1 Heisenberg Equations of Motion

1.1

\[ \partial_t \langle \hat{x} \rangle = \frac{1}{i} \langle \left[ \hat{x}, \hat{H} \right] \rangle \]
\[ = \frac{1}{i} \langle \left[ \hat{x}, \frac{\hat{p}^2}{2m} \right] + \left[ \hat{x}, \frac{1}{2}m\omega_0^2 \hat{x}^2 \right] \rangle \]
\[ = \frac{1}{2mi} \langle \left[ \hat{x}, \hat{p}^2 \right] \rangle \]
\[ = \frac{1}{m} \hat{p} \tag{1} \]

using equation (10) from the problem set to get to the final line.

1.2

\[ \partial_t \langle \hat{p} \rangle = \frac{1}{i} \langle \left[ \hat{p}, \hat{H} \right] \rangle \]
\[ = \frac{1}{i} \langle \left[ \hat{p}, \frac{\hat{p}^2}{2m} \right] + \left[ \hat{p}, \frac{1}{2}m\omega_0^2 \hat{x}^2 \right] \rangle \]
\[ = \frac{1}{2i}m\omega_0^2 \langle \left[ \hat{x}, \hat{p}^2 \right] \rangle \]
\[ = -m\omega_0^2 \langle \hat{x} \rangle \tag{2} \]

using equation (14) for the last line.

1.3

We have the coupled equations:

\[ \dot{X} = \frac{1}{m} P, \tag{3} \]
\[ \dot{P} = -m\omega_0^2 X. \tag{4} \]
Taking a time derivative of the first equation, and then substituting in the second equation, we obtain a second order differential equation for $X$:

$$
\ddot{X} = \frac{1}{m} \dot{P}
$$

$$
= -\omega_0^2 X. \tag{5}
$$

This equation has solution:

$$
X = X_0 \cos(\omega_0 t + \phi), \tag{7}
$$

and for $P$:

$$
P = -\omega_0 m X_0 \sin(\omega_0 t + \phi). \tag{8}
$$

2 Gross-Pitaevskii Equation

2.1

Making the substitution, we get:

$$
i\hbar \partial_t \left( f e^{i\phi} \right) = -\frac{\hbar^2}{2m} \partial_x^2 \left( f e^{i\phi} \right) + V(x) f e^{i\phi} + \hbar N f^3 e^{i\phi} \tag{9}
$$

$$
i\hbar \left( \dot{f} + i f \dot{\phi} \right) e^{i\phi} = -\frac{\hbar^2}{2m} \partial_x \left[ \left( f' + i \phi' f \right) e^{i\phi} \right] + V f e^{i\phi} + gN f^3 e^{i\phi} \tag{10}
$$

$$
\left( i\hbar \ddot{f} - \hbar f \dot{\phi} \right) e^{i\phi} = -\frac{\hbar^2}{2m} \left( f'' + i \phi'' f + 2i \phi' f' - \phi'^2 f \right) e^{i\phi} + V f e^{i\phi} + gN f^3 e^{i\phi} \tag{11}
$$

$$
\frac{\hbar}{2m} \left( f'' + i \phi'' f + 2i \phi' f' - \phi'^2 f \right) e^{i\phi} + V f + gN f^3, \tag{12}
$$

where a dot indicates a time derivative, and a prime indicates an $x$ derivative. The real part gives:

$$
\hbar \dot{f} \dot{\phi} = \frac{\hbar^2}{2m} \left( f'' - \phi'^2 f \right) - V f - gN f^3, \tag{13}
$$

while the imaginary part gives:

$$
\dot{f} = -\frac{\hbar}{2m} \left( \phi'' f + 2\phi' f' \right). \tag{14}
$$

2.2

Multiplying Eq. (14) by $f$ gives:

$$
\dot{f} f = -\frac{\hbar}{2m} \left( \phi'' f^2 + 2\phi' f' f \right)
$$

$$
\frac{1}{2} \partial_x (f^2) = -\partial_x \left( \frac{\hbar}{2m} f^2 \phi' \right). \tag{15}
$$

This has the form of the continuity equation:

$$
\partial_t \rho = -\nabla \cdot (\rho \vec{u}) \tag{16}
$$
if we make the identifications:
\[ \rho = f^2, \quad v_x = \frac{\hbar}{m} \partial_x \phi. \] (17)

In other words, the modulus squared behaves as a (probability) density, with the spatial variation of the phase measuring its ‘fluid velocity’.

2.3

The \( x \) derivative of Eq. (22) of the homework is given by:
\[ \partial_t \phi' = -\frac{\hbar}{2m} \partial_x (\phi'^2) + \frac{\hbar}{2m} \frac{\partial^2 f}{f} - \frac{V}{\hbar} - \frac{g_n}{\hbar}. \] (18)

Replacing \( \phi' \) by \( \frac{v}{\hbar} \) from Eq. (17), and multiplying by a factor of \( \hbar/m \), gives:
\[ \partial_t v(x, t) + \frac{1}{2} \partial_x (v^2) + \partial_x \left( \frac{V(x)}{m} + \frac{gn(x)}{m} - \frac{\hbar^2}{2m^2} \frac{f''}{f} \right). \] (19)

Therefore, we have that the pressure is given by the final term:
\[ p(x, t) = \frac{V(x)}{m} + \frac{gn(x)}{m} - \frac{\hbar^2}{2m^2} \frac{f''}{f}. \] (20)

3 Boundary Conditions

3.1

The solution is given by:
\[ \psi(x) = \sin(kx), \quad \text{with} \quad k = \frac{n\pi}{L}, \quad n = 1, 2, 3, \ldots \] (21)

for integer \( n \geq 1 \). The general solution has a cos piece as well as a sin piece, but the boundary conditions kill the cos. Plugging this into Schrodinger’s equation gives:
\[ E_n = \frac{\hbar^2}{2m} k^2 = \frac{\hbar^2}{2m} \left( \frac{n\pi}{L} \right)^2, \] (22)

and so the first five Eigenvalues are
\[ E = \frac{\hbar^2 \pi^2}{2mL^2} \times \{1, 4, 9, 16, 25\}. \] (23)

3.2

This time, the solutions are:
\[ \psi(x) = e^{ikx}, \quad \text{with} \quad k = \pm \frac{2n\pi}{L}, \quad n = 0, 1, 2, 3, \ldots. \] (24)
Note that compared with the previous solution: (a) there is a zero mode with zero energy, and (b) the excited modes are twofold degenerate. This last fact corresponds to the presence of clockwise and anti-clockwise travelling modes. The first five modes have energies:

\[ E = 4 \frac{\hbar^2 \pi^2}{2mL^2} \times \{0, 1, 1, 4, 4\} \tag{25} \]

**Aside: zero modes and degeneracy**

In order to understand why there is no \( n = 0 \) mode in the hard boundary case, consider what would be the corresponding eigenfunction:

\[ \psi_{n=0}^{\text{hard}} = \sin(0x) = 0. \tag{26} \]

This is clearly not a normalizable state: it is not a state at all. Therefore, the energy levels of the hard box start at \( n = 1 \). In the periodic case, the zero mode is:

\[ \psi_{n=0}^{\text{periodic}} = e^{i0x} = \text{const.} \tag{27} \]

This is normalizable, and satisfies Schrodinger’s equation with \( E = 0 \). It is therefore the lowest lying energy state of the particle on a ring.

The reason that the hard box does not have degenerate states is that the states \( \pm n \) differ only by a constant phase:

\[ \sin \left( -\frac{n\pi x}{L} \right) = -\sin \left( \frac{n\pi x}{L} \right) = e^{i\pi} \sin \left( \frac{n\pi x}{L} \right). \tag{28} \]

They are therefore the same state. On the other hand, in the periodic case there are two distinct states for each non-zero energy that cannot be related simply by multiplication by a phase:

\[ e^{ikx} \neq e^{i\phi} e^{-ikx}. \tag{29} \]

These are therefore distinct states that can be distinguished, for example, by measuring the angular momentum.

### 3.3

We have that:

\[ \frac{\psi_1 - \psi_2}{2i} = \frac{e^{ikx} + e^{-ikx}}{2i} = \cos(kx). \tag{30} \]

This also satisfies the Schrodinger equation, with \( E = \hbar^2 k^2 / 2m \):

\[ -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \cos(kx) = \frac{\hbar^2 k^2}{2m} \cos(kx). \tag{31} \]
3.4

We have that:

\[ E_{\text{periodic}} = \frac{2\hbar^2 \pi^2}{L^2 m} (0 + 1 + 1 + 4 + 4) = 20 \frac{\hbar^2 \pi^2}{L^2 m} \] (32)

\[ E_{\text{hard}} = \frac{\hbar^2 \pi^2}{2L^2 m} (1 + 4 + 9 + 16 + 25) = \frac{55 \hbar^2 \pi^2}{2 L^2 m}, \] (33)

and therefore:

\[ \frac{E_{\text{periodic}} - E_{\text{hard}}}{E_{\text{periodic}} + E_{\text{hard}}} = \frac{40 - 55}{40 + 55} = -\frac{3}{19} \approx -\frac{1}{6}. \] (34)

4 Finite Differences in Time  Part 2

4.1

Starting from:

\[ i\hbar \partial_t \begin{pmatrix} \psi_0(t) \\ \psi_1(t) \end{pmatrix} = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} \psi_0(t) \\ \psi_1(t) \end{pmatrix}, \] (35)

we use Eq. (28) of the homework to get:

\[ i\hbar \frac{\delta t}{\delta t} \begin{pmatrix} \psi_0(t) - \psi_0(t - \delta t) \\ \psi_1(t) - \psi_1(t - \delta t) \end{pmatrix} = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} \psi_0(t) \\ \psi_1(t) \end{pmatrix}. \] (36)

Multiply through be \(-i\delta t/\hbar\) and rearrange terms to get:

\[ \begin{pmatrix} 0 - \frac{i\delta t}{\hbar} & \frac{i\delta t}{\hbar} \\ -\frac{i\delta t}{\hbar} & 0 \end{pmatrix} \begin{pmatrix} \psi_0(t) \\ \psi_1(t) \end{pmatrix} + \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \psi_0(t) \\ \psi_1(t) \end{pmatrix} = \begin{pmatrix} \psi_0(t - \delta t) \\ \psi_1(t - \delta t) \end{pmatrix}. \] (37)

\[ \begin{pmatrix} 1 & -\frac{i\delta t}{\hbar} \\ -\frac{i\delta t}{\hbar} & 1 \end{pmatrix} \begin{pmatrix} \psi_0(t) \\ \psi_1(t) \end{pmatrix} = \begin{pmatrix} \psi_0(t - \delta t) \\ \psi_1(t - \delta t) \end{pmatrix}. \] (38)

Therefore:

\[ \mathbb{W} = \begin{pmatrix} 1 & -\frac{i\delta t}{\hbar} \\ -\frac{i\delta t}{\hbar} & 1 \end{pmatrix}. \] (39)

4.2

Finding the eigenvalues \( s \) amounts to solving the determinant equation:

\[ \begin{vmatrix} 1 - s & -\frac{i\delta t}{\hbar} \\ -\frac{i\delta t}{\hbar} & 1 - s \end{vmatrix} = 0 \] (40)

\[ (1 - s)^2 + \frac{\delta t^2}{\hbar} = 0 \] (41)

\[ s^2 - 2s + 1 + \frac{\delta t^2}{\hbar} = 0 \] (42)
and so:

\[ s = 1 + i \frac{\delta t}{\hbar}, \quad s' = 1 - i \frac{\delta t}{\hbar}, \]

(43)
to first order in \( \delta t \). Now we wish to solve:

\[
\begin{pmatrix}
1 & -i \frac{\delta t}{\hbar} \\
-i \frac{\delta t}{\hbar} & 1
\end{pmatrix}
\begin{pmatrix}
a_0 \\
a_1
\end{pmatrix}
= \begin{pmatrix}
1 + i \frac{\delta t}{\hbar}
\end{pmatrix}
\begin{pmatrix}
a_0 \\
a_1
\end{pmatrix}.
\]

(44)

This has solution:

\[
\begin{pmatrix}
a_0 \\
a_1
\end{pmatrix}
= \begin{pmatrix} 1 \\ -1 \end{pmatrix}.
\]

(45)

Similarly, the Eigenvector equation:

\[
\begin{pmatrix}
1 & -i \frac{\delta t}{\hbar} \\
-i \frac{\delta t}{\hbar} & 1
\end{pmatrix}
\begin{pmatrix}
b_0 \\
b_1
\end{pmatrix}
= \begin{pmatrix}
1 - i \frac{\delta t}{\hbar}
\end{pmatrix}
\begin{pmatrix}
b_0 \\
b_1
\end{pmatrix}.
\]

(46)

has solution:

\[
\begin{pmatrix}
b_0 \\
b_1
\end{pmatrix}
= \begin{pmatrix} 1 \\ 1 \end{pmatrix}.
\]

(47)

4.3

We are given:

\[
\begin{pmatrix}
\psi_0(0) \\
\psi_1(0)
\end{pmatrix}
= \begin{pmatrix} 1 \\ 0 \end{pmatrix}
= \frac{1}{2} \begin{pmatrix} 1 \\ 1 \end{pmatrix} + \frac{1}{2} \begin{pmatrix} 1 \\ -1 \end{pmatrix}.
\]

(48)

We therefore have \( A = B = 1/2 \).

4.4

Putting everything together, and using Eq. (37) of the homework, we arrive at:

\[
\begin{pmatrix}
\psi_0(N\delta t) \\
\psi_1(N\delta t)
\end{pmatrix}
= \frac{1}{2} \left( 1 - i \frac{\delta t}{\hbar} \right)^{-N} \left( 1 + i \frac{\delta t}{\hbar} \right)^{-N} + \frac{1}{2} \left( 1 - i \frac{\delta t}{\hbar} \right)^{-N} \left( 1 + i \frac{\delta t}{\hbar} \right)^{-N}.
\]

(49)

4.5

4.6

With forward Euler the overall probability gradually increased with time, violating unitarity (conservation of probability). We can see that backward Euler has a steadily decreasing overall probability.
Figure 1: Blue: Exact solution; Orange: backwards Euler approximation with $\delta t = 0.1$

Figure 2: Blue: Exact solution; Orange: backwards Euler approximation with $\delta t = 0.01$