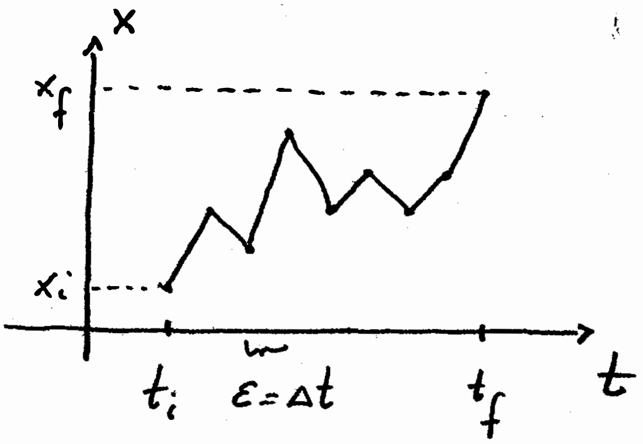
Lectures 3/4/5/6

Feynman Path Integral (continued)



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

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

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

$$\searrow$$

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

Feynman Path Integral

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

zig-zag

Lecture 3/4/5/6

Free particle, harmonic oscillator, Schrodinger equation

Free Particle

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

$i \leftrightarrow a$

$f \leftrightarrow b$

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

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

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

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

$x_0 = x_a\ ,\ t_a = t_0$

$x_N = x_b\ \ t_b = t_N$

Next we multiply this result by

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

and integrate now over x_2 to get:

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

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

$$\left(\frac{m}{2\pi i\hbar\, N\cdot\varepsilon}\right)^{\frac{1}{2}} \; \exp\left[i\frac{m}{2\hbar\, N\cdot\varepsilon}\,(x_N-x_0)^2\right]$$

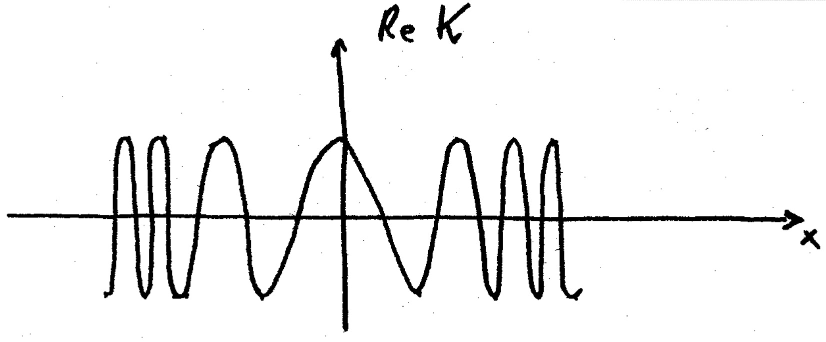
which is identical to the announced result

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

Gaussian

even if α and β are complex

$\mathrm{Re}\,\alpha > 0$ 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:

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

$x \gg \lambda$

$$\lambda = \frac{2\pi\hbar}{m\left(\frac{x}{t}\right)}$$

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:

$$K \sim \exp\left[\frac{i}{\hbar} S_{cl}(b,a)\right]$$

amplitude of particle to arrive at point b

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

$$k = \frac{1}{\hbar} \frac{\partial S_{cl}}{\partial x_b} \longrightarrow p = \hbar k$$

change in phase per unit displacement (wave number)

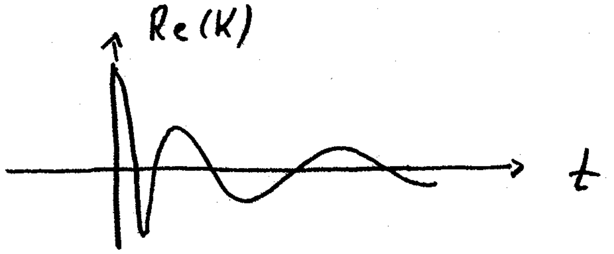
$$k = \frac{2\pi}{\lambda}$$

$$p = \frac{\partial L}{\partial \dot{x}} \qquad \left.\frac{\partial L}{\partial \dot{x}}\right|_{x=x_b} = \frac{\partial S_{cl}}{\partial x_b}$$

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

$p = \frac{h}{\lambda}$ 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

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

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

$$\downarrow$$

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

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 $\sim e^{-i\omega t}$ 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 :

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

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

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

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

$$T = t_b - t_a$$

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

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

reqired to show in hw 2

Proof comes from recursive integration

Schrödinger Equation

rapidly oscillates for large $y-x$

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

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

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

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

integral contributes in $0 \le |\eta| \le \sqrt{\frac{\hbar\varepsilon}{m}}$ range

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

power series

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

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

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

$$\int_{-\infty}^{+\infty} \frac{1}{A} e^{\frac{i m \eta^2}{2\hbar\varepsilon}} \cdot \eta \, d\eta = 0$$

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

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

$$\downarrow$$

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

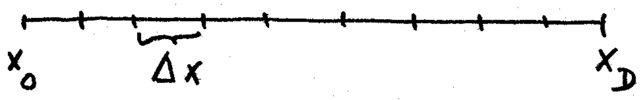
Schrödinger Eq. !

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

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

"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

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

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

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

Harmonic Oscillator

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

$T_0 = 2\pi$ 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 $\psi_0(x)$

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

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

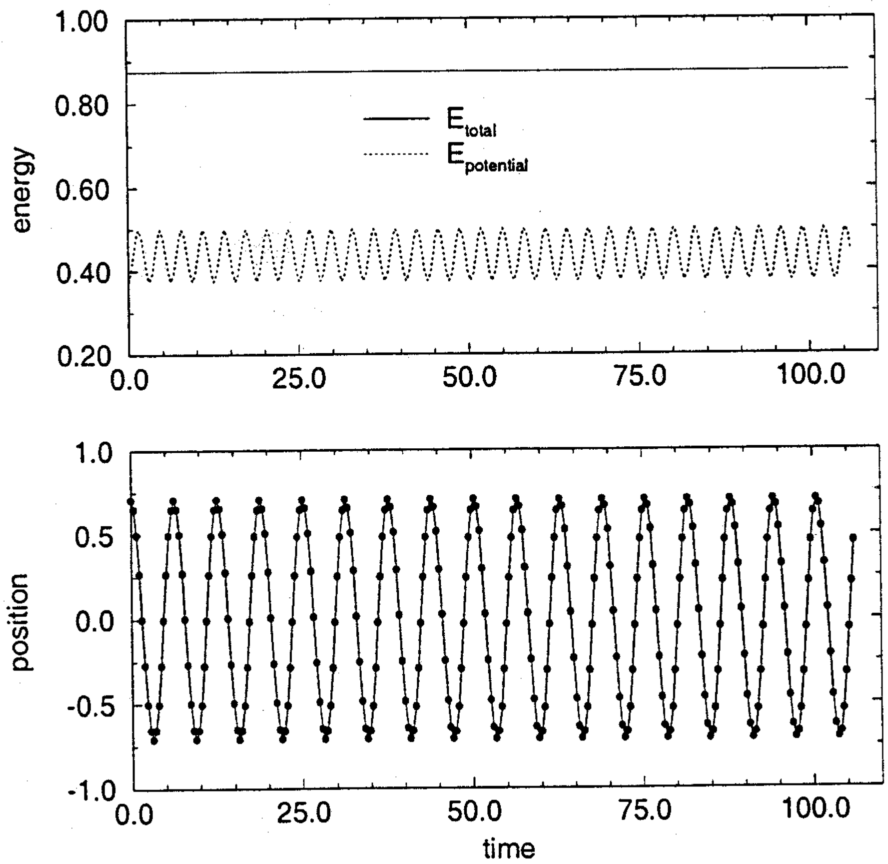
superposition principle for probability amplitudes

Spatial resolution $N_D = 600$

$X_0 = -4$

$X_D = +4$

time evolution becomes matrix multiplication of the propagator matrix



← energy

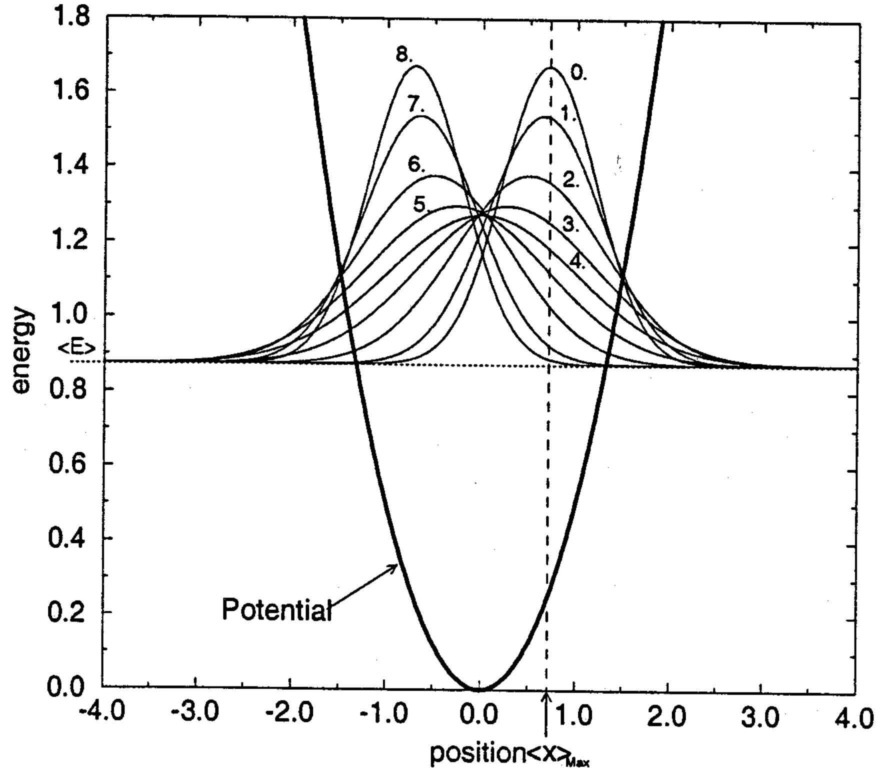
virial theorem is well satisfied

← average position

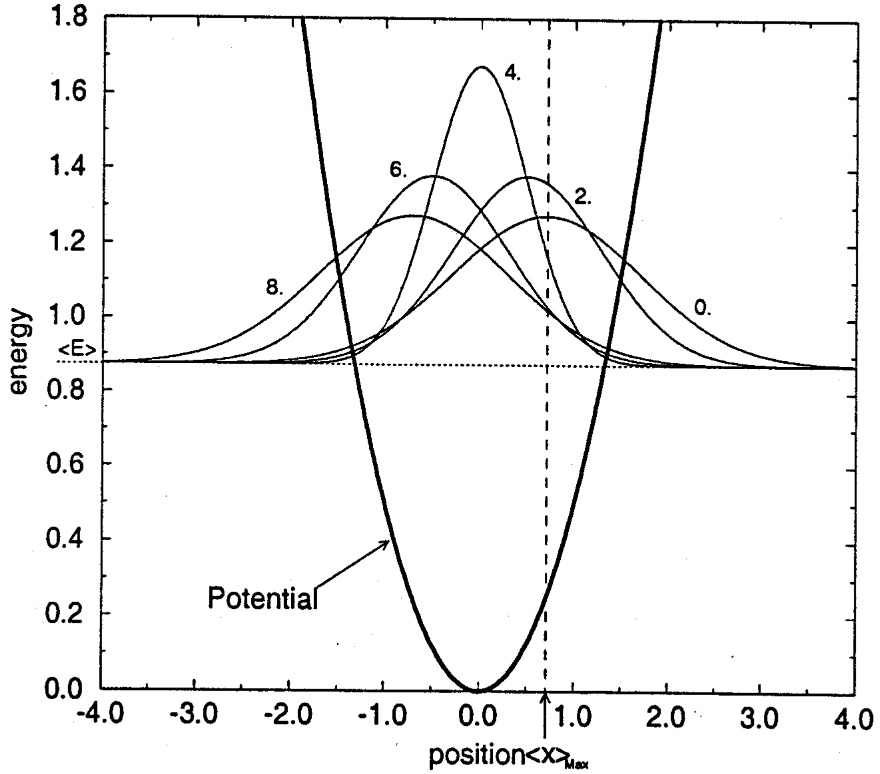
16 samples in each period

solid line is the analytic result of continuum path integral

Time evolution of wave function:

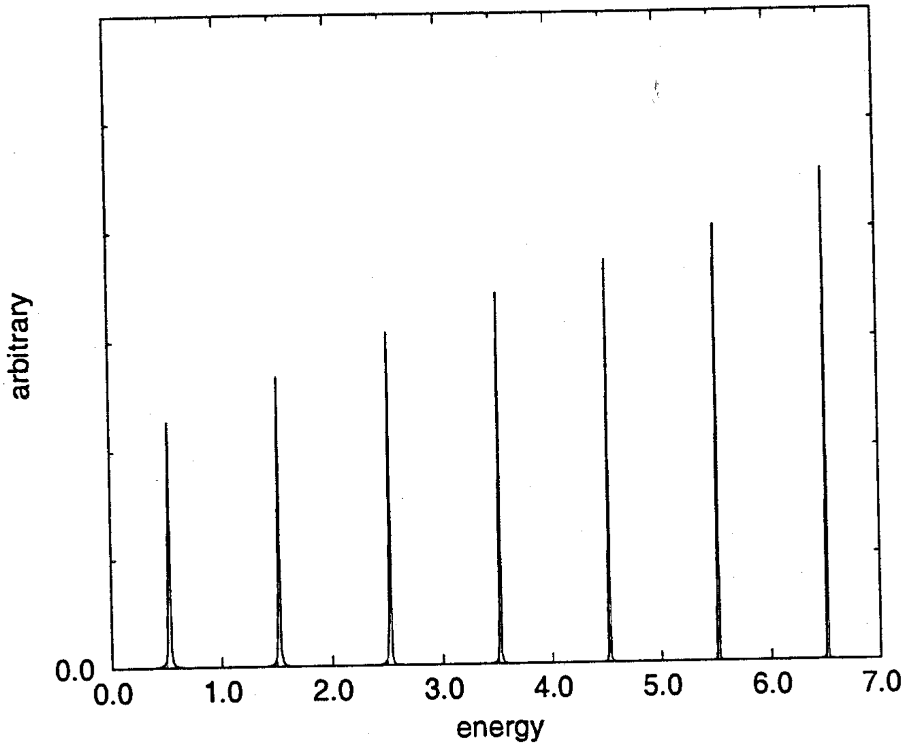


$\alpha = 2$



$\alpha = 0.5$

Energy spectrum (Fourier transformation)



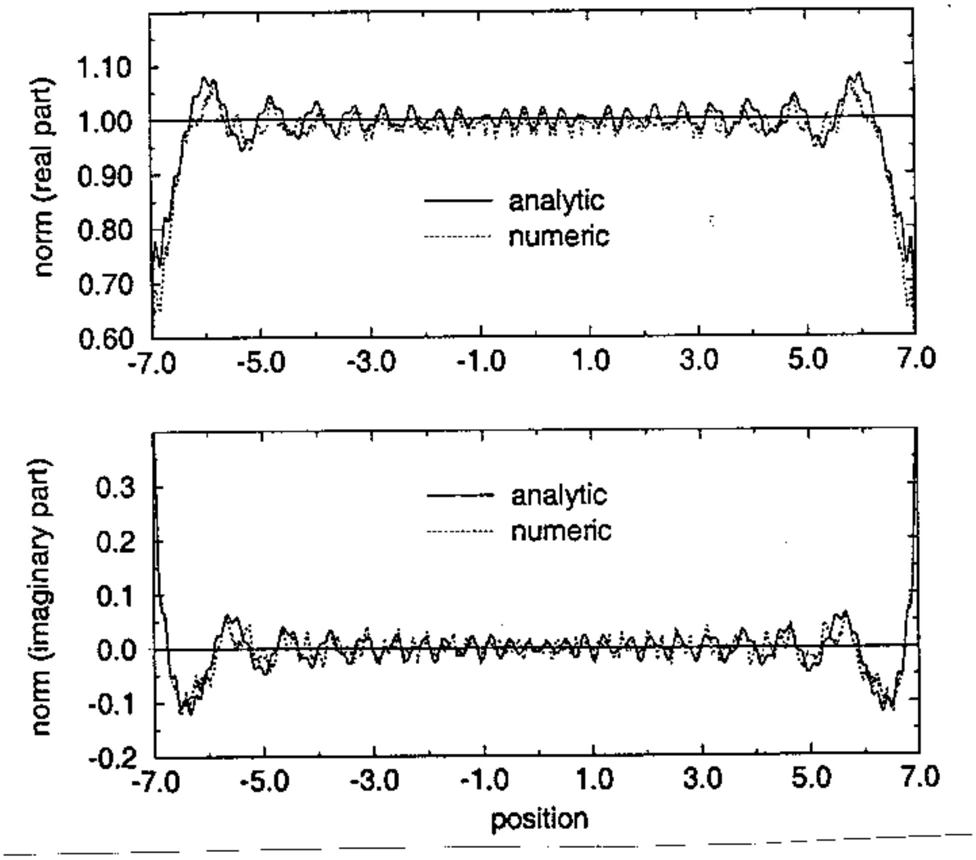
$E_n = n + \frac{1}{2}$

$n = 0, 1, \dots,$

Error of discretization is checked by normalization condition on propagator:

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

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

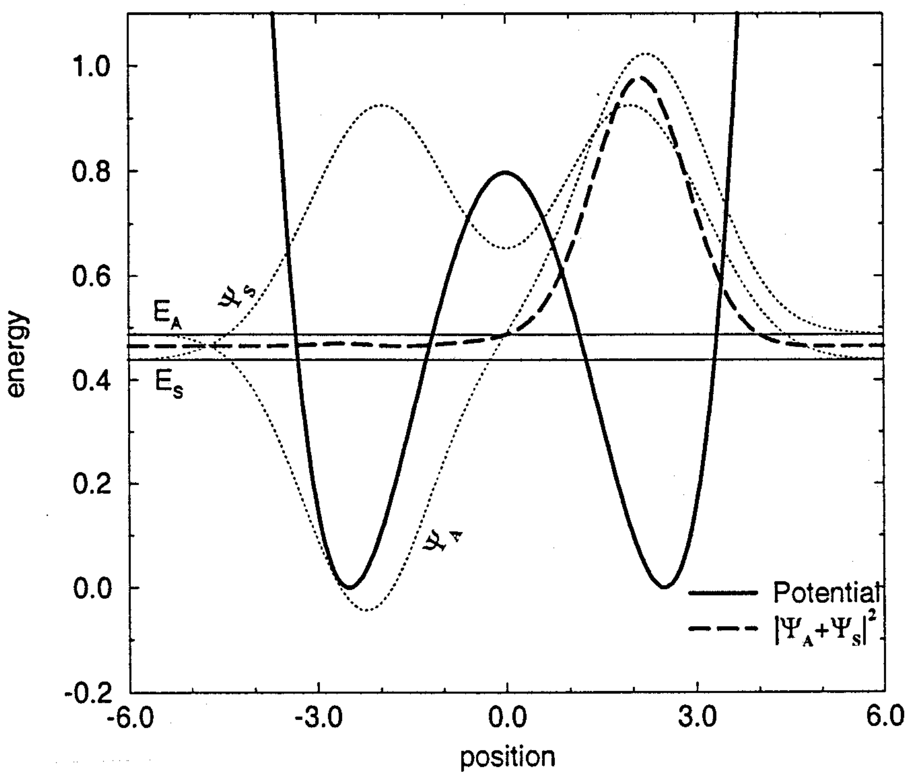


check on error of spatial resolution

Double Well Potential

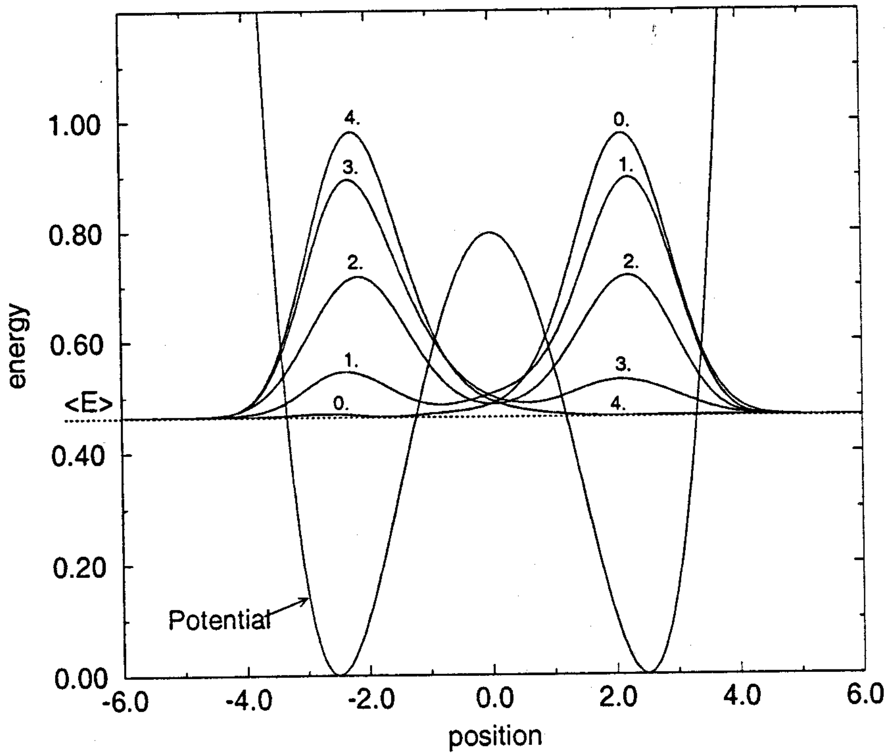
$$L(x, \dot{x}) = \frac{1}{2}\dot{x}^2 - \alpha\,(x - x_{min})^2\,(x + x_{min})^2$$

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



wavefunctions

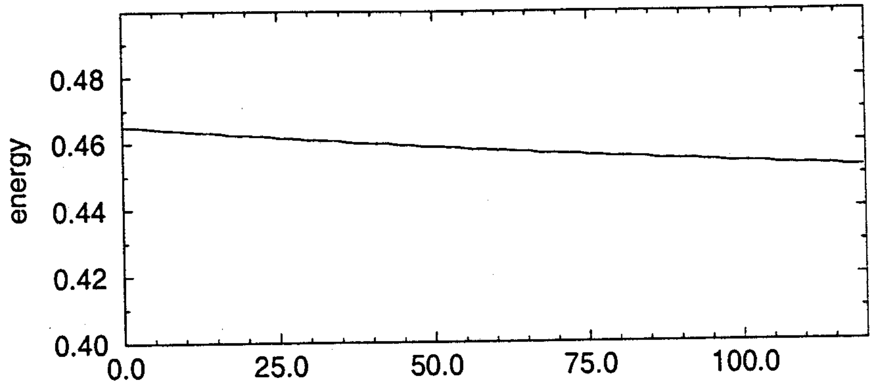
Time evolution :



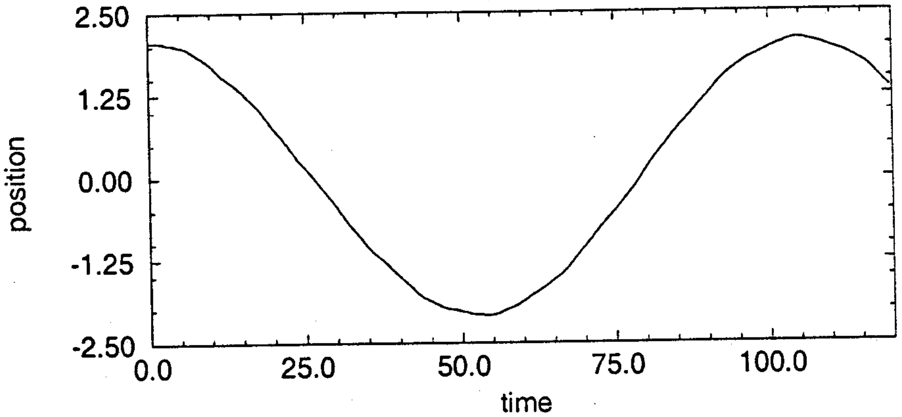
every 55th time step is plotted

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

$T = 54.4$
tunneling time

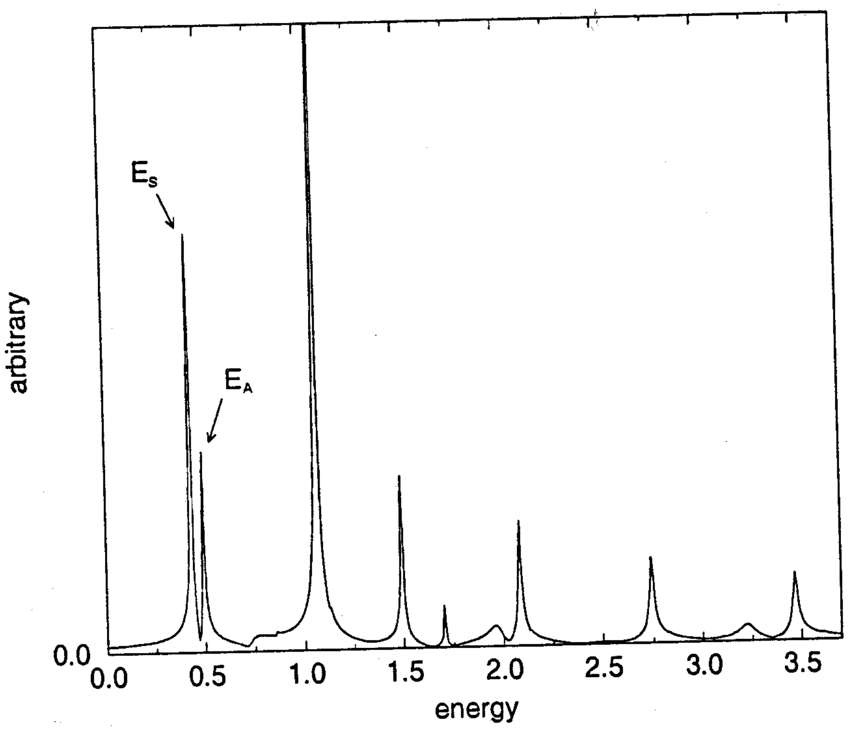


energy



average position

Energy Spectrum :



↑

peaks occur at $E_S = 0.433$

$E_A = 0.494$

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