Quantum dynamics computer assignment 1: wave packet in a box

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I. PARAMETERS

Take a one-dimensional box with $0 < x < a$, where x is the position of the particle and the width of the box is $a = 5\ a_0$. Set the mass of the particle to $\mu = 1\ m_e$. The Hamiltonian in atomic units is given by

$$\hat{H} = -\frac{1}{2}\frac{d^2}{dx^2}. \tag{1}$$

The normalized particle in a box eigen functions (see Fig. 1)are given by

$$\phi_n(x) = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}, \qquad \text{n=1,2,...} \tag{2}$$

The corresponding eigenvalues are

$$E_n = \frac{n^2\pi^2}{2a^2}. \tag{3}$$

Take the normalized initial state χ_0 in the interval $[b, c] = [1, 3]$

$$\chi_0(x) = \sqrt{\frac{2}{3(c-b)}} \left[1 - \cos\left(2\pi\frac{x-b}{c-b}\right)\right] e^{ikx}, \tag{4}$$

and $\chi_0(x) = 0$ otherwise. The momentum $k = 10\ a_0^{-1}$ (see Fig. 2).

Expand the initial state in the basis

$$\chi_0(x) = \sum_{i=1}^{N} c_n\phi_n(x), \tag{5}$$

with $N = 40$. Compute the expectation value of the Hamiltonian

$$E_{\text{av}} = \langle\chi_0|\hat{H}|\chi_0\rangle. \tag{6}$$

Compute the corresponding classical velocity v from

$$E_{\text{av}} = \frac{1}{2}v^2 \tag{7}$$

and the period for one oscillation of a classical particle τ

$$\tau = \frac{2a}{v}. \tag{8}$$

Compute the time dependent wave packet $\Psi(x, t)$ for initial condition

$$\Psi(x, t) = \chi_0(x) \tag{9}$$

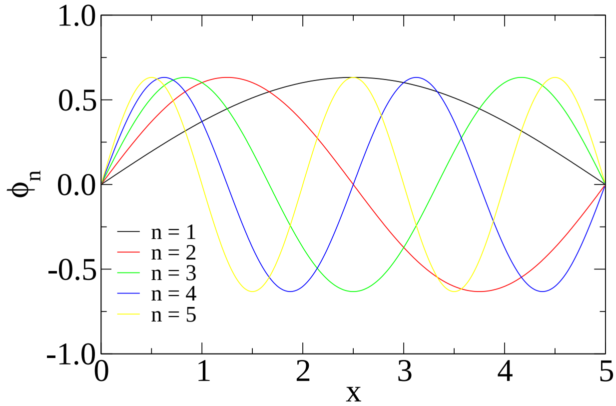

FIG. 1: The first 5 particle in a box functions $\phi_n(x)$

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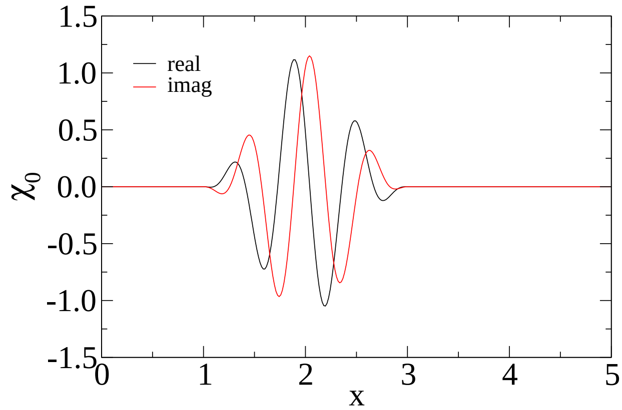

FIG. 2: Real and imaginary parts of initial state $\chi_0(x)$.

for times

$$t_n = \frac{n}{8}\tau, \qquad n = 0, 1, \ldots, 8. \tag{10}$$

as in Fig. 3

Compute the auto correlation function

$$P(t) = \langle\Psi(x, t)|\Psi(x, t = 0)\rangle \tag{11}$$

and plot for $0 < t/\tau < 5$ as in Fig. 4.

Compute the spectrum, i.e., the Fourier transform of the damped auto correlation function

$$\tilde{P}(t) = P(t)e^{-\Gamma|t|}, \tag{12}$$

with $\Gamma = 1$, and

$$F(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \tilde{P}(t)e^{-i\omega t}dt. \tag{13}$$

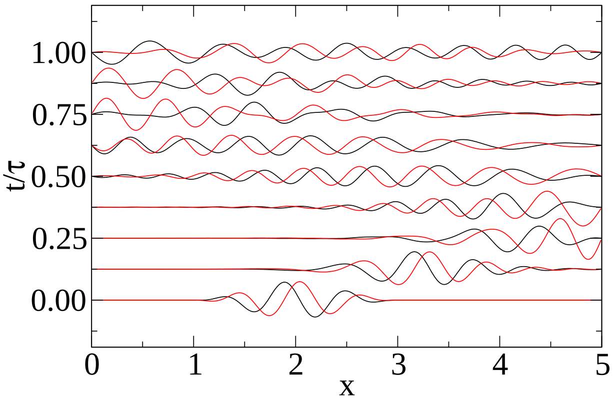

FIG. 3: $\Psi(t_n, x)$ for $n = 0, 1, \ldots, 8$.

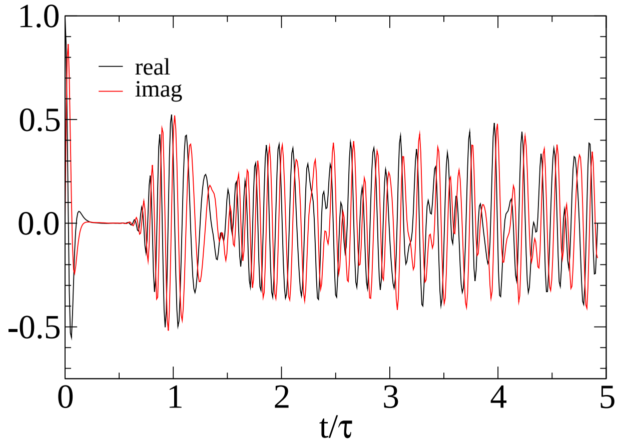

FIG. 4: Auto correlation function $P(t)$.

Also include the stick spectrum as vertical bars at $\hbar\omega = E_n$, with height $|c_n|^2/(\Gamma\sqrt{2\pi})$, as in Fig. 5.

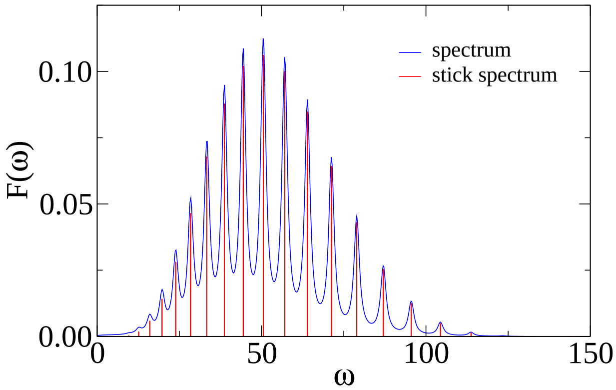

FIG. 5: Spectrum $F(\omega)$ (blue) and stick spectrum (red).