# Principles of Quantum Mechanics

SECOND EDITION

SOLUTION MANUAL

R. Shankar

# Preface

This solution manual is a dedicated companion to the renowned textbook Principles of Quantum Mechanics by R. Shankar. It is designed to provide clear and comprehensive solutions to the problems presented in the original work, aiding students, researchers, and enthusiasts in their pursuit of understanding quantum mechanics.

Quantum mechanics, as a cornerstone of modern physics, challenges intuition with its abstract principles and intricate mathematical framework. The problems in R. Shankar's text are carefully crafted to deepen comprehension and enhance problem-solving skills. This manual seeks to complement that effort by providing detailed and accessible solutions, bridging the gap between theoretical concepts and practical application.

This work is created with the intention of supporting readers at all levels, whether they are delving into quantum mechanics for the first time or revisiting its concepts with a fresh perspective. While every effort has been made to ensure the accuracy and clarity of the solutions, mistakes can occasionally occur.

If you identify any errors or have suggestions for improvement, please do not hesitate to contact me at

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Updates and corrections to this manual will be made available at

https://xumin-liang.net

I hope that this manual serves as a helpful resource, making the journey through quantum mechanics both engaging and rewarding.

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# Contents

# Chapter 1

# Mathematical Introduction

## 1.1 Linear Vector Spaces: Basics

**Exercise 1.1.1.** Verify these claims. For the first consider $|0\rangle + |0'\rangle$ and use the advertised properties of the two null vectors in turn. For the second start with $|0\rangle = (0+1)|V\rangle + |-V\rangle$. For the third, begin with $|V\rangle + (-|V\rangle) = 0|V\rangle = |0\rangle$. For the last, let $|W\rangle$ also satisfy $|V\rangle + |W\rangle = |0\rangle$. Since $|0\rangle$ is unique, this means $|V\rangle + |W\rangle = |V\rangle + |-V\rangle$. Take it from here.

**Solution.**

(1) $|0\rangle$ is unique.

*Proof.* For an arbitrary state ket $|V\rangle$,

(a) $|V\rangle + |0\rangle = |V\rangle$

(b) $|V\rangle + |0'\rangle = |V\rangle$

Set $|V\rangle = |0'\rangle$ in (i) $\Rightarrow |0'\rangle + |0\rangle = |0'\rangle$;
Set $|V\rangle = |0\rangle$ in (ii) $\Rightarrow |0\rangle + |0'\rangle = |0\rangle$; Therefore, by commutativity of vector addition, we have

$$|0'\rangle = |0'\rangle + |0\rangle = |0\rangle + |0'\rangle = |0\rangle$$

□

(2) $0|V\rangle = |0\rangle$

*Proof.* $1|V\rangle = (1+0)|V\rangle = 1|V\rangle + 0|V\rangle$, where $1|V\rangle = |V\rangle$. Therefore

$$|V\rangle = |V\rangle + 0|V\rangle$$

Since $|V\rangle$ is arbitrary here, compared with the definition of $|0\rangle$, which is $|V\rangle + |0\rangle = |V\rangle$ for any $|V\rangle$, plus $|0\rangle$ is unique, we can conclude that

$$0|V\rangle = |0\rangle.$$

□

(3) $|-V\rangle = -|V\rangle$

*Proof.* For arbitrary $|V\rangle$,

$$|V\rangle + (-|V\rangle) = 0|V\rangle = |0\rangle.$$

By definition of $|-V\rangle$, which is $|V\rangle + |-V\rangle = 0$, we can conclude that

$$|-V\rangle = -|V\rangle.$$

□

(4) $|-V\rangle$ is the unique addtive inverse of $|V\rangle$.

*Proof.* Suppose there exists another vector $|W\rangle$, satisfying $|W\rangle = -|V\rangle$, then

$$\begin{aligned}|V\rangle + |W\rangle &= |V\rangle - |V\rangle \\ &= (1-1)|V\rangle \\ &= 0|V\rangle \\ &= |0\rangle\end{aligned}$$

Add $|-V\rangle$ on the both sides, we have

$$\begin{aligned}|V\rangle + |W\rangle + |-V\rangle &= |0\rangle + |-V\rangle \\ |W\rangle + (|V\rangle + |-V\rangle) &= |-V\rangle \\ |W\rangle + |0\rangle &= |-V\rangle\end{aligned}$$

Therefore,

$$|W\rangle = |-V\rangle$$

□

**Exercise 1.1.2.** Consider the set of all entities of the form $(a, b, c)$ where the entries are real numbers. Addition and scalar multiplication are defined as follows:

$$\begin{aligned}(a, b, c) + (d, e, f) &= (a + d, b + e, c + f) \\ \alpha(a, b, c) &= (\alpha a, \alpha b, \alpha c).\end{aligned}$$

Write down the null vector and inverse of $(a, b, c)$. Show that vectors of the form $(a, b, 1)$ do not form a vector space.

**Solution.**

- Null vector of $(a, b, c)$: By definition, for any $|V\rangle$,

$$|V\rangle + |0\rangle = |V\rangle.$$

Set $|0\rangle = (a_0, b_0, c_0)$, $|V\rangle = (a, b, c)$, where $a, b, c$ are arbitrary numbers. Then

$$\begin{aligned}|0\rangle + |V\rangle &= (a_0, b_0, c_0) + (a, b, c) \\ &= (a_0 + a, b_0 + b, c_0 + c) \\ &= |V\rangle \\ &= (a, b, c)\end{aligned}$$

$$\Rightarrow \begin{cases} a_0 + a = a \\ b_0 + b = b \\ c_0 + c = c \end{cases} \Rightarrow \begin{cases} a_0 = 0 \\ b_0 = 0 \\ c_0 = 0 \end{cases}$$

Therefore, the null vector of $(a, b, c)$ is $(0, 0, 0)$.

- Inverse vector of $(a, b, c)$: Suppose the inverse vector of $(a, b, c)$ is $(\bar{a}, \bar{b}, \bar{c})$. By definition,

$$(a, b, c) + (\bar{a}, \bar{b}, \bar{c}) = |0\rangle = (0, 0, 0)$$

$$(a + \bar{a}, b + \bar{b}, c + \bar{c}) = (0, 0, 0)$$

$$\Rightarrow \begin{cases} a + \bar{a} = 0 \\ b + \bar{b} = 0 \\ c + \bar{c} = 0 \end{cases} \Rightarrow \begin{cases} \bar{a} = -a \\ \bar{b} = -b \\ \bar{c} = -c \end{cases}$$

Therefore, the inverse vector of $(a, b, c)$ is $(-a, -b, -c)$.

- $\{(a, b, 1)\}$ does not form a vector space since
  (a) It violates the closure under addition, i.e.

$$(a_1, b_1, 1) + (a_2, b_2, 1) = (a_1 + a_2, b_1 + b_2, 2) \notin \{(a, b, 1)\}.$$

  (b) It violates the closure under scalar multiplication, i.e.

$$\omega(a_1, b_1, 1) = (\omega a_1, \omega b_1, \omega) \notin \{(a, b, 1)\}$$

  as long as $\omega \neq 1$.

  (c) There is no null vector, i.e.

$$(0, 0, 0) \notin \{(a, b, 1)\}.$$

  (d) The inverse does not exist, i.e.

$$(-a, -b, -1) \notin \{(a, b, 1)\}$$

**Exercise 1.1.3.** Do functions that vanish at the end points $x = 0$ and $x = L$ form a vector space? How about periodic functions obeying $f(0) = f(L)$ ? How about functions that obey $f(0) = 4$ ? If the functions do not qualify, list the things that go wrong.

**Solution.**

(1) $\{f(x)\}$, $f(0) = f(L) = 0$, form a vector space.

(2) $\{f(x)\}$, periodic functions obeying $f(0) = f(L)$, form a vector space. If you want to prove the property of closure in this problem, please mention that $f(x) + g(x)$ and $\alpha f(x)$ are also periodic functions. That is, $f(0) + g(0) = f(L) + g(L)$, $\alpha f(0) = \alpha f(L)$.

(3) $\{f(x)\}$, $f(0) = 4$, do not form a vector space, since

  (a) If $g(x), h(x) \in \{f(x)\}$, then $g(x)+h(x) \notin \{f(x)\}$, since $g(0)+h(0) = 8 \neq 4$.

(b) If $g(x) \in \{f(x)\}$, then $\lambda g(x) \notin \{f(x)\}$, since $\lambda g(0) = 4\lambda \neq 4$, as long as $\lambda \neq 1$.

(c) No null vector. $g(x) \equiv 0 \notin \{f(x)\}$, since $g(0) = 0 \neq 4$.

(d) If $g(x) \in \{f(x)\}$, then the inverse $-g(x) \notin \{f(x)\}$, since $-g(0) = -4 \neq 4$.

**Exercise 1.1.4.** Consider three elements from the vector space of real $2 \times 2$ matrices:

$$|1\rangle = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \quad |2\rangle = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix} \quad |3\rangle = \begin{pmatrix} -2 & -1 \\ 0 & -2 \end{pmatrix}$$

Are they linearly independent? Support your answer with details. (Notice we are calling these matrices vectors and using kets to represent them to emphasize their role as elements of a vector space.)

**Solution.** Suppose $\alpha_1|1\rangle + \alpha_2|2\rangle + \alpha_3|3\rangle = 0$. We have

$$\begin{pmatrix} 0 \cdot \alpha_1 + 1 \cdot \alpha_2 + (-2) \cdot \alpha_3 & 1 \cdot \alpha_1 + 1 \cdot \alpha_2 + (-1) \cdot \alpha_3 \\ 0 \cdot \alpha_1 + 0 \cdot \alpha_2 + 0 \cdot \alpha_3 & 0 \cdot \alpha_1 + 1 \cdot \alpha_2 + (-2) \cdot \alpha_3 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$$

$$\Rightarrow \quad \begin{cases} \alpha_2 - 2\alpha_3 = 0 \\ \alpha_1 + \alpha_2 - \alpha_3 = 0 \end{cases}$$

$$\Rightarrow \quad \begin{cases} \alpha_1 = -\alpha_3 \\ \alpha_2 = 2\alpha_3 \end{cases}$$

It is not necessary for $\alpha_1, \alpha_2$ and $\alpha_3$ to be 0 together. Therefore, $|1\rangle$, $|2\rangle$ and $|3\rangle$ are linearly dependent.

**Exercise 1.1.5.** Show that the following row vectors are linearly dependent: $(1,1,0)$, $(1,0,1)$, and $(3,2,1)$. Show the opposite for $(1,1,0), (1,0,1)$, and $(0,1,1)$.

**Solution.** Suppose $\alpha_1(1,1,0) + \alpha_2(1,0,1) + \alpha_3(3,2,1) = 0$. Then

$$\begin{cases} \alpha_1 + \alpha_2 + 3\alpha_3 = 0 \\ \alpha_1 + 2\alpha_3 = 0 \\ \alpha_2 + \alpha_3 = 0 \end{cases} \quad \Rightarrow \quad \begin{cases} \alpha_1 = -2\alpha_3 \\ \alpha_2 = -\alpha_3 \end{cases}$$

When $\alpha_3 \neq 0$. $\alpha_1, \alpha_2, \alpha_3$ can have non-zero values. Therefore, $(1,1,0)$, $(1,0,1)$, $(3,2,1)$ are linearly dependent.

Suppose $\alpha_1(1,1,0) + \alpha_2(1,0,1) + \alpha_3(0,1,1) = 0$. Then

$$\begin{cases} \alpha_1 + \alpha_2 = 0 \\ \alpha_1 + \alpha_3 = 0 \\ \alpha_2 + \alpha_3 = 0 \end{cases} \quad \Rightarrow \quad \begin{cases} \alpha_1 = 0 \\ \alpha_2 = 0 \\ \alpha_3 = 0 \end{cases} \text{ is the only solution.}$$

Therefore, $(1,1,0)$, $(1,0,1)$, $(0,1,1)$ are linearly independent.

## 1.2 Inner Product Spaces

## 1.3 Dual Spaces and the Dirac Notation

**Exercise 1.3.1.** Form an orthonormal basis in two dimensions starting with $\vec{A} = 3\vec{i} + 4\vec{j}$ and $\vec{B} = 2\vec{i} - 6\vec{j}$. Can you generate another orthonormal basis starting with these two vectors? If so, produce another.

**Solution.** Using Gram-Schmidt process here, starting from $\vec{A}$.

$$\vec{e}_1 = \frac{\vec{A}}{|\vec{A}|} = \frac{3\vec{i} + 4\vec{j}}{\sqrt{3^2 + 4^2}} = \frac{3}{5}\vec{i} + \frac{4}{5}\vec{j}$$

$$\begin{aligned}
\vec{e}_2' &= \vec{B} - (\vec{B} \cdot \vec{e}_1)\vec{e}_1 \\
&= (2\vec{i} - 6\vec{j}) - \left(\frac{6}{5} - \frac{24}{5}\right)\left(\frac{3}{5}\vec{i} + \frac{4}{5}\vec{j}\right) \\
&= \left(2 + \frac{54}{25}\right)\vec{i} + \left(-6 + \frac{72}{25}\right)\vec{j} \\
&= \frac{104}{25}\vec{i} - \frac{78}{25}\vec{j}
\end{aligned}$$

$$\vec{e}_2 = \frac{\vec{e}_2'}{|\vec{e}_2'|} = \frac{\frac{104}{25}\vec{i} - \frac{78}{25}\vec{j}}{\sqrt{\left(\frac{104}{25}\right)^2 + \left(\frac{78}{25}\right)^2}} = \frac{4}{5}\vec{i} - \frac{3}{5}\vec{j}$$

Therefore, the new basis is $\vec{e}_1 = \frac{3}{5}\vec{i} + \frac{4}{5}\vec{j}$, $\vec{e}_2 = \frac{4}{5}\vec{i} - \frac{3}{5}\vec{j}$.

**Exercise 1.3.2.** Show how to go from the basis

$$|I\rangle = \begin{pmatrix} 3 \\ 0 \\ 0 \end{pmatrix} \quad |II\rangle = \begin{pmatrix} 0 \\ 1 \\ 2 \end{pmatrix} \quad |III\rangle = \begin{pmatrix} 0 \\ 2 \\ 5 \end{pmatrix}$$

to the orthonormal basis

$$|1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \quad |2\rangle = \begin{pmatrix} 0 \\ 1/\sqrt{5} \\ 2/\sqrt{5} \end{pmatrix} \quad |3\rangle = \begin{pmatrix} 0 \\ -2/\sqrt{5} \\ 1/\sqrt{5} \end{pmatrix}$$

**Solution.**

$$
\begin{aligned}
|1\rangle &= \frac{|I\rangle}{\sqrt{\langle I \mid I\rangle}} = \frac{1}{3}\begin{pmatrix}3\\0\\0\end{pmatrix} = \begin{pmatrix}1\\0\\0\end{pmatrix}\\
|2'\rangle &= |II\rangle - (\langle 1 \mid II\rangle)|1\rangle\\
&= \begin{pmatrix}0\\1\\2\end{pmatrix} - 0\cdot\begin{pmatrix}1\\0\\0\end{pmatrix}\\
&= \begin{pmatrix}0\\1\\2\end{pmatrix}\\
|2\rangle &= \frac{|2'\rangle}{\sqrt{\langle 2' \mid 2'\rangle}} = \frac{1}{\sqrt{5}}\begin{pmatrix}0\\1\\2\end{pmatrix} = \begin{pmatrix}0\\1/\sqrt{5}\\2/\sqrt{5}\end{pmatrix}\\
|3'\rangle &=| III\rangle - (\langle 1 \mid II\rangle)|1\rangle - (\langle 2 \mid III\rangle)|2\rangle\\
&= \begin{pmatrix}0\\2\\5\end{pmatrix} - 0\cdot\begin{pmatrix}1\\0\\0\end{pmatrix} - \left(0 + \frac{2}{\sqrt{5}} + \frac{10}{\sqrt{5}}\right)\begin{pmatrix}0\\1/\sqrt{5}\\2/\sqrt{5}\end{pmatrix}\\
&= \begin{pmatrix}0\\2\\5\end{pmatrix} - \begin{pmatrix}0\\12/5\\24/5\end{pmatrix}\\
&= \begin{pmatrix}0\\-2/5\\1/5\end{pmatrix}\\
|3\rangle &= \frac{|3'\rangle}{\sqrt{\langle 3' \mid 3'\rangle}} = \begin{pmatrix}0\\-2/\sqrt{5}\\1/\sqrt{5}\end{pmatrix}
\end{aligned}
$$

**Exercise 1.3.3.** When will this equality

$$\langle V \mid V\rangle = \frac{\langle W \mid V\rangle\langle V \mid W\rangle}{|W|^2}$$

be satisfied? Does this agree with your experience with arrows?

**Solution.** When $|V\rangle = C|W\rangle$, we have

$$\langle V \mid V\rangle = |C|^2\langle W \mid W\rangle = |C|^2|W|^2$$

Also

$$
\begin{aligned}
\langle W \mid V\rangle\langle V \mid W\rangle &= (C\langle W \mid W\rangle)(C^\star\langle W \mid W\rangle)\\
&= |C|^2\langle W \mid W\rangle\langle W \mid W\rangle\\
&= |C|^2|W|^4
\end{aligned}
$$

Hence,

$$\langle V \mid V\rangle = \frac{\langle W \mid V\rangle\langle V \mid W\rangle}{|W|^2}$$

When two arrows are parallel or anti-parallel with each other, the square of their inner product equals to the product of their norms.

**Exercise 1.3.4.** Prove the triangle inequality starting with $|V + W|^2$. You must use $\mathrm{Re}\langle V|W\rangle \leqslant |\langle V|W\rangle|$ and the Schwarz inequality. Show that the final inequality becomes an equality only if $|V\rangle = a|W\rangle$ where $a$ is a real positive scalar.

**Solution.** $\mathrm{Re}\langle V \mid W\rangle \leqslant |\langle V \mid W\rangle| \leqslant |V||W|$

$$\Rightarrow \quad \mathrm{Re}\langle V \mid W\rangle \leqslant 2|V||W|$$

Add $|V|^2 + |W|^2$ to both sides of the inequality above, we have

$$\langle V \mid V\rangle + 2\mathrm{Re}\langle V \mid W\rangle + \langle W \mid W\rangle \leqslant |V|^2 + |W|^2 + 2|V||W|$$

$$\begin{aligned}
\mathrm{LHS} &= \langle V \mid V\rangle + \langle V \mid W\rangle + \langle W \mid V\rangle + \langle W \mid W\rangle \\
&= \langle V + W \mid V + W\rangle \\
&= |V + W|^2 \\
\mathrm{RHS} &= (|V| + |W|)^2
\end{aligned}$$

Therefore,

$$|V + W|^2 \leqslant (|V| + |W|)^2$$

$$\Rightarrow \quad |V + W| \leqslant |V| + |W| \qquad \text{(the triangular inequality)}$$

Attention: We are supposed to prove the equality holds only if $|V\rangle = \alpha|W\rangle$, where $\alpha$ is a real number.

The equality holds only if the following two equalities hold:

(a) $\langle V \mid W\rangle = |V||W|$

(b) $\mathrm{Re}\langle V \mid W\rangle = |\langle V \mid W\rangle|$

From the proof process of the Schwarz inequality in Shankar, we know that equality (a) holds only if

$$|Z\rangle = |V\rangle - \frac{\langle W \mid V\rangle}{|W|^2}|W\rangle = 0$$

which means $|V\rangle$ must be able to expressed as $\alpha|W\rangle$, where $\alpha$ is a number. To prove that $\alpha$ must be real, we substitude $|V\rangle = \alpha|W\rangle$ into equality (b) above.

$$\langle V \mid W\rangle = \alpha^\star\langle V \mid V\rangle$$

To satisfy equality (b), $\langle V \mid W\rangle$ must be real. Since $\langle V \mid V\rangle$ is real, $\alpha^\star$ must be real. Therefore, $\alpha$ must be a real number.

## 1.4 Subspaces

**Exercise 1.4.1.** In a space $\mathbb{V}^n$, prove that the set of all vectors $\left\{\left|V_\perp^1\right\rangle, \left|V_\perp^2\right\rangle, \ldots\right\}$, orthogonal to any $|V\rangle \neq |0\rangle$, form a subspace $\mathbb{V}^{n-1}$.

**Solution.** Given a vector space $\mathbb{V}^n$, one can start with an arbitrary vector $|V\rangle \neq 0$ and construct $n-1$ other vectors orthogonal to this $|V\rangle$ through Gram-Schmidt process. Since these $n-1$ vectors are linear independent, they span a $\mathbb{V}^{n-1}$ subspace. Now we prove that this subspace $\mathbb{V}^{n-1}$ is the set of all vectors orthogonal to $|V\rangle$.

(1) Every vector in $\mathbb{V}^{n-1}$ is orthogonal to $|V\rangle$: Since every vector in $\mathbb{V}^{n-1}$ can be expressed as a linear combination of the $n-1$ vectors we constructed above $|V_\perp\rangle = \sum_{i=1}^{n-1} \alpha_i |V_i\rangle$, and $\langle V \mid V_\perp\rangle = \sum_{i=1}^{n-1} \alpha_i \langle V \mid V_i\rangle = 0$, because $\langle V \mid V_i\rangle = 0$ for each $V_i$.

(2) Every vector in $\mathbb{V}^n$ but outside $\mathbb{V}^{n-1}$ is not orthogonal to $|V\rangle$: Since this kind of vectors can be expressed as $|W\rangle = \alpha|V\rangle + \sum_{i=1}^{n-1} \alpha_i |V_i\rangle$, where $\alpha \neq 0$. Therefore $\langle V \mid W\rangle = \alpha\langle V \mid V\rangle = \alpha \neq 0$.

**Exercise 1.4.2.** Suppose $\mathbb{V}_1^{n_1}$ and $\mathbb{V}_2^{n_2}$ are two subspaces such that any element of $\mathbb{V}_1$ is orthogonal to any element of $\mathbb{V}_2$. Show that the dimensionality of $\mathbb{V}_1 \oplus \mathbb{V}_2$ is $n_1 + n_2$. (Hint: Theorem 4.)

**Solution.** Since $\mathbb{V}_1^{n_1}$ and $\mathbb{V}_2^{n_2}$ are two subspace orthogonal to each other, we can take the $n_1$ basis vectors of $\mathbb{V}_1^{n_1}$ and the $n_2$ basis vectors of $\mathbb{V}_2^{n_2}$, and put them together. Because these $n_1 + n_2$ vectors are orthogonal to each other, they can span a $\mathbb{V}^{n_1+n_2}$ subspace. We now prove that this $\mathbb{V}^{n_1+n_2}$ is nothing but the $\mathbb{V}_1 \oplus \mathbb{V}_2$.

(1) Every vector in $\mathbb{V}^{n_1+n_2}$ is in $\mathbb{V}_1 \oplus \mathbb{V}_2$:

Since each vector in $\mathbb{V}^{n_1+n_2}$ can be expressed as $|U\rangle = \sum_{i=1}^{n_1} \alpha_i |V_i\rangle + \sum_{j=1}^{n_2} \beta_j |W_j\rangle$, where $\{|V_i\rangle\}$, $\{|W_j\rangle\}$ are basis vectors of $\mathbb{V}_1$ and $\mathbb{V}_2$ respectively. Notice that $\sum_{i=1}^{n_1} \alpha_i |V_i\rangle$ is a vector in $\mathbb{V}_1$, and $\sum_{j=1}^{n_2} b_j |W_j\rangle$ is a vector in $\mathbb{V}_2$. Therefore $|U\rangle$ can be expressed as a combination of vectors from $\mathbb{V}_1$ and $\mathbb{V}_2$. According to the definition of $\mathbb{V}_1 \oplus \mathbb{V}_2$ (Definition 12 in Shankar), $|U\rangle \in \mathbb{V}_1 \oplus \mathbb{V}_2$.

(2) Every vector in $\mathbb{V}_1 \oplus \mathbb{V}_2$ is in $\mathbb{V}^{n_1+n_2}$:

Every vector in $\mathbb{V}_1 \oplus \mathbb{V}_2$ can be expressed as $|Z\rangle = C_1|Z_1\rangle + C_2|Z_2\rangle$, where $|Z_1\rangle \in \mathbb{V}_1^{n_1}$, $|Z_2\rangle \in \mathbb{V}_2^{n_2}$. Therefore, $|Z_1\rangle = \sum_{i=1}^{n_1} p_i |V_i\rangle$, and $|Z_2\rangle = \sum_{j=1}^{n_2} q_j |W_j\rangle$. Thus, $|Z\rangle = \sum_{i=1}^{n_1} C_1 p_i |V_i\rangle + \sum_{j=1}^{n_2} C_2 q_j |W_j\rangle$, which lies in $\mathbb{V}^{n_1+n_2}$.

Therefore, by theorem 4 in Shankar, there are $n_1 + n_2$ orthogonal vectors in $\mathbb{V}_1 \oplus \mathbb{V}_2$, so the dimension of $\mathbb{V}_1 \oplus \mathbb{V}_2$ is $n_1 + n_2$.

## 1.5 Linear Operators

## 1.6 Matrix Elements of Linear Operators

**Exercise 1.6.1.** An operator $\Omega$ is given by the matrix

$$\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$$

What is its action?

**Solution.** To see $\Omega$'s action, let's act on basis vectors:

$$\Omega|1\rangle = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = |2\rangle$$
$$\Omega|2\rangle = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = |3\rangle$$
$$\Omega|3\rangle = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = |1\rangle$$

This is a cyclic permutation of the three basis vectors.
It is equivalent to rotation of the coordinate axis along $(1, 1, 1)$ by $\frac{2\pi}{3}$.

**Exercise 1.6.2.** Given $\Omega$ and $\Lambda$ are Hermitian what can you say about (1) $\Omega\Lambda$; (2) $\Omega\Lambda + \Lambda\Omega$; (3) $[\Omega, \Lambda]$; and (4) $\mathrm{i}[\Omega, \Lambda]$ ?

**Solution.**

(1) Not Hermitian: $(\Omega\Lambda)^\dagger = \Lambda^\dagger\Omega^\dagger = \Lambda\Omega \neq \Omega\Lambda$

(2) Hermitian:
$$\begin{aligned} (\Omega\Lambda + \Lambda\Omega)^\dagger &= (\Omega\Lambda)^\dagger + (\Lambda\Omega)^\dagger \\ &= \Lambda^\dagger\Omega^\dagger + \Omega^\dagger\Lambda^\dagger \\ &= \Lambda\Omega + \Omega\Lambda \\ &= \Omega\Lambda + \Lambda\Omega \end{aligned}$$

(3) Anti-Hermitian:
$$\begin{aligned} [\Omega, \Lambda]^\dagger &= (\Omega\Lambda - \Lambda\Omega)^\dagger \\ &= (\Omega\Lambda)^\dagger - (\Lambda\Omega)^\dagger \\ &= \Lambda^\dagger\Omega^\dagger - \Omega^\dagger\Lambda^\dagger \\ &= \Lambda\Omega - \Omega\Lambda \\ &= -(\Omega\Lambda - \Lambda\Omega) \\ &= -[\Omega, \Lambda] \end{aligned}$$

(4) Hermitian:
$$\begin{aligned} (\mathrm{i}\,[\Omega, \Lambda])^\dagger &= -\mathrm{i}\,[\Omega, \Lambda]^\dagger \\ &= -\mathrm{i} \cdot (-\,[\Omega, \Lambda]) \\ &= [\Omega, \Lambda] \end{aligned}$$

**Exercise 1.6.3.** Show that a product of unitary operator is unitary.

**Solution.** Suppose $U_1, U_2$ are unitary, which means that

$$U_1^\dagger U_1 = \mathbb{I} = U_2^\dagger U_2$$

Therefore,

$$\begin{aligned}(U_1U_2)^\dagger(U_1U_2) &= U_2^\dagger U_1^\dagger U_1U_2\\ &= U_2^\dagger(U_1^\dagger U_1)U_2\\ &= U_2^\dagger \mathbb{I}\, U_2\\ &= U_2^\dagger U_2\\ &= \mathbb{I}\end{aligned}$$

Hence a product of unitary operator is unitary.

**Exercise 1.6.4.** It is assumed that you know (1) what a determinant is, (2) that $\det\Omega^{\mathrm{T}} = \det\Omega$ (T denotes transpose), (3) that the determinant of a product of matrices is the product of the determinants. [If you do not, verify these properties for a two-dimensional case

$$\Omega = \begin{pmatrix}\alpha & \beta\\ \gamma & \delta\end{pmatrix}$$

with $\det\Omega = (\alpha\delta - \beta\gamma)$.] Prove that the determinant of a unitary matrix is a complex number of unit modulus.

**Solution.** Suppose $U$ is the unitary matrix, which means that it satisfies

$$U^\dagger U = \mathbb{I}$$

Take determinant of the both sides, we get

$$\begin{aligned}\det(U^\dagger U) &= \det(\mathbb{I})\\ \det(U^\dagger)\det(U) &= 1\\ \det((U^{\mathrm{T}})^\star)\det(U) &= 1\\ (\det(U^{\mathrm{T}}))^\star\det(U) &= 1\\ (\det(U))^\star\det(U) &= 1\\ |\det(U)|^2 &= 1\\ |\det(U)| &= 1\end{aligned}$$

Therefore, $\det(U)$ is a complex number of unit modulus.

**Exercise 1.6.5.** Verify that $R\left(\frac{1}{2}\pi\mathbf{i}\right)$ is unitary (orthogonal) by examining its matrix.

**Solution.** We know from Example 1.6.1,

$$R\left(\frac{1}{2}\pi\mathbf{i}\right) = \begin{pmatrix}1 & 0 & 0\\ 0 & 0 & -1\\ 0 & 1 & 0\end{pmatrix}$$

Therefore,

$$R\left(\frac{1}{2}\pi\mathbf{i}\right)^\dagger R\left(\frac{1}{2}\pi\mathbf{i}\right) = \begin{pmatrix}1 & 0 & 0\\ 0 & 0 & 1\\ 0 & -1 & 0\end{pmatrix}\begin{pmatrix}1 & 0 & 0\\ 0 & 0 & -1\\ 0 & 1 & 0\end{pmatrix} = \begin{pmatrix}1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 1\end{pmatrix} = \mathbb{I}$$

Hence, $R\left(\frac{1}{2}\pi\mathbf{i}\right)$ is unitary.

**Exercise 1.6.6.** Verify that the following matrices are unitary:

$$\frac{1}{2^{1/2}}\begin{pmatrix}1 & \mathrm{i}\\ \mathrm{i} & 1\end{pmatrix}, \quad \frac{1}{2}\begin{pmatrix}1+\mathrm{i} & 1-\mathrm{i}\\ 1-\mathrm{i} & 1+\mathrm{i}\end{pmatrix}$$

Verify that the determinant is of the form $e^{\mathrm{i}\theta}$ in each case. Are any of the above matrices Hermitian?

**Solution.**

- $\frac{1}{2^{1/2}}\begin{pmatrix}1 & \mathrm{i}\\ \mathrm{i} & 1\end{pmatrix}$ is unitary, since

$$\frac{1}{2^{1/2}}\begin{pmatrix}1 & \mathrm{i}\\ \mathrm{i} & 1\end{pmatrix}^\dagger \cdot \frac{1}{2^{1/2}}\begin{pmatrix}1 & \mathrm{i}\\ \mathrm{i} & 1\end{pmatrix} = \frac{1}{2}\begin{pmatrix}1 & -\mathrm{i}\\ -\mathrm{i} & 1\end{pmatrix}\begin{pmatrix}1 & \mathrm{i}\\ \mathrm{i} & 1\end{pmatrix} = \frac{1}{2}\begin{pmatrix}2 & 0\\ 0 & 2\end{pmatrix} = \mathbb{I}$$

The determinant of $\frac{1}{2^{1/2}}\begin{pmatrix}1 & \mathrm{i}\\ \mathrm{i} & 1\end{pmatrix}$ is of $\mathrm{e}^{\mathrm{i}\theta}$ form, since

$$\det\left[\frac{1}{2^{1/2}}\begin{pmatrix}1 & \mathrm{i}\\ \mathrm{i} & 1\end{pmatrix}\right] = \left(\frac{1}{2^{1/2}}\right)^2 (1\cdot 1 - \mathrm{i}\cdot\mathrm{i}) = 1 = \mathrm{e}^{\mathrm{i}\theta}, \text{ where } \theta = 2k\pi \text{ for } k \in \mathbb{Z}$$

$\frac{1}{2^{1/2}}\begin{pmatrix}1 & \mathrm{i}\\ \mathrm{i} & 1\end{pmatrix}$ is not Hermitian, since

$$\frac{1}{2^{1/2}}\begin{pmatrix}1 & \mathrm{i}\\ \mathrm{i} & 1\end{pmatrix}^\dagger = \frac{1}{2^{1/2}}\begin{pmatrix}1 & -\mathrm{i}\\ -\mathrm{i} & 1\end{pmatrix} \neq \frac{1}{2^{1/2}}\begin{pmatrix}1 & \mathrm{i}\\ \mathrm{i} & 1\end{pmatrix}$$

- $\frac{1}{2}\begin{pmatrix}1+\mathrm{i} & 1-\mathrm{i}\\ 1-\mathrm{i} & 1+\mathrm{i}\end{pmatrix}$ is unitary, since

$$\begin{aligned}\frac{1}{2}\begin{pmatrix}1+\mathrm{i} & 1-\mathrm{i}\\ 1-\mathrm{i} & 1+\mathrm{i}\end{pmatrix}^\dagger \cdot \frac{1}{2}\begin{pmatrix}1+\mathrm{i} & 1-\mathrm{i}\\ 1-\mathrm{i} & 1+\mathrm{i}\end{pmatrix} &= \frac{1}{4}\begin{pmatrix}1-\mathrm{i} & 1+\mathrm{i}\\ 1+\mathrm{i} & 1-\mathrm{i}\end{pmatrix}\begin{pmatrix}1+\mathrm{i} & 1-\mathrm{i}\\ 1-\mathrm{i} & 1+\mathrm{i}\end{pmatrix}\\ &= \frac{1}{4}\begin{pmatrix}4 & 0\\ 0 & 4\end{pmatrix}\\ &= \mathbb{I}\end{aligned}$$

The determinant of $\frac{1}{2}\begin{pmatrix}1+\mathrm{i} & 1-\mathrm{i}\\ 1-\mathrm{i} & 1+\mathrm{i}\end{pmatrix}$ is of $\mathrm{e}^{\mathrm{i}\theta}$ form, since

$$\det\left[\frac{1}{2}\begin{pmatrix}1+\mathrm{i} & 1-\mathrm{i}\\ 1-\mathrm{i} & 1+\mathrm{i}\end{pmatrix}\right] = \left(\frac{1}{2}\right)^2 [(1+\mathrm{i})^2 - (1-\mathrm{i})^2] = \mathrm{i}$$

where $\theta = 2k\pi + \frac{\pi}{2}$ for $k \in \mathbb{Z}$. $\frac{1}{2}\begin{pmatrix}1+\mathrm{i} & 1-\mathrm{i}\\ 1-\mathrm{i} & 1+\mathrm{i}\end{pmatrix}$ is not Hermitian, since

$$\frac{1}{2}\begin{pmatrix}1+\mathrm{i} & 1-\mathrm{i}\\ 1-\mathrm{i} & 1+\mathrm{i}\end{pmatrix}^\dagger = \frac{1}{2}\begin{pmatrix}1-\mathrm{i} & 1+\mathrm{i}\\ 1+\mathrm{i} & 1-\mathrm{i}\end{pmatrix} \neq \frac{1}{2}\begin{pmatrix}1+\mathrm{i} & 1-\mathrm{i}\\ 1-\mathrm{i} & 1+\mathrm{i}\end{pmatrix}$$

## 1.7 Active and Passive Transformations

**Exercise 1.7.1.** The trace of a matrix is defined to be the sum of its diagonal matrix elements

$$\operatorname{Tr}\Omega = \sum_i \Omega_{ii}$$

Show that

(1) $\operatorname{Tr}(\Omega\Lambda) = \operatorname{Tr}(\Lambda\Omega)$.

(2) $\operatorname{Tr}(\Omega\Lambda\theta) = \operatorname{Tr}(\Lambda\theta\Omega) = \operatorname{Tr}(\theta\Omega\Lambda)$ (The permutations are *cyclic*).

(3) The trace of an operator is unaffected by a unitary change of basis $|i\rangle \to U|i\rangle$. [Equivalently, show $\operatorname{Tr}\Omega = \operatorname{Tr}\left(U^\dagger \Omega U\right)$.]

**Solution.**

(1) $\operatorname{Tr}(\Omega\Lambda) = \sum_i (\Omega\Lambda)_{ii} = \sum_i \sum_j \Omega_{ij}\Lambda_{ji} = \sum_j \sum_i \Lambda_{ji}\Omega_{ij} = \sum_j (\Lambda\Omega)_{jj} = \operatorname{Tr}(\Lambda\Omega)$.

(2)

$$\begin{aligned}
\operatorname{Tr}(\Omega\Lambda\theta) &= \sum_i (\Omega\Lambda\theta)_{ii} = \sum_i \sum_j \sum_k \Omega_{ij}\Lambda_{jk}\theta_{ki} \\
&= \sum_j \sum_k \sum_i \Lambda_{jk}\theta_{ki}\Omega_{ij} = \sum_j (\Lambda\theta\Omega)_{jj} = \operatorname{Tr}(\Lambda\theta\Omega) \\
&= \sum_k \sum_i \sum_j \theta_{ki}\Omega_{ij}\Lambda_{jk} = \sum_k (\theta\Omega\Lambda)_{kk} = \operatorname{Tr}(\theta\Omega\Lambda)
\end{aligned}$$

(3) $\operatorname{Tr}(U^\dagger\Omega U) = \operatorname{Tr}(\Omega U U^\dagger) = \operatorname{Tr}(\Omega\mathbb{I}) = \operatorname{Tr}(\Omega)$.

**Exercise 1.7.2.** Show that the determinant of a matrix is unaffected by a unitary change of basis. [Equivalently show $\det\Omega = \det\left(U^\dagger\Omega U\right)$.]

**Solution.**

$$\begin{aligned}
\det\left(U^\dagger\Omega U\right) &= \det U^\dagger \det\Omega \det U \\
&= \det\Omega \left(\det U^\dagger \det U\right) \\
&= \det\Omega \det\left(U^\dagger U\right) \\
&= \det\Omega \cdot 1 \\
&= \det\Omega.
\end{aligned}$$

## 1.8 The Eigenvalue Problem

**Exercise 1.8.1.**

(1) Find the eigenvalues and normalized eigenvectors of the matrix

$$\Omega = \begin{pmatrix} 1 & 3 & 1 \\ 0 & 2 & 0 \\ 0 & 1 & 4 \end{pmatrix}$$

(2) Is the matrix Hermitian? Are the eigenvectors orthogonal?

**Solution.**

(1) To find the eigenvalues and normalized eigenvectors of the matrix $\Omega$, we can compute the characteristic equation

$$\det(\Omega - \omega\mathbb{I}) = \begin{vmatrix} 1-\omega & 3 & 1 \\ 0 & 2-\omega & 0 \\ 0 & 1 & 4-\omega \end{vmatrix} = (1-\omega)(2-\omega)(4-\omega) = 0$$

So the eigenvalues are

$$\omega = 1, 2, 4$$

The eigenvectors corresponding eigenvalues are

$$\omega = 1 : \begin{pmatrix} 0 & 3 & 1 \\ 0 & 1 & 0 \\ 0 & 1 & 3 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = 0 \qquad \Rightarrow \quad |\omega = 1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$

$$\omega = 2 : \begin{pmatrix} -1 & 3 & 1 \\ 0 & 0 & 0 \\ 0 & 1 & 2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = 0 \qquad \Rightarrow \quad |\omega = 2\rangle = \frac{1}{\sqrt{30}} \begin{pmatrix} 5 \\ 2 \\ -1 \end{pmatrix}$$

$$\omega = 4 : \begin{pmatrix} -3 & 3 & 1 \\ 0 & -2 & 0 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = 0 \qquad \Rightarrow \quad |\omega = 4\rangle = \frac{1}{\sqrt{10}} \begin{pmatrix} 1 \\ 0 \\ 3 \end{pmatrix}$$

(2) Matrix $\Omega$ is not Hermitian, since

$$\Omega^\dagger = \begin{pmatrix} 1 & 0 & 0 \\ 3 & 2 & 0 \\ 1 & 0 & 4 \end{pmatrix} \neq \Omega$$

The eigenvectors are not orthogonal, since

$$\langle \omega = 1 \mid \omega = 2 \rangle = 1 \times \frac{5}{\sqrt{30}} + 0 \times \frac{2}{\sqrt{30}} + 0 \times \frac{-1}{\sqrt{30}} = \frac{\sqrt{30}}{6} \neq 0$$

$$\langle \omega = 1 \mid \omega = 4 \rangle = 1 \times \frac{1}{\sqrt{10}} + 0 \times 0 + 0 \times \frac{3}{\sqrt{10}} = \frac{\sqrt{10}}{10} \neq 0$$

$$\langle \omega = 2 \mid \omega = 4 \rangle = \frac{5}{\sqrt{30}} \times \frac{1}{\sqrt{10}} + \frac{2}{\sqrt{30}} \times 0 + \frac{-1}{\sqrt{30}} \times \frac{3}{\sqrt{10}} = \frac{\sqrt{3}}{15} \neq 0$$

**Exercise 1.8.2.** Consider the matrix

$$\Omega = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}$$

(1) Is it Hermitian?

(2) Find its eigenvalues and eigenvectors.

(3) Verify that $U^\dagger \Omega U$ is diagonal, $U$ being the matrix of eigenvectors of $\Omega$.

**Solution.**

(1) Matrix $\Omega$ is Hermitian since

$$\Omega^\dagger = \Omega$$

(2) To find the eigenvalues and eigenvectors of the matrix $\Omega$, we can compute the characteristic equation

$$\det(\Omega - \omega\mathbb{I}) = \begin{vmatrix} -\omega & 0 & 1 \\ 0 & -\omega & 0 \\ 1 & 0 & -\omega \end{vmatrix} = -\omega^3 + \omega = -\omega(\omega+1)(\omega-1) = 0$$

Therefore, eigenvalues are

$$\omega = -1, 0, 1$$

The eigenvectors corresponding to eigenvalues are

$$\begin{aligned} \omega = -1: \begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} &= 0 \qquad \Rightarrow \quad |\omega = -1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} \\ \omega = 0: \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} &= 0 \qquad \Rightarrow \quad |\omega = 0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \\ \omega = 1: \begin{pmatrix} -1 & 0 & 1 \\ 0 & -1 & 0 \\ 1 & 0 & -1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} &= 0 \qquad \Rightarrow \quad |\omega = 1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} \end{aligned}$$

(3) If $U$ is the matrix of eigenvectors of $\Omega$, then

$$U = \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ 0 & 1 & 0 \\ -\frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \end{pmatrix} \qquad U^\dagger = \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} \\ 0 & 1 & 0 \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \end{pmatrix}$$

We can compute

$$\begin{aligned} U^\dagger \Omega U &= \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} \\ 0 & 1 & 0 \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ 0 & 1 & 0 \\ -\frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \end{pmatrix} \\ &= \begin{pmatrix} -\frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ 0 & 0 & 0 \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ 0 & 1 & 0 \\ -\frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \end{pmatrix} \\ &= \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \end{aligned}$$

This is a diagonal matrix.

**Exercise 1.8.3.** Consider the Hermitian matrix

$$\Omega = \frac{1}{2} \begin{pmatrix} 2 & 0 & 0 \\ 0 & 3 & -1 \\ 0 & -1 & 3 \end{pmatrix}$$

(1) Show that $\omega_1 = \omega_2 = 1$; $\omega_3 = 2$.

(2) Show that $|\omega = 2\rangle$ is any vector of the form

$$\frac{1}{(2a^2)^{1/2}}\begin{pmatrix}0\\a\\-a\end{pmatrix}$$

(3) Show that the $\omega = 1$ eigenspace contains all vectors of the form

$$\frac{1}{(b^2+2c^2)^{1/2}}\begin{pmatrix}b\\c\\c\end{pmatrix}$$

either by feeding $\omega = 1$ into the equations or by requiring that the $\omega = 1$ eigenspace be orthogonal to $|\omega = 2\rangle$.

**Solution.**

(1) The characteristic equation is

$$\begin{aligned}
\det(\Omega - \omega\mathbb{I}) &= \begin{vmatrix}1-\omega & 0 & 0\\ 0 & \frac{3}{2}-\omega & -\frac{1}{2}\\ 0 & -\frac{1}{2} & \frac{3}{2}-\omega\end{vmatrix}\\
&= (1-\omega)\left(\frac{3}{2}-\omega\right)^2 - (1-\omega)\left(-\frac{1}{2}\right)^2\\
&= (1-\omega)\left[\left(\frac{3}{2}-\omega\right)^2 - \frac{1}{4}\right] = (1-\omega)(\omega^2-3\omega+2)\\
&= (1-\omega)(\omega-1)(\omega-2) = 0
\end{aligned}$$

Then the eigenvalues are

$$\omega_1 = \omega_2 = 1 \quad \omega_3 = 2$$

(2) To get the eigenvector corresponding to eigenvalue $\omega = 2$, we need to solve the equation

$$\begin{pmatrix}-1 & 0 & 0\\ 0 & -\frac{1}{2} & -\frac{1}{2}\\ 0 & -\frac{1}{2} & -\frac{1}{2}\end{pmatrix}\begin{pmatrix}x_1\\x_2\\x_3\end{pmatrix} = 0 \quad \Rightarrow \quad \begin{cases} x_1 = 0\\ x_2 + x_3 = 0\end{cases}$$

Set $x_2 = a$, we have $x_3 = -a$. Therefore,

$$|\omega = 2\rangle = \frac{1}{\sqrt{2a^2}}\begin{pmatrix}0\\a\\-a\end{pmatrix}$$

(3) For $\omega = 1$:

$$\begin{pmatrix}0 & 0 & 0\\ 0 & \frac{1}{2} & -\frac{1}{2}\\ 0 & -\frac{1}{2} & \frac{1}{2}\end{pmatrix}\begin{pmatrix}x_1\\x_2\\x_3\end{pmatrix} = 0$$

$x_1$ is arbitrary, set $x_1 = b$. $x_2 - x_3 = 0$, set $x_2 = c$, then $x_3 = c$. Therefore, the eigenvector corresponding $\omega = 1$ is of the form

$$|\omega = 1\rangle = \frac{1}{\sqrt{b^2 + 2c^2}} \begin{pmatrix} b \\ c \\ c \end{pmatrix}.$$

**Exercise 1.8.4.** An arbitrary $n \times n$ matrix need not have $n$ eigenvectors. Consider as an example

$$\Omega = \begin{pmatrix} 4 & 1 \\ -1 & 2 \end{pmatrix}$$

(1) Show that $\omega_1 = \omega_2 = 3$.

(2) By feeding in this value show we get only one eigenvector of the form

$$\frac{1}{(2a^2)^{1/2}} \begin{pmatrix} +a \\ -a \end{pmatrix}$$

We cannot find another one that is linear independent.

**Solution.**

(1) The characteristic equation is

$$\det(\Omega - \omega\mathbb{I}) = \begin{vmatrix} 4 - \omega & 1 \\ -1 & 2 - \omega \end{vmatrix} = (4 - \omega)(2 - \omega) + 1 = \omega^2 - 6\omega + 9 = 0$$

Thus the eigenvalues are

$$\omega_1 = \omega_2 = 3$$

(2) By feeding this eigenvalue $\omega = 3$, we get the equation

$$\begin{pmatrix} 1 & 1 \\ -1 & -1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = 0 \qquad \Rightarrow \qquad x_1 + x_2 = 0$$

Set $x_1 = a$, we have $x_2 = -a$. Therefore, the eigenvector is of the form

$$|\omega = 3\rangle = \frac{1}{\sqrt{2a^2}} \begin{pmatrix} a \\ -a \end{pmatrix}.$$

This is the only eigenvector we can find.

**Exercise 1.8.5.** Consider the matrix

$$\Omega = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}$$

(1) Show that it is unitary.

(2) Show that its eigenvalues are $e^{i\theta}$ and $e^{-i\theta}$.

(3) Find the corresponding eigenvectors; show that they are orthogonal.

(4) Verify that $U^\dagger \Omega U =$ (diagonal matrix), where $U$ is the matrix of eigenvectors of $\Omega$.

**Solution.**

(1) Matrix $\Omega$ is unitary, since

$$\begin{aligned}\Omega^\dagger\Omega &= \begin{pmatrix}\cos\theta & -\sin\theta\\ \sin\theta & \cos\theta\end{pmatrix}\begin{pmatrix}\cos\theta & \sin\theta\\ -\sin\theta & \cos\theta\end{pmatrix}\\ &= \begin{pmatrix}\cos^2\theta+\sin^2\theta & \cos\theta\sin\theta-\sin\theta\cos\theta\\ \sin\theta\cos\theta-\cos\theta\sin\theta & \sin^2\theta+\cos^2\theta\end{pmatrix}\\ &= \begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}\\ &= \mathbb{I}\end{aligned}$$

(2) Solve the characteristic equation

$$\det(\Omega-\omega\mathbb{I}) = \begin{vmatrix}\cos\theta-\omega & \sin\theta\\ -\sin\theta & \cos\theta-\omega\end{vmatrix} = \omega^2-2\omega\cos\theta+1=0$$

By Euler's formula, we get the eigenvalues

$$\omega = \cos\theta\pm \mathrm{i}\sin\theta = \mathrm{e}^{\pm\mathrm{i}\theta}$$

(3) By feeding this eigenvalue, we get the equations

$$\begin{aligned}\omega=\mathrm{e}^{-\mathrm{i}\theta}: &\quad \begin{pmatrix}\mathrm{i}\sin\theta & \sin\theta\\ -\sin\theta & \mathrm{i}\sin\theta\end{pmatrix}\begin{pmatrix}x_1\\ x_2\end{pmatrix}=0 \quad\Rightarrow\quad \mathrm{i}x_1+x_2=0\\ \omega=\mathrm{e}^{\mathrm{i}\theta}: &\quad \begin{pmatrix}-\mathrm{i}\sin\theta & \sin\theta\\ -\sin\theta & -\mathrm{i}\sin\theta\end{pmatrix}\begin{pmatrix}x_1\\ x_2\end{pmatrix}=0 \quad\Rightarrow\quad -\mathrm{i}x_1+x_2=0\end{aligned}$$

Thus the corresponding eigenvectors are

$$\begin{aligned}|\omega=\mathrm{e}^{-\mathrm{i}\theta}\rangle &= \frac{1}{\sqrt{2}}\begin{pmatrix}1\\ -\mathrm{i}\end{pmatrix}\\ |\omega=\mathrm{e}^{\mathrm{i}\theta}\rangle &= \frac{1}{\sqrt{2}}\begin{pmatrix}1\\ \mathrm{i}\end{pmatrix}\end{aligned}$$

They are orthogonal since

$$\langle\omega=\mathrm{e}^{-\mathrm{i}\theta}\mid\omega=\mathrm{e}^{\mathrm{i}\theta}\rangle = \frac{1}{2}(1\quad \mathrm{i})\begin{pmatrix}1\\ \mathrm{i}\end{pmatrix} = \frac{1}{2}(1+\mathrm{i}^2)=0$$

(4) The matrix of eigenvectors of $\Omega$ is

$$U = \begin{pmatrix}\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}}\\ -\frac{\mathrm{i}}{\sqrt{2}} & \frac{\mathrm{i}}{\sqrt{2}}\end{pmatrix}$$

Then

$$
\begin{aligned}
U^\dagger \Omega U &= \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{\mathrm{i}}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{\mathrm{i}}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ -\frac{\mathrm{i}}{\sqrt{2}} & \frac{\mathrm{i}}{\sqrt{2}} \end{pmatrix} \\
&= \begin{pmatrix} \frac{1}{\sqrt{2}}(\cos\theta - \mathrm{i}\sin\theta) & \frac{1}{\sqrt{2}}(\sin\theta + \mathrm{i}\cos\theta) \\ \frac{1}{\sqrt{2}}(\cos\theta + \mathrm{i}\sin\theta) & \frac{1}{\sqrt{2}}(\sin\theta - \mathrm{i}\cos\theta) \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ -\frac{\mathrm{i}}{\sqrt{2}} & \frac{\mathrm{i}}{\sqrt{2}} \end{pmatrix} \\
&= \begin{pmatrix} \frac{1}{\sqrt{2}}\mathrm{e}^{-\mathrm{i}\theta} & \frac{\mathrm{i}}{\sqrt{2}}\mathrm{e}^{-\mathrm{i}\theta} \\ \frac{1}{\sqrt{2}}\mathrm{e}^{\mathrm{i}\theta} & -\frac{\mathrm{i}}{\sqrt{2}}\mathrm{e}^{\mathrm{i}\theta} \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ -\frac{\mathrm{i}}{\sqrt{2}} & \frac{\mathrm{i}}{\sqrt{2}} \end{pmatrix} \\
&= \begin{pmatrix} \mathrm{e}^{-\mathrm{i}\theta} & 0 \\ 0 & \mathrm{e}^{\mathrm{i}\theta} \end{pmatrix}
\end{aligned}
$$

is diagonal.

**Exercise 1.8.6.**

(1) We have seen that the determinant of a matrix is unchanged under a unitary change of basis. Argue now that

$$\det\Omega = \text{ product of eigenvalues of } \Omega = \prod_{i=1}^{n} \omega_i$$

for a Hermitian or unitary $\Omega$.

(2) Using the invariance of the trace under the same transformation, show that

$$\operatorname{Tr}\Omega = \sum_{i=1}^{n} \omega_i$$

**Solution.**

(1) Suppose $U$ is the unitary matrix that transforms $\Omega$ into a diagonal matrix $D$ with $\Omega$'s eigenvalues $\omega_i$ on its diagonal. Then

$$\det\Omega = \det(U^\dagger \Omega U) = \det D = \prod_{i=1}^{n} \omega_i$$

(2) By using the same transformation, we have

$$\operatorname{Tr}\Omega = \operatorname{Tr}(U^\dagger \Omega U) = \operatorname{Tr} D = \sum_{i=1}^{n} \omega_i$$

**Exercise 1.8.7.** By using the results on the trace and determinant from the last problem, show that the eigenvalues of the matrix

$$\Omega = \begin{pmatrix} 1 & 2 \\ 2 & 1 \end{pmatrix}$$

are 3 and $-1$. Verify this by explicit computation. Note that the Hermitian nature of the matrix is an essential ingredient.

**Solution.** According to Exercise 1.8.6, we have

$$\begin{cases} \omega_1 \times \omega_2 = \det \Omega = 1 \times 1 - 2 \times 2 = -3 \\ \omega_1 + \omega_2 = 1 + 1 = 2 \end{cases}$$

Solving the equation, we get

$$\begin{cases} \omega_1 = -1 \\ \omega_2 = 3 \end{cases}$$

For verification, we can calculate the characteristic equation

$$\det(\Omega - \omega \mathbb{I}) = \begin{vmatrix} 1-\omega & 2 \\ 2 & 1-\omega \end{vmatrix} = (1-\omega)^2 - 4 = (1-\omega+2)(1-\omega-2) = 0$$

We can get the eigenvalues

$$\begin{cases} \omega_1 = -1 \\ \omega_2 = 3 \end{cases}$$

**Exercise 1.8.8.** Consider Hermitian matrices $M^1, M^2, M^3, M^4$ that obey

$$M^i M^j + M^j M^i = 2\delta^{ij}\mathbb{I}, \quad i, j = 1, \ldots, 4$$

(1) Show that the eigenvalues of $M^i$ are $\pm 1$. (Hint: go to the eigenbasis of $M^i$, and use the equation for $i = j$.)

(2) By considering the relation

$$M^i M^i = -M^j M^i \quad \text{for } i \neq j$$

show that $M^i$ are traceless. [Hint: $\text{Tr}(ACB) = \text{Tr}(CBA)$.]

(3) Show that they cannot be odd-dimensional matrices.

**Solution.**

(1) Start with equation

$$M^i M^j + M^j M^i = 2\delta^{ij}\mathbb{I}$$

Take $i = j$, we get

$$M^i M^i = \mathbb{I}$$

Apply $M^i M^i$ to eigenvector $|\omega\rangle$ of $M^i$, we have

$$M^i M^i |\omega\rangle = M^i(\omega|\omega\rangle) = \omega^2|\omega\rangle$$
$$M^i M^i |\omega\rangle = \mathbb{I}|\omega\rangle = |\omega\rangle$$

Therefore,

$$\omega^2 = 1$$
$$\omega = \pm 1$$

(2) From the relation

$$M^i M^j = -M^j M^i$$
$$M^j M^i M^j = -M^j M^j M^i = -M^i$$

We can take the trace of $M^i$ to get

$$\begin{aligned}\operatorname{Tr} M^i &= \operatorname{Tr}(-M^j M^i M^j)\\ &= -\operatorname{Tr}(M^j M^i M^j)\\ &= -\operatorname{Tr}(M^i M^j M^j)\\ &= -\operatorname{Tr}(M^i \mathbb{I})\\ &= -\operatorname{Tr}(M^i)\\ &= 0\end{aligned}$$

$M^i$ is traceless.

(3) According to 1.8.6,

$$\operatorname{Tr} M^i = \sum_{k=1}^{n} \omega_k$$

where $n$ is the dimension of the matrix. Since $\omega_k = \pm 1$, $\operatorname{Tr} M^i$ can be zero only if $n$ is even[1].

**Exercise 1.8.9.** A collection of masses $m_\alpha$, located at $\mathbf{r}_\alpha$ and rotating with angular velocity $\boldsymbol{\omega}$ around a common axis has an angular momentum

$$\mathbf{l} = \sum_\alpha m_\alpha \left(\mathbf{r}_\alpha \times \mathbf{v}_\alpha\right)$$

where $\mathbf{v}_\alpha = \boldsymbol{\omega} \times \mathbf{r}_\alpha$ is the velocity of $m_\alpha$. By using the identity

$$\mathbf{A} \times (\mathbf{B} \times \mathbf{C}) = \mathbf{B}(\mathbf{A} \cdot \mathbf{C}) - \mathbf{C}(\mathbf{A} \cdot \mathbf{B})$$

show that each Cartesian component $l_i$ of $\mathbf{l}$ is given by

$$l_i = \sum_j M_{ij} \omega_j$$

where

$$M_{ij} = \sum_\alpha m_\alpha \left[ r_\alpha^2 \delta_{ij} - (\mathbf{r}_\alpha)_i (\mathbf{r}_\alpha)_j \right]$$

or in Dirac notation

$$|l\rangle = M|\omega\rangle$$

(1) Will the angular momentum and angular velocity always be parallel?

(2) Show that the moment of inertia matrix $M_{ij}$ is Hermitian.

(3) Argue now that there exist three directions for $\boldsymbol{\omega}$ such that $\mathbf{l}$ and $\boldsymbol{\omega}$ will be parallel. How are these directions to be found?

(4) Consider the moment of inertia matrix of a sphere. Due to the complete symmetry of the sphere, it is clear that every direction is its eigendirection for rotation. What does this say about the three eigenvalues of the matrix $M$?

[1] The sum of an odd number of odd numbers is still odd, and cannot be zero.

**Solution.** Start from the angular momentum

$$
\begin{aligned}
\mathbf{l} &= \sum_\alpha m_\alpha \mathbf{r}_\alpha \times (\boldsymbol{\omega} \times \mathbf{r}_\alpha) \\
&= \sum_\alpha m_\alpha [\boldsymbol{\omega}(\mathbf{r}_\alpha \cdot \mathbf{r}_\alpha) - \mathbf{r}_\alpha(\mathbf{r}_\alpha \cdot \boldsymbol{\omega})] \\
&= \sum_\alpha m_\alpha [\boldsymbol{\omega}\, r_\alpha^2 - \mathbf{r}_\alpha(\mathbf{r}_\alpha \cdot \boldsymbol{\omega})]
\end{aligned}
$$

Writing in components, we get

$$
\begin{aligned}
l_i &= \sum_\alpha m_\alpha [\omega_i\, r_\alpha^2 - (\mathbf{r}_\alpha)_i\, (\mathbf{r}_\alpha \cdot \boldsymbol{\omega})] \\
&= \sum_\alpha m_\alpha [\omega_i\, r_\alpha^2 - (\mathbf{r}_\alpha)_i\, \sum_j (\mathbf{r}_\alpha)_j \omega_j] \\
&= \sum_\alpha m_\alpha [\sum_j \delta_{ij}\omega_j\, r_\alpha^2 - (\mathbf{r}_\alpha)_i\, \sum_j (\mathbf{r}_\alpha)_j \omega_j] \\
&= \sum_j \sum_\alpha m_\alpha [r_\alpha^2\, \delta_{ij} - (\mathbf{r}_\alpha)_i\, (\mathbf{r}_\alpha)_j] \omega_j \\
&\equiv \sum_j M_{ij}\omega_j
\end{aligned}
$$

where $M_{ij} \equiv \sum_\alpha m_\alpha [r_\alpha^2\, \delta_{ij} - (\mathbf{r}_\alpha)_i\, (\mathbf{r}_\alpha)_j]$. Or in Dirac notation,

$$
|l\rangle = M|\omega\rangle
$$

(1) No. The angular momentum and angular velocity are not parallel unless $|\omega\rangle$ is an eigenvector of $M$.

(2) $M_{ji}^\star = (\sum_\alpha m_\alpha [r_\alpha^2\, \delta_{ji} - (\mathbf{r}_\alpha)_j\, (\mathbf{r}_\alpha)_i])^\star = \sum_\alpha m_\alpha [r_\alpha^2\, \delta_{ij} - (\mathbf{r}_\alpha)_i\, (\mathbf{r}_\alpha)_j] = M_{ij}$.

(3) Since $M$ is Hermitian, we can always find three eigenvectors which are orthogonal to each other by solving the eigen-problem $M|\omega\rangle = \omega|\omega\rangle$. And these three eigenvectors denote the three directions for $\boldsymbol{\omega}$ we want to find in the 3-dimensional Euclidean space.

(4) The complete symmetry of sphere means all directions are equivalent eigendirections. Therefore, the eigenvalues are degenerate.

**Exercise 1.8.10.** By considering the commutator, show that the following Hermitian matrices may be simultaneously diagonalized. Find the eigenvectors common to both and verify that under a unitary transformation to this basis, both matrices are diagonalized.

$$
\Omega = \begin{pmatrix} 1 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 1 \end{pmatrix}, \quad \Lambda = \begin{pmatrix} 2 & 1 & 1 \\ 1 & 0 & -1 \\ 1 & -1 & 2 \end{pmatrix}
$$

Since $\Omega$ is degenerate and $\Lambda$ is not, you must be prudent in deciding which matrix dictates the choice of basis.

**Solution.** Since the two Hermitian matrices commute

$$\begin{aligned}[\Omega, \Lambda] &= \Omega\Lambda - \Lambda\Omega \\ &= \begin{pmatrix} 1 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 1 \end{pmatrix}\begin{pmatrix} 2 & 1 & 1 \\ 1 & 0 & -1 \\ 1 & -1 & 2 \end{pmatrix} - \begin{pmatrix} 2 & 1 & 1 \\ 1 & 0 & -1 \\ 1 & -1 & 2 \end{pmatrix}\begin{pmatrix} 1 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 1 \end{pmatrix} \\ &= \begin{pmatrix} 3 & 0 & 3 \\ 0 & 0 & 0 \\ 3 & 0 & 3 \end{pmatrix} - \begin{pmatrix} 3 & 0 & 3 \\ 0 & 0 & 0 \\ 3 & 0 & 3 \end{pmatrix} \\ &= 0 \end{aligned}$$

They can be diagonalized simultaneously. We choose $\Lambda$'s characteristic equation

$$\det(\Lambda - \lambda\mathbb{I}) = \begin{vmatrix} 2-\lambda & 1 & 1 \\ 1 & -\lambda & -1 \\ 1 & -1 & 2-\lambda \end{vmatrix} = (\lambda+1)(2-\lambda)(\lambda-3) = 0$$

The eigenvalues are

$$\lambda = -1, 2, 3$$

Then the eigenvectors corresponding the eigenvalues are

$$\begin{aligned} \lambda = -1: &\quad \begin{pmatrix} 3 & 1 & 1 \\ 1 & 1 & -1 \\ 1 & -1 & 3 \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = 0 \quad \Rightarrow \quad |\lambda = -1\rangle = \frac{1}{\sqrt{6}}\begin{pmatrix} 1 \\ -2 \\ -1 \end{pmatrix} \\ \lambda = 2: &\quad \begin{pmatrix} 0 & 1 & 1 \\ 1 & -2 & -1 \\ 1 & -1 & 0 \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = 0 \quad \Rightarrow \quad |\lambda = 2\rangle = \frac{1}{\sqrt{3}}\begin{pmatrix} 1 \\ 1 \\ -1 \end{pmatrix} \\ \lambda = 3: &\quad \begin{pmatrix} -1 & 1 & 1 \\ 1 & -3 & -1 \\ 1 & -1 & -1 \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = 0 \quad \Rightarrow \quad |\lambda = 3\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} \end{aligned}$$

Then the matrix of eigenvectors of $\Lambda$ is

$$U = \begin{pmatrix} \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{2}} \\ -\frac{2}{\sqrt{6}} & \frac{1}{\sqrt{3}} & 0 \\ -\frac{1}{\sqrt{6}} & -\frac{1}{\sqrt{3}} & \frac{1}{\sqrt{2}} \end{pmatrix}$$

To verify $\Omega$ and $\Lambda$ are simultanelously diagonalized:

$$\begin{aligned} U^\dagger \Omega U &= \begin{pmatrix} \frac{1}{\sqrt{6}} & -\frac{2}{\sqrt{6}} & -\frac{1}{\sqrt{6}} \\ \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \end{pmatrix}\begin{pmatrix} 1 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 1 \end{pmatrix}\begin{pmatrix} \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{2}} \\ -\frac{2}{\sqrt{6}} & \frac{1}{\sqrt{3}} & 0 \\ -\frac{1}{\sqrt{6}} & -\frac{1}{\sqrt{3}} & \frac{1}{\sqrt{2}} \end{pmatrix} \\ &= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ \sqrt{2} & 0 & \sqrt{2} \end{pmatrix}\begin{pmatrix} \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{2}} \\ -\frac{2}{\sqrt{6}} & \frac{1}{\sqrt{3}} & 0 \\ -\frac{1}{\sqrt{6}} & -\frac{1}{\sqrt{3}} & \frac{1}{\sqrt{2}} \end{pmatrix} \\ &= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 2 \end{pmatrix} \end{aligned}$$

$$
\begin{aligned}
U^\dagger \Lambda U &= \begin{pmatrix} \frac{1}{\sqrt{6}} & -\frac{2}{\sqrt{6}} & -\frac{1}{\sqrt{6}} \\ \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} 2 & 1 & 1 \\ 1 & 0 & -1 \\ 1 & -1 & 2 \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{2}} \\ -\frac{2}{\sqrt{6}} & \frac{1}{\sqrt{3}} & 0 \\ -\frac{1}{\sqrt{6}} & -\frac{1}{\sqrt{3}} & \frac{1}{\sqrt{2}} \end{pmatrix} \\
&= \begin{pmatrix} -\frac{1}{\sqrt{6}} & \frac{2}{\sqrt{6}} & \frac{1}{\sqrt{6}} \\ \frac{2}{\sqrt{3}} & \frac{2}{\sqrt{3}} & -\frac{2}{\sqrt{3}} \\ \frac{3}{\sqrt{2}} & 0 & \frac{3}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{2}} \\ -\frac{2}{\sqrt{6}} & \frac{1}{\sqrt{3}} & 0 \\ -\frac{1}{\sqrt{6}} & -\frac{1}{\sqrt{3}} & \frac{1}{\sqrt{2}} \end{pmatrix} \\
&= \begin{pmatrix} -1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 3 \end{pmatrix}
\end{aligned}
$$

**Exercise 1.8.11.** Consider the coupled mass problem discussed above.

(1) Given that the initial state is $|1\rangle$, in which the first mass is displaced by unity and the second is left alone, calculate $|1(t)\rangle$ by following the algorithm.

(2) Compare your result with that following from Eq. (1.8.39).

**Solution.**

(1) Equation of motion

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} -\frac{2k}{m} & \frac{k}{m} \\ \frac{k}{m} & -\frac{2k}{m} \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$$

Set

$$\begin{vmatrix} -\frac{2k}{m} + \omega^2 & \frac{k}{m} \\ \frac{k}{m} & -\frac{2k}{m} + \omega^2 \end{vmatrix} = 0$$

we have

$$\omega_1 = \sqrt{\frac{3k}{m}} \quad \omega_2 = \sqrt{\frac{k}{m}}$$

The corresponding eigenvectors are

$$|\omega_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix} \quad |\omega_2\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

Then the matrix of eigenvectors is

$$\Lambda \equiv \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix}$$

It can diagonalize the original matrix

$$\Lambda^\dagger \begin{pmatrix} -\frac{2k}{m} & \frac{k}{m} \\ \frac{k}{m} & -\frac{2k}{m} \end{pmatrix} \Lambda = \begin{pmatrix} -\omega_1^2 & 0 \\ 0 & -\omega_2^2 \end{pmatrix}$$

In eigenbasis,

$$\begin{pmatrix} \ddot{x}_I \\ \ddot{x}_{II} \end{pmatrix} = \begin{pmatrix} -\omega_1^2 & 0 \\ 0 & -\omega_2^2 \end{pmatrix}\begin{pmatrix} x_I \\ x_{II} \end{pmatrix} \quad \Rightarrow \quad \begin{cases} x_I(t) = x_I(0)\cos\omega_1 t \\ x_{II}(t) = x_{II}(0)\cos\omega_2 t \end{cases} \qquad (\star)$$

In this problem,

$$|1\rangle = \begin{pmatrix} x_1(0) \\ x_2(0) \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

We first transform it into eigenbasis

$$\begin{pmatrix} x_I(t) \\ x_{II}(t) \end{pmatrix} = \Lambda^\dagger \begin{pmatrix} x_1(0) \\ x_2(0) \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}$$

In the eigenbasis, the state evolves according to ($\star$).

$$\begin{pmatrix} x_I(t) \\ x_{II}(t) \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} \cos \omega_1 t \\ \frac{1}{\sqrt{2}} \cos \omega_2 t \end{pmatrix}$$

Then we transform it back to the original basis:

$$\begin{aligned} |1(t)\rangle = \begin{pmatrix} x_1(t) \\ x_2(t) \end{pmatrix} &= \Lambda \begin{pmatrix} x_I(t) \\ x_{II}(t) \end{pmatrix} \\ &= \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} \cos \omega_1 t \\ \frac{1}{\sqrt{2}} \cos \omega_2 t \end{pmatrix} \\ &= \begin{pmatrix} \frac{1}{2} \cos \sqrt{\frac{3k}{m}} t + \frac{1}{2} \cos \sqrt{\frac{k}{m}} t \\ -\frac{1}{2} \cos \sqrt{\frac{3k}{m}} t + \frac{1}{2} \cos \sqrt{\frac{k}{m}} t \end{pmatrix} \end{aligned}$$

(2) By subsitituting $\begin{pmatrix} x_1(0) \\ x_2(0) \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ in equation (1.8.39), we can get the same solution:

$$\begin{pmatrix} x_1(t) \\ x_2(t) \end{pmatrix} = \begin{pmatrix} \frac{1}{2} \cos \sqrt{\frac{3k}{m}} t + \frac{1}{2} \cos \sqrt{\frac{k}{m}} t \\ -\frac{1}{2} \cos \sqrt{\frac{3k}{m}} t + \frac{1}{2} \cos \sqrt{\frac{k}{m}} t \end{pmatrix}$$

**Exercise 1.8.12.** Consider once again the problem discussed in the previous example.

(1) Assuming that

$$|\ddot{x}\rangle = \Omega |x\rangle$$

has a solution

$$|x(t)\rangle = U(t)|x(0)\rangle$$

find the differential equation satisfied by $U(t)$. Use the fact that $|x(0)\rangle$ is arbitrary.

(2) Assuming (as is the case) that $\Omega$ and $U$ can be simultaneously diagonalized, solve for the elements of the matrix $U$ in this common basis and regain Eq. (1.8.43). Assume $|\dot{x}(0)\rangle = 0$.

**Solution.**

(1) Assuming that

$$|\ddot{x}(t)\rangle = \Omega|x(t)\rangle$$

has a solution

$$|x(t)\rangle = U(t)|x(0)\rangle$$

Then we can get

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2}U(t)|x(0)\rangle = \Omega U(t)|x(0)\rangle$$
$$\left(\frac{\mathrm{d}^2}{\mathrm{d}t^2} - \Omega\right)U(t)|x(0)\rangle = 0$$

Since $|x(0)\rangle$ is arbitrary, we get the differential equation

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2}U(t) - \Omega U(t) = 0$$

(2) From Exercise 1.8.11, we know the $\Lambda = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix}$ can diagonalize $\Omega$, and therefore, it can also diagonalize $U$.

In this common basis, we have

$$\begin{pmatrix} \ddot{U}_{11}(t) & 0 \\ 0 & \ddot{U}_{22}(t) \end{pmatrix} - \begin{pmatrix} -\omega_1^2 & 0 \\ 0 & -\omega_2^2 \end{pmatrix}\begin{pmatrix} U_{11}(t) & 0 \\ 0 & U_{22}(t) \end{pmatrix} = 0$$

$$\Rightarrow \begin{cases} \ddot{U}_{11}(t) + \omega_1^2 U_{11}(t) = 0 \\ \ddot{U}_{22}(t) + \omega_2^2 U_{22}(t) = 0 \end{cases}$$

$$\Rightarrow \begin{cases} U_{11} = A_1 \cos\omega_1 t + B_1 \sin\omega_1 t \\ U_{22} = A_2 \cos\omega_2 t + B_2 \sin\omega_2 t \end{cases}$$

Then

$$|\dot{x}(0)\rangle = \frac{\mathrm{d}}{\mathrm{d}t}[U(t)|x(0)\rangle]\bigg|_{t=0} = \left(\frac{\mathrm{d}}{\mathrm{d}t}U(t)\right)\bigg|_{t=0}|x(0)\rangle = 0$$

Since $|x(0)\rangle$ is arbitrary, we have

$$\frac{\mathrm{d}}{\mathrm{d}t}U(t)\bigg|_{t=0} = 0$$

which means

$$\dot{U}_{11}(0) = \dot{U}_{22}(0) = 0$$
$$B_1 = B_2 = 0$$

To satisfy that $U$ is unitary, we have

$$A_1 = A_2 = 1$$

Therefore,

$$U = \begin{pmatrix} \cos\omega_1 t & 0 \\ 0 & \cos\omega_2 t \end{pmatrix}$$

which is the same as equation (1.8.43).

## 1.9 Functions of Operators and Related Concepts

**Exercise 1.9.1.** We know that the series

$$f(x) = \sum_{n=0}^{\infty} x^n$$

may be equated to the function $f(x) = (1-x)^{-1}$ if $|x| < 1$. By going to the eigenbasis, examine when the $q$ number power series

$$f(\Omega) = \sum_{n=0}^{\infty} \Omega^n$$

of a Hermitian operator $\Omega$ may be identified with $(1-\Omega)^{-1}$.

**Solution.** In the eigenbasis,

$$\Omega = \begin{pmatrix} \omega_1 & & & \\ & \omega_2 & & \\ & & \ddots & \\ & & & \omega_m \end{pmatrix}$$

where $\omega_i$ are eigenvalues.

$$f(\Omega) = \sum_{n=0}^{\infty} \Omega^n = \begin{pmatrix} \sum\limits_{n=0}^{\infty} \omega_1^n & & \\ & \ddots & \\ & & \sum\limits_{n=0}^{\infty} \omega_m^n \end{pmatrix} = \begin{pmatrix} \frac{1}{1-\omega_1} & & \\ & \ddots & \\ & & \frac{1}{1-\omega_m} \end{pmatrix} = \frac{1}{1-\Omega}$$

The third equality holds if and only if $|\omega_i| < 1$ for $i = 1, \ldots, m$. Therefore, $f(\Omega)$ can be defined as $\frac{1}{1-\Omega}$ if and only if the absolute value of each of $\Omega$'s eigenvalues is less than 1.

**Exercise 1.9.2.** If $H$ is a Hermitian operator, show that $U = \mathrm{e}^{\mathrm{i}H}$ is unitary. (Notice the analogy with $c$ numbers: if $\theta$ is real, $u = \mathrm{e}^{\mathrm{i}\theta}$ is a number of unit modulus.)

**Solution.** Since $H$ is Hermitian, it satisfies

$$H^\dagger = H$$

We can compute

$$U^\dagger = (\mathrm{e}^{\mathrm{i}H})^\dagger = \mathrm{e}^{-\mathrm{i}H^\dagger} = \mathrm{e}^{-\mathrm{i}H}$$

Then[2]

$$U^\dagger U = \mathrm{e}^{-\mathrm{i}H}\mathrm{e}^{\mathrm{i}H} = \mathrm{e}^{-\mathrm{i}H+\mathrm{i}H} = 1$$

Therefore $U$ is unitary.

[2]The second equality holds only for commuting operators.

**Exercise 1.9.3.** For the case above, show that $\det U = \mathrm{e}^{\mathrm{i}\,\mathrm{Tr}\,H}$.

**Solution.** In the eigenbasis of $H$,

$$U = \mathrm{e}^{\mathrm{i}H} = \begin{pmatrix} \sum\limits_{n=0}^{\infty} \frac{(\mathrm{i}\epsilon_1)^n}{n!} & & \\ & \ddots & \\ & & \sum\limits_{n=0}^{\infty} \frac{(\mathrm{i}\epsilon_m)^n}{n!} \end{pmatrix} = \begin{pmatrix} \mathrm{e}^{\mathrm{i}\epsilon_1} & & \\ & \ddots & \\ & & \mathrm{e}^{\mathrm{i}\epsilon_m} \end{pmatrix}$$

where $\epsilon_1, \ldots, \epsilon_m$ are eigenvalues of $H$, i.e.

$$H = \begin{pmatrix} \epsilon_1 & & \\ & \ddots & \\ & & \epsilon_m \end{pmatrix}$$

Therefore,

$$\det U = \prod_{i=1}^{m} \mathrm{e}^{\mathrm{i}\epsilon_i} = \mathrm{e}^{\mathrm{i}\sum\limits_{i=1}^{m}\epsilon_i} = \mathrm{e}^{\mathrm{i}\,\mathrm{Tr}\,H}$$

## 1.10 Generalization to Infinite Dimensions

**Exercise 1.10.1.** Show that $\delta(ax) = \delta(x)/|a|$. [Consider $\int \delta(ax)\,\mathrm{d}(ax)$. Remember that $\delta(x) = \delta(-x)$.]

**Solution.** Since $\delta(x) = \delta(-x)$, we have

$$\delta(ax) = \delta(|a|x)$$

Therefore,

$$\begin{aligned} \int_{-\infty}^{\infty} \delta(ax)dx &= \int_{-\infty}^{\infty} \delta(|a|x)dx = \int_{-\infty}^{\infty} \delta(|a|x)\cdot\frac{1}{|a|}\mathrm{d}(|a|x) \\ &= \frac{1}{|a|}\int_{-\infty}^{\infty} \delta(|a|x)\,\mathrm{d}(|a|x) \qquad \text{(change } |a|x \text{ to } x\text{)} \\ &= \frac{1}{|a|}\int_{-\infty}^{\infty} \delta(x)\,\mathrm{d}x \end{aligned}$$

Thus,

$$\delta(ax) = \delta(x)/|a|$$

**Exercise 1.10.2.** Show that

$$\delta(f(x)) = \sum_i \frac{\delta\left(x_i - x\right)}{|\mathrm{d}f/\mathrm{d}x_i|}$$

where $x_i$ are the zeros of $f(x)$. Hint: Where does $\delta(f(x))$ blow up? Expand $f(x)$ near such points in a Taylor series, keeping the first nonzero term.

**Solution.** Expand $f(x)$ around $x_i$, where $f(x_i) = 0$:

$$\begin{aligned} f(x) &= f(x_i) + f'(x_i)(x - x_i) + \frac{1}{2} f''(x_i)(x - x_i)^2 + \cdots \\ &= 0 + f'(x_i)(x - x_i) + \mathcal{O}[(x - x_i)^2] \\ &\approx f'(x_i)(x - x_i) \end{aligned}$$

Introduce a test function $g(x)$,[3]

$$\begin{aligned} \int_{-\infty}^{\infty} g(x)\delta(f(x))\mathrm{d}x &= \sum_i \int_{x_i-\epsilon}^{x_i+\epsilon} g(x)\,\delta(f(x))\,\mathrm{d}x \\ &= \sum_i \int_{x_i-\epsilon}^{x_i+\epsilon} g(x)\,\delta\left( \left.\frac{\mathrm{d}f}{\mathrm{d}x}\right|_{x=x_i} (x - x_i) \right) \mathrm{d}x \\ &= \sum_i \int_{x_i-\epsilon}^{x_i+\epsilon} g(x)\, \frac{\delta(x - x_i)}{\left| \left.\frac{\mathrm{d}f}{\mathrm{d}x}\right|_{x=x_i} \right|} \mathrm{d}x \end{aligned}$$

Therefore,

$$\delta(f(x)) = \sum_i \frac{\delta(x - x_i)}{|f'(x_i)|}$$

**Exercise 1.10.3.** Consider the theta function $\theta(x-x')$ which vanishes if $x-x'$ is negative and equals 1 if $x-x'$ is positive. Show that $\delta(x-x') = \frac{\mathrm{d}}{\mathrm{d}x}\theta(x-x')$.

**Solution.** Introduce a test function[4] $g(x)$, we have

$$\begin{aligned} \int_{-\infty}^{\infty} g(x)\,\frac{\mathrm{d}}{\mathrm{d}x}\theta(x - x')\mathrm{d}x &= \int_{-\infty}^{\infty} \mathrm{d}\theta(x - x') \\ &= \theta(x - x')g(x)\Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \theta(x - x')g'(x)\mathrm{d}x \\ &= 1 \cdot g(\infty) - 0 \cdot g(-\infty) - \infty_0^{\infty} g'(x)\mathrm{d}x \\ &= g(\infty) - [g(\infty) - g(0)] \\ &= g(0) \\ &= \int_{-\infty}^{\infty} g(x)\delta(x)\mathrm{d}x \end{aligned}$$

Therefore,

$$\frac{\mathrm{d}}{\mathrm{d}x}\theta(x - x') = \delta(x)$$

**Exercise 1.10.4.** A string is displaced as follows at $t = 0$ :

$$\begin{aligned} \psi(x, 0) &= \frac{2xh}{L}, & 0 \leqslant x \leqslant \frac{L}{2} \\ &= \frac{2h}{L}(L - x), & \frac{L}{2} \leqslant x \leqslant L \end{aligned}$$

[3] We use the Exercise 1.10.1 at the last equality.

[4] $g(-\infty)$ and $g(\infty)$ are finite

Show that

$$\psi(x,t)=\sum_{m=1}^{\infty}\sin\left(\frac{m\pi x}{L}\right)\cos\omega_m t\cdot\left(\frac{8h}{\pi^2m^2}\right)\sin\left(\frac{\pi m}{2}\right)$$

**Solution.** We start from equation (1.10.55)

$$|\psi(t)\rangle=\sum_{m=1}^{\infty}|m\rangle\langle m\mid\psi(0)\rangle\cos\omega_m t,\qquad \omega_m=\frac{m\pi}{L}$$

Then

$$\psi(x,t)=\langle x\mid\psi(t)\rangle=\sum_{in=1}^{\infty}\langle x\mid m\rangle\langle m\mid\psi(0)\rangle\cos\omega_m t$$

From equation (1.10.55), we have

$$\langle x\mid m\rangle=\psi_m(x)=\left(\frac{2}{L}\right)^{\frac{1}{2}}\sin\frac{m\pi x}{L}$$

Therefore,

$$\begin{aligned}\langle m\mid\psi(0)\rangle&=\int_0^L\left(\frac{2}{L}\right)^{\frac{1}{2}}\sin\frac{m\pi x}{L}\cdot\psi(x,0)\,\mathrm{d}x\\&=\left(\frac{2}{L}\right)^{\frac{1}{2}}\left[\int_0^{\frac{L}{2}}\frac{2xh}{L}\sin\frac{m\pi x}{L}\mathrm{d}x+\int_{\frac{L}{2}}^{L}\frac{2h}{L}(L-x)\sin\frac{m\pi x}{L}\mathrm{d}x\right]\end{aligned}$$

where

$$\begin{aligned}\int_0^{\frac{L}{2}}\frac{2xh}{L}\sin\frac{m\pi x}{L}\mathrm{d}x&=-\frac{2h}{L}\cdot\frac{L}{m\pi}\int_0^{\frac{L}{2}}x\mathrm{d}\cos\frac{m\pi x}{L}\\&=-\frac{2h}{L}\cdot\frac{L}{m\pi}x\cos\frac{m\pi x}{L}\Big|_0^{\frac{L}{2}}+\frac{2h}{L}\cdot\frac{L}{m\pi}\int_0^{\frac{L}{2}}\cos\frac{m\pi x}{L}\mathrm{d}x\\&=-\frac{2h}{2}\cdot\frac{L}{2}\cos\frac{m\pi}{2}+\frac{2h}{L}\left(\frac{L}{m\pi}\right)^2\sin\frac{m\pi x}{L}\Big|_0^{\frac{L}{2}}\\&=-\frac{hL}{m\pi}\cos\frac{m\pi}{2}+\frac{2h}{L}\left(\frac{L}{m\pi}\right)^2\sin\frac{m\pi}{2}\end{aligned}$$

$$\int_{\frac{L}{2}}^{L}\frac{2h}{L}(L-x)\sin\frac{m\pi x}{L}\mathrm{d}x=\int_{\frac{L}{2}}^{L}\frac{2h}{L}\cdot L\sin\frac{m\pi x}{L}\mathrm{d}x-\int_{\frac{L}{2}}^{L}\frac{2hx}{L}\sin\frac{m\pi x}{L}\mathrm{d}x$$

$$=-2h\cdot\frac{L}{m\pi}\cos\frac{m\pi x}{L}\Big|_{\frac{L}{2}}^{L}+\frac{2h}{L}\cdot\frac{L}{m\pi}\int_{\frac{L}{2}}^{L}x\mathrm{d}\cos\frac{m\pi x}{L}$$

$$=\frac{2hL}{m\pi}\cos\frac{m\pi}{2}-\frac{2hL}{m\pi}\cos m\pi+\frac{2h}{L}\cdot\frac{L}{m\pi}x\cos\frac{m\pi x}{L}\Big|_{\frac{L}{2}}^{L}-\frac{2h}{m\pi}\int_{\frac{L}{2}}^{L}\cos\frac{m\pi}{L}\mathrm{d}x$$

$$=\frac{2hL}{m\pi}\cos\frac{m\pi}{2}-\cancel{\frac{2hL}{2m\pi}\cos m\pi}+\cancel{\frac{2hL}{2n\pi}\cos m\pi}-\frac{hL}{m\pi}\cos\frac{m\pi}{2}-\frac{2h}{m\pi}\cdot\frac{L}{m\pi}\sin\frac{m\pi x}{L}\Big|_{\frac{L}{2}}^{L}$$

$$=\frac{hL}{m\pi}\cos\frac{m\pi}{2}-\underbrace{\frac{2h}{L}\left(\frac{L}{m\pi}\right)^2\sin m\pi}_{=0}+\frac{2h}{L}\left(\frac{L}{m\pi}\right)^2\sin\frac{m\pi}{2}$$

Then

$$\langle m \mid \psi(0)\rangle = \left(\frac{2}{L}\right)^{\frac{1}{2}} \frac{4h}{L} \left(\frac{L}{m\pi}\right)^{2} \sin\frac{m\pi}{2}$$

Therefore,

$$\begin{aligned} \psi(x,t) &= \sum_{m=1}^{\infty} \left(\frac{2}{L}\right)^{\frac{1}{2}} \sin\frac{m\pi x}{L} \cdot \left(\frac{2}{L}\right)^{\frac{1}{2}} \cdot \frac{4h}{L} \left(\frac{L}{m\pi}\right)^{2} \sin\frac{m\pi}{2} \cos\omega_m t \\ &= \sum_{m=1}^{\infty} \sin\left(\frac{m\pi x}{L}\right) \cos\omega_m t \cdot \left(\frac{8h}{\pi^2 m^2}\right) \sin\left(\frac{\pi m}{2}\right) \end{aligned}$$

# Chapter 2

# Review of Classical Mechanics

## 2.1 The Principle of Least Action and Lagrangian Mechanics

**Exercise 2.1.1.** Consider the following system, called a *harmonic oscillator*. The block has a mass $m$ and lies on a frictionless surface. The spring has a force constant $k$. Write the Lagrangian and get the equation of motion.

**Solution.** The kinetic energy and potential energy are

$$T = \frac{1}{2}m\dot{x}^2$$
$$V = \frac{1}{2}kx^2$$

Then the Lagrangian is

$$\mathscr{L} = T - V = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}kx^2$$

We can compute

$$\frac{\partial \mathscr{L}}{\partial \dot{x}} = m\dot{x}$$
$$\frac{\partial \mathscr{L}}{\partial x} = -kx$$

Therefore, the Euler-Lagrange equation is

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial \mathscr{L}}{\partial \dot{x}}\right) - \frac{\partial \mathscr{L}}{\partial x} = 0$$

The equation of motion is

$$m\ddot{x} + kx = 0$$

**Exercise 2.1.2.** Do the same for the coupled-mass problem discussed at the end of Section 1.8. Compare the equations of motion with Eqs. (1.8.24) and (1.8.25).

**Solution.** The kinetic energy and potential energy of the system are

$$
\begin{aligned}
T &= \frac{1}{2}m\dot{x}_1^2 + \frac{1}{2}m\dot{x}_2^2 \\
V &= \frac{1}{2}kx^2 + \frac{1}{2}k(x_2 - x_1)^2 + \frac{1}{2}kx_2^2
\end{aligned}
$$

Then the Lagrangian is

$$
\mathscr{L} = T - V = \frac{1}{2}m(\dot{x}_1^2 + \dot{x}_2^2) - k(x_1^2 - x_1x_2 + x_2^2)
$$

- The Euler-Lagrange equation of 1:

$$
\begin{aligned}
\frac{\partial \mathscr{L}}{\partial \dot{x}_1} &= m\dot{x}_1 \\
\frac{\partial \mathscr{L}}{\partial x_1} &= -2kx_1 + kx_2 \\
\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial \mathscr{L}}{\partial \dot{x}_1}\right) - \frac{\partial \mathscr{L}}{\partial x_1} &= 0
\end{aligned}
$$

  We get equation of motion

$$
\begin{aligned}
m\ddot{x}_1 + 2kx_1 - kx_2 &= 0 \\
\ddot{x}_1 &= -\frac{2k}{m}x_1 + \frac{k}{m}x_2 \qquad (2.1)
\end{aligned}
$$

- The Euler-Lagrange equation of 2:

$$
\begin{aligned}
\frac{\partial \mathscr{L}}{\partial \dot{x}_2} &= m\dot{x}_2 \\
\frac{\partial \mathscr{L}}{\partial x_1} &= kx_1 - 2kx_2 \\
\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial \mathscr{L}}{\partial \dot{x}_2}\right) - \frac{\partial \mathscr{L}}{\partial x_2} &= 0
\end{aligned}
$$

  We get equation of motion

$$
\begin{aligned}
m\ddot{x}_2 - kx_1 + 2kx_2 &= 0 \\
\ddot{x}_2 &= \frac{k}{m}x_1 - \frac{2k}{m}x_2 \qquad (2.2)
\end{aligned}
$$

(2.1) and (2.2) are the same as Eqs. (1.8.24) and (1.8.25).

**Exercise 2.1.3.** A particle of mass $m$ moves in three dimensions under a potential $V(r, \theta, \phi) = V(r)$. Write its $\mathscr{L}$ and find the equations of motions.

**Solution.** The kinetic energy and potential energy are

$$
\begin{aligned}
T &= \frac{1}{2}m(\dot{r}^2 + r^2\dot{\theta}^2 + r^2\sin^2\theta\dot{\phi}^2) \\
V &= V(r)
\end{aligned}
$$

Then the Lagrangian is

$$
\mathscr{L} = T - V = \frac{1}{2}m(\dot{r}^2 + r^2\dot{\theta}^2 + r^2\sin^2\theta\dot{\phi}^2) - V(r)
$$

- Euler-Lagrange equation of $r$:

$$\frac{\partial \mathscr{L}}{\partial \dot{r}} = m\dot{r}, \quad \frac{\partial \mathscr{L}}{\partial r} = mr\dot{\theta}^2 + mr\sin^2\theta\,\dot{\phi}^2 - \frac{\partial V(r)}{r}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial \mathscr{L}}{\partial \dot{r}}\right) - \frac{\partial \mathscr{L}}{\partial r} = 0$$

The equation of motion is

$$m\ddot{r} - mr\dot{\theta}^2 - mr\sin^2\theta\,\dot{\phi}^2 + \frac{\partial V(r)}{\partial r} = 0$$

- Euler-Lagrange equation of $\theta$:

$$\frac{\partial \mathscr{L}}{\partial \dot{\theta}} = mr^2\dot{\theta}, \quad \frac{\partial \theta}{\partial r} = mr^2\sin\theta\cos\theta\,\dot{\phi}^2$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial \mathscr{L}}{\partial \dot{\theta}}\right) - \frac{\partial \mathscr{L}}{\partial \theta} = 0$$

The equation of motion is

$$mr^2\ddot{\theta} + 2mr\dot{r}\dot{\theta} - mr^2\sin\theta\cos\theta\,\dot{\phi}^2 = 0$$

- Euler-Lagrange equation of $\phi$:

$$\frac{\partial \mathscr{L}}{\partial \dot{\phi}} = mr^2\sin^2\theta\dot{\phi}, \quad \frac{\partial \mathscr{L}}{\partial \phi} = 0$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial \mathscr{L}}{\partial \dot{r}}\right) - \frac{\partial \mathscr{L}}{\partial r} = 0$$

The equation of motion is

$$\frac{\mathrm{d}}{\mathrm{d}t}(mr^2\sin^2\theta\,\dot{\phi}) = 0$$
$$mr^2\sin^2\theta\,\dot{\phi} = l$$
$$\dot{\phi} = \frac{l}{mr^2\sin^2\theta}$$

where $l$ is a contant.

## 2.2 The Electromagnetic Lagrangian

## 2.3 The Two Body Problem

**Exercise 2.3.1.** Derive Eq. (2.3.6) from (2.3.5) by changing variables.

**Solution.** Since

$$\mathbf{r}_1 = \mathbf{r}_{\text{CM}} + \frac{m_2\mathbf{r}}{m_1+m_2} \qquad \dot{\mathbf{r}}_1 = \dot{\mathbf{r}}_{\text{CM}} + \frac{m_2\dot{\mathbf{r}}}{m_1+m_2}$$
$$\mathbf{r}_2 = \mathbf{r}_{\text{CM}} - \frac{m_1\mathbf{r}}{m_1+m_2} \qquad \dot{\mathbf{r}}_2 = \dot{\mathbf{r}}_{\text{CM}} - \frac{m_1\dot{\mathbf{r}}}{m_1+m_2}$$

The Lagrangian becomes

$$
\begin{aligned}
\mathscr{L} &= \frac{1}{2}m_1\left|\dot{\mathbf{r}}_1\right|^2 + \frac{1}{2}m_2\left|\dot{\mathbf{r}}_2\right|^2 - V(\mathbf{r}_1 - \mathbf{r}_2) \\
&= \frac{1}{2}m_1\left(\dot{\mathbf{r}}_{\mathrm{CM}} + \frac{m_2\dot{\mathbf{r}}}{m_1+m_2}\right)^2 + \frac{1}{2}m_2\left(\dot{\mathbf{r}}_{\mathrm{CM}} - \frac{m_1\dot{\mathbf{r}}}{m_1+m_2}\right)^2 - V(\mathbf{r}) \\
&= \frac{1}{2}m_1|\dot{\mathbf{r}}_{\mathrm{CM}}|^2 + \frac{1}{2}\frac{m_1m_2^2}{(m_1+m_2)^2}|\dot{\mathbf{r}}|^2 + \frac{1}{2}m_2|\dot{\mathbf{r}}_{\mathrm{CM}}|^2 + \frac{1}{2}\frac{m_2m_1^2}{(m_1+m_2)^2}|\dot{\mathbf{r}}|^2 - V(\mathbf{r}) \\
&= \frac{1}{2}(m_1+m_2)|\dot{\mathbf{r}}_{\mathrm{CM}}|^2 + \frac{1}{2}\frac{m_1m_2(m_1+m_2)}{(m_1+m_2)^2}|\dot{\mathbf{r}}|^2 - V(\mathbf{r}) \\
&= \frac{1}{2}(m_1+m_2)|\dot{\mathbf{r}}_{\mathrm{CM}}|^2 + \frac{1}{2}\frac{m_1m_2}{m_1+m_2}|\dot{\mathbf{r}}|^2 - V(\mathbf{r})
\end{aligned}
$$

## 2.4 How Smart Is a Particle?

## 2.5 The Hamiltonian Formalism

**Exercise 2.5.1.** Show that if $T = \sum_i \sum_j T_{ij}(q)\dot{q}_i\dot{q}_j$, where $\dot{q}$'s are generalized velocities, $\sum_i p_i\dot{q}_i = 2T$.

**Solution.**

$$
\begin{aligned}
p_s &= \frac{\partial T}{\partial \dot{q}_s} \\
&= \sum_i \sum_j T_{ij}(q)\dot{q}_i\delta_{js} + \sum_i \sum_j T_{ij}(q)\delta_{is}\dot{q}_j \\
&= \sum_i T_{is}(q)\dot{q}_i + \sum_j T_{sj}(q)\dot{q}_j
\end{aligned}
$$

Therefore,

$$
\begin{aligned}
\sum_s p_s\dot{q}_s &= \sum_i T_{is}(q)\dot{q}_i\dot{q}_s + \sum_j T_{sj}(q)\dot{q}_j\dot{q}_s \\
&= T + T \\
&= 2T
\end{aligned}
$$

**Exercise 2.5.2.** Using the conservation of energy, show that the trajectories in phase space for the oscillator are ellipses of the form $(x/a)^2 + (p/b)^2 = 1$, where $a^2 = 2E/k$ and $b^2 = 2mE$.

**Solution.** The Lagrangian is

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

So the momentum is

$$p = \frac{\partial \mathscr{L}}{\partial \dot{x}} = m\dot{x}$$

Hamiltonian is

$$\mathscr{H} = p\dot{x} - \mathscr{L} = \frac{p^2}{2m} + \frac{1}{2}kx^2$$

Since $\mathscr{L}$ is not an explicit function of $t$, $\mathscr{H}$ is conservative. Set $\mathscr{H} = E$, where $E$ is a constant, we have

$$\frac{1}{2}kx^2 + \frac{p^2}{2m} = E$$

If we denote $a^2 = 2E/k$ and $b^2 = 2mE$, we have

$$\left(\frac{x}{a}\right)^2 + \left(\frac{p}{b}\right)^2 = 1$$

**Exercise 2.5.3.** Solve Exercise 2.1.2 using the Hamiltonian formalism.

**Solution.** Start from Lagrangian of the system

$$\mathscr{L} = \frac{1}{2}m(\dot{x}_1^2 + \dot{x}_2^2) - k(x_1^2 + x_2^2 - x_1 x_2)$$

Then the momenta are

$$\begin{aligned} p_1 &= \frac{\partial \mathscr{L}}{\partial \dot{x}_1} = m\dot{x}_1 \quad \Rightarrow \quad \dot{x}_1 = \frac{p_1}{m} \\ p_2 &= \frac{\partial \mathscr{L}}{\partial \dot{x}_2} = m\dot{x}_2 \quad \Rightarrow \quad \dot{x}_2 = \frac{p_2}{m} \end{aligned}$$

Then the Hamiltonian of the system is

$$\begin{aligned} \mathscr{H} &= p_1\dot{x}_1 + p_2\dot{x}_2 - \mathscr{L} \\ &= \frac{p_1^2}{m} + \frac{p_2^2}{m} - \frac{p_1^2}{2m} - \frac{p_2^2}{2m} + k(x_1^2 + x_2^2 - x_1x_2) \\ &= \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + k(x_1^2 + x_2^2 - x_1x_2) \end{aligned}$$

- Hamilton's canonical equations of 1:

$$\begin{cases} \dot{x}_1 = \dfrac{\partial \mathscr{H}}{\partial p_1} = \dfrac{p_1}{m} \\ \dot{p}_1 = -\dfrac{\partial \mathscr{H}}{\partial x_1} = -2kx_1 + kx_2 \end{cases}$$

  From the first equation, we know $p_1 = m\dot{x}_1$. Take the time derivative on the both side, we get $\dot{p}_1 = m\ddot{x}_1$. Substitute it into the second equation, we get

$$\begin{aligned} m\ddot{x}_1 &= -2kx_1 + kx_2 \\ \ddot{x}_1 &= -\frac{2k}{m}x_1 + \frac{k}{m}x_2 \end{aligned}$$

- Hamilton's canonical equations of 2:

$$\begin{cases} \dot{x}_2 = \dfrac{\partial \mathscr{H}}{\partial p_2} = \dfrac{p_2}{m} \\ \dot{p}_2 = -\dfrac{\partial \mathscr{H}}{\partial x_2} = -2kx_2 + kx_1 \end{cases}$$

  From the first equation, we know $p_2 = m\dot{x}_2$. Take the time derivative on the both side, we get $\dot{p}_2 = m\ddot{x}_2$. Substitute it into the second equation, we get

$$\begin{aligned} m\ddot{x}_2 &= -2kx_2 + kx_1 \\ \ddot{x}_2 &= \frac{k}{m}x_1 - \frac{2k}{m}x_2 \end{aligned}$$

**Exercise 2.5.4.** Show that $\mathscr{H}$ corresponding to $\mathscr{L}$ in Eq. (2.3.6) is $\mathscr{H} = |\mathbf{p}_{\rm CM}|^2/2M + |\mathbf{p}|^2/\ 2\mu + V(\mathbf{r})$, where $M$ is the total mass, $\mu$ is the reduced mass, $\mathbf{p}_{\rm CM}$ and $\mathbf{p}$ are the momenta conjugate to $\mathbf{r}_{\rm CM}$ and $\mathbf{r}$, respectively.

**Solution.** Start from Lagrangian

$$\begin{aligned}\mathscr{L} &= \frac{1}{2}(m_1+m_2)|\dot{\mathbf{r}}_{\rm CM}|^2 + \frac{1}{2}\frac{m_1m_2}{m_1+m_2}|\dot{\mathbf{r}}|^2 - V(\mathbf{r})\\ &= \frac{1}{2}M|\dot{\mathbf{r}}_{\rm CM}|^2 + \frac{1}{2}\mu|\dot{\mathbf{r}}|^2 - V(\mathbf{r})\end{aligned}$$

where total mass $M = m_1 + m_2$ and reduced mass $\mu = \frac{m_1m_2}{m_1+m_2}$. Then the momenta satisfy

$$\begin{aligned}|\mathbf{p}_{\rm CM}| &= \frac{\partial\mathscr{L}}{\partial|\dot{\mathbf{r}}_{\rm CM}|} = M|\dot{\mathbf{r}}_{\rm CM}| \qquad &&\Rightarrow\quad |\dot{\mathbf{r}}_{\rm CM}| = \frac{|\mathbf{p}_{\rm CM}|}{M}\\ |\mathbf{p}| &= \frac{\partial\mathscr{L}}{\partial|\dot{\mathbf{r}}|} = \mu|\dot{\mathbf{r}}| &&\Rightarrow\quad |\dot{\mathbf{r}}| = \frac{|\mathbf{p}|}{\mu}\end{aligned}$$

Therefore the Hamiltonian is

$$\begin{aligned}\mathscr{H} &= \mathbf{p}_{\rm CM}\cdot\dot{\mathbf{r}}_{\rm CM} + \mathbf{p}\cdot\dot{\mathbf{r}} - \mathscr{L}\\ &= |\mathbf{p}_{\rm CM}||\dot{\mathbf{r}}_{\rm CM}| + |\mathbf{p}||\dot{\mathbf{r}}| - \frac{1}{2}M|\dot{\mathbf{r}}_{\rm CM}|^2 - \frac{1}{2}\mu|\dot{\mathbf{r}}|^2 + V(\mathbf{r})\\ &= \frac{|\mathbf{p}_{\rm CM}|^2}{M} + \frac{|\mathbf{p}|^2}{\mu} - \frac{1}{2}M\frac{|\mathbf{p}_{\rm CM}|^2}{M^2} - \frac{1}{2}\mu\frac{|\mathbf{p}|^2}{\mu^2} + V(\mathbf{r})\\ &= \frac{|\mathbf{p}_{\rm CM}|^2}{2M} + \frac{|\mathbf{p}|^2}{2\mu} + V(\mathbf{r})\end{aligned}$$

## 2.6 The Electromagnetic Force in the Hamiltonian Scheme

## 2.7 Cyclic Coordinates, Poisson Brackets, and Canonical Transformations

**Exercise 2.7.1.** Show that

$$\begin{aligned}\{\omega,\lambda\} &= -\{\lambda,\omega\}\\ \{\omega,\lambda+\sigma\} &= \{\omega,\lambda\} + \{\omega,\sigma\}\\ \{\omega,\lambda\sigma\} &= \{\omega,\lambda\}\sigma + \lambda\{\omega,\sigma\}\end{aligned}$$

Note the similarity between the above and Eqs. (1.5.10) and (1.5.11) for commutators.

**Solution.**

$$\{\omega,\lambda\} = \sum_i\left(\frac{\partial\omega}{\partial q_i}\frac{\partial\lambda}{\partial p_i} - \frac{\partial\omega}{\partial p_i}\frac{\partial\lambda}{\partial q_i}\right) = -\sum_i\left(\frac{\partial\lambda}{\partial q_i}\frac{\partial\omega}{\partial p_i} - \frac{\partial\lambda}{\partial p_i}\frac{\partial\omega}{\partial q_i}\right) = -\{\lambda,\omega\}$$

$$
\begin{aligned}
\{\omega, \lambda+\sigma\} &= \sum_i \left( \frac{\partial \omega}{\partial q_i} \cdot \frac{\partial(\lambda+\sigma)}{\partial p_i} - \frac{\partial \omega}{\partial p_i} \cdot \frac{\partial(\lambda+\sigma)}{\partial q_i} \right) \\
&= \sum_i \left[ \frac{\partial \omega}{\partial q_i} \cdot \left( \frac{\partial \lambda}{\partial p_i} + \frac{\partial \sigma}{\partial p_i} \right) - \frac{\partial \omega}{\partial p_i} \cdot \left( \frac{\partial \lambda}{\partial q_i} + \frac{\partial \sigma}{\partial q_i} \right) \right] \\
&= \sum_i \left[ \left( \frac{\partial \omega}{\partial q_i} \frac{\partial \lambda}{\partial p_i} - \frac{\partial \omega}{\partial p_i} \frac{\partial \lambda}{\partial q_i} \right) + \left( \frac{\partial \omega}{\partial q_i} \frac{\partial \sigma}{\partial p_i} - \frac{\partial \omega}{\partial p_i} \frac{\partial \sigma}{\partial q_i} \right) \right] \\
&= \sum_i \left( \frac{\partial \omega}{\partial q_i} \frac{\partial \lambda}{\partial p_i} - \frac{\partial \omega}{\partial p_i} \frac{\partial \lambda}{\partial q_i} \right) + \sum_i \left( \frac{\partial \omega}{\partial q_i} \frac{\partial \sigma}{\partial p_i} - \frac{\partial \omega}{\partial p_i} \frac{\partial \sigma}{\partial q_i} \right) \\
&= \{\omega, \lambda\} + \{\omega, \sigma\}
\end{aligned}
$$

$$
\begin{aligned}
\{\omega, \lambda\sigma\} &= \sum_i \left[ \frac{\partial \omega}{\partial q_i} \frac{\partial(\lambda\sigma)}{\partial p_i} - \frac{\partial \omega}{\partial p_i} \cdot \frac{\partial(\lambda\sigma)}{\partial q_i} \right] \\
&= \sum_i \left[ \lambda \frac{\partial \omega}{\partial q_i} \frac{\partial \sigma}{\partial p_i} + \frac{\partial \omega}{\partial q_i} \frac{\partial \lambda}{\partial p_i} \sigma - \lambda \frac{\partial \omega}{\partial p_i} \frac{\partial \sigma}{\partial q_i} - \frac{\partial \omega}{\partial p_i} \frac{\partial \lambda}{\partial q_i} \sigma \right] \\
&= \lambda \sum_i \left( \frac{\partial \omega}{\partial q_i} \frac{\partial \sigma}{\partial p_i} - \frac{\partial \omega}{\partial p_i} \frac{\partial \sigma}{\partial q_i} \right) + \sum_i \left( \frac{\partial \omega}{\partial q_i} \frac{\partial \lambda}{\partial p_i} - \frac{\partial \omega}{\partial p_i} \frac{\partial \lambda}{\partial q_i} \right) \sigma \\
&= \lambda \{\omega, \sigma\} + \{\omega, \lambda\} \sigma.
\end{aligned}
$$

**Exercise 2.7.2.** (i) Verify Eqs. (2.7.4) and (2.7.5). (ii) Consider a problem in two dimensions given by $\mathscr{H} = p_x^2 + p_y^2 + ax^2 + by^2$. Argue that if $a = b, \{l_z, \mathscr{H}\}$ must vanish. Verify by explicit computation.

**Solution.**

(i)

$$
\begin{aligned}
\{q_i, q_j\} &:= \sum_k \left( \frac{\partial q_i}{\partial q_k} \cdot \frac{\partial q_j}{\partial p_k} - \frac{\partial q_i}{\partial p_k} \cdot \frac{\partial q_j}{\partial q_k} \right) = \sum_k \left( \frac{\partial q_i}{\partial q_k} \cdot 0 - 0 \cdot \frac{\partial q_j}{\partial q_k} \right) = 0 \\
\{p_i, p_j\} &:= \sum_k \left( \frac{\partial p_i}{\partial q_k} \cdot \frac{\partial p_j}{\partial p_k} - \frac{\partial p_i}{\partial p_k} \cdot \frac{\partial p_j}{\partial q_k} \right) = \sum_k \left( 0 \cdot \frac{\partial p_j}{\partial p_k} - \frac{\partial p_i}{\partial p_k} \cdot 0 \right) = 0 \\
\{q_i, p_j\} &:= \sum_k \left( \frac{\partial q_i}{\partial q_k} \cdot \frac{\partial p_j}{\partial p_k} - \frac{\partial q_i}{\partial p_k} \cdot \frac{\partial p_j}{\partial q_k} \right) = \sum_k \left( \delta_{ik}\delta_{jk} - 0 \cdot 0 \right) = \delta_{ij}
\end{aligned}
$$

and

$$
\begin{aligned}
\{q_i, \mathscr{H}\} &:= \sum_k \left( \frac{\partial q_i}{\partial q_k} \cdot \frac{\partial \mathscr{H}}{\partial p_k} - \frac{\partial q_i}{\partial p_k} \cdot \frac{\partial \mathscr{H}}{\partial q_k} \right) = \sum_k \left( \delta_{ik} \cdot \frac{\partial \mathscr{H}}{\partial p_k} - 0 \cdot \frac{\partial \mathscr{H}}{\partial q_k} \right) \\
&= \frac{\partial \mathscr{H}}{\partial p_i} = \dot{q}_i \\
\{p_i, \mathscr{H}\} &:= \sum_k \left( \frac{\partial p_i}{\partial q_k} \cdot \frac{\partial \mathscr{H}}{\partial p_k} - \frac{\partial p_i}{\partial p_k} \cdot \frac{\partial \mathscr{H}}{\partial q_k} \right) = \sum_k \left( 0 \cdot \frac{\partial \mathscr{H}}{\partial p_k} - \delta_{ik} \cdot \frac{\partial \mathscr{H}}{\partial q_k} \right) \\
&= -\frac{\partial \mathscr{H}}{\partial q_i} = \dot{p}_i
\end{aligned}
$$

(ii) The Hamiltonian given is $\mathscr{H} = p_x^2 + p_y^2 + ax^2 + by^2$. If $a = b$, $\mathscr{H}$ has a symmetry under simultaneous rotations in the $x - y$ and $p_x - p_y$ planes, under which $l_z$ (the generator) is conserved. Therefore, $\{l_z, \mathscr{H}\} = 0$. We check this as follows:

$$\begin{aligned}\{l_z, \mathscr{H}\} &= \sum_k \left( \frac{\partial l_z}{\partial q_k} \cdot \frac{\partial \mathscr{H}}{\partial p_k} - \frac{\partial l_z}{\partial p_k} \cdot \frac{\partial \mathscr{H}}{\partial q_k} \right) \\ &= \frac{\partial l_z}{\partial x} \cdot \frac{\partial \mathscr{H}}{\partial p_x} + \frac{\partial l_z}{\partial y} \cdot \frac{\partial \mathscr{H}}{\partial p_y} - \frac{\partial l_z}{\partial p_x} \cdot \frac{\partial \mathscr{H}}{\partial x} - \frac{\partial l_z}{\partial p_y} \cdot \frac{\partial \mathscr{H}}{\partial y}\end{aligned}$$

But

$$\begin{aligned}&\frac{\partial \mathscr{H}}{\partial p_k} = 2p_k, \quad \frac{\partial l_z}{\partial p_k} = \frac{\partial \left( x p_y - y p_x \right)}{\partial p_k} = \left( \frac{\partial l_z}{\partial p_x}, \frac{\partial l_z}{\partial p_y} \right) = (-y, x), \\ &\frac{\partial \mathscr{H}}{\partial x_k} = \left( \frac{\partial \mathscr{H}}{\partial x}, \frac{\partial \mathscr{H}}{\partial y} \right) = (2ax, 2by), \quad \frac{\partial l_z}{\partial q_k} = \left( \frac{\partial l_z}{\partial x}, \frac{\partial l_z}{\partial y} \right) = (p_y, -p_x)\end{aligned}$$

So

$$\{l_z, \mathscr{H}\} = p_y \cdot 2p_x + (-p_x) \cdot 2p_y - (-y) \cdot 2ax - x \cdot 2by = 2xy(a - b)$$

which vanishes if $a = b$.

**Exercise 2.7.3.** Fill in the missing steps leading to Eq. (2.7.18) starting from Eq. (2.7.14).

**Solution.** Consider the following transformations:

$$\begin{aligned}\bar{q}_i &= \bar{q}_i(q, p) \\ \bar{p}_i &= \bar{p}_i(q, p)\end{aligned}$$

If this transformation is canonical, then the variables $\bar{q}_i$ and $\bar{p}_i$ satisfy Hamilton's equation:

$$\begin{aligned}\dot{\bar{q}}_i &= \frac{\partial \mathscr{H}}{\partial \bar{p}_i} \\ \dot{\bar{p}}_i &= -\frac{\partial \mathscr{H}}{\partial \bar{q}_i}\end{aligned}$$

If we write Hamiltonian $\mathscr{H}$ as a function of new variables, we can get partial derivatives

$$\begin{aligned}\frac{\partial \mathscr{H}(\bar{q}, \bar{p})}{\partial p_i} &= \sum_k \left( \frac{\partial \mathscr{H}}{\partial \bar{q}_k} \frac{\partial \bar{q}_k}{\partial p_i} + \frac{\partial \mathscr{H}}{\partial \bar{p}_k} \frac{\partial \bar{p}_k}{\partial p_i} \right) \\ \frac{\partial \mathscr{H}(\bar{q}, \bar{p})}{\partial q_i} &= \sum_k \left( \frac{\partial \mathscr{H}}{\partial \bar{q}_k} \frac{\partial \bar{q}_k}{\partial q_i} + \frac{\partial \mathscr{H}}{\partial \bar{p}_k} \frac{\partial \bar{p}_k}{\partial q_i} \right)\end{aligned}$$

The time derivative of any function $\omega$ can be written as a Poisson bracket with Hamiltonian $\mathscr{H}$:

$$\dot{\omega} = \{\omega, \mathscr{H}\}$$

Therefore, for transformed velocities, we have

$$\begin{aligned}
\dot{\bar{q}}_j &= \{\bar{q}_j, \mathscr{H}\} \\
&= \sum_i \left( \frac{\partial \bar{q}_j}{\partial q_i} \frac{\partial \mathscr{H}}{\partial p_i} - \frac{\partial \bar{q}_j}{\partial p_i} \frac{\partial \mathscr{H}}{\partial q_i} \right) \\
&= \sum_i \sum_k \left[ \frac{\partial \bar{q}_j}{\partial q_i} \left( \frac{\partial \mathscr{H}}{\partial \bar{q}_k} \frac{\partial \bar{q}_k}{\partial p_i} + \frac{\partial \mathscr{H}}{\partial \bar{p}_k} \frac{\partial \bar{p}_k}{\partial p_i} \right) - \frac{\partial \bar{q}_j}{\partial p_i} \left( \frac{\partial \mathscr{H}}{\partial \bar{q}_k} \frac{\partial \bar{q}_k}{\partial q_i} + \frac{\partial \mathscr{H}}{\partial \bar{p}_k} \frac{\partial \bar{p}_k}{\partial q_i} \right) \right] \\
&= \sum_k \frac{\partial \mathscr{H}}{\partial \bar{q}_k} \sum_i \left( \frac{\partial \bar{q}_j}{\partial q_i} \frac{\partial \bar{q}_k}{\partial p_i} - \frac{\partial \bar{q}_j}{\partial p_i} \frac{\partial \bar{q}_k}{\partial q_i} \right) + \sum_k \frac{\partial \mathscr{H}}{\partial \bar{p}_k} \sum_i \left( \frac{\partial \bar{q}_j}{\partial q_i} \frac{\partial \bar{p}_k}{\partial p_i} - \frac{\partial \bar{q}_j}{\partial p_i} \frac{\partial \bar{p}_k}{\partial q_i} \right) \\
&= \sum_k \frac{\partial \mathscr{H}}{\partial \bar{q}_k} \{\bar{q}_j, \bar{q}_k\} + \sum_k \frac{\partial \mathscr{H}}{\partial \bar{p}_k} \{\bar{q}_j, \bar{p}_k\}
\end{aligned}$$

In order to satisfy Hamilton's equation, we must have

$$\begin{aligned}
\{\bar{q}_j, \bar{q}_k\} &= 0 \\
\{\bar{q}_j, \bar{p}_k\} &= \delta_{jk}
\end{aligned}$$

We could do the same calculation for the time derivative of transform momentum

$$\begin{aligned}
\dot{\bar{p}}_j &= \{\bar{p}_j, \mathscr{H}\} \\
&= \sum_i \left( \frac{\partial \bar{p}_j}{\partial q_i} \frac{\partial \mathscr{H}}{\partial p_i} - \frac{\partial \bar{p}_j}{\partial p_i} \frac{\partial \mathscr{H}}{\partial q_i} \right) \\
&= \sum_i \sum_k \left[ \frac{\partial \bar{p}_j}{\partial q_i} \left( \frac{\partial \mathscr{H}}{\partial \bar{q}_k} \frac{\partial \bar{q}_k}{\partial p_i} + \frac{\partial \mathscr{H}}{\partial \bar{p}_k} \frac{\partial \bar{p}_k}{\partial p_i} \right) - \frac{\partial \bar{p}_j}{\partial p_i} \left( \frac{\partial \mathscr{H}}{\partial \bar{q}_k} \frac{\partial \bar{q}_k}{\partial q_i} + \frac{\partial \mathscr{H}}{\partial \bar{p}_k} \frac{\partial \bar{p}_k}{\partial q_i} \right) \right] \\
&= \sum_k \frac{\partial \mathscr{H}}{\partial \bar{q}_k} \sum_i \left( \frac{\partial \bar{p}_j}{\partial q_i} \frac{\partial \bar{q}_k}{\partial p_i} - \frac{\partial \bar{p}_j}{\partial p_i} \frac{\partial \bar{q}_k}{\partial q_i} \right) + \sum_k \frac{\partial \mathscr{H}}{\partial \bar{p}_k} \sum_i \left( \frac{\partial \bar{p}_j}{\partial q_i} \frac{\partial \bar{p}_k}{\partial p_i} - \frac{\partial \bar{p}_j}{\partial p_i} \frac{\partial \bar{p}_k}{\partial q_i} \right) \\
&= \sum_k \frac{\partial \mathscr{H}}{\partial \bar{q}_k} \{\bar{p}_j, \bar{q}_k\} + \sum_k \frac{\partial \mathscr{H}}{\partial \bar{p}_k} \{\bar{p}_j, \bar{p}_k\}
\end{aligned}$$

In order to satisfy Hamilton's equation, we must have

$$\begin{aligned}
\{\bar{p}_j, \bar{q}_k\} &= -\delta_{jk} \\
\{\bar{p}_j, \bar{p}_k\} &= 0
\end{aligned}$$

Thus, we can conclude that in order for the transformation to be canonical, the conditions are

$$\begin{aligned}
\{\bar{q}_j, \bar{q}_k\} &= \{\bar{p}_j, \bar{p}_k\} = 0 \\
\{\bar{q}_j, \bar{p}_k\} &= \delta_{jk}
\end{aligned}$$

**Exercise 2.7.4.** Verify that the change to a rotated frame

$$\begin{aligned}
\bar{x} &= x \cos\theta - y \sin\theta \\
\bar{y} &= x \sin\theta + y \cos\theta \\
\bar{p}_x &= p_x \cos\theta - p_y \sin\theta \\
\bar{p}_y &= p_x \sin\theta + p_y \cos\theta
\end{aligned}$$

is a canonical transformation.

**Solution.** To show this is a canonical transformation, we must evaluate the Poisson brackets. Before computing Poisson brackets, we can first compute non-vanishing derivatives

$$\begin{aligned}
\frac{\partial \bar{x}}{\partial x} &= \cos\theta & \frac{\partial \bar{x}}{\partial y} &= -\sin\theta \\
\frac{\partial \bar{y}}{\partial x} &= \sin\theta & \frac{\partial \bar{y}}{\partial y} &= \cos\theta \\
\frac{\partial \bar{p}_x}{\partial p_x} &= \cos\theta & \frac{\partial \bar{p}_x}{\partial p_y} &= -\sin\theta \\
\frac{\partial \bar{p}_y}{\partial p_x} &= \sin\theta & \frac{\partial \bar{p}_y}{\partial p_y} &= \cos\theta
\end{aligned}$$

where $q_1 = x$, $q_2 = y$ and $p_1 = p_x$, $p_2 = p_y$.

$$\{\bar{x}, \bar{y}\} = \sum_i \left( \frac{\partial \bar{x}}{\partial q_i}\frac{\partial \bar{y}}{\partial p_i} - \frac{\partial \bar{x}}{\partial p_i}\frac{\partial \bar{y}}{\partial q_i} \right) = 0$$

since neither coordinate depends on any momentum. Similarly,

$$\{\bar{p}_x, \bar{p}_y\} = 0$$

since Poisson bracket contains derivatives of $\bar{p}_i$ with respect to $q_i$ and these are all zero.

The remaining Poisson brackets are of the form $\{\bar{q}_i, \bar{p}_j\}$.

$$\begin{aligned}
\{\bar{x}, \bar{p}_x\} &= \sum_i \left( \frac{\partial \bar{x}}{\partial q_i}\frac{\partial \bar{p}_x}{\partial p_i} - \frac{\partial \bar{x}}{\partial p_i}\frac{\partial \bar{p}_x}{\partial q_i} \right) \\
&= \frac{\partial \bar{x}}{\partial x}\frac{\partial \bar{p}_x}{\partial p_x} + \frac{\partial \bar{x}}{\partial y}\frac{\partial \bar{p}_x}{\partial p_y} \\
&= \cos^2\theta + \sin^2\theta \\
&= 1 \\
\{\bar{x}, \bar{p}_y\} &= \sum_i \left( \frac{\partial \bar{x}}{\partial q_i}\frac{\partial \bar{p}_y}{\partial p_i} - \frac{\partial \bar{x}}{\partial p_i}\frac{\partial \bar{p}_y}{\partial q_i} \right) \\
&= \frac{\partial \bar{x}}{\partial x}\frac{\partial \bar{p}_y}{\partial p_x} + \frac{\partial \bar{x}}{\partial y}\frac{\partial \bar{p}_y}{\partial p_y} \\
&= \sin\theta\cos\theta - \sin\theta\cos\theta \\
&= 0
\end{aligned}$$

Similarly,

$$\begin{aligned}
\{\bar{y}, \bar{p}_x\} &= \sum_i \left( \frac{\partial \bar{y}}{\partial q_i} \frac{\partial \bar{p}_x}{\partial p_i} - \frac{\partial \bar{y}}{\partial p_i} \frac{\partial \bar{p}_x}{\partial q_i} \right) \\
&= \frac{\partial \bar{y}}{\partial x} \frac{\partial \bar{p}_x}{\partial p_x} + \frac{\partial \bar{y}}{\partial y} \frac{\partial \bar{p}_x}{\partial p_y} \\
&= \sin\theta \cos\theta + \cos\theta(-\sin\theta) \\
&= 0 \\
\{\bar{y}, \bar{p}_y\} &= \sum_i \left( \frac{\partial \bar{y}}{\partial q_i} \frac{\partial \bar{p}_y}{\partial p_i} - \frac{\partial \bar{y}}{\partial p_i} \frac{\partial \bar{p}_y}{\partial q_i} \right) \\
&= \frac{\partial \bar{y}}{\partial x} \frac{\partial \bar{p}_y}{\partial p_x} + \frac{\partial \bar{y}}{\partial y} \frac{\partial \bar{p}_y}{\partial p_y} \\
&= \sin\theta \sin\theta + \cos\theta \cos\theta \\
&= 1
\end{aligned}$$

Therefore, the change of rotated frame is a canonical transformation.

**Exercise 2.7.5.** Show that the polar variables

$$\rho = \left(x^2 + y^2\right)^{1/2}, \quad \phi = \tan^{-1}(y/x)$$
$$p_\rho = \hat{e}_\rho \cdot \mathbf{p} = \frac{x p_x + y p_y}{\left(x^2 + y^2\right)^{1/2}}, \quad p_\phi = x p_y - y p_x \, (= l_z)$$

are canonical. ( $\hat{e}_\rho$ is the unit vector in the radial direction.)

**Solution.** The non-vanishing derivatives are

$$\begin{aligned}
\frac{\partial \rho}{\partial x} &= \frac{x}{\sqrt{x^2 + y^2}} & \frac{\partial \rho}{\partial y} &= \frac{y}{\sqrt{x^2 + y^2}} \\
\frac{\partial \phi}{\partial x} &= \frac{-y}{x^2 + y^2} & \frac{\partial \phi}{\partial y} &= \frac{x}{x^2 + y^2} \\
\frac{\partial p_\rho}{\partial x} &= \frac{y^2 p_x - x y p_y}{(x^2 + y^2)^{3/2}} & \frac{\partial p_\rho}{\partial y} &= \frac{x^2 p_y - x y p_x}{(x^2 + y^2)^{3/2}} \\
\frac{\partial p_\rho}{\partial p_x} &= \frac{x}{\sqrt{x^2 + y^2}} & \frac{\partial p_\rho}{\partial p_y} &= \frac{y}{\sqrt{x^2 + y^2}} \\
\frac{\partial p_\phi}{\partial x} &= p_y & \frac{\partial p_\phi}{\partial y} &= -p_x \\
\frac{\partial p_\phi}{\partial p_x} &= -y & \frac{\partial p_\phi}{\partial p_y} &= x
\end{aligned}$$

Now, let's evaluate Poisson brackets

$$\{\rho, \phi\} = \sum_i \left( \frac{\partial \rho}{\partial q_i} \frac{\partial \phi}{\partial p_i} - \frac{\partial \rho}{\partial p_i} \frac{\partial \phi}{\partial q_i} \right) = 0$$

since coordinates don't depend on the momenta.

$$\begin{aligned}
\{p_\rho, p_\phi\} &= \sum_i \left( \frac{\partial p_\rho}{\partial q_i} \frac{\partial p_\phi}{\partial p_i} - \frac{\partial p_\rho}{\partial p_i} \frac{\partial p_\phi}{\partial q_i} \right) \\
&= \frac{\partial p_\rho}{\partial x} \frac{\partial p_\phi}{\partial p_x} - \frac{\partial p_\rho}{\partial p_x} \frac{\partial p_\phi}{\partial x} + \frac{\partial p_\rho}{\partial y} \frac{\partial p_\phi}{\partial p_y} - \frac{\partial p_\rho}{\partial p_y} \frac{\partial p_\phi}{\partial y} \\
&= \frac{y^2 p_x - xyp_y}{(x^2+y^2)^{3/2}}(-y) - \frac{x}{\sqrt{x^2+y^2}} p_y + \frac{x^2 p_y - xyp_x}{(x^2+y^2)^{3/2}} x - \frac{y}{\sqrt{x^2+y^2}}(-p_x) \\
&= \frac{-y^3 p_x + xy^2 p_y - (x^3 + xy^2) p_y + x^3 p_y - x^2 y p_x + (x^2 y + y^3) p_x}{(x^2+y^2)^{3/2}} \\
&= 0
\end{aligned}$$

The remaining Poisson brackets are of the form $\{\bar{q}_i, \bar{p}_j\}$.

$$\begin{aligned}
\{\rho, p_\rho\} &= \sum_i \left( \frac{\partial \rho}{\partial q_i} \frac{\partial p_\rho}{\partial p_i} - \frac{\partial \rho}{\partial p_i} \frac{\partial p_\rho}{\partial q_i} \right) \\
&= \frac{\partial \rho}{\partial x} \frac{\partial p_\rho}{\partial p_x} - \frac{\partial \rho}{\partial p_x} \frac{\partial p_\rho}{\partial x} + \frac{\partial \rho}{\partial y} \frac{\partial p_\rho}{\partial p_y} - \frac{\partial \rho}{\partial p_y} \frac{\partial p_\rho}{\partial y} \\
&= \frac{x^2}{x^2+y^2} - 0 + \frac{y^2}{x^2+y^2} - 0 \\
&= 1 \\
\{\rho, p_\phi\} &= \sum_i \left( \frac{\partial \rho}{\partial q_i} \frac{\partial p_\phi}{\partial p_i} - \frac{\partial \rho}{\partial p_i} \frac{\partial p_\phi}{\partial q_i} \right) \\
&= \frac{\partial \rho}{\partial x} \frac{\partial p_\phi}{\partial p_x} - \frac{\partial \rho}{\partial p_x} \frac{\partial p_\phi}{\partial x} + \frac{\partial \rho}{\partial y} \frac{\partial p_\phi}{\partial p_y} - \frac{\partial \rho}{\partial p_y} \frac{\partial p_\phi}{\partial y} \\
&= -\frac{xy}{\sqrt{x^2+y^2}} - 0 + \frac{xy}{\sqrt{x^2+y^2}} - 0 \\
&= 0 \\
\{\phi, p_\rho\} &= \sum_i \left( \frac{\partial \phi}{\partial q_i} \frac{\partial p_\rho}{\partial p_i} - \frac{\partial \phi}{\partial p_i} \frac{\partial p_\rho}{\partial q_i} \right) \\
&= \frac{\partial \phi}{\partial x} \frac{\partial p_\rho}{\partial p_x} - \frac{\partial \phi}{\partial p_x} \frac{\partial p_\rho}{\partial x} + \frac{\partial \phi}{\partial y} \frac{\partial p_\rho}{\partial p_y} - \frac{\partial \phi}{\partial p_y} \frac{\partial p_\rho}{\partial y} \\
&= \frac{-y}{x^2+y^2} \frac{x}{\sqrt{x^2+y^2}} - 0 + \frac{x}{x^2+y^2} \frac{y}{\sqrt{x^2+y^2}} - 0 \\
&= 0 \\
\{\phi, p_\phi\} &= \sum_i \left( \frac{\partial \phi}{\partial q_i} \frac{\partial p_\phi}{\partial p_i} - \frac{\partial \phi}{\partial p_i} \frac{\partial p_\phi}{\partial q_i} \right) \\
&= \frac{\partial \phi}{\partial x} \frac{\partial p_\phi}{\partial p_x} - \frac{\partial \phi}{\partial p_x} \frac{\partial p_\phi}{\partial x} + \frac{\partial \phi}{\partial y} \frac{\partial p_\phi}{\partial p_y} - \frac{\partial \phi}{\partial p_y} \frac{\partial p_\phi}{\partial y} \\
&= \frac{-y}{x^2+y^2}(-y) - 0 + \frac{x}{x^2+y^2} x - 0 \\
&= 1
\end{aligned}$$

Thus all the Poisson brackets are correct, so the transformation is canonical.

**Exercise 2.7.6.** Verify that the change from the variables $\mathbf{r}_1, \mathbf{r}_2, \mathbf{p}_1, \mathbf{p}_2$ to $\mathbf{r}_{\text{CM}}, \mathbf{p}_{\text{CM}}, \mathbf{r}$, and $\mathbf{p}$ is a canonical transformation. (See Exercise 2.5.4).

**Solution.** The transformation from the coordinates $\mathbf{r}_1$ and $\mathbf{r}_2$ of the masses $m_1$ and $m_2$ to relative position $\mathbf{r}$ and the position of the center of mass $\mathbf{r}_{CM}$ are

$$\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$$
$$\mathbf{r}_{CM} = \frac{m_1\mathbf{r}_1 + m_2\mathbf{r}_2}{M}$$

where $M := m_1 + m_2$ is the total mass. The conjugate momenta is the original system are

$$\mathbf{p}_i = m_i\dot{\mathbf{r}}_i$$

The conjugate momenta transform according to

$$\mathbf{p} = \mu\dot{\mathbf{r}} = \frac{m_2\mathbf{p}_1 - m_1\mathbf{p}_2}{M}$$
$$\mathbf{p}_{CM} = M\dot{\mathbf{r}}_{CM} = \mathbf{p}_1 + \mathbf{p}_2$$

where $\mu := \frac{m_1 m_2}{M}$ is the reduced mass.

Now we calculate the Poisson brackets to check whether it is a canonical transformation.

Note that the new coordinates depend only on the old coordinates, and conversely, the new momenta depend only on the old momenta. Also notice that $r_i$ depends only on the $i$ components of $\mathbf{r}_1$ and $\mathbf{r}_2$, and $p_j$ depends only on the $j$ components of $\mathbf{p}_1$ and $\mathbf{p}_2$.

Since the Poisson brackets $\{\bar{q}_i, \bar{q}_j\}$ and $\{\bar{p}_i, \bar{p}_j\}$ all invoke taking derivatives of coordinates with respect to momenta or momenta with respect to coordinates, we have

$$\{\bar{q}_i, \bar{q}_j\} = 0$$
$$\{\bar{p}_i, \bar{p}_j\} = 0$$

where $i$ and $j$ takes on the values $x$, $y$ and $z$. Then what we left to check are $\{\bar{q}_i, \bar{p}_j\}$. There are three cases $\{r_i, p_j\}$, $\{r_{CMi}, p_{CMj}\}$, $\{r_{CMi}, p_j\}$ or $\{r_i, p_{CMj}\}$.

(1) $\{r_i, p_j\}$

- $i = j$

$$\begin{aligned}\{r_i, p_i\} &= \sum_\alpha \left(\frac{\partial r_i}{\partial q_\alpha}\frac{\partial p_i}{\partial p_\alpha} - \frac{\partial r_i}{\partial p_\alpha}\frac{\partial p_i}{\partial q_\alpha}\right)\\ &= \sum_\alpha \frac{\partial r_i}{\partial q_\alpha}\frac{\partial p_i}{\partial p_\alpha}\\ &= \frac{\partial r_i}{\partial r_{1i}}\frac{\partial p_i}{\partial p_{1i}} + \frac{\partial r_i}{\partial r_{2i}}\frac{\partial p_i}{\partial p_{2i}}\\ &= 1\cdot\frac{m_2}{M} + (-1)\cdot\left(-\frac{m_1}{M}\right)\\ &= \frac{m_1+m_2}{M}\\ &= 1\end{aligned}$$

where $q_\alpha$ and $p_\alpha$ sum over all 6 components of the original position vectors $\{r_{1x}, r_{1y}, r_{1z}, r_{2x}, r_{2y}, r_{2z}\}$ that we denote as $\{r_{1i}, r_{2i}\}$

and momentum vectors $\{p_{1x}, p_{1y}, p_{1z}, p_{2x}, p_{2y}, p_{2z}\}$ that we denote as $\{p_{1i}, p_{2i}\}$, respectively.

- $i \neq j$

$$\begin{aligned}
\{x_i, y_j\} &= \sum_\alpha \left( \frac{\partial r_i}{\partial q_\alpha}\frac{\partial p_j}{\partial p_\alpha} - \frac{\partial r_i}{\partial p_\alpha}\frac{\partial p_j}{\partial q_\alpha} \right) \\
&= \sum_\alpha \frac{\partial r_i}{\partial q_\alpha}\frac{\partial p_j}{\partial p_\alpha} \\
&= \frac{\partial r_i}{\partial r_{1i}}\frac{\partial p_j}{\partial p_{1i}} + \frac{\partial r_i}{\partial r_{2i}}\frac{\partial p_j}{\partial p_{2i}} + \frac{\partial r_i}{\partial r_{1j}}\frac{\partial p_j}{\partial p_{1j}} + \frac{\partial r_i}{\partial r_{2j}}\frac{\partial p_j}{\partial p_{2j}} \\
&= 1 \cdot 0 + (-1) \cdot 0 + 0 \cdot \frac{m_2}{M} + 0 \cdot \left(-\frac{m_1}{M}\right) \\
&= 0
\end{aligned}$$

(2) $\{r_{CMi}, p_{CMj}\}$

- $i = j$

$$\begin{aligned}
\{r_{CMi}, p_{CMi}\} &= \sum_\alpha \left( \frac{\partial r_{CMi}}{\partial q_\alpha}\frac{\partial p_{CMi}}{\partial p_\alpha} - \frac{\partial r_{CMi}}{\partial p_\alpha}\frac{\partial p_{CMi}}{\partial q_\alpha} \right) \\
&= \sum_\alpha \frac{\partial r_{CMi}}{\partial q_\alpha}\frac{\partial p_{CMi}}{\partial p_\alpha} \\
&= \frac{\partial r_{CMi}}{\partial r_{1i}}\frac{\partial p_{CMi}}{\partial p_{1i}} + \frac{\partial r_{CMi}}{\partial r_{2i}}\frac{\partial p_{CMi}}{\partial p_{2i}} \\
&= \frac{m_1}{M} \cdot 1 + \frac{m_2}{M} \cdot 1 \\
&= \frac{m_1 + m_2}{M} \\
&= 1
\end{aligned}$$

- $i \neq j$

$$\begin{aligned}
\{r_{CMi}, p_{CMj}\} &= \sum_\alpha \left( \frac{\partial r_{CMi}}{\partial q_\alpha}\frac{\partial p_{CMj}}{\partial p_\alpha} - \frac{\partial r_{CMi}}{\partial p_\alpha}\frac{\partial p_{CMj}}{\partial q_\alpha} \right) \\
&= \sum_\alpha \frac{\partial r_{CMi}}{\partial q_\alpha}\frac{\partial p_{CMj}}{\partial p_\alpha} \\
&= \frac{\partial r_{CMi}}{\partial r_{1i}}\frac{\partial p_{CMj}}{\partial p_{1i}} + \frac{\partial r_{CMi}}{\partial r_{2i}}\frac{\partial p_{CMj}}{\partial p_{2i}} + \frac{\partial r_{CMi}}{\partial r_{1j}}\frac{\partial p_{CMj}}{\partial p_{1j}} + \frac{\partial r_{CMi}}{\partial r_{2j}}\frac{\partial p_{CMj}}{\partial p_{2j}} \\
&= 0
\end{aligned}$$

(3) $\{r_{CMi}, p_j\}$ or $\{r_i, p_{CMj}\}$

- $i = j$

$$\begin{aligned}
\{r_{CMi}, p_j\} &= \sum_\alpha \left( \frac{\partial r_{CMi}}{\partial q_\alpha} \frac{\partial p_i}{\partial p_\alpha} - \frac{\partial r_{CMi}}{\partial p_\alpha} \frac{\partial p_i}{\partial q_\alpha} \right) \\
&= \sum_\alpha \frac{\partial r_{CMi}}{\partial q_\alpha} \frac{\partial p_i}{\partial p_\alpha} \\
&= \frac{\partial r_{CMi}}{\partial r_{1i}} \frac{\partial p_i}{\partial p_{1i}} + \frac{\partial r_{CMi}}{\partial r_{2i}} \frac{\partial p_i}{\partial p_{2i}} \\
&= \frac{m_1}{M} \cdot \frac{m_2}{M} + \frac{m_2}{M} \cdot \left( -\frac{m_1}{M} \right) \\
&= 0
\end{aligned}$$

$$\begin{aligned}
\{r_i, p_{CMj}\} &= \sum_\alpha \left( \frac{\partial r_i}{\partial q_\alpha} \frac{\partial p_{CMi}}{\partial p_\alpha} - \frac{\partial r_i}{\partial p_\alpha} \frac{\partial p_{CMi}}{\partial q_\alpha} \right) \\
&= \sum_\alpha \frac{\partial r_i}{\partial q_\alpha} \frac{\partial p_{CMi}}{\partial p_\alpha} \\
&= \frac{\partial r_i}{\partial r_{1i}} \frac{\partial p_{CMi}}{\partial p_{1i}} + \frac{\partial r_i}{\partial r_{2i}} \frac{\partial p_{CMi}}{\partial p_{2i}} \\
&= 1 \cdot 1 + (-1) \cdot 1 \\
&= 0
\end{aligned}$$

- $i \neq j$

$$\begin{aligned}
\{r_{CMi}, p_j\} &= \sum_\alpha \left( \frac{\partial r_{CMi}}{\partial q_\alpha} \frac{\partial p_j}{\partial p_\alpha} - \frac{\partial r_{CMi}}{\partial p_\alpha} \frac{\partial p_j}{\partial q_\alpha} \right) \\
&= \sum_\alpha \frac{\partial r_{CMi}}{\partial q_\alpha} \frac{\partial p_j}{\partial p_\alpha} \\
&= \frac{\partial r_{CMi}}{\partial r_{1i}} \frac{\partial p_j}{\partial p_{1i}} + \frac{\partial r_{CMi}}{\partial r_{2i}} \frac{\partial p_j}{\partial p_{2i}} + \frac{\partial r_{CMi}}{\partial r_{1j}} \frac{\partial p_j}{\partial p_{1j}} + \frac{\partial r_{CMi}}{\partial r_{2j}} \frac{\partial p_j}{\partial p_{2j}} \\
&= 0
\end{aligned}$$

$$\begin{aligned}
\{r_i, p_{CMj}\} &= \sum_\alpha \left( \frac{\partial r_i}{\partial q_\alpha} \frac{\partial p_{CMj}}{\partial p_\alpha} - \frac{\partial r_i}{\partial p_\alpha} \frac{\partial p_{CMj}}{\partial q_\alpha} \right) \\
&= \sum_\alpha \frac{\partial r_i}{\partial q_\alpha} \frac{\partial p_{CMj}}{\partial p_\alpha} \\
&= \frac{\partial r_i}{\partial r_{1i}} \frac{\partial p_{CMj}}{\partial p_{1i}} + \frac{\partial r_i}{\partial r_{2i}} \frac{\partial p_{CMj}}{\partial p_{2i}} + \frac{\partial r_i}{\partial r_{1j}} \frac{\partial p_{CMj}}{\partial p_{1j}} + \frac{\partial r_i}{\partial r_{2j}} \frac{\partial p_{CMj}}{\partial p_{2j}} \\
&= 0
\end{aligned}$$

Thus all the Poisson brackets are correct, so the transformation is canonical.

**Exercise 2.7.7.** Verify that

$$\begin{aligned}
\bar{q} &= \ln \left( q^{-1} \sin p \right) \\
\bar{p} &= q \cot p
\end{aligned}$$

is a canonical transformation.

**Solution.** The partial derivatives are

$$\frac{\partial \bar{q}}{\partial q} = -q^{-1} \qquad \frac{\partial \bar{q}}{\partial p} = \cot p$$
$$\frac{\partial \bar{p}}{\partial q} = \cot p \qquad \frac{\partial \bar{p}}{\partial p} = -q(1+\cot^2 p)$$

The only remaining term to verify is

$$\begin{aligned}\{\bar{q}, \bar{p}\} &= \frac{\partial \bar{q}}{\partial q}\frac{\partial \bar{p}}{\partial p} - \frac{\partial \bar{q}}{\partial p}\frac{\partial \bar{p}}{\partial q} \\ &= -q^{-1}(-q(1+\cot^2 p)] - \cot^2 p \\ &= 1\end{aligned}$$

Thus the transformation is canonical.

**Exercise 2.7.8.** We would like to derive here Eq. (2.7.9), which gives the transformation of the momenta under a coordinate transformation in configuration space:

$$q_i \to \bar{q}_i(q_1, \ldots, q_n)$$

(1) Argue that if we invert the above equation to get $q = q(\bar{q})$, we can derive the following counterpart of Eq. (2.7.7):

$$\dot{q}_i = \sum_j \frac{\partial q_i}{\partial \bar{q}_j}\dot{\bar{q}}_j$$

(2) Show from the above that

$$\left(\frac{\partial \dot{q}_i}{\partial \dot{\bar{q}}_j}\right)_{\bar{q}} = \frac{\partial q_i}{\partial \bar{q}_j}$$

(3) Now calculate

$$\bar{p}_i = \left[\frac{\partial \mathscr{L}(\bar{q}, \dot{\bar{q}})}{\partial \dot{\bar{q}}_i}\right]_{\bar{q}} = \left[\frac{\partial \mathscr{L}(q, \dot{q})}{\partial \dot{\bar{q}}_i}\right]_{\bar{q}}$$

Use the chain rule and the fact that $q = q(\bar{q})$ and not $q(\bar{q}, \dot{\bar{q}})$ to derive Eq. (2.7.9).

(4) Verify, by calculating the Poisson braket in Eq. (2.7.18), that the point transformation is canonical.

**Solution.**

(1) Since $q_i = q_i(\bar{q}_1, \ldots, \bar{q}_n)$,

$$\dot{q}_i = \frac{\mathrm{d}q_i}{\mathrm{d}t} = \sum_j \frac{\partial q_i}{\partial \bar{q}_j}\frac{\mathrm{d}\bar{q}_j}{\mathrm{d}t} = \sum_j \frac{\partial q_i}{\partial \bar{q}_j}\dot{\bar{q}}_j$$

(2) Since the velocities $\dot{\bar{q}}_j$ are independent variables, if we hold the coordinates $\bar{q}$ constant, we will have

$$\left(\frac{\partial \dot{q}_i}{\partial \dot{\bar{q}}_j}\right)_{\bar{q}} = \frac{\partial}{\partial \dot{\bar{q}}_j}\left(\sum_l \frac{\partial q_i}{\partial \bar{q}_k}\dot{\bar{q}}_k\right) = \sum_k \frac{\partial q_i}{\partial \bar{q}_k}\frac{\partial \dot{\bar{q}}_k}{\partial \dot{\bar{q}}_j} = \sum_k \frac{\partial q_i}{\partial \bar{q}_k}\delta_{kj} = \frac{\partial q_i}{\partial \bar{q}_j} \quad (2.3)$$

(3) We can use the Lagrangian to see how the momenta $p_i$ transform under the coordinate change. The definition of the canonical momentum is

$$p_i := \frac{\partial \mathscr{L}}{\partial \dot{q}_i}$$

If we write the Lagrangian in terms of the new coordinates and velocities $\mathscr{L} = \mathscr{L}(\bar{q}, \dot{\bar{q}})$, then the momenta in the new coordinate system are

$$\bar{p}_i = \frac{\partial \mathscr{L}(\bar{q}, \dot{\bar{q}})}{\partial \dot{\bar{q}}_i}$$

At this point, it's worth noting that although $\mathscr{L}(\bar{q}, \dot{\bar{q}})$ and $\mathscr{L}(q, \dot{q})$ are different functions, they have the same value at each point in the configuration space. That is, if we choose some point that has the coordinates $(q, \dot{q})$ in the $q$ system and coordinates $(\bar{q}, \dot{\bar{q}})$ in the $\bar{q}$ system, then, numerically at that one point, we must have $\mathscr{L}(\bar{q}, \dot{\bar{q}}) = \mathscr{L}(q, \dot{q})$. Because of this, we can write

$$\bar{p}_i = \left(\frac{\partial \mathscr{L}(\bar{q}, \dot{\bar{q}})}{\partial \dot{\bar{q}}_i}\right)_{\bar{q}} = \left(\frac{\partial \mathscr{L}(q, \dot{q})}{\partial \dot{\bar{q}}_i}\right)_{\bar{q}}$$

That is, if we are keeping $\bar{q}$ constant, the derivative of $\mathscr{L}$ with respect to $\dot{\bar{q}}_i$ must be the same (numerically) no matter what coordinates we are using to write $\mathscr{L}$. Therefore, we can use the latter form and then use the chain rule to write out the derivative:

$$\bar{p}_i = \left(\frac{\partial L(q, \dot{q})}{\partial \dot{\bar{q}}_i}\right)_{\bar{q}} = \sum_j \left[\frac{\partial L}{\partial q_j}\frac{\partial q_j}{\partial \dot{\bar{q}}_i} + \frac{\partial L}{\partial \dot{q}_j}\frac{\partial \dot{q}_j}{\partial \dot{\bar{q}}_i}\right]$$

Because the coordinates $q$ don't depend on the velocities $\dot{\bar{q}}$, the first term on the RHS is zero. We can use (2.3) in the second term, and we have

$$\begin{aligned}\bar{p}_i &= \sum_j \frac{\partial L}{\partial \dot{q}_j}\frac{\partial \dot{q}_j}{\partial \dot{\bar{q}}_i} \\ &= \sum_j \frac{\partial L}{\partial \dot{q}_j}\frac{\partial q_j}{\partial \bar{q}_i} \\ &= \sum_j \frac{\partial q_j}{\partial \bar{q}_i} p_j\end{aligned}$$

where we used the definition of canonical momentum at the last equality. We have derived Eq. (2.7.9).

(4) Point transformation is given by

$$\begin{aligned}\bar{q}_i &= \bar{q}_i(q_1, \ldots, q_n) \\ \bar{p}_i &= \sum_j \frac{\partial q_j}{\partial \bar{q}_i} p_j\end{aligned}$$

In this case, the coordinate transformation to $\bar{q}$ is completely arbitrary, but the momentum transformation must follow the formula given. The derivatives $\frac{\partial q_i}{\partial \bar{q}_j}$ in the formula for $\bar{p}_i$ are taken at constant $\bar{q}$. Since the coordinate formulas depend only on the old coordinates, and the momentum formulas depend only on the old momenta, the Poisson brackets satisfy

$$\{\bar{q}_i, \bar{q}_j\} = \{\bar{p}_i, \bar{p}_j\} = 0$$

For the mixed brackets, we have

$$\begin{aligned}
\{\bar{q}_i, \bar{p}_j\} &= \sum_k \left( \frac{\partial \bar{q}_i}{\partial q_k} \frac{\partial \bar{p}_j}{\partial p_k} - \frac{\partial \bar{q}_i}{\partial p_k} \frac{\partial \bar{p}_j}{\partial q_k} \right) \\
&= \sum_k \frac{\partial \bar{q}_i}{\partial q_k} \left( \frac{\partial}{\partial p_k} \left( \sum_l \frac{\partial q_l}{\partial \bar{q}_j} p_l \right) \right) \\
&= \sum_k \frac{\partial \bar{q}_i}{\partial q_k} \left( \sum_l \frac{\partial q_l}{\partial \bar{q}_j} \frac{\partial p_l}{\partial p_k} \right) \\
&= \sum_k \frac{\partial \bar{q}_i}{\partial q_k} \left( \sum_l \frac{\partial q_l}{\partial \bar{q}_j} \delta_{lk} \right) \\
&= \sum_k \frac{\partial \bar{q}_i}{\partial q_k} \frac{\partial q_k}{\partial \bar{q}_j} \\
&= \frac{\partial \bar{q}_i}{\partial \bar{q}_j} \\
&= \delta_{ij}
\end{aligned}$$

Thus the point transformation is a canonical transformation.

**Exercise 2.7.9.** Verify Eq. (2.7.19) by direct computation. Use the chain rule to go from $q, p$ derivatives to $\bar{q}, \bar{p}$ derivatives. Collect terms that represent Poisson braket of the latter.

**Solution.** The Poisson bracket of two functions is defined as

$$\{\omega, \sigma\} = \sum_i \left( \frac{\partial \omega}{\partial q_i} \frac{\partial \sigma}{\partial p_i} - \frac{\partial \omega}{\partial p_i} \frac{\partial \sigma}{\partial q_i} \right)$$

Calculating the Poisson bracket requires knowing $\omega$ and $\sigma$ as functions of the coordinates $q_i$ and momenta $p_i$ in the particular coordinate system we're using.

The simplest way of finding out is to write the canonical transformation as

$$\begin{aligned}
\bar{q}_i &= \bar{q}_i(q, p) \\
\bar{p}_i &= \bar{p}(q, p)
\end{aligned}$$

We can then write the Poisson bracket in the new coordinates as

$$\{\omega, \sigma\}_{\bar{q},\bar{p}} = \sum_j \left( \frac{\partial \omega}{\partial \bar{q}_j} \frac{\partial \sigma}{\partial \bar{p}_j} - \frac{\partial \omega}{\partial \bar{p}_j} \frac{\partial \sigma}{\partial \bar{q}_j} \right)$$

Assuming the transformation is invertible, we can use the chain rule to calculate the derivatives with respect to the barred coordinates. This gives the following

(Here we use Einstein summation convention):

$$
\begin{aligned}
\{\omega, \sigma\}_{\bar{q},\bar{p}} =& \left(\frac{\partial \omega}{\partial q_i}\frac{\partial q_i}{\partial \bar{q}_j} + \frac{\partial \omega}{\partial p_i}\frac{\partial p_i}{\partial \bar{q}_j}\right)\left(\frac{\partial \sigma}{\partial q_k}\frac{\partial q_k}{\partial \bar{p}_j} + \frac{\partial \sigma}{\partial p_k}\frac{\partial p_k}{\partial \bar{p}_j}\right) \\
&- \left(\frac{\partial \omega}{\partial q_i}\frac{\partial q_i}{\partial \bar{p}_j} + \frac{\partial \omega}{\partial p_i}\frac{\partial p_i}{\partial \bar{p}_j}\right)\left(\frac{\partial \sigma}{\partial q_k}\frac{\partial q_k}{\partial \bar{q}_j} + \frac{\partial \sigma}{\partial p_k}\frac{\partial p_k}{\partial \bar{q}_j}\right) \\
=& \frac{\partial \omega}{\partial q_i}\frac{\partial \sigma}{\partial p_k}\left(\frac{\partial q_i}{\partial \bar{q}_j}\frac{\partial p_k}{\partial \bar{p}_j} - \frac{\partial q_i}{\partial \bar{p}_j}\frac{\partial p_k}{\partial \bar{q}_j}\right) + \frac{\partial \omega}{\partial p_i}\frac{\partial \sigma}{\partial q_k}\left(\frac{\partial p_i}{\partial \bar{q}_j}\frac{\partial q_k}{\partial \bar{p}_j} - \frac{\partial p_i}{\partial \bar{p}_j}\frac{\partial q_k}{\partial \bar{q}_j}\right) \\
&+ \frac{\partial \omega}{\partial q_i}\frac{\partial \sigma}{\partial q_k}\left(\frac{\partial q_i}{\partial \bar{q}_j}\frac{\partial q_k}{\partial \bar{p}_j} - \frac{\partial q_i}{\partial \bar{p}_j}\frac{\partial q_k}{\partial \bar{q}_j}\right) + \frac{\partial \omega}{\partial p_i}\frac{\partial \sigma}{\partial p_k}\left(\frac{\partial p_i}{\partial \bar{q}_j}\frac{\partial p_k}{\partial \bar{p}_j} - \frac{\partial p_i}{\partial \bar{p}_j}\frac{\partial p_k}{\partial \bar{q}_j}\right) \\
=& \frac{\partial \omega}{\partial q_i}\frac{\partial \sigma}{\partial p_k}\{q_i, p_k\} + \frac{\partial \omega}{\partial p_i}\frac{\partial \sigma}{\partial q_k}\{p_i, q_k\} + \frac{\partial \omega}{\partial q_i}\frac{\partial \sigma}{\partial q_k}\{q_i, q_k\} + \frac{\partial \omega}{\partial p_i}\frac{\partial \sigma}{\partial p_k}\{p_i, p_k\}
\end{aligned}
$$

For a canonical transformation, the Poisson brackets in the last equation satisfy

$$
\begin{aligned}
\{q_i, p_k\} &= -\{p_i, q_k\} = \delta_{ik} \\
\{q_i, q_k\} &= \{p_i, p_k\} = 0
\end{aligned}
$$

Applying these conditions to the above, we find

$$
\begin{aligned}
\{\omega, \sigma\}_{\bar{q},\bar{p}} &= \left(\frac{\partial \omega}{\partial q_i}\frac{\partial \sigma}{\partial p_k} - \frac{\partial \omega}{\partial p_i}\frac{\partial \sigma}{\partial q_k}\right)\delta_{ik} \\
&= \frac{\partial \omega}{\partial q_i}\frac{\partial \sigma}{\partial p_i} - \frac{\partial \omega}{\partial p_i}\frac{\partial \sigma}{\partial q_i} \\
&= \{\omega, \sigma\}_{q,p}
\end{aligned}
$$

Thus the Poisson bracket is invariant under a canonical transformation.

## 2.8 Symmetries and Their Consequences

**Exercise 2.8.1.** Show that $p = p_1 + p_2$, the total momentum, is the generator of infinitesimal translations for a two-particle system.

**Solution.** Since $g = p_1 + p_2$, it generates the infinitesimal transformations

$$
\begin{aligned}
\delta x_1 &= +\varepsilon \tfrac{\partial g}{\partial p_1} = +\varepsilon, \quad \delta p_1 = -\varepsilon \tfrac{\partial g}{\partial x_1} = 0 \\
\delta x_2 &= +\varepsilon \tfrac{\partial g}{\partial p_2} = +\varepsilon, \quad \delta p_2 = -\varepsilon \tfrac{\partial g}{\partial x_2} = 0
\end{aligned}
$$

So to order $\varepsilon$, these give the canonical transformations $x_i \to \bar{x}_i(x_j, p_j)$ and $p_i \to \bar{p}_i(x_j, p_j)$ with

$$
\begin{aligned}
\bar{x}_1 &= x_1 + \varepsilon, \quad \bar{p}_1 = p_1, \\
\bar{x}_2 &= x_2 + \varepsilon, \quad \bar{p}_2 = p_2,
\end{aligned}
$$

which is precisely a spatial transformation of the whole system by an amount $\varepsilon$.

**Exercise 2.8.2.** Verify that the infinitesimal transformation generated by any dynamical variable $g$ is a canonical transformation. (Hint: Work, as usual, to first order in $\varepsilon$.)

**Solution.** If the coordinates and momenta after the infinitesimal transformation generated by dynamical variable $g$ becomes

$$\bar{q}_i = q_i + \varepsilon \frac{\partial g}{\partial p_i}$$
$$\bar{p}_j = p_j - \varepsilon \frac{\partial g}{\partial q_j}$$

Then the Poisson brackets between new coordinate and momentum is

$$\begin{aligned}
\{\bar{q}_i, \bar{p}_j\} &= \sum_k \left( \frac{\partial \bar{q}_i}{\partial q_k} \frac{\partial \bar{p}_j}{\partial p_k} - \frac{\partial \bar{q}_i}{\partial p_k} \frac{\partial \bar{p}_j}{\partial q_k} \right) \\
&= \sum_k \left[ \left( \delta_{ik} + \varepsilon \frac{\partial^2 g}{\partial p_i \partial q_k} \right) \left( \delta_{jk} + \varepsilon \frac{\partial^2 g}{\partial q_j \partial p_k} \right) - \varepsilon \frac{\partial^2 g}{\partial p_i \partial p_k} \cdot \varepsilon \frac{\partial^2 g}{\partial q_i \partial q_k} \right] \\
&= \sum_k \left[ \delta_{ik}\delta_{jk} + \varepsilon \frac{\partial^2 g}{\partial p_i \partial q_k} \cdot \delta_{jk} - \delta_{ik} \cdot \varepsilon \frac{\partial^2 g}{\partial q_j \partial p_k} + \mathcal{O}(\varepsilon^2) \right] \\
&= \delta_{ij} + \varepsilon \frac{\partial^2 g}{\partial p_i \partial q_j} - \varepsilon \frac{\partial^2 g}{\partial q_j \partial p_i} + \mathcal{O}(\varepsilon^2) \\
&= \delta_{ij} + \mathcal{O}(\varepsilon^2) \\
&\approx \delta_{ij}
\end{aligned}$$

Therefore, the infinitesimal transformation generated by any dynamical variable $g$ is a canonical transformation.

**Exercise 2.8.3.** Consider

$$\mathscr{H} = \frac{p_x^2 + p_y^2}{2m} + \frac{1}{2} m\omega^2 \left(x^2 + y^2\right)$$

whose invariance under the rotation of the coordinates and momenta leads to the conservation of $l_z$. But $\mathscr{H}$ is also invariant under the rotation of *just the coordinates*. Verify that this is a *noncanonical* transformation. Convince yourself that in this case it is not possible to write $\delta\mathscr{H}$ as $\varepsilon\{\mathscr{H}, g\}$ for any $g$, i.e., that no conservation law follows.

**Solution.** Rotation of just the coordinates:

$$\begin{cases} \bar{x} = x\cos\theta - y\sin\theta \\ \bar{y} = x\sin\theta + y\cos\theta \end{cases} \qquad \begin{cases} \bar{p}_x = p_x \\ \bar{p}_y = p_y \end{cases}$$

Then the Poisson brackets are

$$\begin{aligned}
\{\bar{x},\bar{y}\} &= \frac{\partial\bar{x}}{\partial x}\frac{\partial\bar{y}}{\partial p_x} - \frac{\partial\bar{x}}{\partial p_x}\frac{\partial\bar{y}}{\partial x} + \frac{\partial\bar{x}}{\partial y}\frac{\partial\bar{y}}{\partial p_y} - \frac{\partial\bar{x}}{\partial p_y}\frac{\partial\bar{y}}{\partial y} = 0 \\
\{\bar{p}_x,\bar{p}_y\} &= \{p_x,p_y\} = 0 \\
\{\bar{x},\bar{p}_x\} &= \frac{\partial\bar{x}}{\partial x}\frac{\partial\bar{p}_x}{\partial p_x} - \frac{\partial\bar{x}}{\partial p_x}\frac{\partial\bar{p}_x}{\partial x} + \frac{\partial\bar{x}}{\partial y}\frac{\partial\bar{p}_x}{\partial p_y} - \frac{\partial\bar{x}}{\partial p_y}\frac{\partial\bar{p}_x}{\partial y} = \cos\theta \neq 1 \\
\{\bar{x},\bar{p}_y\} &= \frac{\partial\bar{x}}{\partial x}\frac{\partial\bar{p}_y}{\partial p_x} - \frac{\partial\bar{x}}{\partial p_x}\frac{\partial\bar{p}_y}{\partial x} + \frac{\partial\bar{x}}{\partial y}\frac{\partial\bar{p}_y}{\partial p_y} - \frac{\partial\bar{x}}{\partial p_y}\frac{\partial\bar{p}_y}{\partial y} = -\sin\theta \neq 0 \\
\{\bar{y},\bar{p}_x\} &= \frac{\partial\bar{y}}{\partial x}\frac{\partial\bar{p}_x}{\partial p_x} - \frac{\partial\bar{y}}{\partial p_x}\frac{\partial\bar{p}_x}{\partial x} + \frac{\partial\bar{y}}{\partial y}\frac{\partial\bar{p}_x}{\partial p_y} - \frac{\partial\bar{y}}{\partial p_y}\frac{\partial\bar{p}_x}{\partial y} = \sin\theta \neq 0 \\
\{\bar{y},\bar{p}_y\} &= \frac{\partial\bar{y}}{\partial x}\frac{\partial\bar{p}_y}{\partial p_x} - \frac{\partial\bar{y}}{\partial p_x}\frac{\partial\bar{p}_y}{\partial x} + \frac{\partial\bar{y}}{\partial y}\frac{\partial\bar{p}_y}{\partial p_y} - \frac{\partial\bar{y}}{\partial p_y}\frac{\partial\bar{p}_y}{\partial y} = \cos\theta \neq 1
\end{aligned}$$

Thus, rotation of just the coordinates is not a canonical transformation.

If $\delta\mathscr{H} = \varepsilon\{\mathscr{H},g\} = \varepsilon\left(\frac{\partial\mathscr{H}}{\partial x}\frac{\partial g}{\partial p_x} - \frac{\partial\mathscr{H}}{\partial p_x}\frac{\partial g}{\partial x} + \frac{\partial\mathscr{H}}{\partial y}\frac{\partial g}{\partial p_y} - \frac{\partial\mathscr{H}}{\partial p_y}\frac{\partial g}{\partial y}\right)$, we have

$$\begin{aligned}
\delta x &= \varepsilon\frac{\partial g}{\partial p_x} & \delta p_x &= -\varepsilon\frac{\partial g}{\partial x}, \\
\delta y &= \varepsilon\frac{\partial g}{\partial p_y} & \delta p_y &= -\varepsilon\frac{\partial g}{\partial y}.
\end{aligned}$$

which means that

$$\begin{cases} \bar{x} = x + \varepsilon\dfrac{\partial g}{\partial p_x} \\ \bar{y} = y + \varepsilon\dfrac{\partial g}{\partial p_y} \end{cases} \qquad \begin{cases} \bar{p}_x = p_x - \varepsilon\dfrac{\partial g}{\partial x} \\ \bar{p}_y = p_y - \varepsilon\dfrac{\partial g}{\partial y} \end{cases}$$

According to last exercise, this is a canonical transformation. Therefore, there doesn't exists any $g$, such that $\delta\mathscr{H} = \varepsilon\{\mathscr{H},g\}$.

**Exercise 2.8.4.** Consider $\mathscr{H} = \frac{1}{2}p^2 + \frac{1}{2}x^2$, which is invariant under infinitesimal rotations in phase space (the $x-p$ plane). Find the generator of this transformation (after verifying that it is canonical). (You could have guessed the answer based on Exercise 2.5.2.).

**Solution.** Consider a one-dimensitonal system with

$$\mathscr{H} = \frac{1}{2}(p^2 + x^2)$$

and perform a infinitesimal rotation in phase space $x-p$ plane:

$$\begin{aligned}
\delta x &= \varepsilon p \\
\delta p &= -\varepsilon x
\end{aligned}$$

This is a canonical transformation since

$$\begin{aligned}
\{\bar{x},\bar{p}\} &= \{x,p\} + \varepsilon\{\delta x,p\} + \varepsilon\{x,\delta p\} + \mathcal{O}(\varepsilon^2) \\
&= \{x,p\} \\
&= 1
\end{aligned}$$

If $g(x, p)$ is the generator

$$\delta x = \varepsilon\{x, g\} = \varepsilon \frac{\partial g}{\partial p} = \varepsilon p \Rightarrow \frac{\partial g}{\partial p} = p$$
$$\delta p = \varepsilon\{p, g\} = -\varepsilon \frac{\partial g}{\partial x} = -\varepsilon x \Rightarrow \frac{\partial g}{\partial x} = x$$

The solution of these two equations is

$$g(x, p) = \frac{1}{2}(p^2 + x^2) + C$$

where $C$ is a constant of integration. The equality is just the Hamiltonian itself.

In fact, the canonical transformation is just the time evolution with $\theta = t$.

**Exercise 2.8.5.** Why is it that a noncanonical transformation that leaves $\mathscr{H}$ invariant does not map a solution into another? Or, in view of the discussions on consequence II, why is it that an experiment and its transformed version do not give the same result when the transformation that leaves $\mathscr{H}$ invariant is not canonical? It is best to consider an example. Consider the potential given in Exercise 2.8.3. Suppose I release a particle at $(x = a, y = 0)$ with $(p_x = b, p_y = 0)$ and you release one in the transformed state in which $(x = 0, y = a)$ and $(p_x = b, p_y = 0)$, i.e., you rotate the coordinates but not the momenta. This is a noncanonical transformation that leaves $\mathscr{H}$ invariant. Convince yourself that at later times the states of the two particles are not related by the same transformation. Try to understand what goes wrong in the general case.

**Solution.** If the Hamiltonian is invariant under a regular canonical transformation and we can find a generator $g$ such that an infinitesimal version of this transformation is given by

$$\bar{q}_i = q_i + \varepsilon \frac{\partial g}{\partial p_i} \equiv q_i + \delta q_i$$
$$\bar{p}_i = p_i - \varepsilon \frac{\partial g}{\partial q_i} \equiv p_i + \delta p_i$$

then $g$ is conserved.

If we are dealing with a finite regular canonical transformation where we go from $(q, p) \to (\bar{q}, \bar{p})$, and the Hamiltonian is invariant under this transformation, then it turns out that if a trajectory $(q(t), p(t))$ satisfies Hamilton's equations of motion:

$$\frac{\partial H}{\partial p_i} = \dot{q}_i$$
$$-\frac{\partial H}{\partial q_i} = \dot{p}_i$$

then the trajectory obtained by transforming every point in the original trajectory $(q(t), p(t))$ to the barred system $(\bar{q}(t), \bar{p}(t))$ is also a solution of Hamilton's equations in the sense that

$$\frac{\partial H}{\partial \bar{p}_i} = \dot{\bar{q}}_i \tag{2.4}$$
$$-\frac{\partial H}{\partial \bar{q}_i} = \dot{\bar{p}}_i \tag{2.5}$$

The proof of this is a bit subtle, but goes as follows. To begin, review the derivation of the conditions for a transformation to be canonical. This derivation applied to a passive transformation, in which the two sets of parameters $(q,p) \to (\bar{q},\bar{p})$ refer to the same point in phase space. The transformation we're considering here is an active transformation, in which $(q,p) \to (\bar{q},\bar{p})$ actually moves the point in phase space. The original derivation (for passive transformations) relied on the fact that the numerical value of the Hamiltonian is the same in both coordinate systems, since both $(q,p)$ and $(\bar{q},\bar{p})$ refer to the same point in phase space. However, for our active transformation, we're assuming that the Hamiltonian is invariant under the transformation, that is $H(\bar{q},\bar{p}) = H(q,p)$, where $(q,p)$ and $(\bar{q},\bar{p})$ now refer to different points in phase space. Since the assumption that the Hamiltonian satisfies $H(\bar{q},\bar{p}) = H(q,p)$ was all that we used in the original derivation, the same derivation works both for passive transformations (always) and for active transformations (if the Hamiltonian is invariant under the active transformation). We therefore end up with the equations

$$\dot{\bar{q}}_j = \sum_k \frac{\partial H}{\partial \bar{q}_k}\{\bar{q}_j,\bar{q}_k\} + \sum_k \frac{\partial H}{\partial \bar{p}_k}\{\bar{q}_j,\bar{p}_k\} \tag{2.6}$$

$$\dot{\bar{p}}_j = \sum_k \frac{\partial H}{\partial \bar{q}_k}\{\bar{p}_j,\bar{q}_k\} + \sum_k \frac{\partial H}{\partial \bar{p}_k}\{\bar{p}_j,\bar{p}_k\} \tag{2.7}$$

Since the transformation is specified to be canonical, the conditions on the Poisson brackets apply here:

$$\{\bar{q}_j,\bar{q}_k\} = \{\bar{p}_j,\bar{p}_k\} = 0 \tag{2.8}$$

$$\{\bar{q}_j,\bar{p}_k\} = \delta_{jk} \tag{2.9}$$

The result is that the transformed trajectory also satisfies Hamilton's equations (2.4) and (2.5).

We can now revisit the 2-d harmonic oscillator to show that a noncanonical transformation violates these results. The Hamiltonian is

$$H = \frac{1}{2m}\left(p_x^2 + p_y^2\right) + \frac{1}{2}m\omega^2\left(x^2+y^2\right)$$

and we consider the transformation where we rotate the coordinates but not the momenta. The transformation is

$$\begin{aligned}\bar{x} &= x\cos\theta - y\sin\theta\\ \bar{y} &= x\sin\theta + y\cos\theta\\ \bar{p}_x &= p_x\\ \bar{p}_y &= p_y\end{aligned}$$

As we've seen, this is a noncanonical transformation. To see what happens, we'll consider the initial conditions

$$\begin{aligned}x(0) &= a\\ p_x(0) &= b\\ y(0) &= p_y(0) = 0\end{aligned}$$

The mass is started off at a point on the $x$ axis with a momentum only in the $x$ direction. In this case, the mass behaves like a one-dimensional harmonic oscillator, moving along the $x$ axis only. To be precise, we can work out Hamilton's equations of motion:

$$\dot{p}_x = -\frac{\partial H}{\partial x} = -m\omega^2 x \tag{2.10}$$

$$\dot{x} = \frac{\partial H}{\partial p_x} = \frac{p_x}{m} \tag{2.11}$$

The equations for $y$ and $p_y$ are the same, with $x$ replaced by $y$ everywhere. We can solve these ODEs in the usual way, by differentiating the first one and substituting the second one into the first to get

$$\ddot{p}_x = -m\omega^2 \dot{x} = -\omega^2 p_x$$

This has the general solution

$$p_x(t) = A\cos\omega t + B\sin\omega t$$

We can do the same for $x$ and get

$$x(t) = C\cos\omega t + D\sin\omega t$$

Applying the initial conditions, we get

$$\begin{aligned} p_x(0) &= A = b \\ x(0) &= C = a \end{aligned}$$

Plugging these into the equations of motion (2.10) and (2.11) and solving for $B$ and $D$ we get the final solution

$$\begin{aligned} p_x(t) &= b\cos\omega t - m\omega a\sin\omega t \\ x(t) &= a\cos\omega t + \frac{b}{m\omega}\sin\omega t \\ y(t) &= p_y(t) = 0 \end{aligned}$$

Now suppose we start off with $x(0) = 0$, $y(0) = a$, $p_x(0) = b$ and $p_y(0) = 0$. That is, we have rotated the coordinates through $\frac{\pi}{2}$, but not the momenta. We now begin with the mass on the $y$ axis, but moving in the $x$ direction, so as time progresses, it will have components of momentum in both the $x$ and $y$ directions. Although it's fairly obvious that this motion will not be simply the motion in the first case rotated through $\frac{\pi}{2}$, let's go through the equations. By the same technique as above, we can solve the equations to get

$$\begin{aligned} p_x(t) &= b\cos\omega t \\ p_y(t) &= -m\omega a\sin\omega t \\ x(t) &= \frac{b}{m\omega}\sin\omega t \\ y(t) &= a\cos\omega t \end{aligned}$$

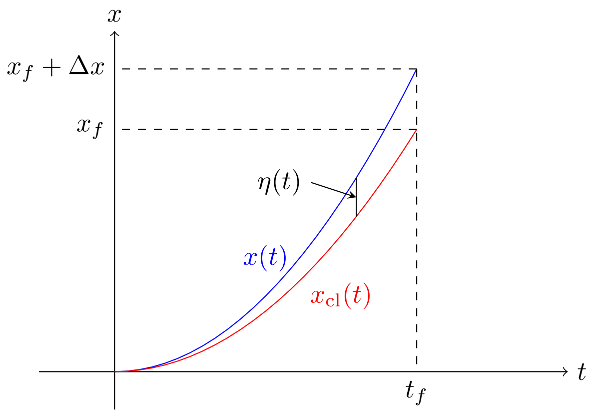
If we look at the system at, say, $t = \frac{\pi}{2\omega}$, then $\cos\omega t = 0$ and $\sin\omega t = 1$. The mass that started off on the $x$ axis will be at position $(x, y) = \left(\frac{b}{m\omega}, 0\right)$ and so will the mass that started off on the $y$ axis. Since the two masses are in the same place, obviously one is not the rotated version of the other.

Another, probably easier, way to see this is that since the first mass moves only along the $x$ axis, if the rotated version of the trajectory was also to be a solution, the rotated trajectory would have to lie entirely along the $y$ axis, which is certainly not true for the mass that starts off on the $y$ axis, but with a momentum $p_x \neq 0$.

In the general case, if the transformation is noncanonical, then the Poisson brackets in (2.6) and (2.7) don't satisfy the conditions (2.8) and (2.9), with the result that Hamilton's equations aren't satisfied in the $(\bar{q},\bar{p})$ coordinates. (There may be a deeper, physical interpretation that I've missed, but from a mathematical point of view, that's what goes wrong.)

**Exercise 2.8.6.** Show that $\partial S_{\text{cl}}/\partial x_f = p(t_f)$.

**Solution.** The situation is as shown in the following diagram:




The two trajectories now take the same time, but in the modified trajectory, the particle moves a distance $\Delta x$ further. Since both paths take the same time, there is no extra contribution $\mathscr{L}\Delta t$. In this case $\eta(t)>0$, since the new (blue) curve $x(t)$ is above the old (red) one $x_{\text{cl}}(t)$. The total variation in the action is now

$$\delta S_{\text{cl}} = \frac{\partial\mathscr{L}}{\partial\dot{x}}\eta(t)\bigg|_{t_f}$$

At $t=t_f$, $\eta(t_f)=\Delta x$, we get

$$\delta S_{\text{cl}} = \frac{\partial\mathscr{L}}{\partial\dot{x}}\bigg|_{t_f}\Delta x$$

$$\frac{\partial S_{\text{cl}}}{\partial x_f} = \frac{\partial\mathscr{L}}{\partial\dot{x}}\bigg|_{t_f} = p(t_f)$$

**Exercise 2.8.7.** Consider the harmonic oscillator, for which the general solution is

$$x(t) = A\cos\omega t + B\sin\omega t.$$

Express the energy in terms of $A$ and $B$ and note that it does not depend on time. Now choose $A$ and $B$ such that $x(0)=x_1$ and $x(T)=x_2$. Write down the energy in terms of $x_1, x_2$, and $T$. Show that the action for the trajectory connecting $x_1$ and $x_2$ is

$$S_{\text{cl}}(x_1, x_2, T) = \frac{m\omega}{2\sin\omega T}\left[\left(x_1^2 + x_2^2\right)\cos\omega T - 2x_1x_2\right]$$

Verify that $\partial S_{\text{cl}}/\partial T = -E$.

**Solution.** For the case of the one-dimensional harmonic oscillator, we have

$$\frac{\partial S_{\text{cl}}}{\partial t_f} = -H(t_f)$$

The general solution for the position is given by

$$\begin{aligned} x(t) &= A\cos\omega t + B\sin\omega t \\ \dot{x}(t) &= -A\omega\sin\omega t + B\omega\cos\omega t \end{aligned}$$

The total energy is given by

$$\begin{aligned} E &= \frac{1}{2}m\dot{x}^2 + \frac{1}{2}m\omega^2x^2 \\ &= \frac{m}{2}\left((-A\omega\sin\omega t + B\omega\cos\omega t)^2 + \omega^2(A\cos\omega t + B\sin\omega t)^2\right) \\ &= \frac{m\omega^2}{2}\left(A^2 + B^2\right) \end{aligned} \tag{2.12}$$

where we just multiplied out the second line, cancelled terms and used $\cos^2 x + \sin^2 x = 1$.

To get the action, we need the Lagrangian:

$$\begin{aligned} L &= T - V \\ &= \frac{1}{2}m\dot{x}^2 - \frac{1}{2}m\omega^2x^2 \\ &= \frac{m}{2}\left((-A\omega\sin\omega t + B\omega\cos\omega t)^2 - \omega^2(A\cos\omega t + B\sin\omega t)^2\right) \\ &= \frac{m\omega^2}{2}\left[A^2\left(\sin^2\omega t - \cos^2\omega t\right) + B^2\left(\cos^2\omega t - \sin^2\omega t\right) - 4AB\sin\omega t\cos\omega t\right] \\ &= \frac{m\omega^2}{2}\left(\left(B^2 - A^2\right)\cos 2\omega t - 2AB\sin 2\omega t\right) \end{aligned}$$

The action for a trajectory from $t = 0$ to $t = T$ is then

$$\begin{aligned} S &= \int_0^T L dt \\ &= \frac{m\omega}{4}\left[\left(B^2 - A^2\right)\sin 2\omega t + 2AB\cos 2\omega t\right]_0^T \\ &= \frac{m\omega}{4}\left[\left(B^2 - A^2\right)\sin 2\omega T + 2AB(\cos 2\omega T - 1)\right] \\ &= \frac{m\omega}{2}\left[\left(B^2 - A^2\right)\sin\omega T\cos\omega T + AB\left(\cos^2\omega T - \sin^2\omega T - 1\right)\right] \\ &= \frac{m\omega}{2}\left[\left(B^2 - A^2\right)\sin\omega T\cos\omega T - 2AB\sin^2\omega T\right] \end{aligned} \tag{2.13}$$

To proceed further, we need to specify $A$ and $B$, since these depend on the boundary conditions (that is, on where we require the mass to be at $t = 0$ and $t = T$ ). If we require $x(0) = x_1$ and $x(T) = x_2$, then

$$
\begin{aligned}
A &= x_1 \\
x_1 \cos \omega T + B \sin \omega T &= x_2 \\
B &= \frac{x_2 - x_1 \cos \omega T}{\sin \omega T}
\end{aligned}
$$

Plugging these into (2.12) gives the energy as

$$
\begin{aligned}
E &= \frac{m\omega^2}{2} \left( x_1^2 + \left( \frac{x_2 - x_1 \cos \omega T}{\sin \omega T} \right)^2 \right) \\
&= \frac{m\omega^2}{2 \sin^2 \omega T} \left( x_1^2 + x_2^2 - 2x_1 x_2 \cos \omega T \right)
\end{aligned}
$$

Plugging $A$ and $B$ into (2.13), we get:

$$
\begin{aligned}
S &= \frac{m\omega}{2 \sin \omega T} \left[ (x_2 - x_1 \cos \omega T)^2 \cos \omega T - x_1 \sin^2 \omega T \cos \omega T - 2x_1 \sin^2 \omega T \, (x_2 - x_1 \cos \omega T) \right] \\
&= \frac{m\omega}{2 \sin \omega T} \left[ \left( x_2^2 - 2x_1 x_2 \cos \omega T + x_1^2 \cos^2 \omega T \right) \cos \omega T - x_1^2 \sin^2 \omega T \cos \omega T - 2x_1 x_2 \sin^2 \omega T + 2x_1 \sin^2 \omega T \cos \right. \\
&= \frac{m\omega}{2 \sin \omega T} \left[ \left( x_1^2 + x_2^2 \right) \cos \omega T - 2x_1 x_2 \right]
\end{aligned}
$$

Taking the derivative, we get

$$
\begin{aligned}
\frac{\partial S}{\partial T} &= \frac{m\omega}{2 \sin^2 \omega T} \left[ -\omega \left( x_1^2 + x_2^2 \right) \sin^2 \omega T - \left( \left( x_1^2 + x_2^2 \right) \cos \omega T - 2x_1 x_2 \right) \omega \cos \omega T \right] \\
&= \frac{m\omega^2}{2 \sin^2 \omega T} \left[ - \left( x_1^2 + x_2^2 \right) + 2x_1 x_2 \cos \omega T \right] \\
&= -\frac{m\omega^2}{2 \sin^2 \omega T} \left( x_1^2 + x_2^2 - 2x_1 x_2 \cos \omega T \right) \\
&= -E
\end{aligned}
$$

Thus the result is verified for the harmonic oscillator.

## Chapter 3

# All Is Not Well with Classical Mechanics

# Chapter 4

# The Postulates——a General Discussion

## 4.1 The Postulates

## 4.2 Discussion of Postulates I-III

**Exercise 4.2.1.** Consider the following operators on a Hilbert space $\mathbb{V}^3(C)$:

$$L_x = \frac{1}{2^{1/2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \qquad L_y = \frac{1}{2^{1/2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix} \qquad L_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

(1) What are the possible values one can obtain if $L_z$ is measured?

(2) Take the state in which $L_z = 1$. In this state what are $\langle L_x \rangle$, $\langle L_x^2 \rangle$ and $\Delta L_x$?

(3) Find the normalized eigenstates and the eigenvalues of $L_x$ in the $L_z$ basis.

(4) If the particle is in the state with $L_z = -1$, and $L_x$ is measured, what are the possible outcomes and their probabilities?

(5) Consider the state

$$|\psi\rangle = \begin{pmatrix} 1/2 \\ 1/2 \\ 1/2^{1/2} \end{pmatrix}$$

in the $L_z$ basis. If $L_z^2$ is measured in this state and a result $+1$ is obtained, what is the state after the measurement? How probable was this result? If $L_z$ is measured, what are the outcomes and respective probabilities?

(6) A particle is in a state for which the probabilities are $P(L_z = 1) = 1/4$, $P(L_z = 0) = 1/2$, and $P(L_z = -1) = 1/4$. Convince yourself that the most general, normalized state with this property is

$$|\psi\rangle = \frac{e^{i\delta_1}}{2} |L_z = 1\rangle + \frac{e^{i\delta_2}}{2^{1/2}} |L_z = 0\rangle + \frac{e^{i\delta_3}}{2} |L_z = -1\rangle$$

It was stated earlier on that if $|\psi\rangle$ is a normalized state then the state $e^{i\theta}|\psi\rangle$ is a physically equivalent normalized state. Does this mean that the factors $e^{i\delta_i}$ multiplying the $L_z$ eigenstates are irrelevant? [Calculate for example $P(L_x = 0)$.]

**Solution.**

(1) The possible values one can obtain if $L_z$ is measured are its eigenvalues

$$L_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

Eigenvalues are $1, 0, -1$.

(2) The state in which $L_z|\psi\rangle = 1 \cdot |\psi\rangle$ is the corresponding eigenvector

$$|\psi\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$

Then in $|\psi\rangle$

$$\langle L_x\rangle = \langle\psi|L_x|\psi\rangle = (1\ 0\ 0)\frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}}(1\ 0\ 0)\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = 0$$

$$\langle L_x^2\rangle = \langle\psi|L_x^2|\psi\rangle = (1\ 0\ 0)\frac{1}{2}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \frac{1}{2}(0\ 1\ 0)\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = \frac{1}{2}$$

$$\Delta L_x = \sqrt{\langle L_x^2\rangle - (\langle L_x\rangle)^2} = \sqrt{\left(\frac{1}{2}\right) - 0^2} = \frac{1}{\sqrt{2}}$$

(3) The characteristic equation for $L_x$ is

$$0 = \det(L_x - \lambda) = \det\begin{pmatrix} -\lambda & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & -\lambda & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & -\lambda \end{pmatrix} = \lambda - \lambda^3 \qquad \Rightarrow \qquad \lambda \in \{1, 0, -1\}.$$

The corresponding eigenvectors $|\lambda\rangle$, then satisfy

$$0 = (L_x - \lambda I)|\lambda\rangle = \begin{pmatrix} -\lambda & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & -\lambda & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & -\lambda \end{pmatrix}\begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} -\lambda a + \frac{b}{\sqrt{2}} \\ \frac{a}{\sqrt{2}} - \lambda b + \frac{c}{\sqrt{2}} \\ \frac{b}{\sqrt{2}} - \lambda a \end{pmatrix}$$

where we have parameterized the components of $|\lambda\rangle$ by $(a\ b\ c)$. For $\lambda = 1$, we can solve for $b$ and $c$ in terms of $a$ by solving the following equations:

$$\begin{cases} -a + \dfrac{b}{\sqrt{2}} = 0 \\ \dfrac{a}{\sqrt{2}} - b + \dfrac{c}{\sqrt{2}} = 0 \\ \dfrac{b}{\sqrt{2}} - a = 0 \end{cases}$$

We get

$$\begin{cases} b = \sqrt{2}a \\ c = a \end{cases}$$

We then determine $a$ by normalizing $|\lambda = 1\rangle$:

$$|\lambda = 1\rangle = \begin{pmatrix} a \\ \sqrt{2}a \\ a \end{pmatrix}$$

$$\Rightarrow \quad 1 = \langle \lambda = 1|\lambda = 1\rangle = (a^* \ \sqrt{2}a^* \ a^*) \begin{pmatrix} a \\ \sqrt{2}a \\ a \end{pmatrix} = 4|a|^2$$

$$\Rightarrow \quad a = \frac{1}{2}$$

(where I have chosen the arbitrary phase to be 1).

We could do the same thing for $\lambda = 0$:

$$\begin{cases} \dfrac{b}{\sqrt{2}} = 0 \\ \dfrac{a}{\sqrt{2}} + \dfrac{c}{\sqrt{2}} = 0 \\ \dfrac{b}{\sqrt{2}} = 0 \end{cases}$$

has a solution:

$$\begin{cases} b = 0 \\ c = -a \end{cases}$$

Normalizing:

$$|\lambda = 0\rangle = \begin{pmatrix} a \\ 0 \\ -a \end{pmatrix}$$

$$\Rightarrow \quad 1 = \langle \lambda = 0|\lambda = 0\rangle = (a^* \ 0 \ -a^*) \begin{pmatrix} a \\ 0 \\ -a \end{pmatrix} = 2|a|^2$$

$$\Rightarrow \quad a = \frac{1}{\sqrt{2}}$$

And for $\lambda = -1$:

$$\begin{cases} a + \dfrac{b}{\sqrt{2}} = 0 \\ \dfrac{a}{\sqrt{2}} + b + \dfrac{c}{\sqrt{2}} = 0 \\ \dfrac{b}{\sqrt{2}} + a = 0 \end{cases}$$

We get

$$\begin{cases} b = -\sqrt{2}a \\ c = a \end{cases}$$

Normalizing:

$$|\lambda=-1\rangle = \begin{pmatrix} a \\ -\sqrt{2}a \\ a \end{pmatrix}$$

$$\Rightarrow \quad 1 = \langle\lambda=-1|\lambda=-1\rangle = (a^* \quad -\sqrt{2}a^* \quad a^*) \begin{pmatrix} a \\ -\sqrt{2}a \\ a \end{pmatrix} = 4|a|^2$$

$$\Rightarrow \quad a = \frac{1}{2}$$

Therefore,

$$|\lambda=1\rangle = \frac{1}{2}\begin{pmatrix} 1 \\ \sqrt{2} \\ 1 \end{pmatrix} \quad |\lambda=0\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} \quad |\lambda=-1\rangle = \frac{1}{2}\begin{pmatrix} 1 \\ -\sqrt{2} \\ 1 \end{pmatrix}$$

Next, we should compute the components of these 3 $L_x$-eigenstate in the $\{|1\rangle, |0\rangle, |-1\rangle\}$-basis of $L_z$-eigenstates. But since $L_z$ is diagonal in the basis in which $L_x$, $L_y$ and $L_z$ are given, the basis that Shankar used to write down the matrix elements of $L_x$, $L_y$, $L_z$ is the $L_z$-eigenbasis. So the components of $|L_x = 1, 0, -1\rangle$ in the given basis that we just calculated are their components in the $L_z$-eigenbasis.

(4) The eigenvectors of $L_z$ corresponding to $L_z = -1$ is $\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$. If we measure $L_x$ in any state, the possible outcomes are any one of the eigenvalues $L_x = \pm 1, 0$.

The probabilities for $L_x = \pm 1, 0$ in the state $|-1\rangle = |L_z = -1\rangle$ are:

$$P(L_x = 1) = |\langle L_x = 1|L_z = -1\rangle|^2 = \left|(\frac{1}{2} \ \frac{1}{\sqrt{2}} \ \frac{1}{2}) \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}\right|^2 = \frac{1}{4}$$

$$P(L_x = 0) = |\langle L_x = 0|L_z = -1\rangle|^2 = \left|(\frac{1}{\sqrt{2}} \ 0 \ -\frac{1}{\sqrt{2}}) \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}\right|^2 = \frac{1}{2}$$

$$P(L_x = -1) = |\langle L_x = -1|L_z = -1\rangle|^2 = \left|(\frac{1}{2} \ -\frac{1}{\sqrt{2}} \ \frac{1}{2}) \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}\right|^2 = \frac{1}{4}$$

(5) Consider the state

$$|\psi\rangle = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{\sqrt{2}} \end{pmatrix}$$

in the $L_z$ basis.

Since $L_z^2$ is measured to be $+1$, $L_z$ can be $+1$ or $-1$. The state after the measurement is

$$\begin{aligned}
|\psi\rangle_{\text{after}} &= \mathcal{N}(|L_z=+1\rangle\langle L_z=+1| + |L_z=-1\rangle\langle L_z=-1|)|\psi\rangle \\
&= \mathcal{N}\left(\begin{pmatrix}1\\0\\0\end{pmatrix}(1\ 0\ 0) + \begin{pmatrix}0\\0\\1\end{pmatrix}(0\ 0\ 1)\right)\begin{pmatrix}\frac{1}{2}\\\frac{1}{2}\\\frac{1}{\sqrt{2}}\end{pmatrix} \\
&= \mathcal{N}\begin{pmatrix}1&0&0\\0&0&0\\0&0&1\end{pmatrix}\begin{pmatrix}\frac{1}{2}\\\frac{1}{2}\\\frac{1}{\sqrt{2}}\end{pmatrix} = \mathcal{N}\begin{pmatrix}\frac{1}{2}\\0\\\frac{1}{\sqrt{2}}\end{pmatrix} \\
&= \frac{1}{\sqrt{\left(\frac{1}{2}\right)^2 + \left(\frac{1}{\sqrt{2}}\right)^2}}\begin{pmatrix}\frac{1}{2}\\0\\\frac{1}{\sqrt{2}}\end{pmatrix} \\
&= \frac{2}{\sqrt{3}}\begin{pmatrix}\frac{1}{2}\\0\\\frac{1}{\sqrt{2}}\end{pmatrix} \\
&= \begin{pmatrix}\frac{1}{\sqrt{3}}\\0\\\sqrt{\frac{2}{3}}\end{pmatrix}
\end{aligned}$$

where $\mathcal{N}$ normalizes the state. The probability of this result is

$$\begin{aligned}
P(L_z^2=+1) &= P(L_z=+1) + P(L_z=-1) \\
&= |\langle L_z=+1|\psi\rangle|^2 + |\langle L_z=-1|\psi\rangle|^2 \\
&= \left|(1\ 0\ 0)\begin{pmatrix}\frac{1}{2}\\ simpletex\frac{1}{2}\\\frac{1}{\sqrt{2}}\end{pmatrix}\right|^2 + \left|(0\ 0\ 1)\begin{pmatrix}\frac{1}{2}\\\frac{1}{2}\\\frac{1}{\sqrt{2}}\end{pmatrix}\right|^2 \\
&= \left|\frac{1}{2}\right|^2 + \left|\frac{1}{\sqrt{2}}\right|^2 \\
&= \frac{1}{4} + \frac{1}{2} \\
&= \frac{3}{4}
\end{aligned}$$

If $L_z$ is measured after $L_z^2$ was measured and $L_z^2 = +1$ was found, the possible outcomes and relative probabilities are:

$$P(L_z=+1)_{\text{after}} = |\langle L_z=+1|\psi\rangle_{\text{after}}|^2 = \left|(1\ 0\ 0)\begin{pmatrix}\frac{1}{\sqrt{3}}\\0\\\sqrt{\frac{2}{3}}\end{pmatrix}\right|^2 = \frac{1}{3}$$

$$P(L_z=0)_{\text{after}} = |\langle L_z=0|\psi\rangle_{\text{after}}|^2 = \left|(0\ 1\ 0)\begin{pmatrix}\frac{1}{\sqrt{3}}\\0\\\sqrt{\frac{2}{3}}\end{pmatrix}\right|^2 = 0$$

$$P(L_z=-1)_{\text{after}} = |\langle L_z=-1|\psi\rangle_{\text{after}}|^2 = \left|(0\ 0\ 1)\begin{pmatrix}\frac{1}{\sqrt{3}}\\0\\\sqrt{\frac{2}{3}}\end{pmatrix}\right|^2 = \frac{2}{3}$$

(6) A particle is in a state for which the probabilities are $P(L_z=1)=1/4$, $P(L_z=0)=1/2$, and $P(L_z=-1)=1/4$. Suppose it has the following form

$$|\psi\rangle = C_1|L_z=+1\rangle + C_2|L_z=0\rangle + C_3|L_z=-1\rangle$$

where $C_1$, $C_2$ and $C_3$ are complex numbers. Then we have

$$\begin{aligned}
|C_1|^2 &= C_1^*C_1 = P(L_z=+1) = \frac{1}{4} && \Rightarrow\ C_1 = \frac{1}{2}e^{i\delta_1}\\
|C_2|^2 &= C_2^*C_2 = P(L_z=0) = \frac{1}{2} && \Rightarrow\ C_2 = \frac{1}{\sqrt{2}}e^{i\delta_2}\\
|C_3|^2 &= C_3^*C_3 = P(L_z=-1) = \frac{1}{4} && \Rightarrow\ C_3 = \frac{1}{2}e^{i\delta_3}
\end{aligned}$$

where $\delta_1$, $\delta_2$ and $\delta_3$ are arbitrary real numbers. Therefore, it has the form

$$|\psi\rangle = \frac{e^{i\delta_1}}{2}|L_z=1\rangle + \frac{e^{i\delta_2}}{2^{1/2}}|L_z=0\rangle + \frac{e^{i\delta_3}}{2}|L_z=-1\rangle$$

The values of the phases matter when measuring an observable that is incompatible with $L_z$, as an example:

$$\langle L_x=0|L_z=1\rangle = \frac{1}{\sqrt{2}}(1\ 0\ -1)\begin{pmatrix}1\\0\\0\end{pmatrix} = \frac{1}{\sqrt{2}}$$

$$\langle L_x=0|L_z=0\rangle = \frac{1}{\sqrt{2}}(1\ 0\ -1)\begin{pmatrix}0\\1\\0\end{pmatrix} = 0$$

$$\langle L_x=0|L_z=-1\rangle = \frac{1}{\sqrt{2}}(1\ 0\ -1)\begin{pmatrix}0\\0\\1\end{pmatrix} = -\frac{1}{\sqrt{2}}$$

$$
\begin{aligned}
P(L_x = 0) &= |\langle L_x = 0|\psi\rangle|^2 \\
&= \left| \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} \frac{e^{i\delta_1}}{2} \\ \frac{e^{i\delta_2}}{\sqrt{2}} \\ \frac{e^{i\delta_3}}{2} \end{pmatrix} \right|^2 \\
&= \frac{1}{8}|e^{i\delta_1} - e^{i\delta_3}|^2 \\
&= \frac{1}{8}(e^{i\delta_1} - e^{i\delta_3})(e^{-i\delta_1} - e^{-i\delta_3}) \\
&= \frac{1}{8}(1 - e^{i(\delta_1-\delta_3)} - e^{-i(\delta_1-\delta_3)} + 1) \\
&= \frac{1}{8}(2 - 2 \cdot \frac{e^{i(\delta_1-\delta_3)} + e^{-i(\delta_1-\delta_3)}}{2}) \\
&= \frac{1}{4}(1 - \cos(\delta_1 - \delta_3))
\end{aligned}
$$

It depends on phases and can be measured by experiment.

**Exercise 4.2.2.** Show that for a real wave function $\psi(x)$, the expectation value of momentum $\langle P\rangle = 0$. (Hint: Show that the probabilities for the momenta $\pm p$ are equal.) Generalize this result to the case $\psi = c\psi_r$, where $\psi_r$ is real and $c$ an arbitrary (real or complex) constant. (Recall that $|\psi\rangle$ and $\alpha|\psi\rangle$ are physically equivalent.)

**Solution.** Since $\psi(x)$ is real, $\psi^*(x) = \psi(x)$.

$$
\begin{aligned}
\langle P\rangle &= \int_{-\infty}^{+\infty} \psi^*(x) \left(-i\hbar\frac{\partial}{\partial x}\right) \psi(x)\; dx \\
&= -i\hbar \int_{-\infty}^{+\infty} \psi(x)\frac{\partial}{\partial x}\psi(x)\; dx \\
&= -\frac{1}{2}i\hbar \int_{-\infty}^{+\infty} \frac{\partial}{\partial x}\psi^2(x)\; dx \\
&= -\frac{1}{2}i\hbar\psi^2(x)\Big|_{-\infty}^{+\infty} \\
&= 0
\end{aligned}
$$

Since $\psi(x) \to 0$, as $x \to \pm\infty$.

For general case,

$$
\begin{aligned}
\langle P\rangle &= \int_{-\infty}^{+\infty} [c\psi_r(x)]^* \left(-i\hbar\frac{\partial}{\partial x}\right) [c\psi_r(x)] \\
&= |c|^2 \int_{-\infty}^{+\infty} \psi_r(x) \left(-i\hbar\frac{\partial}{\partial x}\right) \psi_r(x)\; dx \\
&= |c|^2 \cdot 0 \\
&= 0
\end{aligned}
$$

**Exercise 4.2.3.** Show that if $\psi(x)$ has mean momentum $\langle P\rangle$, $e^{ip_0x/\hbar}\psi(x)$ has mean momentum $\langle P\rangle + p_0$.

**Solution.**

$$
\begin{aligned}
\langle P\rangle &= -i\hbar\int_{-\infty}^{+\infty}\psi^*(x)\frac{\partial}{\partial x}\psi(x)\ dx\\
\langle P'\rangle &= -i\hbar\int_{-\infty}^{+\infty}[e^{-ip_0x/\hbar}\psi^*(x)]\frac{\partial}{\partial x}[e^{ip_0x/\hbar}\psi(x)]\ dx\\
&= -i\hbar\int_{-\infty}^{+\infty}[e^{-ip_0x/\hbar}\psi^*(x)][e^{ip_0x/\hbar}\cdot ip_0/\hbar\cdot\psi(x)+e^{ip_0x/\hbar}\frac{\partial}{\partial x}\psi(x)]\ dx\\
&= -i\hbar\int_{-\infty}^{+\infty}e^{-ip_0x/\hbar}\psi^*(x)\cdot e^{ip_0x/\hbar}\cdot ip_0/\hbar\cdot\psi(x)\ dx\\
&\quad - i\hbar\int_{-\infty}^{+\infty}e^{-ip_0x/\hbar}\psi^*(x)\cdot e^{ip_0x/\hbar}\frac{\partial}{\partial x}\psi(x)\ dx\\
&= p_0\int_{-\infty}^{+\infty}\psi^*(x)\psi(x)\ dx - i\hbar\int_{-\infty}^{+\infty}\psi^*(x)\cdot\frac{\partial}{\partial x}\psi(x)\ dx\\
&= \langle P\rangle + p_0
\end{aligned}
$$

## 4.3 The Schrödinger Equation (Dotting Your $i$s and Crossing your $\hbar$s)

# Chapter 5

# Simple Problems in One Dimension

## 5.1 The Free Particle

**Exercise 5.1.1.** Show that Eq. (5.1.9) may be rewritten as an integral over $E$ and a sum over the $\pm$ index as

$$U(t) = \sum_{\alpha=\pm} \int_0^\infty \left[\frac{m}{(2mE)^{1/2}}\right] |E,\alpha\rangle\langle E,\alpha| \mathrm{e}^{-\mathrm{i}Et/\hbar} \mathrm{d}E$$

**Solution.** $E = \dfrac{p^2}{2m} \to p = \alpha\sqrt{2mE}$

$$\mathrm{d}p = \frac{\alpha m}{\sqrt{2mE}} \mathrm{d}E$$

where $\alpha = \pm 1$. Hence

$$\begin{aligned}
U(t) &= \int_{-\infty}^{+\infty} \mathrm{d}p\, |p\rangle\langle p| \mathrm{e}^{-\mathrm{i}Et/\hbar} \\
&= \int_{-\infty}^{0} \mathrm{d}p\, |p\rangle\langle p| \mathrm{e}^{-\mathrm{i}Et/\hbar} + \int_{0}^{+\infty} \mathrm{d}p\, |p\rangle\langle p| \mathrm{e}^{-\mathrm{i}Et/\hbar} \\
&= \int_{-\infty}^{0} \mathrm{d}E \frac{-m}{\sqrt{2mE}} |E,-\rangle\langle E,-| \mathrm{e}^{-\mathrm{i}Et/\hbar} + \int_{0}^{+\infty} \mathrm{d}E \frac{m}{\sqrt{2mE}} |E,+\rangle\langle E,+| \mathrm{e}^{-\mathrm{i}Et/\hbar} \\
&= \int_{0}^{+\infty} \mathrm{d}E \frac{m}{\sqrt{2mE}} |E,-\rangle\langle E,-| \mathrm{e}^{-\mathrm{i}Et/\hbar} + \int_{0}^{+\infty} \mathrm{d}E \frac{m}{\sqrt{2mE}} |E,+\rangle\langle E,+| \mathrm{e}^{-\mathrm{i}Et/\hbar} \\
&= \sum_{\alpha=\pm} \int_0^\infty \left[\frac{m}{(2mE)^{1/2}}\right] |E,\alpha\rangle\langle E,\alpha| \mathrm{e}^{-\mathrm{i}Et/\hbar} \mathrm{d}E
\end{aligned}$$

**Exercise 5.1.2.** By solving the eigenvalue equation (5.1.3) in the $X$ basis, regain Eq. (5.1.8), i.e., show that the general solution of energy $E$ is

$$\psi_E(x) = \beta \frac{\exp\left[i(2mE)^{1/2}x/\hbar\right]}{(2\pi\hbar)^{1/2}} + \gamma \frac{\exp\left[-i(2mE)^{1/2}x/\hbar\right]}{(2\pi\hbar)^{1/2}}$$

[The factor $(2\pi\hbar)^{-1/2}$ is arbitrary and may be absorbed into $\beta$ and $\gamma$.] Though $\psi_E(x)$ will satisfy the equation even if $E < 0$, are these functions in the Hilbert space?

**Solution.** In $X$ basis, equation (5.1.3) is

$$\langle x \mid H \mid E\rangle = E\langle x \mid E\rangle$$

which becomes

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi_E(x) = E\psi_E(x)$$

The most general solution is

$$\psi_E(x) = A_+\mathrm{e}^{+\frac{\mathrm{i}}{\hbar}\sqrt{2mE}x} + A_-\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\sqrt{2mE}x}$$

where

$$\langle x \mid E\rangle = \beta\langle x \mid E, +\rangle + \gamma\langle x \mid E, -\rangle$$
$$\beta = A_+\sqrt{2\pi\hbar}$$
$$\gamma = A_-\sqrt{2\pi\hbar}$$

If $E < 0$, these solutions are not in the Hilbert space, since then the two terms grow exponentially as $x \to \pm\infty$.

**Exercise 5.1.3.** We have seen that there exists another formula for $U(t)$, namely, $U(t) = e^{-iHt/\hbar}$. For a free particle this becomes

$$U(t) = \exp\left[\frac{i}{\hbar}\left(\frac{\hbar^2 t}{2m}\frac{d^2}{dx^2}\right)\right] = \sum_{n=0}^{\infty}\frac{1}{n!}\left(\frac{i\hbar t}{2m}\right)^n\frac{d^{2n}}{dx^{2n}} \tag{5.1.18}$$

Consider the initial state in Eq. (5.1.14) with $p_0 = 0$, and set $\Delta = 1, t' = 0$ :

$$\psi(x, 0) = \frac{e^{-x^2/2}}{(\pi)^{1/4}}$$

Find $\psi(x, t)$ using Eq. (5.1.18) above and compare with Eq. (5.1.15).
Hints : (1) Write $\psi(x, 0)$ as a power series:

$$\psi(x, 0) = (\pi)^{-1/4}\sum_{n=0}^{\infty}\frac{(-1)^n x^{2n}}{n!(2)^n}$$

(2) Find the action of a few terms

$$1, \quad \left(\frac{i\hbar t}{2m}\right)\frac{d^2}{dx^2}, \quad \frac{1}{2!}\left(\frac{i\hbar t}{2m}\frac{d^2}{dx^2}\right)^2$$

etc., on this power series.
(3) Collect terms with the same power of $x$.
(4) Look for the following series expansion in the coefficient of $x^{2n}$ :

$$\left(1 + \frac{it\hbar}{m}\right)^{-n-12} = 1 - (n + 1/2)\left(\frac{i\hbar t}{m}\right) + \frac{(n + 1/2)(n + 3/2)}{2!}\left(\frac{it\hbar}{m}\right)^2 + \cdots$$

(5) Juggle around till you get the answer.

**Solution.**

**Exercise 5.1.4.** Consider the wave function

$$\begin{aligned}\psi(x,0) &= \sin\left(\frac{\pi x}{L}\right), \quad & |x| \leqslant L/2 \\ &= 0, & |x| > L/2\end{aligned}$$

It is clear that when this function is differentiated any number of times we get another function confined to the interval $|x| \leqslant L/2$. Consequently the action of

$$U(t) = \exp\left[\frac{i}{\hbar}\left(\frac{\hbar^2 t}{2m}\right)\frac{d^2}{dx^2}\right]$$

on this function is to give a function confined to $|x| \leqslant L/2$. What about the spreading of the wave packet?

## 5.2 The Particle in a Box

**Exercise 5.2.1.** A particle is in the ground state of a box of length $L$. Suddenly the box expands (symmetrically) to twice its size, leaving the wave function undisturbed. Show that the probability of finding the particle in the ground state of the new box is $(8/3\pi)^2$.

**Exercise 5.2.2.** (a) Show that for any normalized $|\psi\rangle, \langle\psi|H|\psi\rangle \geqslant E_0$, where $E_0$ is the lowest-energy eigenvalue. (Hint : Expand $|\psi\rangle$ in the eigenbasis of $H$.)

(b) Prove the following theorem: Every attractive potential in one dimension has at least one bound state. Hint: Since $V$ is attractive, if we define $V(\infty) = 0$, it follows that $V(x) = -|V(x)|$ for all $x$. To show that there exists a bound state with $E < 0$, consider

$$\psi_\alpha(x) = \left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\alpha x^2/2}$$

and calculate

$$E(\alpha) = \langle\psi_\alpha|H|\psi_\alpha\rangle\,, \quad H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - |V(x)|$$

Show that $E(\alpha)$ can be made negative by a suitable choice of $\alpha$. The desired result follows from the application of the theorem proved above.

**Exercise 5.2.3.** Consider $V(x) = -aV_0\delta(x)$. Show that it admits a bound state of energy $E = -ma^2V_0^2/2\hbar^2$. Are there any other bound states? Hint: Solve Schrödinger's equation outside the potential for $E < 0$, and keep only the solution that has the right behavior at infinity and is continuous at $x = 0$. Draw the wave function and see how there is a cusp, or a discontinuous change of slope at $x = 0$. Calculate the change in slope and equate it to

$$\int_{-\varepsilon}^{+\varepsilon}\left(\frac{d^2\psi}{dx^2}\right)dx$$

(where $\varepsilon$ is infinitesimal) determined from Schrödinger's equation.

**Exercise 5.2.4.** Consider a particle of mass $m$ in the state $|n\rangle$ of a box of length $L$. Find the force $F = -\partial E/\partial L$ encountered when the walls are slowly pushed in, assuming the particle remains in the $n$th state of the box as its size changes. Consider a classical particle of energy $E_n$ in this box. Find its velocity, the frequency of collision on a given wall, the momentum transfer per collision, and hence the average force. Compare it to $-\partial E/\partial L$ computed above.

**Exercise 5.2.5.** If the box extends from $x = 0$ to $L$ (instead of $-L/2$ to $L/2$) show that $\psi_n(x) = (2/L)^{1/2}\sin(n\pi x/L), n = 1, 2, \ldots, \infty$ and $E_n = \hbar^2\pi^2 n^2/2mL^2$.

**Exercise 5.2.6.** Square Well Potential. Consider a particle in a square well potential:

$$V(x) = \begin{cases} 0, & |x| \leqslant a \\ V_0, & |x| \geqslant a \end{cases}$$

Since when $V_0 \to \infty$, we have a box, let us guess what the lowering of the walls does to the states. First of all, all the bound states (which alone we are interested in), will have $E \leq V_0$. Second, the wave functions of the low-lying levels will look like those of the particle in a box, with the obvious difference that $\psi$ will not vanish at the walls but instead spill out with an exponential tail. The eigenfunctions will still be even, odd, even, etc.

(1) Show that the even solutions have energies that satisfy the transcendental equation

$$k \tan ka = \kappa \tag{5.2.23}$$

while the odd ones will have energies that satisfy

$$k \cot ka = -\kappa \tag{5.2.24}$$

where $k$ and $i\kappa$ are the real and complex wave numbers inside and outside the well, respectively. Note that $k$ and $\kappa$ are related by

$$k^2 + \kappa^2 = 2mV_0/\hbar^2 \tag{5.2.25}$$

Verify that as $V_0$ tends to $\infty$, we regain the levels in the box.

(2) Equations (5.2.23) and (5.2.24) must be solved graphically. In the ($\alpha = ka, \beta = \kappa a$) plane, imagine a circle that obeys Eq. (5.2.25). The bound states are then given by the intersection of the curve $\alpha \tan \alpha = \beta$ or $\alpha \cot \alpha = -\beta$ with the circle. (Remember $\alpha$ and $\beta$ are positive.)

(3) Show that there is always one even solution and that there is no odd solution unless $V_0 \geqslant \hbar^2\pi^2/8ma^2$. What is $E$ when $V_0$ just meets this requirement? Note that the general result from Exercise 5.2.2b holds.

## 5.3 The Continuity Equation for Probability

**Exercise 5.3.1.** Consider the case where $V = V_r - iV_i$, where the imaginary part $V_i$ is a constant. Is the Hamiltonian Hermitian? Go through the derivation of the continuity equation and show that the total probability for finding the particle decreases exponentially as $e^{-2V_i t/\hbar}$. Such complex potentials are used to describe processes in which particles are absorbed by a sink.

**Exercise 5.3.2.** Convince yourself that if $\psi = c\tilde{\psi}$, where $c$ is constant (real or complex) and $\tilde{\psi}$ is real, the corresponding $\mathbf{j}$ vanishes.

**Exercise 5.3.3.** Consider

$$\psi_{\mathbf{p}} = \left(\frac{1}{2\pi\hbar}\right)^{3/2} e^{i(\mathbf{p}\cdot\mathbf{r})/\hbar}$$

Find $\mathbf{j}$ and $P$ and compare the relation between them to the electromagnetic equation $\mathbf{j} = \rho\mathbf{v}$, $\mathbf{v}$ being the velocity. Since $\rho$ and $\mathbf{j}$ are constant, note that the continuity Eq. (5.3.7) is trivially satisfied.

**Exercise 5.3.4.** Consider $\psi = Ae^{ipx/\hbar} + Be^{-ipx/\hbar}$ in one dimension. Show that $j = \left(|A|^2 - |B|^2\right) p/m$. The absence of cross terms between the right- and left-moving pieces in $\psi$ allows us to associate the two parts of $j$ with corresponding parts of $\psi$.

## 5.4 The Single-Step Potential: A Problem in Scattering

**Exercise 5.4.1.** Evaluate the third piece in Eq. (5.416) and compare the resulting $T$ with Eq. (5.4.21). [Hint: Expand the factor $\left(k_1^2 - 2mV_0/\hbar^2\right)^{1/2}$ near $k_1 = k_0$, keeping just the first derivative in the Taylor series.]

**Exercise 5.4.2.** (a) Calculate $R$ and $T$ for scattering of a potential $V(x) = V_0 a\delta(x)$. (b) Do the same for the case $V = 0$ for $|x| > a$ and $V = V_0$ for $|x| < a$. Assume that the energy is positive but less than $V_0$.

**Exercise 5.4.3.** Consider a particle subject to a constant force $f$ in one dimension. Solve for the propagator in momentum space and get

$$U\left(p, t; p', 0\right) = \delta\left(p - p' - ft\right) e^{i\left(p'^3 - p^3\right)/6m\hbar f}$$

Transform back to coordinate space and obtain

$$U\left(x, t; x', 0\right) = \left(\frac{m}{2\pi\hbar i t}\right)^{1/2} \exp\left\{\frac{i}{\hbar}\left[\frac{m\left(x - x'\right)^2}{2t} + \frac{1}{2} ft\left(x + x'\right) - \frac{f^2 t^3}{24m}\right]\right\}$$

[Hint: Normalize $\psi_E(p)$ such that $\langle E \mid E' \rangle = \delta\left(E - E'\right)$. Note that $E$ is not restricted to be positive.]

## 5.5 The Double-Slit Experiment

## 5.6 Some Theorems

# Chapter 6

# The Classical Limit