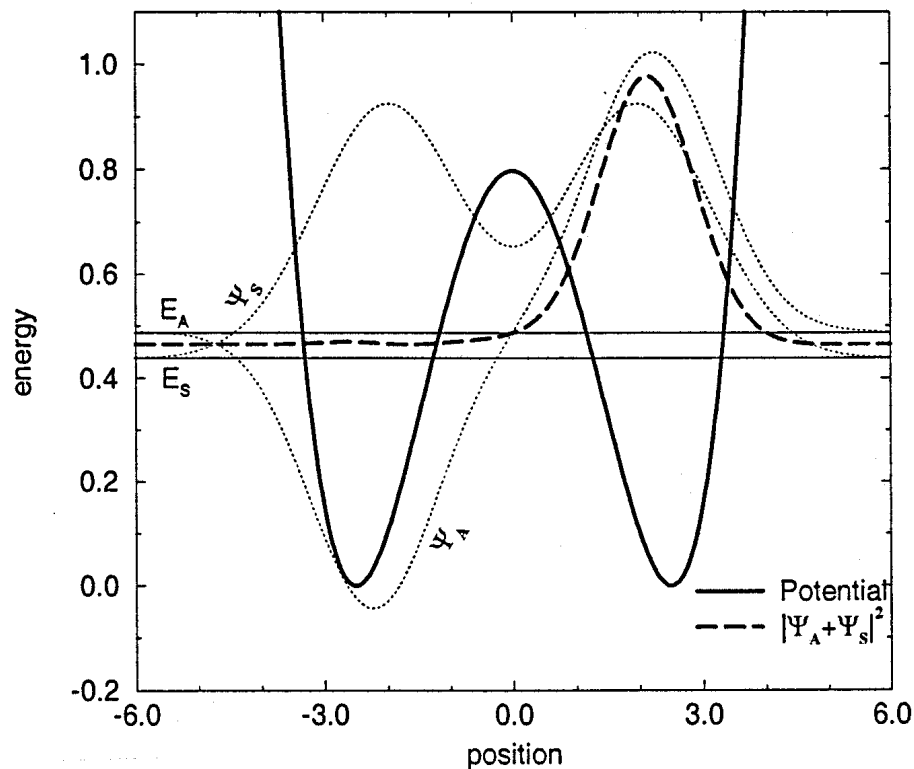
check on error
of spatial resolution



Double Well Potential

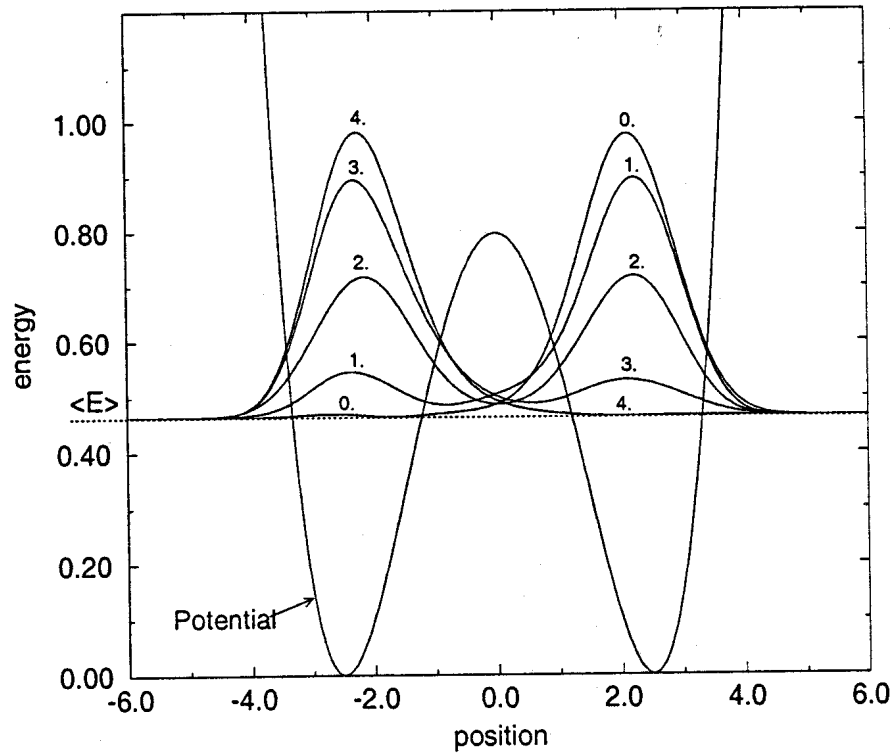
$$L(x, \dot{x}) = \frac{1}{2} \dot{x}^2 - d \left((x - x_{\min})^2 (x + x_{\min})^2 \right)$$

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



wavefunctions

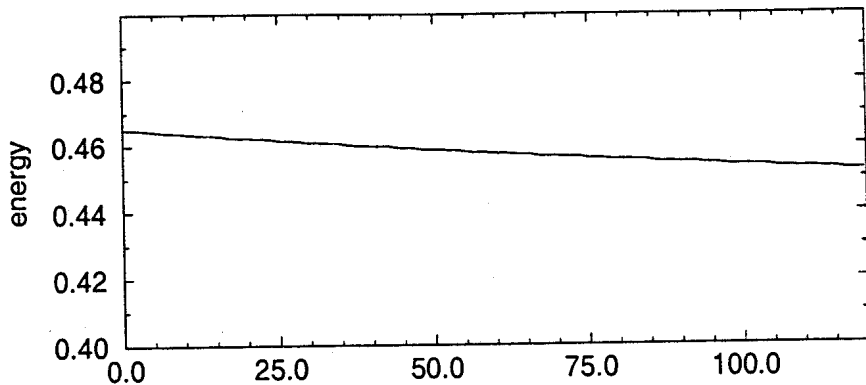
Time evolution :



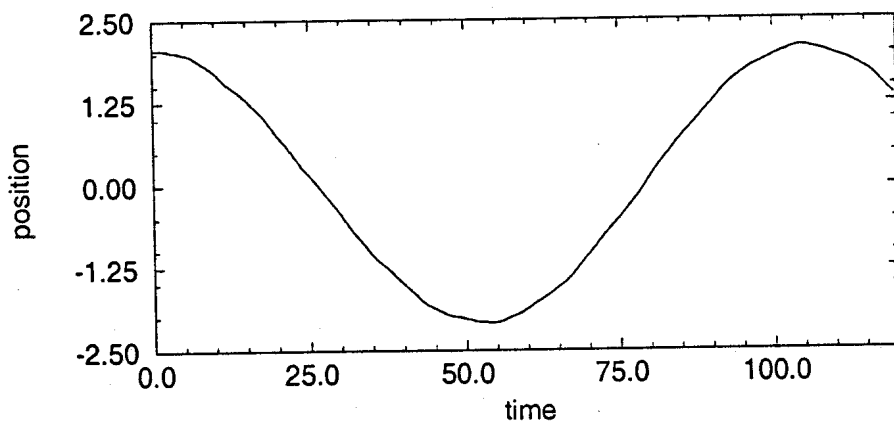
every 55th time
step is plotted

$$\psi_m = \hat{K}^{55} \psi_0$$

$T = 54.4$
hopping time

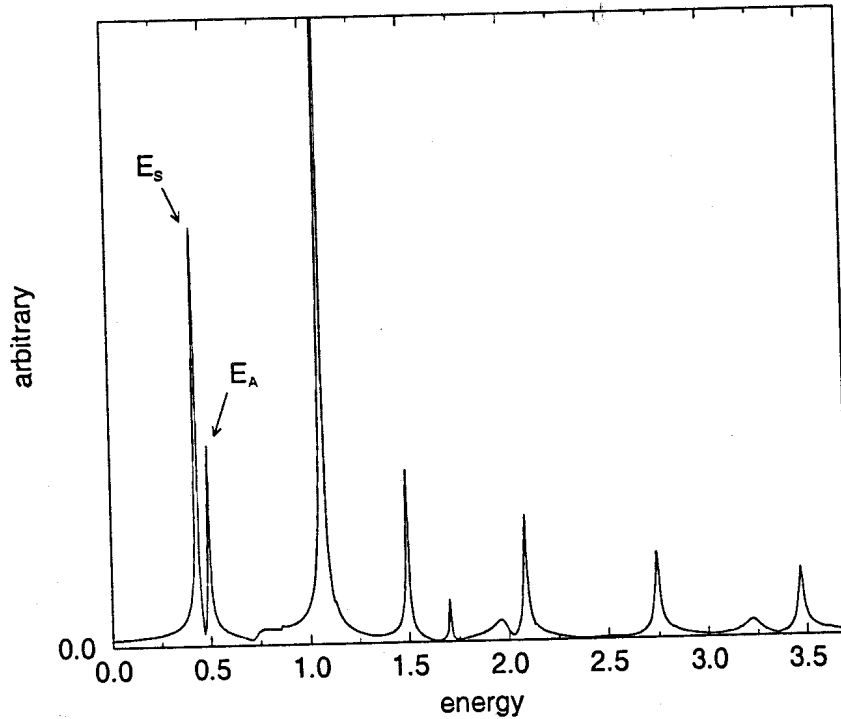


energy



average
position

Energy Spectrum :



↑
peaks occur at $E_S = 0.433$

$$E_A = 0.494$$

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