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 $a = 5a_0$. Set the mass of the particle to $\mu = 1 m_e$. The Hamiltonian in atomic units is given by

$$\hat{H} = -\frac{1}{2} \frac{d^2}{dx^2}. \quad (1)$$

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

$$\phi_n(x) = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}, \quad n=1,2,\ldots \quad (2)$$

The corresponding eigenvalues are

$$E_n = \frac{n^2 \pi^2}{2a^2}. \quad (3)$$

Take the normalized initial state $\chi_0(x)$ in the interval $[b, c] = [1, 3]$ \(\chi_0(x) = \sqrt{\frac{2}{3(c-b)}} \left[ 1 - \cos \left( \frac{2\pi x - b}{c-b} \right) \right] e^{ikx}, \quad (4)\)

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

Expand the initial state in the basis $\chi_0(x) = \sum_{i=1}^{N} c_n \phi_n(x), \quad (5)$

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

$$E_{av} = \langle \chi_0 | \hat{H} | \chi_0 \rangle. \quad (6)$$

Compute the corresponding classical velocity $v$ from

$$E_{av} = \frac{1}{2} v^2 \quad (7)$$

and the period for one oscillation of a classical particle $\tau$

$$\tau = \frac{2a}{v}. \quad (8)$$

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

$$\Psi(x,t) = \chi_0(x) \quad (9)$$

for times

$$t_n = \frac{n}{8} \tau, \quad n = 0, 1, \ldots, 8. \quad (10)$$

as in Fig. 3

Compute the auto correlation function

$$P(t) = \langle \Psi(x,t) | \Psi(x,t = 0) \rangle \quad (11)$$

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

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

with $\Gamma = 1$, and

$$F(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \hat{P}(t)e^{-i\omega t} dt. \quad (13)$$
FIG. 3: $\Psi(t_n, x)$ for $n = 0, 1, \ldots, 8$.

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

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

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.