Notes on Quantum Mechanics

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1. These are notes prepared for the benefit of students enrolled in Quantum Mechanics (PHYS-530A and PHYS-530-B) at Southern Illinois University–Carbondale. It will be updated periodically, and will evolve during the semester. It is not a substitute for standard textbooks, but a supplement prepared as a study-guide.

2. The following textbooks were extensively used in this compilation.

   (a) *Principles of Quantum Mechanics*, by P. A. M. Dirac.

   (b) *Quantum Mechanics: Symbolism of Atomic Measurements*, by J. Schwinger, edited by B.-G. Englert.

   (c) Schwinger's Quantum Action Principle, by K. A. Milton, http://arxiv.org/abs/1503.08091.

   (d) *Introduction to Quantum Mechanics*, lecture notes by K. A. Milton, available at http://www.nhn.ou.edu/∼milton/p3803-12.html and http://www.nhn.ou.edu/∼milton/p4803-12.html.

   (e) *Quantum Mechanics*, by L. I. Schiff.

   (f) Classical Electrodynamics, Julian Schwinger, Lester L. Deraad Jr., Kimball A. Milton, and Wu-yang Tsai.

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Contents

Chapter 1

Matrix algebra

1.1 Matrix diagonalization

Problems

1. (**20 points.**) A 3×3 matrix A satisfies the equation

$$A^3 = 1. \tag{1.1}$$

   Given that the eigenvalues of A are non-degenerate, find all eigenvalues of A.

2. (**20 points.**) Consider the matrix

$$\mathbf{A} = \begin{pmatrix} \cosh\theta & \sinh\theta \\ \sinh\theta & \cosh\theta \end{pmatrix}. \tag{1.2}$$

   (a) Find the eigenvalues of the matrix $\mathbf{A}$.

   (b) Find the normalized eigenvectors of matrix $\mathbf{A}$.

   (c) Determine the matrix that diagonalizes the matrix $\mathbf{A}$.

   (d) What can you then conclude about the eigenvalues and eigenvectors of $\ln \mathbf{A}$? Find them.

3. (**20 points.**) Consider the rotation matrix

$$\mathbf{A} = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}. \tag{1.3}$$

   (a) Find the eigenvalues of the matrix $\mathbf{A}$.

   (b) Find the normalized eigenvectors of matrix $\mathbf{A}$.

   (c) Determine the matrix that diagonalizes the matrix $\mathbf{A}$.

   (d) What can you then conclude about the eigenvalues and eigenvectors of $\mathbf{A}^{107}$? Find them.

4. (**20 points.**) Consider the matrix

$$A = \begin{pmatrix} \cos\theta & \sin\theta \\ \sin\theta & -\cos\theta \end{pmatrix}. \tag{1.4}$$

   (a) Find all the eigenvalues of the matrix A.

   (b) Find the normalized eigenvectors associated with all the eigenvalues of matrix A. (Simplification is achieved by writing the trignometric functions in terms of half angles. $1 - \cos\theta = 2\sin^2\theta/2$, $1 + \cos\theta = 2\cos^2\theta/2$, $\sin\theta = 2\sin\theta/2\cos\theta/2$.)

   (c) Determine the matrix that diagonalizes the matrix A.

5. (**20 points.**) Two matrices A and B satisfy the relation

$$AB - BA = 1. \tag{1.5}$$

   (a) Prove that this cannot be true in a finite dimensional vector space.
   Hint: Take trace.

   (b) Nevertheless, construct infinite dimensional matrices A and B that satisfy the above relation.
   Hint: The answer is not unique. For example,

$$A = \begin{bmatrix} 0 & \sqrt{1} & 0 & 0 & 0 & \cdots \\ 0 & 0 & \sqrt{2} & 0 & 0 & \cdots \\ 0 & 0 & 0 & \sqrt{3} & 0 & \cdots \\ 0 & 0 & 0 & 0 & \sqrt{4} & \cdots \\ 0 & 0 & 0 & 0 & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}, \qquad B = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & \cdots \\ \sqrt{1} & 0 & 0 & 0 & 0 & \cdots \\ 0 & \sqrt{2} & 0 & 0 & 0 & \cdots \\ 0 & 0 & \sqrt{3} & 0 & 0 & \cdots \\ 0 & 0 & 0 & \sqrt{4} & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}. \tag{1.6}$$

   Construct another example with

$$A = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & \sqrt{1} & 0 & 0 & 0 & \cdots \\ \sqrt{1} & 0 & \sqrt{2} & 0 & 0 & \cdots \\ 0 & \sqrt{2} & 0 & \sqrt{3} & 0 & \cdots \\ 0 & 0 & \sqrt{3} & 0 & \sqrt{4} & \cdots \\ 0 & 0 & 0 & \sqrt{4} & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}. \tag{1.7}$$

   These examples exploit the counterintuitive properties of divergent series.

1.2 Pauli matrices

1.2.1 Properties

1. (**20 points.**) The Pauli matrices are traceless Hermitian matrices that satisfy

$$\sigma_i \sigma_j = \delta_{ij} + i\varepsilon_{ijk}\sigma_k, \tag{1.8}$$

where i, j, are either $1, 2$, or 3. Evaluate the commutation relation

$$\big[\sigma_i, \sigma_j\big]. \tag{1.9}$$

Then, evaluate the anti-commutation relation

$$\big\{\sigma_i, \sigma_j\big\}. \tag{1.10}$$

Evaluate

$$\Big[\sigma_i, \big[\sigma_j, \sigma_k\big]\Big]. \tag{1.11}$$

Further, evaluate the relations

$$\big[\sigma_i^n, \sigma_j^m\big] \quad \text{and} \quad \big\{\sigma_i^n, \sigma_j^m\big\} \tag{1.12}$$

for positive integers n and m.

2. (**20 points.**) The Pauli matrices are traceless Hermitian matrices that satisfy

$$\sigma_i \sigma_j = \delta_{ij} + i\varepsilon_{ijk}\sigma_k, \tag{1.13}$$

where i, j, are either $1, 2$, or 3. Evaluate the traces,

$$\operatorname{tr}(\sigma_i \sigma_j) = 2\delta_{ij} \tag{1.14}$$

and

$$\operatorname{tr}(\sigma_i \sigma_j \sigma_k) = 2i\varepsilon_{ijk} \tag{1.15}$$

and

$$\operatorname{tr}(\sigma_i \sigma_m \sigma_j \sigma_n) = 2(\delta_{im}\delta_{jn} - \delta_{ij}\delta_{mn} + \delta_{in}\delta_{jm}). \tag{1.16}$$

3. (**20 points.**) (Based on Milton's lecture notes.) The vector product is defined by

$$(\mathbf{A} \times \mathbf{B})_3 = A_1 B_2 - A_2 B_1, \tag{1.17}$$

and similarly (cyclically) for the 1 and 2 components. If $A_{1,2,3}$ are elements of a non-commutative algebra, the components of $\mathbf{A}$ do not commute, and $\mathbf{A} \times \mathbf{A} \neq 0$ in general. Show that

$$\frac{\boldsymbol{\sigma}}{2} \times \frac{\boldsymbol{\sigma}}{2} = i\frac{\boldsymbol{\sigma}}{2}. \tag{1.18}$$

This is a special case of the angular momentum statement

$$\mathbf{J} \times \mathbf{J} = i\hbar\mathbf{J}. \tag{1.19}$$

4. (**20 points.**) If $\boldsymbol{\sigma}$ is the vector constructed out of Pauli matrices and $\mathbf{a}$, $\mathbf{b}$, are (numerical) vectors, show that

$$(\boldsymbol{\sigma} \cdot \mathbf{a})(\boldsymbol{\sigma} \cdot \mathbf{b}) = \mathbf{a} \cdot \mathbf{b} + i\boldsymbol{\sigma} \cdot (\mathbf{a} \times \mathbf{b}). \tag{1.20}$$

Further, for numerical vector $\boldsymbol{\theta}$, show that

$$e^{i\boldsymbol{\sigma}\cdot\boldsymbol{\theta}} = \cos\theta + i(\boldsymbol{\sigma} \cdot \hat{\boldsymbol{\theta}})\sin\theta, \tag{1.21}$$

where $\theta = |\boldsymbol{\theta}|$ and $\hat{\boldsymbol{\theta}} = \boldsymbol{\theta}/\theta$. Next, evaluate

(a)
$$\operatorname{tr}\cos(\boldsymbol{\sigma} \cdot \boldsymbol{\theta}). \tag{1.22}$$

(b)
$$\operatorname{tr}\sin(\boldsymbol{\sigma} \cdot \boldsymbol{\theta}). \tag{1.23}$$

(c)
$$\operatorname{tr}\tan(\boldsymbol{\sigma} \cdot \boldsymbol{\theta}). \tag{1.24}$$

(d)
$$\operatorname{tr} e^{i\boldsymbol{\sigma}\cdot\boldsymbol{\theta}}. \tag{1.25}$$

Hint: $\operatorname{tr} f(A) = \sum_i f(a_i)$.

5. (**20 points.**) Evaluate

$$[(\boldsymbol{\sigma} \cdot \mathbf{a})(\boldsymbol{\sigma} \cdot \mathbf{b})]\,(\boldsymbol{\sigma} \cdot \mathbf{c}). \tag{1.26}$$

Then evaluate

$$(\boldsymbol{\sigma} \cdot \mathbf{a})\,[(\boldsymbol{\sigma} \cdot \mathbf{b})(\boldsymbol{\sigma} \cdot \mathbf{c})]\,. \tag{1.27}$$

Are they equal?

1.2.2 Properties under rotation: Vector

6. (**20 points.**) Consider the operator construction

$$K(\lambda) = e^{-\lambda A} B e^{\lambda A} \tag{1.28}$$

in terms of two operators A and B, λ being a number. Show that

$$\frac{\partial K}{\partial \lambda} = [K, A]. \tag{1.29}$$

Evaluate the higher derivatives

$$\frac{\partial^n K}{\partial \lambda^n} \tag{1.30}$$

recursively. Thus, using Taylor expansion around $\lambda = 0$, show that

$$K(\lambda) = B + \lambda[B, A] + \frac{\lambda^2}{2!}[[B, A], A] + \frac{\lambda^3}{3!}[[[B, A], A], A] + \dots. \tag{1.31}$$

Then, for $\lambda = 1$, we have

$$e^{-A} B e^{A} = B + [B, A] + \frac{1}{2!}[[B, A], A] + \frac{1}{3!}[[[B, A], A], A] + \dots. \tag{1.32}$$

This is the Baker-Campbell-Hausdorff formula. Using this evaluate

$$\sigma_{x'} = e^{-\frac{i}{2}\phi\sigma_z} \sigma_x e^{\frac{i}{2}\phi\sigma_z}, \tag{1.33a}$$

$$\sigma_{y'} = e^{-\frac{i}{2}\phi\sigma_z} \sigma_y e^{\frac{i}{2}\phi\sigma_z}, \tag{1.33b}$$

$$\sigma_{z'} = e^{-\frac{i}{2}\phi\sigma_z} \sigma_z e^{\frac{i}{2}\phi\sigma_z}, \tag{1.33c}$$

where σ_x, σ_y, and σ_z, are Pauli matrices and ϕ is a number representing an angle of rotation. In particular, show that

$$\sigma_{x'} = \sigma_x \cos\phi + \sigma_y \sin\phi, \tag{1.34a}$$

$$\sigma_{y'} = -\sigma_x \sin\phi + \sigma_y \cos\phi, \tag{1.34b}$$

$$\sigma_{z'} = \sigma_z. \tag{1.34c}$$

What is the physical interpretation?

7. (**20 points.**) (Based on Milton's lecture notes.) Consider a rotation of the coordinate system about the z-axis through an angle ϕ:

$$x' = x\cos\phi + y\sin\phi, \tag{1.35a}$$

$$y' = -x\sin\phi + y\cos\phi, \tag{1.35b}$$

$$z' = z. \tag{1.35c}$$

Pauli matrices, $\boldsymbol{\sigma}$, transform like a vector. The components of Pauli matrices transform as

$$\sigma_{x'} = \sigma_x \cos\phi + \sigma_y \sin\phi, \tag{1.36a}$$

$$\sigma_{y'} = -\sigma_x \sin\phi + \sigma_y \cos\phi, \tag{1.36b}$$

$$\sigma_{z'} = \sigma_z. \tag{1.36c}$$

Verify that the transformed components of Pauli matrices have the same algebraic properties as the original components:

$$\sigma_{x'}^2 = \sigma_{y'}^2 = 1, \qquad \sigma_{x'}\sigma_{y'} = i\sigma_{z'}. \tag{1.37}$$

1.2.3 Eigenbasis dependent properties

8. (**30 points.**) The Pauli matrices are traceless Hermitian matrices that satisfy

$$\sigma_i\sigma_j = \delta_{ij} + i\varepsilon_{ijk}\sigma_k, \tag{1.38}$$

where i, j, are either $1, 2$, or 3. Show that these correspond to the following nine explicit equations.

$$\sigma_1^2 = 1, \tag{1.39a}$$
$$\sigma_2\sigma_1 = -i\sigma_3, \tag{1.39b}$$
$$\sigma_3\sigma_1 = i\sigma_2, \tag{1.39c}$$
$$\sigma_1\sigma_2 = i\sigma_3, \tag{1.39d}$$
$$\sigma_2^2 = 1, \tag{1.39e}$$
$$\sigma_3\sigma_2 = -i\sigma_1, \tag{1.39f}$$
$$\sigma_1\sigma_3 = -i\sigma_2, \tag{1.39g}$$
$$\sigma_2\sigma_3 = i\sigma_1, \tag{1.39h}$$
$$\sigma_3^2 = 1. \tag{1.39i}$$

Let us realize the Pauli matrices in the eigenbasis of σ_3. Using Eq. (1.39i) we have the eigenvalues

$$\sigma_3' = \pm 1. \tag{1.40}$$

The corresponding eigenvectors are $|\sigma_3' = +1\rangle$ and $|\sigma_3' = -1\rangle$. The eigenbasis of σ_3 is often the default basis used in the literature, and we shall often use the simpler notation $|+\rangle$ and $|-\rangle$ to represent them. These eigenvectors satisfy the completeness relation

$$|+\rangle\langle+| \;+\; |-\rangle\langle-| = 1. \tag{1.41}$$

The representation of an operator in a particular basis is obtained by using the completeness relation to invoke all possible projections. Thus,

$$\begin{aligned}
\sigma_3 = 1\sigma_3 1 &= (|+\rangle\langle+| \;+\; |-\rangle\langle-|)\sigma_3(|+\rangle\langle+| \;+\; |-\rangle\langle-|) && (1.42)\\
&= |+\rangle\langle+|\sigma_3|+\rangle\langle+| \;+\; |+\rangle\langle+|\sigma_3|-\rangle\langle-| && (1.43)\\
&\quad + \; |-\rangle\langle-|\sigma_3|+\rangle\langle+| \;+\; |-\rangle\langle-|\sigma_3|-\rangle\langle-| && (1.44)
\end{aligned}$$

9. (**40 points.**) Consider the eigenvalue equation

$$\sigma_x|\sigma_x'\rangle = \sigma_x'|\sigma_x'\rangle, \tag{1.45}$$

where primes denote eigenvalues.

(a) Find the eigenvalues and normalized eigenvectors (up to a phase) of

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \tag{1.46}$$

For reference we shall call these eigenvectors $|\sigma_x' = +\rangle$ and $|\sigma_x' = -\rangle$.

(b) Now compute the new matrix

$$\bar{\sigma}_x = \begin{pmatrix} \langle\sigma_x' = +|\sigma_x|\sigma_x' = +\rangle & \langle\sigma_x' = +|\sigma_x|\sigma_x' = -\rangle \\ \langle\sigma_x' = -|\sigma_x|\sigma_x' = +\rangle & \langle\sigma_x' = -|\sigma_x|\sigma_x' = -\rangle \end{pmatrix}. \tag{1.47}$$

(c) Similarly, compute the new matrices

$$\bar{\sigma}_y = \begin{pmatrix} \langle\sigma_x' = +|\sigma_y|\sigma_x' = +\rangle & \langle\sigma_x' = +|\sigma_y|\sigma_x' = -\rangle \\ \langle\sigma_x' = -|\sigma_y|\sigma_x' = +\rangle & \langle\sigma_x' = -|\sigma_y|\sigma_x' = -\rangle \end{pmatrix}, \quad \text{where} \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \tag{1.48}$$

and

$$\bar{\sigma}_z = \begin{pmatrix} \langle\sigma_x' = +|\sigma_z|\sigma_x' = +\rangle & \langle\sigma_x' = +|\sigma_z|\sigma_x' = -\rangle \\ \langle\sigma_x' = -|\sigma_z|\sigma_x' = +\rangle & \langle\sigma_x' = -|\sigma_z|\sigma_x' = -\rangle \end{pmatrix}, \quad \text{where} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{1.49}$$

(d) Find the product of the last two matrices, $\bar{\sigma}_y\bar{\sigma}_z$, and express it in terms of $\bar{\sigma}_x$.

10. (**20 points.**) In the eigenbasis,

$$|\sigma'_y = +\rangle = \frac{e^{i\alpha_1}}{\sqrt{2}}\begin{pmatrix} i \\ -1 \end{pmatrix} \quad \text{and} \quad |\sigma'_y = -\rangle = \frac{e^{i\alpha_2}}{\sqrt{2}}\begin{pmatrix} i \\ 1 \end{pmatrix}, \tag{1.50}$$

of

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \tag{1.51}$$

where we included the arbitrariness in the phases as α_1 and α_2, the Pauli matrices are

$$\bar{\sigma}_x = \begin{pmatrix} 0 & -ie^{-i(\alpha_1-\alpha_2)} \\ ie^{i(\alpha_1-\alpha_2)} & 0 \end{pmatrix}, \tag{1.52a}$$

$$\bar{\sigma}_y = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{1.52b}$$

$$\bar{\sigma}_z = \begin{pmatrix} 0 & e^{-i(\alpha_1-\alpha_2)} \\ e^{i(\alpha_1-\alpha_2)} & 0 \end{pmatrix}. \tag{1.52c}$$

Thus, these representations of Pauli matrices depend on the arbitrary choice of phases. Do we loose the ability to predict the outcome of an experiment due to this arbitrariness? Verify that

$$\bar{\sigma}_x\bar{\sigma}_y = i\bar{\sigma}_z, \tag{1.53a}$$

$$\bar{\sigma}_y\bar{\sigma}_z = i\bar{\sigma}_x, \tag{1.53b}$$

$$\bar{\sigma}_z\bar{\sigma}_x = i\bar{\sigma}_y. \tag{1.53c}$$

Thus, the algebra of the Pauli matrices is independent of the arbitrariness in the phases. This will ensure that no measurable quantity depends on the choice of phases.

11. (**45 points.**) A particular representation of Pauli matrices is

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{1.54}$$

(In particular, these are Pauli matrices in the eigenbasis of σ_z.) Find the eigenvalues, normalized eigenvectors, and diagonalizing matrix, for each of the three Pauli matrix. Verify that your results satisfy the eigenvalue equation.

12. (**20 points.**) Construct the matrix

$$\boldsymbol{\sigma}\cdot\hat{\mathbf{r}}, \tag{1.55}$$

where

$$\boldsymbol{\sigma} = \sigma_x\hat{\mathbf{i}} + \sigma_y\hat{\mathbf{j}} + \sigma_z\hat{\mathbf{k}}, \tag{1.56}$$

$$\hat{\mathbf{r}} = \sin\theta\cos\phi\hat{\mathbf{i}} + \sin\theta\sin\phi\hat{\mathbf{j}} + \cos\theta\hat{\mathbf{k}}. \tag{1.57}$$

Use the following representation of Pauli matrices,

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{1.58}$$

Find the eigenvalues of the matrix $\boldsymbol{\sigma}\cdot\hat{\mathbf{r}}$.

13. (**20 points.**) The Pauli matrix
$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{1.59}$$
is written in the eigenbasis of
$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{1.60}$$
Write σ_x in the eigenbasis of
$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}. \tag{1.61}$$
Note that this representation has the arbitraryness of the choice of phase in the eigenvectors.

14. (**30 points.**) The Pauli matrices satisfy
$$\sigma_i \sigma_j = \delta_{ij} + i\varepsilon_{ijk}\sigma_k. \tag{1.62}$$
A particular representation of Pauli matrices is
$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{1.63}$$
In particular, these are Pauli matrices in the eigenbasis of σ_z.

(a) Construct the matrix
$$\sigma_{\theta,\phi} = \boldsymbol{\sigma} \cdot \hat{\mathbf{n}}(\theta, \phi) = \begin{pmatrix} \cos\theta & \sin\theta\, e^{-i\phi} \\ \sin\theta\, e^{i\phi} & -\cos\theta \end{pmatrix}, \tag{1.64}$$
where
$$\boldsymbol{\sigma} = \sigma_x \hat{\mathbf{i}} + \sigma_y \hat{\mathbf{j}} + \sigma_z \hat{\mathbf{k}}, \tag{1.65}$$
$$\hat{\mathbf{n}}(\theta, \phi) = \sin\theta\cos\phi \hat{\mathbf{i}} + \sin\theta\sin\phi \hat{\mathbf{j}} + \cos\theta \hat{\mathbf{k}}. \tag{1.66}$$
Find the eigenvalues $\sigma'_{\theta,\phi}$ and the normalized eigenvectors, $|\sigma'_{\theta,\phi} = +1\rangle$ and $|\sigma'_{\theta,\phi} = -1\rangle$, (up to a phase) of the matrix $\sigma_{\theta,\phi}$.

(b) Now compute the matrices
$$\bar{\sigma}_x = \begin{pmatrix} \langle\sigma'_{\theta,\phi} = +1|\sigma_x|\sigma'_{\theta,\phi} = +1\rangle & \langle\sigma'_{\theta,\phi} = +1|\sigma_x|\sigma'_{\theta,\phi} = -1\rangle \\ \langle\sigma'_{\theta,\phi} = -1|\sigma_x|\sigma'_{\theta,\phi} = +1\rangle & \langle\sigma'_{\theta,\phi} = -1|\sigma_x|\sigma'_{\theta,\phi} = -1\rangle \end{pmatrix}, \tag{1.67}$$
$$\bar{\sigma}_y = \begin{pmatrix} \langle\sigma'_{\theta,\phi} = +1|\sigma_y|\sigma'_{\theta,\phi} = +1\rangle & \langle\sigma'_{\theta,\phi} = +1|\sigma_y|\sigma'_{\theta,\phi} = -1\rangle \\ \langle\sigma'_{\theta,\phi} = -1|\sigma_y|\sigma'_{\theta,\phi} = +1\rangle & \langle\sigma'_{\theta,\phi} = -1|\sigma_y|\sigma'_{\theta,\phi} = -1\rangle \end{pmatrix}, \tag{1.68}$$
$$\bar{\sigma}_z = \begin{pmatrix} \langle\sigma'_{\theta,\phi} = +1|\sigma_z|\sigma'_{\theta,\phi} = +1\rangle & \langle\sigma'_{\theta,\phi} = +1|\sigma_z|\sigma'_{\theta,\phi} = -1\rangle \\ \langle\sigma'_{\theta,\phi} = -1|\sigma_z|\sigma'_{\theta,\phi} = +1\rangle & \langle\sigma'_{\theta,\phi} = -1|\sigma_z|\sigma'_{\theta,\phi} = -1\rangle \end{pmatrix}. \tag{1.69}$$
These matrices are representation of the Pauli matrices in the eigenbasis of $\sigma_{\theta,\phi}$.

(c) Show that
$$\bar{\sigma}_i \bar{\sigma}_j = \delta_{ij} + i\varepsilon_{ijk}\bar{\sigma}_k. \tag{1.70}$$

15. (**20 points.**) For operator σ that satisfies
$$\sigma^2 = 1 \tag{1.71}$$
show that the two states obtained using the construction
$$|\pm\rangle = \left(\frac{1 \pm \sigma}{2}\right) |\;\rangle \tag{1.72}$$
are eigenvectors of the operator σ. That is,
$$\sigma|\pm\rangle = \pm|\pm\rangle. \tag{1.73}$$
In the following, let us further assume σ to be Hermitian. Refer Dirac's QM book (4th edition, page 34).

(a) Show that

$$\left(\frac{1\pm\sigma}{2}\right)^2 = \left(\frac{1\pm\sigma}{2}\right). \tag{1.74}$$

(b) Show that for arbitrary non-zero $|\;\rangle$ we have

$$|\;\rangle = |+\rangle + |-\rangle. \tag{1.75}$$

Further, show that for arbitrary non-zero $|\;\rangle$ we have

$$\sigma|\;\rangle = |+\rangle - |-\rangle. \tag{1.76}$$

Also, show that

$$\langle\;|\;\rangle = \langle+|+\rangle + \langle-|-\rangle = 2, \tag{1.77a}$$

$$\langle\;|\sigma|\;\rangle = \langle+|+\rangle - \langle-|-\rangle = 0. \tag{1.77b}$$

(c) Show that these states orthogonal. That is,

$$\langle+|-\rangle = 0, \qquad \langle+|+\rangle = 1, \qquad \langle-|-\rangle = 1. \tag{1.78}$$

(d) Show that

$$\langle\;|\pm\rangle = 1, \qquad \langle\pm|\;\rangle = 1. \tag{1.79}$$

Using these verify that

$$\Big(|+\rangle\langle+| + |-\rangle\langle-|\Big)|\;\rangle = |\;\rangle, \tag{1.80a}$$

$$\langle\;|\Big(|+\rangle\langle+| + |-\rangle\langle-|\Big) = \langle\;|, \tag{1.80b}$$

and

$$\Big(|+\rangle\langle+| + |-\rangle\langle-|\Big)|\;\rangle\langle\;|\Big(|+\rangle\langle+| + |-\rangle\langle-|\Big) = |\;\rangle\langle\;|. \tag{1.81}$$

Thus, verify that these states form a complete set?

1.3 Unitary evolution using eigenbasis

1. (**20 points.**) Let $\mathbf{e}^i$, for $i = 1, 2$, be an eigenbasis set, such that

$$\mathbf{e}^1\mathbf{e}_1 + \mathbf{e}^2\mathbf{e}_2 = \mathbf{1}. \tag{1.82}$$

We have

$$\mathbf{e}_i = (\mathbf{e}^i)^\dagger. \tag{1.83}$$

Let $\mathbf{g}^i$, for $i = 1, 2$, be another eigenbasis set, such that

$$\mathbf{g}^1\mathbf{g}_1 + \mathbf{g}^2\mathbf{g}_2 = \mathbf{1}. \tag{1.84}$$

Using the above two eigenbases we can construct the operator

$$\mathbf{U} = \mathbf{g}^1\mathbf{e}_1 + \mathbf{g}^2\mathbf{e}_2. \tag{1.85}$$

Show that

$$\mathbf{U}\cdot\mathbf{e}^1 = \mathbf{g}^1, \tag{1.86a}$$

$$\mathbf{U}\cdot\mathbf{e}^2 = \mathbf{g}^2. \tag{1.86b}$$

Thus, the operator $\mathbf{U}$ is the transformation matrix taking us from the eigenbasis $\mathbf{e}^i$ to $\mathbf{g}^i$. What is the associated inverse transformation? To this end, using

$$(\mathbf{g}^i \cdot \mathbf{e}_j)^\dagger = \mathbf{e}_j^\dagger \cdot \mathbf{g}^{i\,\dagger} = \mathbf{e}^j \cdot \mathbf{g}_i \tag{1.87}$$

show that

$$\mathbf{U}^\dagger = \mathbf{e}^1\mathbf{g}_1 + \mathbf{e}^2\mathbf{g}_2, \tag{1.88}$$

and verify

$$\mathbf{U}^\dagger \cdot \mathbf{g}^1 = \mathbf{e}^1, \tag{1.89a}$$

$$\mathbf{U}^\dagger \cdot \mathbf{g}^2 = \mathbf{e}^2. \tag{1.89b}$$

Thus, $\mathbf{U}^\dagger$ is the inverse transformation matrix taking us from the eigenbasis $\mathbf{g}^i$ back to $\mathbf{e}^i$. Further, verify that

$$\mathbf{U}^\dagger \cdot \mathbf{U} = \mathbf{1}, \tag{1.90a}$$

$$\mathbf{U} \cdot \mathbf{U}^\dagger = \mathbf{1}, \tag{1.90b}$$

which states that $\mathbf{U}$ is an unitary operator. Repeat this for i running from 1 to 3. Does it go through? Repeat this for i running from 1 to n. Does it go through?

2. (**20 points.**) Given two eigenbases $\mathbf{e}^i$ and $\mathbf{g}^i$ we can construct an unitary operator

$$\mathbf{U} = \mathbf{g}^i\mathbf{e}_i. \tag{1.91}$$

A Schwinger periodic unitary operator is constructed by choosing the second eigenbasis $\mathbf{g}^i$ to be the same as the original eigenbasis set $\mathbf{e}^i$ but in a different order. That is,

$$\mathbf{g}^i = \begin{cases} \mathbf{e}^{i+1}, & \text{if} \quad i \neq n, \\ \mathbf{e}^1, & \text{if} \quad i = n, \end{cases} \tag{1.92}$$

such that the unitary operator is

$$\mathbf{U} = \mathbf{e}^{i+1}\mathbf{e}_i. \tag{1.93}$$

(a) Show that

$$\mathbf{U} \cdot \mathbf{e}^i = \begin{cases} \mathbf{e}^{i+1}, & \text{if} \quad i \neq n, \\ \mathbf{e}^1, & \text{if} \quad i = n. \end{cases} \tag{1.94}$$

Verify that the transformation is cyclic, that is,

$$\mathbf{U} \cdot \mathbf{e}^1 = \mathbf{e}^2, \tag{1.95a}$$

$$\mathbf{U}^2 \cdot \mathbf{e}^1 = \mathbf{e}^3, \tag{1.95b}$$

$$\vdots$$

$$\mathbf{U}^{n-1} \cdot \mathbf{e}^1 = \mathbf{e}^n, \tag{1.95c}$$

$$\mathbf{U}^n \cdot \mathbf{e}^1 = \mathbf{e}^1. \tag{1.95d}$$

The cyclic nature of the transformation of the eigenbasis is illustrated in Figure 1.1 and generated by the periodic unitary operator $\mathbf{U}$.

(b) Show that the periodic unitary operator satisfies

$$\mathbf{U}^n = \mathbf{1}, \tag{1.96}$$

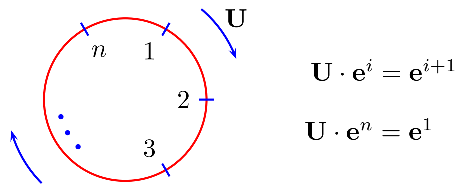

Figure 1.1: A periodic unitary operator.

where n is called the period of $\mathbf{U}$. Consider the eigenvalue equation

$$\mathbf{U}\cdot\mathbf{u}^k = u'_k\mathbf{u}^k, \qquad \text{no sum on } k. \tag{1.97}$$

The eigenvalues u'_k of the operator $\mathbf{U}$ satisfy

$$(u'_k)^n = 1, \tag{1.98}$$

where u'_k is the k-th eigenvalue, $k = 1, 2, \ldots, n$. An immediate observation, then, is that the eigenvalues are the n-th roots of unity,

$$u'_k = e^{i\frac{2\pi}{n}k}, \qquad k = 1, 2, \ldots, n. \tag{1.99}$$

To determine the eigenvectors $\mathbf{u}^k$ in the eigenbasis of $\mathbf{e}^i$ start by writing

$$\mathbf{u}^k = \mathbf{1}\cdot\mathbf{u}^k \tag{1.100a}$$

$$= \sum_{l=1}^{n}\mathbf{e}^l\mathbf{e}_l\cdot\mathbf{u}^k \tag{1.100b}$$

$$= \sum_{l=1}^{n}\mathbf{U}^l\cdot\mathbf{e}^n\,(\mathbf{e}_l\cdot\mathbf{u}^k). \tag{1.100c}$$

where we used

$$\mathbf{e}^l = \mathbf{U}^l\cdot\mathbf{e}^n. \tag{1.101}$$

Operating from the left leads to

$$\mathbf{u}_{\bar{k}}\cdot\mathbf{u}^k = \sum_{l=1}^{n}\mathbf{u}_{\bar{k}}\cdot\mathbf{U}^l\cdot\mathbf{e}^n\,(\mathbf{e}_l\cdot\mathbf{u}^k). \tag{1.102a}$$

Starting from the eigenvalue equation for $\mathbf{U}$, operate $\mathbf{U}^\dagger$ on both sides, deduce

$$\mathbf{U}^\dagger\cdot\mathbf{u}^k = (u'_k)^*\mathbf{u}^k, \qquad \text{no sum on } k, \tag{1.103}$$

which leads to the reciprocal statement

$$\mathbf{u}_k\cdot\mathbf{U} = u'_k\mathbf{u}_k, \qquad \text{no sum on } k. \tag{1.104}$$

Thus, we have

$$\mathbf{u}_k\cdot\mathbf{U}^l = e^{i\frac{2\pi}{n}kl}\mathbf{u}_k. \tag{1.105}$$

In conjunction with the orthogonality relations of the eigenvectors,

$$\mathbf{u}_{\bar{k}}\cdot\mathbf{u}^k = \delta_{\bar{k}}{}^k, \tag{1.106}$$

show that

$$\frac{\delta_{\bar{k}}{}^{k}}{(\mathbf{u}_{\bar{k}}\cdot\mathbf{e}^{n})}=\sum_{l=1}^{n}e^{i\frac{2\pi}{n}\bar{k}l}(\mathbf{e}_{l}\cdot\mathbf{u}^{k}). \tag{1.107}$$

Recognize the discrete Fourier transform in the above expression. Then, invert the equations to derive

$$(\mathbf{e}_{l}\cdot\mathbf{u}^{k})=\frac{1}{n}\frac{e^{-i\frac{2\pi}{n}kl}}{(\mathbf{u}_{k}\cdot\mathbf{e}^{n})}. \tag{1.108}$$

For $l=n$, we have

$$(\mathbf{e}_{l}\cdot\mathbf{u}^{k})(\mathbf{u}_{k}\cdot\mathbf{e}^{n})=\frac{1}{n}, \tag{1.109}$$

so that

$$(\mathbf{u}_{k}\cdot\mathbf{e}^{n})=\frac{1}{\sqrt{n}} \tag{1.110}$$

up to a phase, and

$$(\mathbf{e}_{l}\cdot\mathbf{u}^{k})=\frac{1}{\sqrt{n}}e^{-i\frac{2\pi}{n}kl}. \tag{1.111}$$

Thus, show that the eigenvectors $\mathbf{u}^{k}$ in the eigenbasis of $\mathbf{e}^{i}$ are given by

$$\mathbf{u}^{k}=\frac{1}{\sqrt{n}}\sum_{l=1}^{n}e^{-i\frac{2\pi}{n}kl}\mathbf{e}^{l}. \tag{1.112}$$

(c) Repeat the above exercise for another periodic operator constructed out of $\mathbf{u}^{i}$ in the form

$$\mathbf{V}=\mathbf{u}^{i}\mathbf{u}_{i+1}. \tag{1.113}$$

Show that

$$\mathbf{u}_{i}\cdot\mathbf{V}=\begin{cases}\mathbf{u}_{i+1}, & \text{if} \quad i\neq n,\\ \mathbf{u}_{1}, & \text{if} \quad i=n.\end{cases} \tag{1.114}$$

Repeat the steps that we carried out for $\mathbf{U}$ now for $\mathbf{V}$. Define the eigenvalue equation to act to the left, $\mathbf{v}_{k}\cdot\mathbf{V}=v_{k}'\mathbf{v}_{k}$. In particular, show that

$$\mathbf{V}^{n}=\mathbf{1}, \tag{1.115}$$

eigenvalues v_{k}' are given by

$$v_{k}'=e^{i\frac{2\pi}{n}k}, \qquad k=1,2,\ldots,n, \tag{1.116}$$

and the eigenvectors are

$$\mathbf{v}_{k}=\frac{1}{\sqrt{n}}\sum_{l=1}^{n}e^{-i\frac{2\pi}{n}kl}\mathbf{u}_{k}. \tag{1.117}$$

(d) Show that

$$\mathbf{v}^{i}=\mathbf{e}^{i}. \tag{1.118}$$

Thus, recognize that the eigenvectors of the periodic operators $\mathbf{U}$ and $\mathbf{V}$ are related to each other by discrete Fourier transformation,

$$\mathbf{u}^{k}=\frac{1}{\sqrt{n}}\sum_{l=1}^{n}e^{-i\frac{2\pi}{n}kl}\mathbf{v}^{l}, \tag{1.119a}$$

$$\mathbf{v}^{l}=\frac{1}{\sqrt{n}}\sum_{k=1}^{n}e^{i\frac{2\pi}{n}kl}\mathbf{u}^{k}. \tag{1.119b}$$

(e) Verify that

$$\mathbf{U}\cdot\mathbf{V}\cdot\mathbf{v}^k = \mathbf{v}^{k+1} e^{i\frac{2\pi}{n}k} \tag{1.120}$$

and

$$\mathbf{V}\cdot\mathbf{U}\cdot\mathbf{v}^k = \mathbf{v}^{k+1} e^{i\frac{2\pi}{n}(k+1)}. \tag{1.121}$$

Thus, derive

$$\mathbf{U}\cdot\mathbf{V} = e^{i\frac{2\pi}{n}}\mathbf{V}\cdot\mathbf{U}. \tag{1.122}$$

(f) For $n = 2$ we have

$$\mathbf{U}^2 = \mathbf{1}, \qquad \mathbf{V}^2 = \mathbf{1}, \quad \text{and} \quad \mathbf{U}\cdot\mathbf{V} = -\mathbf{V}\cdot\mathbf{U}. \tag{1.123}$$

These constitute four independent operators, $\mathbf{1}$, $\mathbf{U}$, $\mathbf{V}$, and $\mathbf{U}\cdot\mathbf{V}$, which have the same algebra as that of 1, σ_x, σ_y, and σ_z.

3. (**20 points.**) Consider an operator U that is defined using the following operations,

$$U|a_1\rangle = |a_2\rangle, \tag{1.124a}$$
$$U|a_2\rangle = |a_3\rangle, \tag{1.124b}$$
$$U|a_3\rangle = |a_1\rangle. \tag{1.124c}$$

Find the eigenvalues of the operator U.

1.4 Linear vector space over a complex field

1. (**Adjoint operator.**) The adjoint of an operator A, denoted by

$$A^\dagger, \tag{1.125}$$

is defined by the relation, for arbitrary two states $|1\rangle$ and $|2\rangle$,

$$\langle 1|\Big(A|2\rangle\Big) = \Big(\langle 1|A^\dagger\Big)|2\rangle. \tag{1.126}$$

2. (**Hermitian operator.**) A self-adjoint, or a Hermitian, operator is one for which

$$A^\dagger = A. \tag{1.127}$$

That is, for arbitrary two states $|1\rangle$ and $|2\rangle$,

$$\langle 1|\Big(A|2\rangle\Big) = \Big(\langle 1|A\Big)|2\rangle. \tag{1.128}$$

3. (**20 points.**) Prove that if A is Hermitian,

$$A = A^\dagger, \tag{1.129}$$

then, $\langle\ |A|\ \rangle$, for an arbitrary state $|\ \rangle$, is real.
Hint: An Hermitian operator has real eigenvalues A'_i. Thus, we have

$$\langle\ |A|\ \rangle = \langle\ |\left(\sum_i |A'_i\rangle\langle A'_i|\right) A \left(\sum_j |A'_j\rangle\langle A'_j|\right)|\ \rangle \tag{1.130a}$$

$$= \sum_i A'_i |\langle A'_i|\ \rangle|^2. \tag{1.130b}$$

4. (**20 points.**) The projection operator that projects a state $|\ \rangle$ into $|1\rangle$ is defined as

$$P_1 = \frac{|1\rangle\langle 1|}{\langle 1|1\rangle}, \tag{1.131}$$

with the operation

$$P_1|\ \rangle = |1\rangle \frac{\langle 1|\ \rangle}{\langle 1|1\rangle}. \tag{1.132}$$

Show that P_1 is a Hermitian operator. That is, show that, for arbitrary two states $|2\rangle$ and $|3\rangle$,

$$\langle 3|\Big(P_1|2\rangle\Big) = \Big(\langle 3|P_1\Big)|2\rangle. \tag{1.133}$$

5. (**20 points.**) The momentum operator $\mathbf{p}$ is a Hermitian operator. That is, $\mathbf{p}^\dagger = \mathbf{p}$. When the system is described by the state vector $|\ \rangle$, the expectation value of the momentum operator is given by

$$\mathbf{u_p} = \langle\ |\mathbf{p}|\ \rangle. \tag{1.134}$$

In the position-basis we have

$$\mathbf{u_p} = \int d^3x' \langle\ |\mathbf{x}'\rangle\langle \mathbf{x}'|\mathbf{p}|\ \rangle = \int d^3x' \psi^*(\mathbf{x}') \frac{\hbar}{i} \boldsymbol{\nabla}\psi(\mathbf{x}'), \tag{1.135}$$

where the wavefunction $\psi(\mathbf{x}') = \langle\ |\mathbf{x}'\rangle$ is the projection of the state vector in the position-basis. Using the position-basis representation of $\mathbf{u_p}$ given by the second equality in Eq. (1.135) show that

$$\mathbf{u_p}^* = \mathbf{u_p}. \tag{1.136}$$

(Hint: Use integration by parts.)

The orbital angular momentum is given by the operator construction

$$\mathbf{L} = \mathbf{r} \times \mathbf{p} \tag{1.137}$$

in terms of the position operator $\mathbf{r}$ and the momentum operator $\mathbf{p}$, each being Hermitian. Show that orbital angular momentum is Hermitian. That is, $\mathbf{L}^\dagger = \mathbf{L}$. The expectation value of the angular momentum, in the position-basis representation, is given by

$$\mathbf{u_L} = \int d^3x' \psi^*(\mathbf{x}') \frac{\hbar}{i} (\mathbf{r} \times \boldsymbol{\nabla})\psi(\mathbf{x}'). \tag{1.138}$$

Show that

$$\mathbf{u_L}^* = \mathbf{u_L}. \tag{1.139}$$

6. *Refer Schwinger lecture notes for more problems. They need to recasted using the Dirac notation.* (**20 points.**) The requirement for an operator to be unitary is

$$(A\psi, A\psi) = (\psi, \psi) \tag{1.140}$$

for any ψ. Show that this implies

$$(A\phi, A\psi) = (\phi, \psi). \tag{1.141}$$

1.5 Linear transformation on a vector space

Problems

1. (**40 points.**) A unitary matrix is defined by

$$U^\dagger U = 1, \tag{1.142}$$

where † stands for transpose and complex conjugation.

(a) Show that

$$U = e^{iH} \tag{1.143}$$

is unitary if H is Hermitian, that is $H^\dagger = H$.

(b) Show that

$$U = \frac{1+iA}{1-iA} \tag{1.144}$$

is unitary if A is Hermitian.

(c) Using

$$\tan^{-1} A = \frac{i}{2} \ln \left(\frac{1-iA}{1+iA} \right) \tag{1.145}$$

show that

$$H = 2\tan^{-1} A. \tag{1.146}$$

(d) Show that

$$U = \frac{1-iB}{1+iB} \tag{1.147}$$

is unitary if B is Hermitian.

2. (**20 points.**) Show that the combination $X^\dagger X$ is Hermitian, irrespective of X being Hermitian. Use this to deduce that the eigenvalues of $X^\dagger X$ are non-negative.

3. (**20 points.**) Prove that Hermitian operators have real eigenvalues. Further, show that any two eigenfunctions belonging to distinct (unequal) eigenvalues of a Hermitian operator are mutually orthogonal.

4. (**10 points.**) A is a matrix with eigenvalues $a_1, a_2, \ldots$, such that

$$\text{tr} A = \sum_i a_i, \tag{1.148}$$

exists. Prove that, for a function f,

$$\text{tr} f(A) = \sum_i f(a_i). \tag{1.149}$$

Chapter 2

Measurement algebra

2.1 Stern-Gerlach experiment

Problems

2.1.1 Stern Gerlach experiment

1. (**20 points.**) (Ref: Milton's notes.) The energy of a charge e moving with velocity $\mathbf{v}$ in an external electromagnetic field is

$$E = e\phi - \frac{e}{c}\mathbf{v}\cdot\mathbf{A}, \tag{2.1}$$

where ϕ is the scalar potential and $\mathbf{A}$ is the vector potential. The relation between $\mathbf{A}$ and the magnetic field $\mathbf{H}$ is

$$\mathbf{H} = \boldsymbol{\nabla}\times\mathbf{A}. \tag{2.2}$$

For a constant (homogenous in space) magnetic field $\mathbf{H}$, verify that

$$\mathbf{A} = \frac{1}{2}\mathbf{H}\times\mathbf{r} \tag{2.3}$$

is a possible vector potential. Then, by looking at the energy, identify the magnetic moment $\boldsymbol{\mu}$ of the moving charge.

2. (**20 points.**) Consider an atom entering a Stern-Gerlach apparatus. Deflection upward begins as soon as the atom enters the inhomogeneous field. By the time the atom leaves the field, it has been deflected upward by a net amount Δz. Compute Δz for

$$\mu_z = 10^{-27}\frac{\mathrm{J}}{\mathrm{G}}, \quad \frac{\partial H_z}{\partial z} = 10^6\frac{\mathrm{G}}{\mathrm{m}}, \quad l = 10\,\mathrm{cm}, \quad \frac{1}{2}mv_x^2 = kT, \quad T = 10^3\,\mathrm{K}. \tag{2.4}$$

3. (**20 points.**) (Ref: Milton's notes.) A silver atom has mass (actually the stable isotopes are Ag^{107}, Ag^{109})

$$m = 108\times 1.67\times 10^{-27}\,\mathrm{kg}, \tag{2.5}$$

and speed

$$v = 10^2\,\mathrm{m/s}. \tag{2.6}$$

Compute the reduced de Broglie wavelength, $\lambdabar$, and the corresponding diffraction angle $\delta\theta$ when a beam of such atoms passes through a slit of width $10^{-2}\,\mathrm{cm}$. (See Fig. 3.3 in Milton's notes and discussion of Eq. (3.26) there.) Compare this diffraction angle with the deflection angle produced in a Stern-Gerlach experiment.

2.1.2 Probabilities

4. (**20 points.**) Using the notation for the probability for a measurement in the Stern-Gerlach experiment, introduced in the class, show that

$$p\big([+;\theta_1,\phi_1] \to [-;\theta_2,\phi_2]\big) = \frac{1-\cos\Theta}{2}, \tag{2.7}$$

where

$$\cos\Theta = \cos\theta_1\cos\theta_2 + \sin\theta_1\sin\theta_2\cos(\phi_1-\phi_2). \tag{2.8}$$

5. (**20 points.**) The probabilities in a series setup of Stern-Gerlach experiment can be described using the notation

$$p([A=a'] \to [B=b'] \to [C=c']), \tag{2.9}$$

where $[A=a']$ denotes the selection of the beam corresponding to the eigenvalue a'. For spin-$\frac{1}{2}$ the operators A, B, and C, are given by $\boldsymbol{\sigma}\cdot\hat{\mathbf{n}}$, where $\hat{\mathbf{n}}$ is the direction of the magnetic field. Connecting with the notation introduced in class, we have, for example, $[\sigma_x=+1]=[+;\theta=\frac{\pi}{2},\phi=0]$. Show that

$$p([A=a'] \to [B=b'] \to [C=c']) = p([A=a'] \to [B=b'])p([B=b'] \to [C=c']). \tag{2.10}$$

6. (**20 points.**) Using the notation for the probability for a measurement in the Stern-Gerlach experiment, introduced in the class, evaluate

$$p\left([+;0,0] \to [+;\frac{\pi}{2},0] \to [+;\frac{\pi}{2},\frac{\pi}{2}] \to [+;0,0]\right), \tag{2.11}$$

which is also written as

$$p\left([\sigma_z=+1] \to [\sigma_x=+1] \to [\sigma_y=+1] \to [\sigma_z=+1]\right). \tag{2.12}$$

7. (**20 points.**) The eigenvectors for the Stern-Gerlach Hamiltonian are

$$|+;\theta,\phi\rangle = \begin{pmatrix} \cos\frac{\theta}{2}\,e^{-i\frac{\phi}{2}} \\ \sin\frac{\theta}{2}\,e^{i\frac{\phi}{2}} \end{pmatrix} \quad\text{and}\quad |-;\theta,\phi\rangle = \begin{pmatrix} -\sin\frac{\theta}{2}\,e^{-i\frac{\phi}{2}} \\ \cos\frac{\theta}{2}\,e^{i\frac{\phi}{2}} \end{pmatrix}. \tag{2.13}$$

   (a) Show that $|-;\pi-\theta,\phi+\pi\rangle = |+;\theta,\phi\rangle$, up to a phase.

   (b) What is the physical interpretation?

8. (**20 points.**) The eigenvectors for the Stern-Gerlach Hamiltonian, choosing $\phi=0$, are

$$|+;\theta\rangle = \begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2} \end{pmatrix} \quad\text{and}\quad |-;\theta\rangle = \begin{pmatrix} -\sin\frac{\theta}{2} \\ \cos\frac{\theta}{2} \end{pmatrix}. \tag{2.14}$$

Also, we have

$$|+;\theta\rangle\langle+;\theta| = \frac{1}{2}\begin{pmatrix} 1+\cos\theta & \sin\theta \\ \sin\theta & 1-\cos\theta \end{pmatrix} \quad\text{and}\quad |-;\theta\rangle\langle-;\theta| = \frac{1}{2}\begin{pmatrix} 1-\cos\theta & -\sin\theta \\ -\sin\theta & 1+\cos\theta \end{pmatrix}. \tag{2.15}$$

Using the notation for the probability for a measurement in the Stern-Gerlach experiment, introduced in the class, evaluate

$$p\big([+;0] \to [-;\frac{\pi}{3}] \to [+;0]\big). \tag{2.16}$$

2.1.3 Interference

9. (**20 points.**) Show that
$$p\big([+;0,0] \to [+;\pi,0]\big) = 0. \tag{2.17}$$
Further, show that
$$p\big([+;0,0] \to [\pm;\theta,\phi] \to [+;\pi,0]\big) = 0, \tag{2.18}$$
which is a statement of destructive interference. Compare this with the probability for
$$p\big([+;0,0] \to [+;\theta,\phi] \to [+;\pi,0]\big) \tag{2.19}$$
and
$$p\big([+;0,0] \to [-;\theta,\phi] \to [+;\pi,0]\big). \tag{2.20}$$

10. (**20 points.**) Show that
$$p\big([+;0,0] \to [-;\pi,0]\big) = 1. \tag{2.21}$$
Further, show that
$$p\big([+;0,0] \to [\pm;\theta,\phi] \to [-;\pi,0]\big) = 1, \tag{2.22}$$
which is a statement of constructive interference. Compare this with the probability for
$$p\big([+;0,0] \to [+;\theta,\phi] \to [-;\pi,0]\big) \tag{2.23}$$
and
$$p\big([+;0,0] \to [-;\theta,\phi] \to [-;\pi,0]\big). \tag{2.24}$$

2.1.4 Measurement disturbs the system

11. (**20 points.**) Let us temporarily write θ for $[+;\theta,0]$, where the supression of information will not have a consequence because we shall always select the + beam and always have $\phi = 0$. Thus, for example, we shall denote $p_2 = p(0,\pi/2,\pi) = p([+;0,0] \to [+;\pi/2,0]) \to [+;\pi,0])$. Show that
$$p_1 = p(0,\pi) = p([+;0,0] \to [+;\pi,0]) = 0. \tag{2.25}$$
A measurement disturbs the system. More measurements disturb the system further more. As the number of intermediate measurement increases, the original null probably approaches the opposite limit of 1.

    (a) Show that
$$p_2 = p(0,\pi/2,\pi) = \left(\cos\frac{\pi}{2\times 2}\right)^{2\times 2} \sim 0.25, \tag{2.26}$$
$$p_3 = p(0,\frac{\pi}{3},2\frac{\pi}{3},\pi) = \left(\cos\frac{\pi}{2\times 3}\right)^{2\times 3} \sim 0.42, \tag{2.27}$$
$$p_4 = p(0,\frac{\pi}{4},2\frac{\pi}{4},3\frac{\pi}{4},\pi) = \left(\cos\frac{\pi}{2\times 4}\right)^{2\times 4} \sim 0.53, \tag{2.28}$$
$$p_5 = p(0,\frac{\pi}{4},2\frac{\pi}{5},3\frac{\pi}{5},4\frac{\pi}{5},\pi) = \left(\cos\frac{\pi}{2\times 5}\right)^{2\times 5} \sim 0.61. \tag{2.29}$$

    (b) The sequence is rather slowly converging to 1. Show that
$$p_{100} \sim 0.98. \tag{2.30}$$

    (c) Show that
$$p_n = p(0,\frac{\pi}{n},\ldots,\pi) = \left(\cos\frac{\pi}{2n}\right)^{2n}. \tag{2.31}$$

    (d) Show that
$$\lim_{n\to\infty} p_n = 1. \tag{2.32}$$

2.1.5 Operator forms

12. (**20 points.**) Using the properties of Pauli matrices,

$$\sigma_i \sigma_j = \delta_{ij} + i\varepsilon_{ijk}\sigma_k, \tag{2.33}$$

and the Euler formula

$$e^{ix} = \cos x + i \sin x, \tag{2.34}$$

evaluate

$$e^{-i\theta\frac{\sigma_x}{2}} \sigma_y e^{i\theta\frac{\sigma_x}{2}}. \tag{2.35}$$

(Hint: Use series expansion for the trignometric functions.) What is the physical interpretation of this operation?

13. (**20 points.**) The probability for a measurement in the Stern-Gerlach experiment is given by

$$p\big([+;\theta_1,\phi_1] \to [\pm;\theta_2,\phi_2]\big) = \frac{1 \pm \cos\Theta}{2}, \tag{2.36}$$

where

$$\cos\Theta = \cos\theta_1 \cos\theta_2 + \sin\theta_1 \sin\theta_2 \cos(\phi_1 - \phi_2). \tag{2.37}$$

Verify that

$$\text{tr}\left(\frac{1 + \boldsymbol{\sigma}\cdot\hat{\mathbf{n}}(\theta_1,\phi_1)}{2}\right)\left(\frac{1 \pm \boldsymbol{\sigma}\cdot\hat{\mathbf{n}}(\theta_2,\phi_2)}{2}\right) = \frac{1 \pm \cos\Theta}{2}. \tag{2.38}$$

14. (**20 points.**) The probabilities in a series setup of Stern-Gerlach experiment, for spin-$\frac{1}{2}$, is given by

$$p([A = a'] \to [B = b'] \to [C = c']) = \text{tr}\left(\frac{1 + a'A}{2}\right)\left(\frac{1 + b'B}{2}\right) \text{tr}\left(\frac{1 + b'B}{2}\right)\left(\frac{1 + c'C}{2}\right), \tag{2.39}$$

where $[A = a']$ denotes the selection of the beam corresponding to the eigenvalue a'. Find the following probabilities:

(a) $p([\sigma_x = +1] \to [\sigma_x = +1])$

(b) $p([\sigma_x = +1] \to [\sigma_y = +1] \to [\sigma_x = +1])$

2.2 Complementary variables

1. (**20 points.**) The probabilities in a series setup of Stern-Gerlach experiment can be described using the notation

$$p([A = a'] \to [B = b'] \to [C = c']), \tag{2.40}$$

where $[A = a']$ denotes the selection of the beam corresponding to the eigenvalue a'. For spin-$\frac{1}{2}$ the operators A, B, and C, are given by $\boldsymbol{\sigma}\cdot\hat{\mathbf{n}}$, where $\hat{\mathbf{n}}$ is the direction of the magnetic field. Connecting with the notation introduced in class, we have, for example, $[\sigma_x = +1] = [+;\theta = \frac{\pi}{2}, \phi = 0]$.

(a) Verify the following probabilities:

$$p([\sigma_x = +1] \to [\sigma_x = +1]) = 1, \tag{2.41a}$$

$$p([\sigma_x = +1] \to [\sigma_y = +1] \to [\sigma_x = +1]) = \frac{1}{4}, \tag{2.41b}$$

$$p([\sigma_x = +1] \to [\sigma_y = +1] \to [\sigma_x = -1]) = \frac{1}{4}, \tag{2.41c}$$

$$p([\sigma_x = +1] \to [\sigma_y = -1] \to [\sigma_x = +1]) = \frac{1}{4}, \tag{2.41d}$$

$$p([\sigma_x = +1] \to [\sigma_y = -1] \to [\sigma_x = -1]) = \frac{1}{4}. \tag{2.41e}$$

Does the measurement of σ_y *completely* wipe out the prior knowledge of the measurement of σ_x? If yes, why? If no, why not? (Hint: Argue that the measurement of σ_y has completely randomized the information content of σ_x, and thus wiped out the prior knowledge of the measurement of σ_x.) Are σ_x and σ_y complementary?

(b) An experiment is capable of measuring the following six physical variables:

$$J_x, J_y, J_z, J_x^2, J_y^2, J_z^2, \tag{2.42}$$

where

$$\mathbf{J} = \frac{\hbar}{2}\boldsymbol{\sigma}. \tag{2.43}$$

Out of the 15 distinct pairs of variables above, list the pairs that can be measured simultaneously. That is, list those for which the measurement of one variable in a pair does not disturb the measurement of the other–the measurements are compatible.

(c) Are the remaining pairs in the list complementary sets? Remember, complementary variables have optimal incompatibility. Complementary variables are pairs that are needed to describe the system, but the measurement of one variable completely (and maximally) wipes out the prior knowledge of the other.

2. (**20 points.**) For a positive integer n the equation

$$(u_k')^n = 1 \tag{2.44}$$

is satisfied by n roots of unity,

$$u_k' = e^{i\frac{2\pi}{n}k}, \qquad k = 1, 2, \ldots, n. \tag{2.45}$$

Using the periodicity property show that $u_{n+l}' = u_l'$, for positive integer $l \leq n$. The n-th roots of unity satisfy

$$\sum_{k=1}^{n} u_k' = 0 \tag{2.46}$$

and, for integer r,

$$\frac{1}{n}\sum_{k=1}^{n}(u_k')^r = \begin{cases} 1 & \text{for} \quad r = 0, n, 2n, \ldots, \\ 0 & \text{otherwise.} \end{cases} \tag{2.47}$$

3. (**20 points.**) An eigenbasis that spans an n-dimensional space consists of eigenvectors $\hat{\mathbf{e}}_i$, where $i = 1, 2, \ldots, n$. These eigenvectors have n components that can be indexed using $a, b = 1, 2, \ldots, n$. That is, $\hat{\mathbf{e}}_i = \mathrm{e}_i^a$. Thus, using Einstein summation convention, the orthonormality conditions can be stated as

$$\hat{\mathbf{e}}_i^\dagger \cdot \hat{\mathbf{e}}_j = \delta_{ij}, \qquad \text{or} \qquad \mathrm{e}_i^{a\dagger}\mathrm{e}_j^a = \delta_{ij}, \tag{2.48}$$

and the completeness relation can be stated as

$$\hat{\mathbf{e}}_1\hat{\mathbf{e}}_1^\dagger + \ldots + \hat{\mathbf{e}}_n\hat{\mathbf{e}}_n^\dagger = \mathbf{1}, \qquad \text{or} \qquad \mathrm{e}_i^a\mathrm{e}_i^{b\dagger} = \delta^{ab}. \tag{2.49}$$

In this spirit, consider the following eigenbasis, constructed using n-th roots of unity,

$$\mathrm{e}_k^l = \frac{1}{\sqrt{n}}(u_k')^l = \frac{1}{\sqrt{n}}e^{i\frac{2\pi}{n}kl}, \qquad k, l = 1, 2, \ldots, n. \tag{2.50}$$

Show that

$$\sum_{k=1}^{n} e^{i\frac{2\pi}{n}k(l-l')} = n\,\delta_{ll'}, \tag{2.51}$$

and using this relation verify that the eigenbasis satisfies the completeness and orthonormality relations. For $n = 2$, the eigenvectors are

$$\hat{\mathbf{e}}_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} -1 \\ 1 \end{pmatrix}, \qquad \hat{\mathbf{e}}_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}. \tag{2.52}$$

Show that these eigenvectors satisfy the orthonormality and completeness relations. Determine the eigenvectors for $n = 3$ and verify the corresponding completeness and orthonormality relations. Caution: Do not forget the complex conjugation.
Solution:

$$\hat{\mathbf{e}}_1 = \frac{1}{\sqrt{3}} \begin{pmatrix} u_1' \\ u_2' \\ 1 \end{pmatrix}, \qquad \hat{\mathbf{e}}_2 = \frac{1}{\sqrt{3}} \begin{pmatrix} u_2' \\ u_1' \\ 1 \end{pmatrix}, \qquad \hat{\mathbf{e}}_3 = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}. \tag{2.53}$$

4. (**20 points.**) An n-dimensional vector $\mathbf{r}$ can be expressed in the following way

$$\mathbf{r} = \mathbf{1} \cdot \mathbf{r} = \sum_{k=1}^{n} \hat{\mathbf{e}}_k \, (\hat{\mathbf{e}}_k^\dagger \cdot \mathbf{r}) = \sum_{k=1}^{n} \hat{\mathbf{e}}_k \, \tilde{r}_k, \tag{2.54}$$

where $\tilde{r}_k = (\hat{\mathbf{e}}_k^\dagger \cdot \mathbf{r})$. Then, indexing the components of the vectors $\mathbf{r}$ and $\hat{\mathbf{e}}_k$ we have

$$r_l = \frac{1}{\sqrt{n}} \sum_{k=1}^{n} e^{i\frac{2\pi}{n}kl} \, \tilde{r}_k, \tag{2.55}$$

which can be inverted to give

$$\tilde{r}_k = \frac{1}{\sqrt{n}} \sum_{l=1}^{n} e^{-i\frac{2\pi}{n}kl} \, r_k. \tag{2.56}$$

5. (**20 points.**) Prove that, upto a phase,

$$\langle v_l' | u_k' \rangle = \frac{1}{\sqrt{n}} e^{-i\frac{2\pi}{n}kl}. \tag{2.57}$$

6. (**20 points.**) Show that the action of a unitary operator U on a function $f(A)$, where A is an operator, satisfies

$$U f(A) U^{-1} = f(U A U^{-1}). \tag{2.58}$$

Problems

1. (**20 points.**) Consider an operator U that produces the same set of a vectors but in different order, as produced by numbering them: $a_1, a_2, \ldots, a_n$, and then, cyclically permuting them. That is,

$$U|a_k\rangle = |a_{k+1}\rangle, \qquad \text{for } k \neq n, \tag{2.59}$$

$$U|a_n\rangle = |a_1\rangle. \tag{2.60}$$

Find the eigenvalues of the operator U.
Hint: We have the simplest example of this in σ_x:

$$\sigma_x|-\rangle = |+\rangle, \qquad \sigma_x|+\rangle = |-\rangle. \tag{2.61}$$

In this example, repetition gives unity, $\sigma_x^2 = 1$.

2. (**20 points.**) Show that, for integer $n > 0$,

$$z^n - 1 = (z - 1)(1 + z + z^2 + \ldots + z^{n-1}). \tag{2.62}$$

If z's are the n-th roots of unity,

$$z^n = 1, \tag{2.63}$$

with u'_k being the roots,

$$u'_k = e^{i\frac{2\pi}{n}k}, \quad k = 1, 2, \ldots, n, \tag{2.64}$$

show that

$$z^n - 1 = \left(\frac{z}{u'_k}\right)^n - 1 = \left(\frac{z}{u'_k} - 1\right)\left[1 + \left(\frac{z}{u'_k}\right) + \left(\frac{z}{u'_k}\right)^2 + \ldots + \left(\frac{z}{u'_k}\right)^{n-1}\right]. \tag{2.65}$$

3. (**20 points.**) In terms of the eigenvectors of the complementary variables, U and V, introduced in class, evaluate

$$\sum_{k=1}^{n} \langle v'_l | u'_k \rangle \langle u'_k | v'_m \rangle. \tag{2.66}$$

Thus, derive

$$\sum_{k=1}^{n} e^{i\frac{2\pi}{n}k(m-l)} = n\delta_{lm}. \tag{2.67}$$

(a) What do you learn about the n-th roots of unity from this relation?

(b) For, n=7, verify the (seven) relations after setting $l = n$.

(c) (Optional. Will not be graded.) Muse on the connection of the above relation with Ramanujan's sum.

(d) (Optional. Will not be graded.) Muse on the connection of the above relation with the discussion on 'Constructible polygons' in Wikipedia.

Chapter 3

Uncertainty states

3.1 Notation

- $|\ \rangle$: State vector describing the state of a system.
- A, a: Measurable quantities, in general an operator.
- A', a': Eigenvalues.
- $|A'\rangle$, $|a'\rangle$: Eigenvectors.
- $\langle A'|\ \rangle$: Wavefunction, describing the state of the system in the eigenbasis of operator A.

3.2 Intrinsic uncertainty in position and momentum

3.3 Heisenberg's uncertainty relation

1. (**60 points.**) Let A and B be Hermitian operators. Consider the expectation or average values of A and B in the physical state $|\ \rangle$,

$$\langle A\rangle = \langle\ |A|\ \rangle, \qquad \langle B\rangle = \langle\ |B|\ \rangle, \tag{3.1}$$

and the mean square deviation from these averages,

$$(\delta A)^2 = \langle\ |(A-\langle A\rangle)^2|\ \rangle \equiv \langle 1|1\rangle, \tag{3.2}$$

$$(\delta B)^2 = \langle\ |(B-\langle B\rangle)^2|\ \rangle \equiv \langle 2|2\rangle, \tag{3.3}$$

where

$$\langle 1| = \langle\ |(A-\langle A\rangle), \qquad |2\rangle = (B-\langle B\rangle)|\ \rangle, \tag{3.4}$$

(a) (Prove the Schwarz inequality.) Use the Schwarz inequality to learn

$$(\delta A)^2(\delta B)^2 = \langle 1|1\rangle\langle 2|2\rangle \geq |\langle 1|2\rangle|^2, \tag{3.5}$$

where the equal sign applies only when $|1\rangle$ is parallel to $|2\rangle$.

(b) Show that the antisymmetric product of two Hermitian operators X and Y,

$$C = \frac{1}{i}(XY - YX) = \frac{1}{i}\big[X, Y\big], \tag{3.6}$$

is also Hermitian, that is, $C^\dagger = C$. Further, show that the symmetric construction,

$$(XY + YX) = \big\{X, Y\big\}, \tag{3.7}$$

is also Hermitian. Thus, the product XY, which is not Hermitian, can be expressed as a combination of two Hermitian operators,

$$XY = \frac{1}{2}(XY + YX) + \frac{i}{2}C. \tag{3.8}$$

Remember that the expectation values of Hermitian operators are real.

(c) Let

$$X = A - \langle A \rangle, \qquad Y = B - \langle B \rangle. \tag{3.9}$$

Thus, derive

$$|\langle \,|(XY)|\, \rangle|^2 = \frac{1}{4}|\langle \,|(XY + YX)|\, \rangle|^2 + \frac{1}{4}|\langle \,|C|\, \rangle|^2. \tag{3.10}$$

(d) Using Eq. (3.10) in Eq. (3.5) derive Robertson's generalization of Heisenberg's uncertainty relation

$$(\delta A)(\delta B) \geq \frac{1}{2}|\langle C \rangle|. \tag{3.11}$$

(e) Apply this to the pairs $(A, B) = (q, p)$ and $(A, B) = (\sigma_x, \sigma_y)$.

3.4 Uncertainty relation for angular momentum

1. (**60 points.**) Consider a normalized state

$$|\,\rangle = \begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} x_1 + i x_2 \\ y_1 + i y_2 \end{pmatrix}, \qquad |u|^2 + |v|^2 = 1. \tag{3.12}$$

(a) Show that the expectation value of the Pauli matrices with respect to the above state satisfies

$$\langle \sigma_x \rangle^2 + \langle \sigma_y \rangle^2 + \langle \sigma_z \rangle^2 = 1. \tag{3.13}$$

Thus, conclude that the magnitude of the expectation value of each of the Pauli matrix is less than or equal to unity.

(b) Define the errors in the measurement of the Pauli matrices to be

$$(\delta\sigma'_x)^2 = \langle \,|\big\{\sigma_x - \langle \sigma_x \rangle\big\}^2|\, \rangle, \tag{3.14a}$$
$$(\delta\sigma'_y)^2 = \langle \,|\big\{\sigma_y - \langle \sigma_y \rangle\big\}^2|\, \rangle, \tag{3.14b}$$
$$(\delta\sigma'_z)^2 = \langle \,|\big\{\sigma_z - \langle \sigma_z \rangle\big\}^2|\, \rangle. \tag{3.14c}$$

Show that

$$(\delta\sigma'_x)^2 = 1 - \langle \sigma_x \rangle^2, \tag{3.15a}$$
$$(\delta\sigma'_y)^2 = 1 - \langle \sigma_y \rangle^2, \tag{3.15b}$$
$$(\delta\sigma'_z)^2 = 1 - \langle \sigma_z \rangle^2. \tag{3.15c}$$

Thus, conclude that the errors in the measurement of each of the Pauli matrix is less than or equal to unity. Show that

$$(\delta\sigma'_x)^2 + (\delta\sigma'_y)^2 + (\delta\sigma'_z)^2 = 2. \tag{3.16}$$

(c) Using Robertson's generalization of Heisenberg's uncertainty relation

$$(\delta A)(\delta B) \geq \frac{1}{2}|\langle C \rangle|, \qquad C = \frac{1}{i}\big[A, B\big], \tag{3.17}$$

deduce the uncertainty relations for the Pauli matrices to be

$$(\delta\sigma'_x)^2(\delta\sigma'_y)^2 \geq \langle\sigma_z\rangle^2, \tag{3.18a}$$
$$(\delta\sigma'_y)^2(\delta\sigma'_z)^2 \geq \langle\sigma_x\rangle^2, \tag{3.18b}$$
$$(\delta\sigma'_z)^2(\delta\sigma'_x)^2 \geq \langle\sigma_y\rangle^2. \tag{3.18c}$$

Combine these uncertainty relations to derive an uncertainty relation involving all the three Pauli matrices,

$$(\delta\sigma'_x)^2(\delta\sigma'_y)^2 + (\delta\sigma'_y)^2(\delta\sigma'_z)^2 + (\delta\sigma'_z)^2(\delta\sigma'_x)^2 \geq 1. \tag{3.19}$$

(d) Show that minimal uncertainty in each of the above relations is attained, if

$$\langle\sigma_x\rangle\langle\sigma_y\rangle = 0, \tag{3.20a}$$
$$\langle\sigma_y\rangle\langle\sigma_z\rangle = 0, \tag{3.20b}$$
$$\langle\sigma_z\rangle\langle\sigma_x\rangle = 0. \tag{3.20c}$$

Since the expectation value of the Pauli matrices satisfy Eq. (3.13) all three of the expectation value of Pauli matrices can not be zero for a given state. But, two of them can be zero, which is sufficient for minimizing all the above uncertainty relations. For example, a state satisfying

$$\langle\sigma_x\rangle = \langle\sigma_y\rangle = 0 \tag{3.21}$$

minimizes all the four uncertainty relations above.

(e) Show that

$$|\text{min}\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{3.22}$$

is such a state. Evaluate $\langle\sigma_x\rangle$, $\langle\sigma_y\rangle$, $\langle\sigma_z\rangle$, $\langle\sigma_x^2\rangle$, $\langle\sigma_y^2\rangle$, $\langle\sigma_z^2\rangle$, $\delta\sigma'_x$, $\delta\sigma'_y$, and $\delta\sigma'_z$, when the system is in this state.

(f) Understand the Stern-Gerlach experiment in this light.

2. (**20 points.**) In light of Eq. (3.16), it seems we could conclude that there exits a state $|\ \rangle$ for which

$$\delta\sigma'_x = \delta\sigma'_y = 0, \quad \text{and} \quad \delta\sigma'_z = \sqrt{2}. \tag{3.23}$$

Is this statement correct? If yes, find the state, else, explain why such a state does not exist.
Solution: Such a state does not exist, because it is not compatible with Eq. (3.15c). Thus, not all points on the sphere represented by Eq. (3.16) are allowed. The physical implication of this needs to be explored. Does this have any connection with the CHSH inequality?

3. (**20 points.**) Thoughts:

(a) Refer
L. Dammeier, René Schwonnek, R. F. Werner, Uncertainty relations for angular momentum, New J. Phys. **17** 093046 (2015).
P. Busch, P. Lahti, and R. F. Werner, Colloquium: Quantum root-mean-square error and measurement uncertainty relations, Rev. Mod. Phys. **86** 1261 (2014).

(b) Derive the CHSH inequality, in this context, which seems to involve the correlation $\langle(\boldsymbol{\sigma}\cdot\mathbf{a})(\boldsymbol{\sigma}\cdot\mathbf{b})\rangle$.

3.5 Minimum uncertainty state

1. (**40 points.**) Note dated 20170915: Requiring $\langle \sigma_z \rangle = 0$ in Eq. (3.31) is artificial, but not wrong. Robertson's generalization of Heisenberg's uncertainty relation

$$(\delta A)(\delta B) \geq \frac{1}{2} |\langle C \rangle|, \qquad C = \frac{1}{i}\big[A, B\big], \tag{3.24}$$

for $(A, B) = (\sigma_x, \sigma_y)$ reads

$$(\delta \sigma_x)(\delta \sigma_y) \geq |\langle \sigma_z \rangle|. \tag{3.25}$$

The minimal uncertainty states $|\text{min}\rangle$, are characterized by the equality

$$(\delta \sigma_x)(\delta \sigma_y) = |\langle \sigma_z \rangle|. \tag{3.26}$$

(a) Show that the minimum uncertainty states satisfy the relations,

$$\big\{\sigma_y - \langle \sigma_y \rangle\big\} |\text{min}\rangle = \lambda \big\{\sigma_x - \langle \sigma_x \rangle\big\} |\text{min}\rangle \tag{3.27a}$$

and

$$\langle \text{min}| \big\{\sigma_y - \langle \sigma_y \rangle, \sigma_x - \langle \sigma_x \rangle\big\} |\text{min}\rangle = 0. \tag{3.27b}$$

(b) Show that λ is pure imaginary, $\lambda = i\gamma$, for real γ. Further, show that

$$\gamma = \pm \frac{\delta \sigma_y}{\delta \sigma_x}. \tag{3.28}$$

(c) Using Eq. (3.27b) show that, for minimum uncertainty states,

$$\langle \sigma_x \rangle \langle \sigma_y \rangle = 0. \tag{3.29}$$

(Hint: Use $\sigma_x \sigma_y + \sigma_y \sigma_x = 0$.) Using Eq. (3.29) in Eq. (3.26) show that

$$1 - \langle \sigma_x \rangle^2 - \langle \sigma_y \rangle^2 = |\langle \sigma_z \rangle|^2. \tag{3.30}$$

(Hint: Use $\sigma_x^2 = 1$ and $\sigma_y^2 = 1$.) In the eigenbasis of σ_z we will have $\langle \sigma_z \rangle = 1$, which then leads to

$$\langle \sigma_x \rangle^2 + \langle \sigma_y \rangle^2 = 0. \tag{3.31}$$

Using Eq. (3.29) and Eq. (3.31) show that

$$\langle \sigma_x \rangle = \langle \sigma_y \rangle = 0 \quad \text{and} \quad \langle \delta \sigma_x \rangle = \langle \delta \sigma_y \rangle = 1. \tag{3.32}$$

(d) Thus, show that the minimum unceertainty states satisfy the equations

$$(\sigma_x \pm i \sigma_y) |\text{min}\rangle = 0. \tag{3.33}$$

Solve these matrix equations to determine the two (normalized) minimum uncertainty states $|\text{min}\rangle$. Are linear combinations of the two states minimal uncertainty states?

(e) Evaluate $\langle \sigma_x \rangle$, $\langle \sigma_y \rangle$, $\langle \sigma_z \rangle$, $\langle \sigma_x^2 \rangle$, $\langle \sigma_y^2 \rangle$, $\langle \sigma_z^2 \rangle$, $\delta \sigma_x$, $\delta \sigma_y$, and $\delta \sigma_z$, when the system is in the minimum uncertainty state. Verify Eq. (3.26).

(f) What is the physical interpretation?

2. (**20 points.**) The minimum uncertainty state for Heisenberg's uncertainty relation

$$\delta q \delta p \geq \frac{1}{2} \tag{3.34}$$

in the position eigenbasis is, for $\langle q \rangle = \langle p \rangle = 0$ and $\delta q = \delta p = 1/\sqrt{2}$,

$$\psi_0(q') = \frac{1}{\pi^{\frac{1}{4}}} e^{-\frac{1}{2}q'^2}. \tag{3.35}$$

Evaluate the minimum uncertainty state in the momentum eigenbasis, $\psi_0(p')$, by evaluating the integral for the Fourier transform

$$\psi_0(p') = \int_{-\infty}^{\infty} \frac{dq'}{\sqrt{2\pi}} e^{-iq'p'} \psi_0(q'). \tag{3.36}$$

3. (**30 points.**) Show that

$$\delta(q' - \langle q \rangle) = \lim_{\delta q \to 0} \frac{1}{\sqrt{\pi}} \frac{1}{2\delta q} e^{-\left(\frac{q' - \langle q \rangle}{2\delta q}\right)^2} \tag{3.37}$$

is a suitable representation for the Dirac δ-function. That is, verify that it satisfies

$$\delta(q' - \langle q \rangle) \to 0, \qquad \text{for} \qquad q' \neq \langle q \rangle, \tag{3.38a}$$

$$\delta(q' - \langle q \rangle) \to \infty, \qquad \text{for} \qquad q' = \langle q \rangle, \tag{3.38b}$$

and

$$\int_{-\infty}^{\infty} dq' \delta(q' - \langle q \rangle) = 1. \tag{3.39}$$

3.6 Stationary uncertainty state

Chapter 4

Commutation relations

4.1 Einsteinian relativity

In Einsteinian relativity the new feature is the finiteness of c, speed of light, which requires the abandonment of absolute simultaneity. For infinitesimal Poincaré transformations, Einsteinian relativity is characterized by

$$t' = t - \frac{1}{c}\delta\varepsilon^0 - \frac{1}{c^2}\delta\mathbf{v}\cdot\mathbf{r}, \tag{4.1a}$$

$$\mathbf{r}' = \mathbf{r} - \delta\boldsymbol{\varepsilon} - \delta\boldsymbol{\omega}\times\mathbf{r} - \delta\mathbf{v}t, \tag{4.1b}$$

where $\delta\varepsilon^0/c$ corresponds to translation in time, $\delta\boldsymbol{\varepsilon}$ corresponds to translation in space, $\delta\boldsymbol{\omega}$ corresponds to a rotation, and $\delta\mathbf{v}$ corresponds to boost.

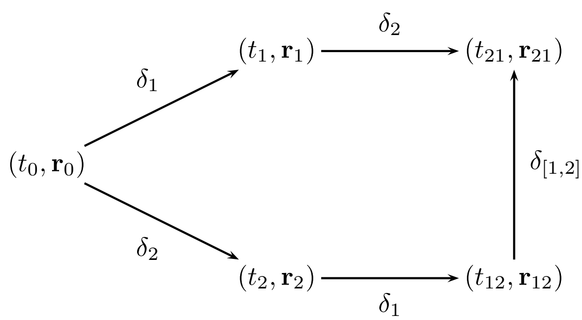

Figure 4.1: Group transformation

Problems

1. Derive the composition properties of the Poincaré group:

$$\delta_{[1,2]}\varepsilon^0 = \frac{1}{c}(\delta_1\mathbf{v}\cdot\delta_2\boldsymbol{\varepsilon} - \delta_2\mathbf{v}\cdot\delta_1\boldsymbol{\varepsilon}), \tag{4.2a}$$

$$\delta_{[1,2]}\boldsymbol{\varepsilon} = (\delta_1\boldsymbol{\omega}\times\delta_2\boldsymbol{\varepsilon} - \delta_2\boldsymbol{\omega}\times\delta_1\boldsymbol{\varepsilon}) + \frac{1}{c}(\delta_1\mathbf{v}\delta_2\varepsilon^0 - \delta_2\mathbf{v}\delta_1\varepsilon^0), \tag{4.2b}$$

$$\delta_{[1,2]}\boldsymbol{\omega} = \delta_1\boldsymbol{\omega}\times\delta_2\boldsymbol{\omega} - \frac{1}{c^2}\delta_1\mathbf{v}\times\delta_2\mathbf{v}, \tag{4.2c}$$

$$\delta_{[1,2]}\mathbf{v} = (\delta_1\mathbf{v}\times\delta_2\boldsymbol{\omega} - \delta_2\mathbf{v}\times\delta_1\boldsymbol{\omega}). \tag{4.2d}$$

2. The generators of the unitary transformation induced by the above infinitesimal coordinate transformations are comprised in

$$G = -\frac{1}{c}\delta\varepsilon^0 cP^0 + \delta\boldsymbol{\varepsilon}\cdot\mathbf{P} + \delta\boldsymbol{\omega}\cdot\mathbf{J} + \delta\mathbf{v}\cdot\mathbf{N} + \delta\phi 1. \tag{4.3}$$

The generator of time translation in Einsteinian relativity is cP^0, which corresponds with the Galilean generator for time translation H, the Hamiltonian, by the relation

$$cP^0 = H + Mc^2. \tag{4.4}$$

Using the group commutation relations

$$\frac{1}{i\hbar}\big[G_1, G_2\big] = \delta_{[1,2]}G \tag{4.5}$$

derive

$$\begin{aligned}
\frac{1}{i\hbar}\Big[-\delta_1\varepsilon^0 P^0 \;+\; &\delta_1\boldsymbol{\varepsilon}\cdot\mathbf{P} + \delta_1\boldsymbol{\omega}\cdot\mathbf{J} + \delta_1\mathbf{v}\cdot\mathbf{N},\; -\delta_2\varepsilon^0 P^0 + \delta_2\boldsymbol{\varepsilon}\cdot\mathbf{P} + \delta_2\boldsymbol{\omega}\cdot\mathbf{J} + \delta_2\mathbf{v}\cdot\mathbf{N}\Big] \\
&= -\delta_{[1,2]}\varepsilon^0 P^0 + \delta_{[1,2]}\boldsymbol{\varepsilon}\cdot\mathbf{P} + \delta_{[1,2]}\boldsymbol{\omega}\cdot\mathbf{J} + \delta_{[1,2]}\mathbf{v}\cdot\mathbf{N} &\text{(4.6a)}\\
&= -\frac{1}{c}(\delta_1\mathbf{v}\cdot\delta_2\boldsymbol{\varepsilon} - \delta_2\mathbf{v}\cdot\delta_1\boldsymbol{\varepsilon})P^0 \\
&\quad +(\delta_1\boldsymbol{\omega}\times\delta_2\boldsymbol{\varepsilon} - \delta_2\boldsymbol{\omega}\times\delta_1\boldsymbol{\varepsilon})\cdot\mathbf{P} + \frac{1}{c}(\delta_1\mathbf{v}\delta_2\varepsilon^0 - \delta_2\mathbf{v}\delta_1\varepsilon^0)\cdot\mathbf{P} \\
&\quad +(\delta_1\boldsymbol{\omega}\times\delta_2\boldsymbol{\omega})\cdot\mathbf{J} - \frac{1}{c^2}(\delta_1\mathbf{v}\times\delta_2\mathbf{v})\cdot\mathbf{J} \\
&\quad +(\delta_1\mathbf{v}\times\delta_2\boldsymbol{\omega} - \delta_2\mathbf{v}\times\delta_1\boldsymbol{\omega})\cdot\mathbf{N}. &\text{(4.6b)}
\end{aligned}$$

Here we have used

$$\delta_{[1,2]}\phi = 0, \tag{4.7}$$

see [1].

3. (a) Show that the response of the generators under time translation is given by

$$\frac{1}{i\hbar}\big[-\delta_1\varepsilon^0 P^0, -\delta_2\varepsilon^0 P^0\big] = 0, \tag{4.8a}$$
$$\frac{1}{i\hbar}\big[\delta_1\boldsymbol{\varepsilon}\cdot\mathbf{P}, -\delta_2\varepsilon^0 P^0\big] = 0, \tag{4.8b}$$
$$\frac{1}{i\hbar}\big[\delta_1\boldsymbol{\omega}\cdot\mathbf{J}, -\delta_2\varepsilon^0 P^0\big] = 0, \tag{4.8c}$$
$$\frac{1}{i\hbar}\big[\delta_1\mathbf{v}\cdot\mathbf{N}, -\delta_2\varepsilon^0 P^0\big] = \frac{1}{c}\delta_2\varepsilon^0\delta_1\mathbf{v}\cdot\mathbf{P}. \tag{4.8d}$$

(b) Show that the response of the generators under translation in space is given by

$$\frac{1}{i\hbar}\big[-\delta_1\varepsilon^0 P^0, \delta_2\boldsymbol{\varepsilon}\cdot\mathbf{P}\big] = 0, \tag{4.9a}$$
$$\frac{1}{i\hbar}\big[\delta_1\boldsymbol{\varepsilon}\cdot\mathbf{P}, \delta_2\boldsymbol{\varepsilon}\cdot\mathbf{P}\big] = 0, \tag{4.9b}$$
$$\frac{1}{i\hbar}\big[\delta_1\boldsymbol{\omega}\cdot\mathbf{J}, \delta_2\boldsymbol{\varepsilon}\cdot\mathbf{P}\big] = (\delta_1\boldsymbol{\omega}\times\delta_2\boldsymbol{\varepsilon})\cdot\mathbf{P}, \tag{4.9c}$$
$$\frac{1}{i\hbar}\big[\delta_1\mathbf{v}\cdot\mathbf{N}, \delta_2\boldsymbol{\varepsilon}\cdot\mathbf{P}\big] = -\frac{1}{c}\delta_1\mathbf{v}\cdot\delta_2\boldsymbol{\varepsilon}P^0. \tag{4.9d}$$

(c) Show that the response of the generators under rotation is given by

$$\frac{1}{i\hbar}\big[-\delta_1\varepsilon^0 P^0, \delta_2\boldsymbol{\omega}\cdot\mathbf{J}\big] = 0, \tag{4.10a}$$

$$\frac{1}{i\hbar}\big[\delta_1\boldsymbol{\varepsilon}\cdot\mathbf{P}, \delta_2\boldsymbol{\omega}\cdot\mathbf{J}\big] = (\delta_1\boldsymbol{\varepsilon}\times\delta_2\boldsymbol{\omega})\cdot\mathbf{P}, \tag{4.10b}$$

$$\frac{1}{i\hbar}\big[\delta_1\boldsymbol{\omega}\cdot\mathbf{J}, \delta_2\boldsymbol{\omega}\cdot\mathbf{J}\big] = (\delta_1\boldsymbol{\omega}\times\delta_2\boldsymbol{\omega})\cdot\mathbf{J}, \tag{4.10c}$$

$$\frac{1}{i\hbar}\big[\delta_1\mathbf{v}\cdot\mathbf{N}, \delta_2\boldsymbol{\omega}\cdot\mathbf{J}\big] = (\delta_1\mathbf{v}\times\delta_2\boldsymbol{\omega})\cdot\mathbf{N}. \tag{4.10d}$$

(d) Show that the response of the generators under boost is given by

$$\frac{1}{i\hbar}\big[-\delta_1\varepsilon^0 P^0, \delta_2\mathbf{v}\cdot\mathbf{N}\big] = -\frac{1}{c}\delta_1\varepsilon^0\delta_2\mathbf{v}\cdot\mathbf{P}, \tag{4.11a}$$

$$\frac{1}{i\hbar}\big[\delta_1\boldsymbol{\varepsilon}\cdot\mathbf{P}, \delta_2\mathbf{v}\cdot\mathbf{N}\big] = \frac{1}{c}\delta_1\boldsymbol{\varepsilon}\cdot\delta_2\mathbf{v}P^0, \tag{4.11b}$$

$$\frac{1}{i\hbar}\big[\delta_1\boldsymbol{\omega}\cdot\mathbf{J}, \delta_2\mathbf{v}\cdot\mathbf{N}\big] = (\delta_1\boldsymbol{\omega}\times\delta_2\mathbf{v})\cdot\mathbf{N}, \tag{4.11c}$$

$$\frac{1}{i\hbar}\big[\delta_1\mathbf{v}\cdot\mathbf{N}, \delta_2\mathbf{v}\cdot\mathbf{N}\big] = -\frac{1}{c^2}(\delta_1\mathbf{v}\times\delta_2\mathbf{v})\cdot\mathbf{J}. \tag{4.11d}$$

4. Compare the commutation relations in Einsteinian relativity with the Galilean ones. Thus, show that in Galilean relativity, $\mathbf{J}/c^2$ is neglected, and H is neglected relative to Mc^2, giving the effective replacement of the operator P^0/c by the number M.

5. We observed that the generator of a unitary transformation is arbitrary upto a phase $\delta\phi$. We shall determine the structure of the phase in this exercise. The generator is given by the expression

$$G = -H\delta t + \mathbf{P}\cdot\delta\boldsymbol{\varepsilon} + \mathbf{J}\cdot\delta\boldsymbol{\omega} + \mathbf{N}\cdot\delta\mathbf{v} + \hbar\delta\phi. \tag{4.12}$$

Our goal will be to construct the bilinear form $\delta_{[1,2]}\phi$.

(a) Argue that $\delta_{[1,2]}\phi$ has to be antisymmetric in 12,

$$\delta_{[1,2]}\phi = -\delta_{[2,1]}\phi. \tag{4.13}$$

(b) Argue that $\delta_{[1,2]}$ has to be a scalar.

(c) Show that the most general bilinear form for $\delta_{[1,2]}\phi$ is

$$\delta_{[1,2]}\phi = K(\delta_1\boldsymbol{\omega}\cdot\delta_2\boldsymbol{\varepsilon} - \delta_2\boldsymbol{\omega}\cdot\delta_1\boldsymbol{\varepsilon}) + L(\delta_1\boldsymbol{\omega}\cdot\delta_2\mathbf{v} - \delta_2\boldsymbol{\omega}\cdot\delta_1\mathbf{v}) + M(\delta_1\boldsymbol{\varepsilon}\cdot\delta_2\mathbf{v} - \delta_2\boldsymbol{\varepsilon}\cdot\delta_1\mathbf{v}), \tag{4.14}$$

where K, L, and M are constants.

(d) The Jacobi identity, applied to three sets of infinitesimal transformations, implies that

$$\begin{aligned} & K[\delta_{[1,2]}\boldsymbol{\omega}\cdot\delta_3\boldsymbol{\varepsilon} - \delta_3\boldsymbol{\omega}\cdot\delta_{[1,2]}\boldsymbol{\varepsilon} + \text{cycl. perm.}] \\ +\ & L[\delta_{[1,2]}\boldsymbol{\omega}\cdot\delta_3\mathbf{v} - \delta_3\boldsymbol{\omega}\cdot\delta_{[1,2]}\mathbf{v} + \text{cycl. perm.}] \\ +\ & M[\delta_{[1,2]}\boldsymbol{\varepsilon}\cdot\delta_3\mathbf{v} - \delta_3\boldsymbol{\varepsilon}\cdot\delta_{[1,2]}\mathbf{v} + \text{cycl. perm.}] = 0. \end{aligned} \tag{4.15}$$

i. Verify that the coefficient of M vanishes identically.
ii. Determine the simplified expression for the non-vanishing coefficient of K.
iii. Determine the simplified expression for the non-vanishing coefficient of L.
iv. Hence conclude that K and L must be zero.

(e) Thus, conclude that

$$\delta_{[1,2]}\phi = M(\delta_1\boldsymbol{\varepsilon}\cdot\delta_2\mathbf{v} - \delta_2\boldsymbol{\varepsilon}\cdot\delta_1\mathbf{v}). \tag{4.16}$$

Chapter 5

Harmonic oscillator

5.1 Harmonic oscillator

1. Any system obeying the Newtonian equation of motion

$$\frac{dp}{dt} = -kx \tag{5.1}$$

is broadly termed a simple harmonic oscillator. Here x and t is position and time of the system, $p = mv$ is momentum, and k is a constant. Recognizing that the associated restoring force is a conservative force, we can write

$$\frac{dp}{dt} = -\frac{\partial}{\partial x}\left(\frac{1}{2}kx^2\right), \tag{5.2}$$

which states that the associated force is a manifestation of the system trying to reduce the energy. This allows us to identify the potential energy associated with a harmonic oscillator as

$$U = \frac{1}{2}kx^2. \tag{5.3}$$

The Hamiltonian for the harmonic oscillator is

$$H(x,p) = \frac{p^2}{2m} + \frac{1}{2}kx^2. \tag{5.4}$$

The Hamilton equations of motion are

$$\frac{dx}{dt} = \frac{\partial H}{\partial p} = \frac{p}{m}, \tag{5.5a}$$

$$\frac{dp}{dt} = -\frac{\partial H}{\partial x} = -kx. \tag{5.5b}$$

These first order equations in conjunction leads to the Newtonian equation of mation.

2. We upgrade to quantum mechanics from the classical picture by imposing the commutation relations

$$[x,x] = 0, \qquad [p,p] = 0, \qquad [x,p] = i\hbar, \tag{5.6}$$

on the dynamical variables x and p. Since these variables donot commute with each other they can not be numbers anymore and are instead operators. The correspondence with the classical picture is made by requiring the eigenvalues of these dynamical operators to relate to their classical counterparts. This is traditionally achieved by requiring the operators to be Hermitian,

$$x^\dagger = x, \quad p^\dagger = p, \tag{5.7}$$

such that the eigenvalues are certainly real.

The Hamilton equations of motion for the dynamical variables are obtained from their classical counterparts simply by generalizing the variables to operators. Further, the Heisenberg equations of motion, which are given in terms of commutation relations between the operators with the Hamiltonian, are

$$\frac{dx}{dt} = \frac{\partial H}{\partial p} = \frac{1}{i\hbar}\big[x, H\big], \tag{5.8a}$$

$$\frac{dp}{dt} = -\frac{\partial H}{\partial x} = \frac{1}{i\hbar}\big[p, H\big]. \tag{5.8b}$$

Verify that

$$\frac{1}{i\hbar}\big[x, H\big] = \frac{p}{m}, \tag{5.9a}$$

$$\frac{1}{i\hbar}\big[p, H\big] = -kx. \tag{5.9b}$$

Thus, the equations of motion are identical, whether we use the Hamiltonian equations of motion or the Heisenberg equations of motion.

3. The eigenvalues H' of the Hamiltonian operator H is defined using the eigenvalue equation

$$H|H'\rangle = H'|H'\rangle. \tag{5.10}$$

Since energy is often denoted by E we will use H' and E interchangably to represent energy. It is desired to project states on a position eigenstate $\langle x'|$, which leads to

$$\langle x'|H|H'\rangle = H'\langle x'|H'\rangle. \tag{5.11}$$

Using the projection of a momentum eigenstate $|p'\rangle$ on a position eigenstate $|x'\rangle$ to be given by

$$\langle x'|p'\rangle = \frac{e^{\frac{i}{\hbar}x'p'}}{\sqrt{2\pi}} \qquad \text{and} \qquad \langle p'|x'\rangle = \frac{e^{-\frac{i}{\hbar}p'x'}}{\sqrt{2\pi}}, \tag{5.12}$$

show that

$$\langle x'|x|H'\rangle = x'\langle x'|H'\rangle \tag{5.13}$$

and

$$\langle x'|p|H'\rangle = \frac{\hbar}{i}\frac{\partial}{\partial x'}\langle x'|H'\rangle. \tag{5.14}$$

Then, using these in the expression for the Hamiltonian derive the time-independent Schrödinger equation for the harmonic oscillator,

$$\left[\frac{1}{2m}\left(\frac{\hbar}{i}\frac{\partial}{\partial x'}\right)^2 + \frac{1}{2}k{x'}^2\right]\psi(x') = E\,\psi(x'), \tag{5.15}$$

where

$$\psi(x') = \langle x'|H'\rangle \tag{5.16}$$

is the projection of an energy eigenstate $|H'\rangle$ on a position eigenstate $\langle x'|$, the energy wavefunction.

4. In terms of the non-Hermitian operators,

$$y = \frac{1}{\sqrt{2\hbar\omega}}\left(\sqrt{k}\,x + i\frac{p}{\sqrt{m}}\right), \tag{5.17a}$$

$$y^\dagger = \frac{1}{\sqrt{2\hbar\omega}}\left(\sqrt{k}\,x - i\frac{p}{\sqrt{m}}\right), \tag{5.17b}$$

where $\omega = \sqrt{k/m}$, verify that

$$\big[y, y^\dagger\big] = 1, \qquad \big[y, y\big] = 0, \qquad \big[y^\dagger, y^\dagger\big] = 0. \tag{5.18}$$

Show that the Hamiltonian for a harmonic oscillator is given by

$$H(y, y^\dagger) = \hbar\omega \left(y^\dagger y + \frac{1}{2} \right). \tag{5.19}$$

Evaluate the content of the Heisenberg equations of motion

$$\frac{dy}{dt} = \frac{1}{i\hbar}\big[y, H\big], \tag{5.20a}$$

$$\frac{dy^\dagger}{dt} = \frac{1}{i\hbar}\big[y^\dagger, H\big]. \tag{5.20b}$$

5. The harmonic oscillator is described by the number operator

$$n = a^\dagger a \tag{5.21}$$

constructed out of a non-Hermitian operator a and it's Hermitian conjugate $a^\dagger$ that satisfy the commutation relation

$$\big[a, a^\dagger\big] = 1. \tag{5.22}$$

(a) A suitable basis for describing the harmonic oscillator are the eigenvecotrs $|n'\rangle$ labeled by the respective eigenvalues n' of the number operator defined using the eigenvalue equation

$$n|n'\rangle = n'|n'\rangle. \tag{5.23}$$

These eigenstates of the number operator n satisfy the completeness relation

$$\sum_{n'} |n'\rangle\langle n'| = 1 \tag{5.24}$$

and the orthonormality relations

$$\langle n'|m'\rangle = \delta_{n'm'}. \tag{5.25}$$

(b) By taking the trace on both sides of Eq. (5.22) argue that $a^\dagger a$ can not be represented using finite dimensional matrices. Thus, deduce that the eigenvalues n' must be infinite of them.

(c) Show that the number operator n is a Hermitian operator. Thus, the eigenvalues n' must be real. Further, because n is a bilinear construction of Hermitian conjugated operators, deduce that the eigenvalues n' are non-negative. That is,

$$n' \geq 0. \tag{5.26}$$

(d) Starting from the commutation relation in Eq. (5.22) show that

$$\big[n, a^\dagger\big] = a^\dagger, \tag{5.27a}$$

$$\big[n, a\big] = -a. \tag{5.27b}$$

Using Eqs. (5.27) derive

$$n\Big\{a^\dagger|n'\rangle\Big\} = (n'+1)\Big\{a^\dagger|n'\rangle\Big\}, \tag{5.28a}$$

$$n\Big\{a|n'\rangle\Big\} = (n'-1)\Big\{a|n'\rangle\Big\}. \tag{5.28b}$$

Thus, deduce that a is a lowering operator, that is,

$$a|n'\rangle = c'_{n'}|n'-1\rangle, \tag{5.29}$$

where $c'_{n'}$ is to be determined. Further, conclude, if n' is an eigenvalue, then $(n'-1)$ is also an eigenvalue. Similarly, deduce that $a^\dagger$ is a raising operator, that is,

$$a^\dagger|n'\rangle = d'_{n'}|n'+1\rangle, \tag{5.30}$$

where $d'_{n'}$ is to be determined. Thus, conclude, if n' is an eigenvalue, then $(n'+1)$ is also an eigenvalue.

(e) Starting from Eq. (5.29) we can construct

$$\langle n'|a^\dagger = {c'_{n'}}^*\langle n'-1|. \tag{5.31}$$

Together, they imply

$$n' = |c'_{n'}|^2. \tag{5.32}$$

Thus, upto a phase

$$c'_{n'} = \sqrt{n'}. \tag{5.33}$$

Similarly, starting from Eq. (5.30) we can construct

$$\langle n'|a = {d'_{n'}}^*\langle n'+1|. \tag{5.34}$$

Together, they imply

$$(n'+1) = |d'_{n'}|^2. \tag{5.35}$$

Thus, upto a phase

$$d'_{n'} = \sqrt{n'+1}. \tag{5.36}$$

Thus, we derive the action of the lowering and raising operators explitcitly,

$$a^\dagger|n'\rangle = \sqrt{n'+1}|n'+1\rangle, \tag{5.37a}$$
$$a|n'\rangle = \sqrt{n'}|n'-1\rangle. \tag{5.37b}$$

(f) Since all the eigenvalues have to be non-negative, the lowering operator cannot indefinitely lower the sate. This is accomplished by requiring the eigenvalues n' to be discrete, take on non-negative integral values, such that the smallest value for n' is 0. Thus, argue the existance of the ground eigenstate that satisfies

$$a|0\rangle = 0. \tag{5.38}$$

That is, $n'=0$ corresponds to the eigenstate for the ground state.

6. To determine $d_{n'}$ we construct an eigenstate in terms of the ground state,

$$|n'\rangle = \frac{(y^\dagger)^{n'}}{D_{n'}}|0\rangle, \qquad D_{n'} = d_0 d_1 \ldots d_{n'-1}. \tag{5.39}$$

Presuming the eigenstates are normalized, use

$$\langle m'|n'\rangle = \delta_{m'n'} \tag{5.40}$$

to learn that

$$|D_{n'}|^2 = \langle 0|y^{n'}(y^\dagger)^{n'}|0\rangle. \tag{5.41}$$

Show that

$$\langle 0|y^{n'}(y^\dagger)^{n'}|0\rangle = n'\,\langle 0|y^{n'-1}(y^\dagger)^{n'-1}|0\rangle. \tag{5.42}$$

(Hint: Show that $\left[y, (y^\dagger)^{n'}\right] = n'(y^\dagger)^{n'-1}$.) Thus, deduce that $|D_{n'}| = \sqrt{n!}$ and $|d_{n'}| = \sqrt{n'+1}$. Thus, we have

$$y^\dagger|n'\rangle = \sqrt{n'+1}|n'+1\rangle. \tag{5.43}$$

Operate the lowering operator y on both sides of the above equation and decipher the statement

$$y|n'\rangle = \sqrt{n'}|n'-1\rangle \tag{5.44}$$

to learn that $c_{n'} = \sqrt{n'}$.

7. The projection of the eigenstates $|n'\rangle$ on the position eigenstates $\langle x'|$ leads to the construction of the corresponding wavefunctions

$$\psi_{n'}(x') = \langle x'|n'\rangle. \tag{5.45}$$

We will set $k = m = 1$ by suitable scaling of x and p and further set $\hbar = 1$ to avoid clutter in the equations. We shall also drop the primes to represent the eigenvalues.

(a) Starting from Eq. (5.38) deduce the differential equation satisfied by the ground state to be

$$\left(x + \frac{\partial}{\partial x}\right)\psi_0(x) = 0. \tag{5.46}$$

Thus, show that

$$\psi_0(x) = \pi^{-\frac{1}{4}} e^{-\frac{1}{2}x^2}. \tag{5.47}$$

Plot $\psi_0(x)$.

(b) Starting from the statement in Eq (5.39),

$$|n\rangle = \frac{(y^\dagger)^n}{\sqrt{n!}}|0\rangle, \tag{5.48}$$

deduce the relation

$$\psi_n(x) = \frac{1}{\sqrt{2^n n!}}\left(x - \frac{\partial}{\partial x}\right)^n \psi_0(x). \tag{5.49}$$

(c) Verify that

$$\left(x - \frac{\partial}{\partial x}\right) f(x) = \left(-e^{\frac{1}{2}x^2}\frac{\partial}{\partial x}e^{-\frac{1}{2}x^2}\right) f(x). \tag{5.50}$$

Thus, show that

$$\left(x - \frac{\partial}{\partial x}\right)^n f(x) = e^{\frac{1}{2}x^2}\left(-\frac{\partial}{\partial x}\right)^n e^{-\frac{1}{2}x^2} f(x). \tag{5.51}$$

(d) The Hermite polynomials are defined as

$$H_n(x) = e^{x^2}\left(-\frac{\partial}{\partial x}\right)^n e^{-x^2}. \tag{5.52}$$

Evaluate $H_n(x)$ for $n = 0, 1, 2, 3, 4$. Thus, derive

$$\psi_n(x) = \frac{1}{\sqrt{2^n n!}}\psi_0(x)H_n(x). \tag{5.53}$$

Plot $\psi_n(x)$ for $n = 0, 1, 2, 3, 4$.

Problems

1. (**50 points.**) A quantum harmonic oscillator can be constructed out of two non-Hermitian operators, y and $y^\dagger$, that satisfy the commutation relation

$$[y, y^\dagger] = 1. \tag{5.54}$$

The eigenstate spectrum of the (Hermitian) number operator, $n = y^\dagger y$, represented by $|n'\rangle$, where $n' = 0, 1, 2, \ldots$, satisfy

$$n|n'\rangle = n'|n'\rangle, \qquad y|n'\rangle = \sqrt{n'}|n'-1\rangle, \qquad y^\dagger|n'\rangle = \sqrt{n'+1}|n'+1\rangle. \tag{5.55}$$

(a) Build the matrix representation of the lowering operator y using

$$y = \begin{bmatrix} \langle 0|y|0\rangle & \langle 0|y|1\rangle & \langle 0|y|2\rangle & \langle 0|y|3\rangle & \langle 0|y|4\rangle & \cdots \\ \langle 1|y|0\rangle & \langle 1|y|1\rangle & \langle 1|y|2\rangle & \langle 1|y|3\rangle & \langle 1|y|4\rangle & \cdots \\ \langle 2|y|0\rangle & \langle 2|y|1\rangle & \langle 2|y|2\rangle & \langle 2|y|3\rangle & \langle 2|y|4\rangle & \cdots \\ \langle 3|y|0\rangle & \langle 3|y|1\rangle & \langle 3|y|2\rangle & \langle 3|y|3\rangle & \langle 3|y|4\rangle & \cdots \\ \langle 4|y|0\rangle & \langle 4|y|1\rangle & \langle 4|y|2\rangle & \langle 4|y|3\rangle & \langle 4|y|4\rangle & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}. \tag{5.56}$$

Kindly calculate the first 5×5 block of the infinite dimensional matrix to report the pattern in the following questions.

(b) Similarly, build the matrix representation of the raising operator $y^\dagger$.

(c) Build the matrix representation of the number operator n.

(d) Using the constructions

$$y = \frac{1}{\sqrt{2\hbar}}(x + ip) \quad \text{and} \quad y^\dagger = \frac{1}{\sqrt{2\hbar}}(x - ip), \tag{5.57}$$

determine the matrix representations for the Hermitian operators, x and p. Check that x and p are indeed Hermitian matrices.

(e) Determine the matrices for the operators xp and px, and verify the commutation relation

$$\frac{1}{i\hbar}[x, p] = 1. \tag{5.58}$$

2. (**10 points.**) Using the asymptotic form for Hermite polynomials for large n,

$$e^{-\frac{x^2}{2}} H_n(x) \xrightarrow{n \gg 1} \frac{2^n}{\sqrt{\pi}} \Gamma\left(\frac{n+1}{2}\right) \cos\left(x\sqrt{2n} - n\frac{\pi}{2}\right), \tag{5.59}$$

discuss the manner in which the harmonic oscillator eigenfunctions

$$\psi_n(x) = \frac{1}{\sqrt{2^n \hbar^n \sqrt{\pi} n!}} e^{-\frac{m\omega}{\hbar}\frac{x^2}{2}} H_n\left(\sqrt{\frac{m\omega}{\hbar}} x\right) \tag{5.60}$$

approach those of the free particle, satisfying the differential equation

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\phi_n(x) = E_n \phi_n(x) \tag{5.61}$$

with eigenfunctions

$$\phi_n(x) = A \cos\left(\sqrt{\frac{2mE_n}{\hbar^2}} x + \delta\right), \tag{5.62}$$

in the limit when the frequency of oscillations $\omega \to 0$.

3. (**40 points.**) (Set $\hbar = 1$.) Starting from

$$y|n\rangle = \sqrt{n}|n-1\rangle \tag{5.63}$$

and by projecting this on the position eigenstate derive

$$\frac{d}{dx}H_n(x) = 2nH_{n-1}(x). \tag{5.64}$$

Check this for $n = 4, 3, 2, 1, 0$. Similarly, starting from

$$y^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle \tag{5.65}$$

and by projecting this on the position eigenstate derive

$$\left(2x - \frac{d}{dx}\right)H_n(x) = H_{n+1}(x). \tag{5.66}$$

Add the two statements to obtain

$$2xH_n(x) = H_{n+1}(x) + 2nH_{n-1}(x). \tag{5.67}$$

This recursion relation gives a way of recursively calculating $H_{n+1}(x)$ in terms of $H_n(x)$ and $H_{n-1}(x)$. Check this for $n = 3, 2, 1, 0$.

4. (**20 points.**) Use the results of Problem 3 to deduce the differential equation

$$\left(\frac{d^2}{dx^2} - 2x\frac{d}{dx} + 2n\right)H_n(x) = 0. \tag{5.68}$$

Show the equivalence of this with

$$\left(\frac{d^2}{dx^2} - x^2 + 2n + 1\right)\psi_n(x) = 0. \tag{5.69}$$

This is the "time-independent Schrödinger equation" for the harmonic oscillator.

5. (**20 points.**) The ground eigenstate of a harmonic oscillator satisfies the equation

$$y|0\rangle = 0, \tag{5.70}$$

where

$$y = \frac{1}{\sqrt{2}}(x + ip). \tag{5.71}$$

Construct the differential equation satisfied by the ground eigenstate in the momentum basis,

$$\psi_0(p') = \langle p'|0\rangle. \tag{5.72}$$

Solve the differential equation and find the normalized ground eigenstate.

Chapter 6

A charge in a uniform magnetic field

6.1 Lorentz force

1. (**40 points.**) A particle of mass m and charge q moving in a uniform magnetic field $\mathbf{B}$ experiences a velocity dependent force $\mathbf{F}$ given by the expression

$$m\frac{d\mathbf{v}}{dt} = q\mathbf{v} \times \mathbf{B}, \tag{6.1}$$

where $\mathbf{v}(t) = d\mathbf{x}/dt$ is the velocity of the particle in terms of its position $\mathbf{x}(t)$. Choose the magnetic field to be along the positive z direction, $\mathbf{B} = B\hat{\mathbf{z}}$.

(a) For the case when the particle starts at rest at the origin at time $t = 0$, use the initial conditions

$$\mathbf{v}(0) = 0\,\hat{\mathbf{x}} + v_0\,\hat{\mathbf{y}} + 0\,\hat{\mathbf{z}}, \tag{6.2}$$

$$\mathbf{x}(0) = 0\,\hat{\mathbf{x}} + 0\,\hat{\mathbf{y}} + 0\,\hat{\mathbf{z}}, \tag{6.3}$$

to solve the differential equation in Eq. (6.1) to find the position $\mathbf{x}(t)$ and velocity $\mathbf{v}(t)$ as a function of time. Use $\omega = qB/m$.
Hint: Second-order differential equations for v_x and v_y introduce two arbitrary constants each. Integrations of these equations, to construct the respective positions, leads to another two arbitrary constants. Thus, there are a total of six arbitrary constants. Four of these are determined by the initial conditions. The remaining two are determined by the coupling in the components of the velocity, given by the first-order differential equations in Eq. (6.1).

(b) In particular, prove that the particle takes a circular path. What is the radius of the circle? Determine the coordinates of the center of the circle?

(c) Repeat the above exercise for the initial conditions

$$\mathbf{v}(0) = -\frac{v_0}{\sqrt{2}}\,\hat{\mathbf{x}} + \frac{v_0}{\sqrt{2}}\,\hat{\mathbf{y}} + 0\,\hat{\mathbf{z}}, \tag{6.4}$$

$$\mathbf{x}(0) = 0\,\hat{\mathbf{x}} + 0\,\hat{\mathbf{y}} + 0\,\hat{\mathbf{z}}. \tag{6.5}$$

6.2 Lagrangian and Hamiltonian

1. The force on a charge particle in an electric and magnetic field experiences the Lorentz force

$$\mathbf{F} = m\frac{d\mathbf{v}}{dt} = q\mathbf{E} + q\mathbf{v} \times \mathbf{B}. \tag{6.6}$$

(a) To identify the Lagrangian we compare the equations of motion with the Euler-Lagrange equation

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \mathbf{v}}\right) = \frac{\partial L}{\partial \mathbf{r}}. \tag{6.7}$$

(b) To this end, we use

$$\mathbf{E} = -\boldsymbol{\nabla}\phi - \frac{\partial \mathbf{A}}{\partial t}, \tag{6.8}$$

$$\mathbf{B} = \boldsymbol{\nabla} \times \mathbf{A}, \tag{6.9}$$

to write

$$\frac{d}{dt}\left(m\mathbf{v} + q\mathbf{A}\right) = -\boldsymbol{\nabla}\left(q\phi - q\mathbf{v}\cdot\mathbf{A}\right). \tag{6.10}$$

Thus, after integrating, identify the Lagrangian

$$L(\mathbf{x}, \mathbf{v}) = \frac{1}{2}mv^2 - \left(q\phi - q\mathbf{v}\cdot\mathbf{A}\right). \tag{6.11}$$

2. The canonical momentum is defined as

$$\mathbf{p} = \frac{\partial L}{\partial \mathbf{v}} = m\mathbf{v} + q\mathbf{A}. \tag{6.12}$$

Thus, using $H = \mathbf{p}\cdot\mathbf{v} - L$, construct the Hamiltonian

$$H(\mathbf{x}, \mathbf{p}) = \frac{1}{2m}(\mathbf{p} - q\mathbf{A})^2 + q\phi. \tag{6.13}$$

3. Evaluate the commutation relations in the Hamilton equations of motion

$$\frac{d\mathbf{x}}{dt} = \frac{1}{i\hbar}\left[\mathbf{x}, H\right], \tag{6.14}$$

$$\frac{d\mathbf{p}}{dt} = \frac{1}{i\hbar}\left[\mathbf{p}, H\right], \tag{6.15}$$

to obtain the equations of motion

$$m\mathbf{v} = \mathbf{p} - q\mathbf{A}, \tag{6.16}$$

$$\frac{d\mathbf{p}}{dt} = ? \tag{6.17}$$

These involve the commutation relation $\left[\mathbf{p}, \phi\right] = -i\hbar(\boldsymbol{\nabla}\phi)$ and $\left[\mathbf{p}^i, \mathbf{A}^j\right] = -i\hbar(\boldsymbol{\nabla}^i A^j)$, in the position basis.

4. A homogeneous magnetic field $\mathbf{B}$ is characterized by the vector potential

$$\mathbf{A} = \frac{1}{2}\mathbf{B} \times \mathbf{r}. \tag{6.18}$$

(a) Evaluate $\boldsymbol{\nabla} \times \mathbf{A}$. (Hint: $\boldsymbol{\nabla} \times \mathbf{A} = \mathbf{B}$.)

(b) Evaluate $\boldsymbol{\nabla} \cdot \mathbf{A}$.

(c) Is this construction unique? (Hint: Remember the freedom of gauge transformation.)

(d) Now, for the case of $\mathbf{B} = (0, 0, B)$, pointing in the z direction, show that $\mathbf{A} = (0, Bx, 0)$ is a solution. Find another solution.

5. A charge in a uniform magnetic field, in the absence of an electric field, is described by the Hamiltonian

$$H(\mathbf{x},\mathbf{p}) = \frac{1}{2m}(\mathbf{p} - q\mathbf{A})^2, \tag{6.19}$$

where

$$\mathbf{A} = \frac{1}{2}\mathbf{B}\times\mathbf{r}. \tag{6.20}$$

Evaluate the commutation relations in the Hamilton equations of motion

$$\frac{d\mathbf{x}}{dt} = \frac{1}{i\hbar}\big[\mathbf{x}, H\big], \tag{6.21}$$

$$\frac{d\mathbf{p}}{dt} = \frac{1}{i\hbar}\big[\mathbf{p}, H\big], \tag{6.22}$$

to obtain the equations of motion

$$m\mathbf{v} = \mathbf{p} - q\mathbf{A}, \tag{6.23}$$

$$\frac{d\mathbf{p}}{dt} = \frac{1}{2}q\mathbf{v}\times\mathbf{B}. \tag{6.24}$$

Further, show that

$$\frac{d\mathbf{A}}{dt} = -\frac{1}{2}q\mathbf{v}\times\mathbf{B}. \tag{6.25}$$

Thus,

$$m\frac{d\mathbf{v}}{dt} = q\mathbf{v}\times\mathbf{B}. \tag{6.26}$$

6. A charge in a uniform magnetic field in the absence of an electric field is described by the Hamiltonian

$$H(\mathbf{x},\mathbf{p}) = \frac{1}{2m}(\mathbf{p} - q\mathbf{A})^2, \tag{6.27}$$

where

$$\mathbf{A} = \frac{1}{2}\mathbf{B}\times\mathbf{r}. \tag{6.28}$$

Using the commutation relations

$$\frac{1}{i\hbar}\big[\mathbf{x},\mathbf{x}\big] = 0, \qquad \frac{1}{i\hbar}\big[\mathbf{x},\mathbf{p}\big] = \mathbf{1}, \qquad \frac{1}{i\hbar}\big[\mathbf{p},\mathbf{p}\big] = 0, \tag{6.29}$$

complete the set

$$\frac{1}{i\hbar}\big[\mathbf{x},\mathbf{x}\big] = 0, \qquad \frac{1}{i\hbar}\big[\mathbf{v},\mathbf{x}\big] = -\frac{1}{m}, \qquad \frac{1}{i\hbar}\big[\mathbf{p},\mathbf{x}\big] = -\mathbf{1}, \qquad \frac{1}{i\hbar}\big[H,\mathbf{x}\big] = -\mathbf{v}, \tag{6.30a}$$

$$\frac{1}{i\hbar}\big[\mathbf{x},\mathbf{v}\big] = \frac{1}{m}, \qquad \frac{1}{i\hbar}\big[\mathbf{v},\mathbf{v}\big] = \frac{q}{m^2}\varepsilon^{ijm}B^m, \qquad \frac{1}{i\hbar}\big[\mathbf{p},\mathbf{v}\big] =, \qquad \frac{1}{i\hbar}\big[H,\mathbf{v}\big] =, \tag{6.30b}$$

$$\frac{1}{i\hbar}\big[\mathbf{x},\mathbf{p}\big] = \mathbf{1}, \qquad \frac{1}{i\hbar}\big[\mathbf{v},\mathbf{p}\big] =, \qquad \frac{1}{i\hbar}\big[\mathbf{p},\mathbf{p}\big] = 0, \qquad \frac{1}{i\hbar}\big[H,\mathbf{p}\big] =, \tag{6.30c}$$

$$\frac{1}{i\hbar}\big[\mathbf{x},H\big] = \mathbf{v}, \qquad \frac{1}{i\hbar}\big[\mathbf{v},H\big] =, \qquad \frac{1}{i\hbar}\big[\mathbf{p},H\big] =, \qquad \frac{1}{i\hbar}\big[H,H\big] = 0. \tag{6.30d}$$

6.3 Landau levels

Chapter 7

Laser: Spontaneous emission

7.1 Jaynes-Cummings model

1. (**40 points.**) Consider the operator constructions

$$\sigma_+ = \frac{1}{2}(\sigma_x + i\sigma_y) \quad \text{and} \quad \sigma_- = \frac{1}{2}(\sigma_x - i\sigma_y). \tag{7.1}$$

   (a) Show that

$$\sigma_+|-\rangle = |+\rangle, \qquad \sigma_+|+\rangle = 0, \tag{7.2a}$$
$$\sigma_-|-\rangle = 0, \qquad \sigma_-|+\rangle = |-\rangle. \tag{7.2b}$$

   (b) Evaluate σ_+^2, σ_-^2, $\sigma_+\sigma_-$, $\sigma_-\sigma_+$, the commutation relation $\big[\sigma_+, \sigma_-\big]$, and the anti-commutation relation $\big\{\sigma_+, \sigma_-\big\}$.

2. (**40 points.**) Consider the operator

$$\gamma_0 = y\sigma_+ + y^\dagger\sigma_-, \tag{7.3}$$

   where $\sigma_+ = (\sigma_x + i\sigma_y)/2$ and $\sigma_- = (\sigma_x - i\sigma_y)/2$.

   (a) Let $|n', \pm 1\rangle$, $n' = 0, 1, 2, \ldots$, be the common eigenvectors of $y^\dagger y$ and σ_z. Consider the subspace spanned by the eigenvectors $|n', +1\rangle$ and $|n'+1, -1\rangle$. Construct the matrix representation of the operator γ_0 in this subspace by evaluating the elements in

$$\gamma_0 = \begin{bmatrix} \langle n', +1|\gamma_0|n', +1\rangle & \langle n', +1|\gamma_0|n'+1, -1\rangle \\ \langle n'+1, -1|\gamma_0|n', +1\rangle & \langle n'+1, -1|\gamma_0|n'+1, -1\rangle \end{bmatrix}. \tag{7.4}$$

   Solution:

$$\gamma_0 = \begin{bmatrix} 0 & \sqrt{n'+1} \\ \sqrt{n'+1} & 0 \end{bmatrix}. \tag{7.5}$$

   (b) Find the eigenvalues of the operator γ_0. (Solution: $\pm\sqrt{n'+1}$.)

   (c) Find the two normalized eigenvectors (upto a phase) of the operator γ_0 in the subspace discussed above, and express them in terms of the respective common eigenvectors.
   Solution:

$$|\gamma_0' = +\rangle = \frac{1}{\sqrt{2}}|n', +1\rangle + \frac{1}{\sqrt{2}}|n'+1, -1\rangle, \tag{7.6a}$$
$$|\gamma_0' = -\rangle = \frac{1}{\sqrt{2}}|n', +1\rangle - \frac{1}{\sqrt{2}}|n'+1, -1\rangle. \tag{7.6b}$$

(d) Evaluate γ_0^2. In particular, show that

$$\gamma_0^2 = \left(y^\dagger y + \frac{1}{2}\right) + \frac{1}{2}\sigma_z. \tag{7.6c}$$

3. (**20 points.**) Given

$$\bar{\gamma} = \sigma_x + \epsilon\sigma_z. \tag{7.7}$$

Let $\bar{\gamma} = \epsilon\gamma$, so that

$$\gamma = \sigma_z + \tan\alpha\,\sigma_x, \qquad \tan\alpha = \frac{1}{\epsilon}. \tag{7.8}$$

Verify the following probabilities:

$$p([\gamma = +] \to [\sigma_z = -1]) = \sin^2\frac{\alpha}{2} = \frac{1}{2}\left(1 - \frac{\epsilon}{\sqrt{1+\epsilon^2}}\right), \tag{7.9a}$$

$$p([\gamma = +] \to [\sigma_x = +1]) = \cos^2\frac{\alpha}{2} = \frac{1}{2}\left(1 + \frac{\epsilon}{\sqrt{1+\epsilon^2}}\right). \tag{7.9b}$$

Plot these probabilities as a function of ϵ.

4. (**40 points.**) Consider the operator

$$\gamma = y\sigma_+ + y^\dagger\sigma_- + \epsilon\sigma_z, \tag{7.10}$$

where $\sigma_+ = (\sigma_x + i\sigma_y)/2$ and $\sigma_- = (\sigma_x - i\sigma_y)/2$.

(a) Let $|n', \pm 1\rangle$, $n' = 0, 1, 2, \ldots$, be the common eigenvectors of $y^\dagger y$ and σ_z. Consider the subspace spanned by the eigenvectors $|n', +1\rangle$ and $|n'+1, -1\rangle$. Construct the matrix representation of the operator γ in this subspace by evaluating the elements in

$$\gamma = \begin{bmatrix} \langle n', +1|\gamma|n', +1\rangle & \langle n', +1|\gamma|n'+1, -1\rangle \\ \langle n'+1, -1|\gamma|n', +1\rangle & \langle n'+1, -1|\gamma|n'+1, -1\rangle \end{bmatrix}. \tag{7.11}$$

Solution:

$$\gamma = \begin{bmatrix} \epsilon & \sqrt{n'+1} \\ \sqrt{n'+1} & -\epsilon \end{bmatrix}. \tag{7.12}$$

(b) Find the eigenvalues of the operator γ. (Solution: $\pm\sqrt{\epsilon^2 + n' + 1}$.)

(c) Find the two normalized eigenvectors (upto a phase) of the operator γ in the subspace discussed above, and express them in terms of the respective common eigenvectors. In particular, show that

$$|\gamma' = +\rangle = \cos\frac{\alpha_n}{2}|n', +1\rangle + \sin\frac{\alpha_n}{2}|n'+1, -1\rangle, \tag{7.13a}$$

$$|\gamma' = -\rangle = -\sin\frac{\alpha_n}{2}|n', +1\rangle + \cos\frac{\alpha_n}{2}|n'+1, -1\rangle, \tag{7.13b}$$

where

$$\tan\alpha_n = \frac{\sqrt{n'+1}}{\epsilon}. \tag{7.14}$$

(d) Find the following probabilities:

$$p([\gamma_0 = +] \to [\gamma = +] \to [\gamma_0 = +]), \tag{7.15a}$$

$$p([\gamma_0 = +] \to [\gamma = +] \to [\gamma_0 = -]), \tag{7.15b}$$

$$p([\gamma_0 = +] \to [\gamma = -] \to [\gamma_0 = +]), \tag{7.15c}$$

$$p([\gamma_0 = +] \to [\gamma = -] \to [\gamma_0 = -]). \tag{7.15d}$$

Plot these probabilities as a function of ϵ, and as a function of n'.

Chapter 8

Angular momentum

8.1 Eigenvalues of angular momentum

1. (**20 points.**) The components J_i $(i = 1, 2, 3)$ of angular momentum $\mathbf{J}$ satisfy the commutation relations

$$\frac{1}{i\hbar}\big[J_i, J_j\big] = \varepsilon_{ijk} J_k. \tag{8.1}$$

The general properties of angular momentum can be deduced from these commutation relations. Since $\mathbf{J}^2$ is a scalar, it commutes with angular momentum $\mathbf{J}$. That is,

$$\big[\mathbf{J}\cdot\mathbf{J}, \mathbf{J}\big] = 0. \tag{8.2}$$

Thus, the common eigenvectors of $\mathbf{J}^2$ and J_z constitute a suitable set of basis vectors for discussing a dynamical system involving only the angular momentum. Let us denote the eigenvalues of these operators by the labeling scheme ${\mathbf{J}'}^2 = j(j+1)\hbar^2$, and ${J_z}' = m\hbar$. Thus, we write

$$\frac{1}{\hbar^2}\mathbf{J}^2|j,m\rangle = j(j+1)|j,m\rangle, \tag{8.3a}$$

$$\frac{1}{\hbar}J_z|j,m\rangle = m|j,m\rangle. \tag{8.3b}$$

Let us also construct (non-Hermitian) operators

$$J_\pm = J_x \pm iJ_y. \tag{8.4}$$

Observe that

$$J_\pm^\dagger = J_\mp. \tag{8.5}$$

(a) Show that

$$\frac{1}{\hbar}J_z\Big\{J_+|j,m\rangle\Big\} = (m+1)\Big\{J_+|j,m\rangle\Big\}. \tag{8.6}$$

Thus deduce that if m is an eigenvalue of J_z, then $(m+1)$ is also an eigenvlaue of J_z. Similarly, show that

$$\frac{1}{\hbar}J_z\Big\{J_-|j,m\rangle\Big\} = (m-1)\Big\{J_-|j,m\rangle\Big\}. \tag{8.7}$$

Thus deduce that if m is an eigenvalue of J_z, then $(m-1)$ is also an eigenvlaue of J_z.

(b) Show that

$$J_+J_- = \mathbf{J}^2 - J_z^2 + \hbar J_z \tag{8.8}$$

is a Hermitian operator. A Hermitian operator has real eigenvalues, but, since $J_+J_- = J_-^\dagger J_-$, infer further that it has non-negative eigenvalues. Thus, deduce that

$$j(j+1) - m(m-1) \geq 0, \tag{8.9}$$

and then infer
$$-j \leq m \leq j+1. \tag{8.10}$$
Similarly, show how that
$$J_-J_+ = \mathbf{J}^2 - J_z^2 - \hbar J_z \tag{8.11}$$
is a Hermitian operator, and deduce that
$$j(j+1) - m(m+1) \geq 0, \tag{8.12}$$
and then infer
$$-j-1 \leq m \leq j. \tag{8.13}$$
Using Eqs. (8.10) and (8.13) in conjunction, show that
$$-j \leq m \leq j. \tag{8.14}$$
(Refer Sec. 36 Dirac's QM book.)

(c) Using Eq. (8.14) infer that
$$j \geq 0. \tag{8.15}$$
Note that $\mathbf{J}^2$ being the square of a Hermitian operator implies $j(j+1) \geq 0$, but it does not imply that j should be non-negative.

(d) The $2j$ transitions from $m = -j$ to $m = j$ happen in $n = 0, 1, 2, \ldots$ steps. Thus, $2j = n$. Thus, conclude that
$$j = 0, \frac{1}{2}, 1, \frac{3}{2}, \ldots, \tag{8.16a}$$
$$m = -j, -j+1, \ldots, j. \tag{8.16b}$$

(e) Repeat the above analysis starting from the labeling scheme
$$\mathbf{J}'^2 = \beta\hbar^2, \quad \text{and} \quad J_z{}' = m\hbar. \tag{8.17}$$

8.2 Orbital anglular momentum

1. (**20 points.**) Orbital angular momentum $\mathbf{L}$ also transforms like angular momentum $\mathbf{J}$. (The eigenvalues of the orbital angular momentum are necessarily integers, because $m = 0$ is necessarily an allowed state due to the fact that $\mathbf{r} \cdot \mathbf{L} = 0$, corresponding to the fact that rotation about $\mathbf{r}$ has no effect. This rules out half-integral values for the eigenvalues.) The orbital angular momentum has the operator construction
$$\mathbf{L} = \mathbf{r} \times \mathbf{p}, \tag{8.18}$$
where $\mathbf{r}$ is the position operator and $\mathbf{p}$ is the linear momentum operator which satisfies the Heisenberg uncertainty relation
$$\frac{1}{i\hbar}\big[\mathbf{r}, \mathbf{p}\big] = \mathbf{1}. \tag{8.19}$$
Show that
$$\mathbf{L}^\dagger = -\mathbf{p} \times \mathbf{r}. \tag{8.20}$$
Evaluate
$$\mathbf{L} - \mathbf{L}^\dagger. \tag{8.21}$$
Is orbital angular momentum $\mathbf{L}$ self-adjoint (Hermitian)?
Caution: Use index notation to avoid pitfalls while using vector operators.

2. (**20 points.**) Using the commutation relations involving the position vector $\mathbf{r}$, the linear momentum vector $\mathbf{p}$, and the orbital angular momentum vector $\mathbf{L} = \mathbf{r} \times \mathbf{p}$, show that

$$\frac{1}{i\hbar}\big(\mathbf{p} \times \mathbf{L} + \mathbf{L} \times \mathbf{p}\big) = a\mathbf{p}, \tag{8.22}$$

where a is a number. Report the numerical value for a.
Caution: Using index notation might be less error prone here.

3. (**100 points.**) The angular momentum can be decomposed as

$$\mathbf{J} = \mathbf{S} + \mathbf{L}, \tag{8.23}$$

where $\mathbf{S}$ is the spin or internal angular momentum, and $\mathbf{L} = \mathbf{r} \times \mathbf{p}$ is the orbital or external angular momentum. For the case $\mathbf{S} = 0$ the eigenvalues of angular momentum are necessarily integer valued, because $\mathbf{r} \cdot \mathbf{L} = 0$. Let us denote the eigenvalues by the labeling scheme $\mathbf{L}'^2 = \hbar^2 l(l+1)$ and $L'_z = \hbar m$, such that

$$\mathbf{L}^2|l,m\rangle = \hbar^2 l(l+1)|l,m\rangle, \tag{8.24a}$$
$$L_z|l,m\rangle = \hbar m|l,m\rangle, \tag{8.24b}$$

where

$$l = 0, 1, 2, \ldots, \tag{8.25a}$$
$$m = -l, -l+1, \ldots, l. \tag{8.25b}$$

The eigenvectors of orbital angular momentum are suitably realized by functions on the surface of a unit sphere, coordinated by spherical polar coordinates θ' and ϕ' or the unit vector $\hat{\mathbf{r}}'$. These wavefunctions defined using the projections

$$\langle\hat{\mathbf{r}}'|l,m\rangle = Y_{lm}(\theta', \phi') \tag{8.26}$$

are the spherical harmonics.

(a) Show that in the position basis, here restricted to the surface of a unit sphere, we have

$$\langle\hat{\mathbf{r}}'|\mathbf{L}|\ \rangle = \langle\hat{\mathbf{r}}'|\mathbf{r} \times \mathbf{p}|\ \rangle = \frac{\hbar}{i}(\mathbf{r}' \times \boldsymbol{\nabla}')\langle\hat{\mathbf{r}}'|\ \rangle. \tag{8.27}$$

Using Eq. (8.27) in Eqs. (8.24) show that the differential equations for spherical harmonics are given by

$$-(\mathbf{r}' \times \boldsymbol{\nabla}') \cdot (\mathbf{r}' \times \boldsymbol{\nabla}')Y_{lm}(\theta', \phi') = l(l+1)Y_{lm}(\theta', \phi'), \tag{8.28a}$$
$$\frac{1}{i}\hat{\mathbf{z}}' \cdot (\mathbf{r}' \times \boldsymbol{\nabla}')Y_{lm}(\theta', \phi') = mY_{lm}(\theta', \phi'). \tag{8.28b}$$

(b) Show that the raising and lowering operators defined using

$$L_\pm = L_x \pm iL_y, \tag{8.29}$$

leading to raising and lowering operations

$$L_\pm|l,m\rangle = \hbar\sqrt{(l \mp m)(l \pm m + 1)}|l, m \pm 1\rangle, \tag{8.30}$$

correspond to the differential equations

$$\frac{1}{i}\Big[\hat{\mathbf{x}}' \cdot (\mathbf{r}' \times \boldsymbol{\nabla}') \pm i\hat{\mathbf{y}}' \cdot (\mathbf{r}' \times \boldsymbol{\nabla}')\Big]Y_{lm}(\theta', \phi') = \sqrt{(l \mp m)(l \pm m + 1)}Y_{l,m\pm1}(\theta', \phi'). \tag{8.31}$$

(c) Using the differential operator in spherical polar coordinates,

$$\boldsymbol{\nabla}' = \hat{\mathbf{r}}'\frac{\partial}{\partial r'} + \hat{\boldsymbol{\theta}}'\frac{1}{r'}\frac{\partial}{\partial\theta'} + \hat{\boldsymbol{\phi}}'\frac{1}{r'\sin\theta'}\frac{\partial}{\partial\phi'}, \tag{8.32}$$

where

$$\begin{aligned} \hat{\mathbf{r}}' &= \hat{\mathbf{x}}'\sin\theta'\cos\phi' + \hat{\mathbf{y}}'\sin\theta'\sin\phi' + \hat{\mathbf{z}}'\cos\theta', && (8.33a)\\ \hat{\boldsymbol{\theta}}' &= \hat{\mathbf{x}}'\cos\theta'\cos\phi' + \hat{\mathbf{y}}'\cos\theta'\sin\phi' - \hat{\mathbf{z}}'\sin\theta', && (8.33b)\\ \hat{\boldsymbol{\phi}}' &= -\hat{\mathbf{x}}'\sin\phi' + \hat{\mathbf{y}}'\cos\phi', && (8.33c) \end{aligned}$$

show that

$$\begin{aligned} \mathbf{r}'\times\boldsymbol{\nabla}' &= \hat{\boldsymbol{\phi}}'\frac{\partial}{\partial\theta'} - \hat{\boldsymbol{\theta}}'\frac{1}{\sin\theta'}\frac{\partial}{\partial\phi'} && (8.34a)\\ &= \hat{\mathbf{x}}'\left[-\sin\phi'\frac{\partial}{\partial\theta'} - \cos\phi'\cot\theta'\frac{\partial}{\partial\phi'}\right] + \hat{\mathbf{y}}'\left[\cos\phi'\frac{\partial}{\partial\theta'} - \sin\phi'\cot\theta'\frac{\partial}{\partial\phi'}\right] + \hat{\mathbf{z}}'\frac{\partial}{\partial\phi'}. && (8.34b) \end{aligned}$$

Thus, show the correspondence

$$\begin{aligned} L_z:&\quad \hat{\mathbf{z}}'\cdot\frac{\hbar}{i}(\mathbf{r}'\times\boldsymbol{\nabla}') = \frac{\hbar}{i}\frac{\partial}{\partial\phi'}, && (8.35a)\\ L_x:&\quad \hat{\mathbf{x}}'\cdot\frac{\hbar}{i}(\mathbf{r}'\times\boldsymbol{\nabla}') = \frac{\hbar}{i}\left[-\sin\phi'\frac{\partial}{\partial\theta'} - \cos\phi'\cot\theta'\frac{\partial}{\partial\phi'}\right], && (8.35b)\\ L_y:&\quad \hat{\mathbf{y}}'\cdot\frac{\hbar}{i}(\mathbf{r}'\times\boldsymbol{\nabla}') = \frac{\hbar}{i}\left[\cos\phi'\frac{\partial}{\partial\theta'} - \sin\phi'\cot\theta'\frac{\partial}{\partial\phi'}\right]. && (8.35c) \end{aligned}$$

Further, verify the correspondence

$$\begin{aligned} L^2:&\quad \frac{\hbar}{i}(\mathbf{r}'\times\boldsymbol{\nabla}')\cdot\frac{\hbar}{i}(\mathbf{r}'\times\boldsymbol{\nabla}') = \frac{\hbar^2}{i^2}\left[\frac{1}{\sin\theta'}\frac{\partial}{\partial\theta'}\sin\theta'\frac{\partial}{\partial\theta'} + \frac{1}{\sin^2\theta'}\frac{\partial^2}{\partial\phi'^2}\right], && (8.36a)\\ L_z^2:&\quad \frac{\hbar^2}{i^2}\Big[\hat{\mathbf{z}}'\cdot(\mathbf{r}'\times\boldsymbol{\nabla}')\Big]^2 = \frac{\hbar^2}{i^2}\frac{\partial^2}{\partial\phi'^2}, && (8.36b)\\ L_\pm:&\quad \frac{\hbar}{i}\Big[\hat{\mathbf{x}}'\cdot(\mathbf{r}'\times\boldsymbol{\nabla}') \pm i\hat{\mathbf{y}}'\cdot(\mathbf{r}'\times\boldsymbol{\nabla}')\Big] = \frac{\hbar}{i}e^{\pm i\phi}\left[\pm i\frac{\partial}{\partial\theta'} - \cot\theta'\frac{\partial}{\partial\phi'}\right], && (8.36c) \end{aligned}$$

(d) Thus, show that the eigenfunctions of angular momentum in the position basis, the spherical harmonics, satisfy the differential equations given by

$$\begin{aligned} L_z:&\quad \frac{1}{i}\frac{\partial}{\partial\phi'}Y_{lm}(\theta',\phi') = mY_{lm}(\theta',\phi'), && (8.37a)\\ L^2:&\quad -\left[\frac{1}{\sin\theta'}\frac{\partial}{\partial\theta'}\sin\theta'\frac{\partial}{\partial\theta'} + \frac{1}{\sin^2\theta'}\frac{\partial^2}{\partial\phi'^2}\right]Y_{lm}(\theta',\phi') = l(l+1)Y_{lm}(\theta',\phi'), && (8.37b)\\ L_\pm:&\quad \frac{i}{i}e^{\pm i\phi}\left[\pm i\frac{\partial}{\partial\theta'} - \cot\theta'\frac{\partial}{\partial\phi'}\right]Y_{lm}(\theta',\phi') = \sqrt{(l\mp m)(l\pm m+1)}Y_{l,m\pm1}(\theta',\phi'). && (8.37c) \end{aligned}$$

Further, verify

$$L_+L_-: \quad -\left[\frac{1}{\sin\theta'}\frac{\partial}{\partial\theta'}\sin\theta'\frac{\partial}{\partial\theta'} + \frac{1}{\sin^2\theta'}\frac{\partial^2}{\partial\phi'^2} - \frac{\partial^2}{\partial\phi'^2} - \frac{1}{i}\frac{\partial}{\partial\phi'}\right]Y_{lm}(\theta',\phi') = \big[l(l+1) - m(m-1)\big]Y_{lm}(\theta',\phi'), \tag{8.38a}$$

$$L_-L_+: \quad -\left[\frac{1}{\sin\theta'}\frac{\partial}{\partial\theta'}\sin\theta'\frac{\partial}{\partial\theta'} + \frac{1}{\sin^2\theta'}\frac{\partial^2}{\partial\phi'^2} - \frac{\partial^2}{\partial\phi'^2} + \frac{1}{i}\frac{\partial}{\partial\phi'}\right]Y_{lm}(\theta',\phi') = \big[l(l+1) - m(m+1)\big]Y_{lm}(\theta',\phi'), \tag{8.38b}$$

$$L_x^2 + L_y^2: \quad -\left[\frac{1}{\sin\theta'}\frac{\partial}{\partial\theta'}\sin\theta'\frac{\partial}{\partial\theta'} + \cot^2\theta'\frac{\partial^2}{\partial\phi'^2}\right]Y_{lm}(\theta',\phi') = \big[l(l+1) - m^2\big]Y_{lm}(\theta',\phi'). \tag{8.38c}$$

8.3 Linear vector space over a complex field

Problems

1. (**50 points.**) (Ref. Milton's notes.)

   (a) Consider three numerical vectors, **a**, **b**, **c**. Show that

   $$\mathbf{a}\times(\mathbf{b}\times\mathbf{c}) + \mathbf{b}\times(\mathbf{c}\times\mathbf{a}) + \mathbf{c}\times(\mathbf{a}\times\mathbf{b}) = 0. \tag{8.39}$$

   (b) Now consider operators A, B, C. Show that

   $$[A,[B,C]] + [B,[C,A]] + [C,[A,B]] = 0. \tag{8.40}$$

   (c) The multiplication property of the Pauli spin matrices can be written as

   $$(\boldsymbol{\sigma}\cdot\mathbf{a})(\boldsymbol{\sigma}\cdot\mathbf{b}) = \mathbf{a}\cdot\mathbf{b} + i\boldsymbol{\sigma}\cdot(\mathbf{a}\times\mathbf{b}). \tag{8.41}$$

   From this, show that

   $$\frac{1}{i\hbar}\left[\frac{\hbar}{2}\boldsymbol{\sigma}\cdot\mathbf{a}, \frac{\hbar}{2}\boldsymbol{\sigma}\cdot\mathbf{b}\right] = \frac{\hbar}{2}\boldsymbol{\sigma}\cdot(\mathbf{a}\times\mathbf{b}). \tag{8.42}$$

   (d) More generally, what is

   $$\frac{1}{i\hbar}[\mathbf{J}\cdot\mathbf{a}, \mathbf{J}\cdot\mathbf{b}]? \tag{8.43}$$

   (e) Use

   $$A = \frac{1}{2}\boldsymbol{\sigma}\cdot\mathbf{a}, \qquad B = \frac{1}{2}\boldsymbol{\sigma}\cdot\mathbf{b}, \qquad \text{and} \qquad C = \frac{1}{2}\boldsymbol{\sigma}\cdot\mathbf{c} \tag{8.44}$$

   in the result of problem (1b) to derive the result of problem (1a).

2. (**20 points.**) A vector operator **V** is defined by the transformation property

$$\frac{1}{i\hbar}[\mathbf{V}, \delta\boldsymbol{\omega}\cdot\mathbf{J}] = \delta\boldsymbol{\omega}\times\mathbf{V}, \tag{8.45}$$

which states the commutation relations of components of **V** with those of angular momentum **J**. Since a scalar operator S does not change under rotations it is defined by the corresponding transformation

$$\frac{1}{i\hbar}[S, \delta\boldsymbol{\omega}\cdot\mathbf{J}] = 0. \tag{8.46}$$

(a) Using Eq. (8.45), show that the scalar product of two vectors $\mathbf{V}_1$ and $\mathbf{V}_2$ is a scalar. That is,

$$\frac{1}{i\hbar}\left[\mathbf{V}_1\cdot\mathbf{V}_2, \delta\boldsymbol{\omega}\cdot\mathbf{J}\right] = 0. \tag{8.47}$$

(b) Using Eq. (8.45), show that the vector product of vectors $\mathbf{V}_1$ and $\mathbf{V}_2$ is a vector. That is,

$$\frac{1}{i\hbar}\left[\mathbf{V}_1\times\mathbf{V}_2, \delta\boldsymbol{\omega}\cdot\mathbf{J}\right] = \delta\boldsymbol{\omega}\times(\mathbf{V}_1\times\mathbf{V}_2). \tag{8.48}$$

(c) How does $\mathbf{V}_1\cdot(\mathbf{V}_2\times\mathbf{V}_3)$ transform?

(d) How does $\mathbf{V}_1\times(\mathbf{V}_2\times\mathbf{V}_3)$ transform?

3. (**20 points.**) Given that $\mathbf{V}_1$, $\mathbf{V}_2$, and $\mathbf{V}_3$, are operators that transform like a vector, what can you conclude about the commutation relation of the operator

$$\mathbf{V}_1\cdot(\mathbf{V}_2\times\mathbf{V}_3) \tag{8.49}$$

with angular momentum $\mathbf{J}$? That is,

$$\big[\mathbf{V}_1\cdot(\mathbf{V}_2\times\mathbf{V}_3), \mathbf{J}\big] = ? \tag{8.50}$$

4. (**50 points.**) For $j = 1$:

(a) Determine the matrix representantion for

$$J_z, J_x, J_y, J_+, J_-, \text{and } J^2. \tag{8.51}$$

For example,

$$J_z = \begin{bmatrix} \langle j,j|J_z|j,j\rangle & \langle j,j|J_z|j,j-1\rangle & \cdots & \langle j,j|J_z|j,-j\rangle \\ \langle j,j-1|J_z|j,j\rangle & \langle j,j-1|J_z|j,j-1\rangle & \cdots & \langle j,j-1|J_z|j,-j\rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle j,-j|J_z|j,j\rangle & \langle j,-j|J_z|j,j-1\rangle & \cdots & \langle j,-j|J_z|j,-j\rangle \end{bmatrix}. \tag{8.52}$$

(b) Evaluate

$$\text{Tr}(J_k), \quad \text{Tr}(J_kJ_l), \quad \text{and} \quad \text{Tr}(J_k^2J_l^2), \quad \text{for} \quad k,l = x,y,z. \tag{8.53}$$

5. (**20 points.**) Using the properties of Pauli matrices show that

$$(\boldsymbol{\sigma}\cdot\hat{\mathbf{n}})^2 = 1. \tag{8.54}$$

Then, prove the identity

$$e^{i\frac{\theta}{2}(\boldsymbol{\sigma}\cdot\hat{\mathbf{n}})} = \cos\frac{\theta}{2} + i(\boldsymbol{\sigma}\cdot\hat{\mathbf{n}})\sin\frac{\theta}{2}, \tag{8.55}$$

where $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ is a vector constructed out of Pauli matrices, and $\hat{\mathbf{n}}$ is an arbitrary (numerical) unit vector. This represents a unitary transformation due to a rotation by angle θ about the axis $\hat{\mathbf{n}}$ for a spin-$\frac{1}{2}$ particle. Show that the wavefunctions differ by a sign under a rotation of $\theta = 2\pi$. But, how can physical measurements differ for rotations of $\theta = 2\pi$? Show that it does not, because physical quantities involve product of two wave functions.

6. (**30 points.**) Consider the construction

$$K(\lambda) = e^{-\lambda A}Be^{\lambda A} \tag{8.56}$$

in terms of two operators A and B. Show that

$$\frac{\partial K}{\partial \lambda} = [K, A]. \tag{8.57}$$

Evaluate the higher derivatives

$$\frac{\partial^n K}{\partial \lambda^n} \tag{8.58}$$

recursively. Thus, using Taylor expansion around $\lambda = 0$, show that

$$K(\lambda) = B + \lambda [B, A] + \frac{\lambda^2}{2!}[[B, A], A] + \frac{\lambda^3}{3!}[[[B, A], A], A] + \ldots. \tag{8.59}$$

Then, for $\lambda = 1$, we have

$$e^{-A} B e^{A} = B + [B, A] + \frac{1}{2!}[[B, A], A] + \frac{1}{3!}[[[B, A], A], A] + \ldots. \tag{8.60}$$

This is the Baker-Campbell-Hausdorff formula.

7. (**20 points.**) Using the Baker-Campbell-Hausdorff formula,

$$e^{-A} B e^{A} = B + [B, A] + \frac{1}{2!}[[B, A], A] + \frac{1}{3!}[[[B, A], A], A] + \ldots \tag{8.61}$$

evaluate

$$e^{-\frac{i}{\hbar}\phi J_z} J_x e^{\frac{i}{\hbar}\phi J_z}, \tag{8.62}$$

where J_x, J_y, and J_z, are components of the angular momentum vector (operator), and ϕ is a number representing an angle of rotation.

8. (**40 points.**) Consider the following unitary transformations,

$$J_x(\phi) = e^{-\frac{i}{\hbar}\phi J_z} J_x e^{\frac{i}{\hbar}\phi J_z} \tag{8.63}$$

and

$$J_y(\phi) = e^{-\frac{i}{\hbar}\phi J_z} J_y e^{\frac{i}{\hbar}\phi J_z}. \tag{8.64}$$

By differentiating with respect to ϕ, and solving the resulting differential equations, derive

$$J_x(\phi) = J_x \cos\phi + J_y \sin\phi, \tag{8.65a}$$
$$J_y(\phi) = -J_x \sin\phi + J_y \cos\phi. \tag{8.65b}$$

Further, derive

$$J_+(\phi) = e^{-i\phi} J_+ \quad \text{and} \quad J_-(\phi) = e^{i\phi} J_-. \tag{8.66}$$

9. (**20 points.**) The transformation function relating the angular momentum eigenvectors between two coordinate frames, related by rotations described using Euler angles (ψ, θ, ϕ), is

$$\langle j, m | U(\psi, \theta, \phi) | j', m' \rangle = \delta_{jj'} e^{im\psi} U^{(j)}_{m,m'}(\theta) e^{im'\phi}, \tag{8.67}$$

where $U^{(j)}_{m,m'}(\theta)$ are generated by the relation

$$\frac{\bar{y}_+^{j+m}}{\sqrt{(j+m)!}} \frac{\bar{y}_-^{j-m}}{\sqrt{(j-m)!}} = \sum_{m'=-j}^{j} e^{im\psi} U^{(j)}_{m,m'}(\theta) e^{im'\phi} \frac{y_+^{j+m'}}{\sqrt{(j+m')!}} \frac{y_-^{j-m'}}{\sqrt{(j-m')!}}, \tag{8.68}$$

where

$$\begin{bmatrix} \bar{y}_+ \\ \bar{y}_- \end{bmatrix} = \begin{bmatrix} e^{i\frac{\psi}{2}} \cos\frac{\theta}{2} e^{i\frac{\phi}{2}} & e^{i\frac{\psi}{2}} \sin\frac{\theta}{2} e^{-i\frac{\phi}{2}} \\ -e^{-i\frac{\psi}{2}} \sin\frac{\theta}{2} e^{i\frac{\phi}{2}} & e^{-i\frac{\psi}{2}} \cos\frac{\theta}{2} e^{-i\frac{\phi}{2}} \end{bmatrix} \begin{bmatrix} y_+ \\ y_- \end{bmatrix}. \tag{8.69}$$

The above transformation function gives the probability amplitude relating measurements of angular momentum, or magnetic dipole moment, in two different directions related by the Euler angles.

(a) Extract the probability amplitudes relating measurements of angular momentum for $j = \frac{3}{2}$.

(b) Extract the probabilities

$$p(m, m'; \theta) = |\langle j, m|U(\psi, \theta, \phi)|j', m'\rangle|^2 \tag{8.70}$$

relating measurements of angular momentum for $j = \frac{3}{2}$.

Chapter 9

Spin assembly

9.1 Harmonic oscillator

Harmonic oscillator is decribed by the number operator

$$n_a = a^\dagger a \tag{9.1}$$

and the commutation relation

$$\left[a, a^\dagger\right] = 1 \tag{9.2}$$

constructed out of a non-Hermitian operator a and it's Hermitian conjugate $a^\dagger$. A suitable basis is the eigenbasis of the number operator, labeled by $n'_a = 0, 1, 2, \ldots$, and characterized by raising and lowering operations

$$a^\dagger |n'_a\rangle = \sqrt{n'_a + 1}|n'_a\rangle, \tag{9.3a}$$

$$a|n'_a\rangle = \sqrt{n'_a}|n'_a\rangle. \tag{9.3b}$$

Chapter 10

Angular momentum addition

10.1 Angular momentum addition

Composition of two uncoupled angular momentum $\mathbf{J}_1$ and $\mathbf{J}_2$ are described by the relations

$$\mathbf{J} = \mathbf{J}_1 + \mathbf{J}_2 \tag{10.1}$$

and

$$\mathbf{J}_z = \mathbf{J}_{1z} + \mathbf{J}_{2z}. \tag{10.2}$$

They can be represented in the eigenbasis built from the product of individual angular momentum states

$$|j_1, m_1\rangle_{①} |j_2, m_2\rangle_{②}, \tag{10.3}$$

and in eigenbasis built from the sum of the total angular momentum states

$$|j_1, j_2; j, m\rangle. \tag{10.4}$$

The subscripts ① and ② might seem reduntant, but it is beneficial when m_1 and m_2 take on specific values. For example, the subscripts in the state $|3,1\rangle_{①}|1,0\rangle_{②}$ are helpful unless we specify that the first ket is associated to the first angular momentum and the second ket is with the second angular momentum.

We shall use a shorthand notation where we supress j_1 and j_2, that is,

$$|j_1, m_1\rangle_{①} |j_2, m_2\rangle_{②} \to |m_1\rangle_{①} |m_2\rangle_{②}, \tag{10.5a}$$

$$|j_1, j_2; j, m\rangle \to |j, m\rangle. \tag{10.5b}$$

For given j_1 and j_2, the first individual angular momentum has $(2j_1 + 1)$ states and the second individual angular momentum has $(2j_2 + 1)$ states, such that the product of the individual angular momentum states have a total of $(2j_1 + 1)(2j_2 + 1)$ states. For given j_1 and j_2, the allowed total angular momentum states are

$$|j_1 - j_2| \leq j \leq j_1 + j_2 \tag{10.6}$$

so that they total

$$\sum_{j=|j_1-j_2|}^{j_1+j_2} (2j+1) = (2j_1 + 1)(2j_2 + 1). \tag{10.7}$$

Problems

1. (**20 points.**) A composite system is built out of two angular momenta $j_1 = 7, j_2 = \frac{3}{2}$. Determine the total number of angular momentum states for the composite system.

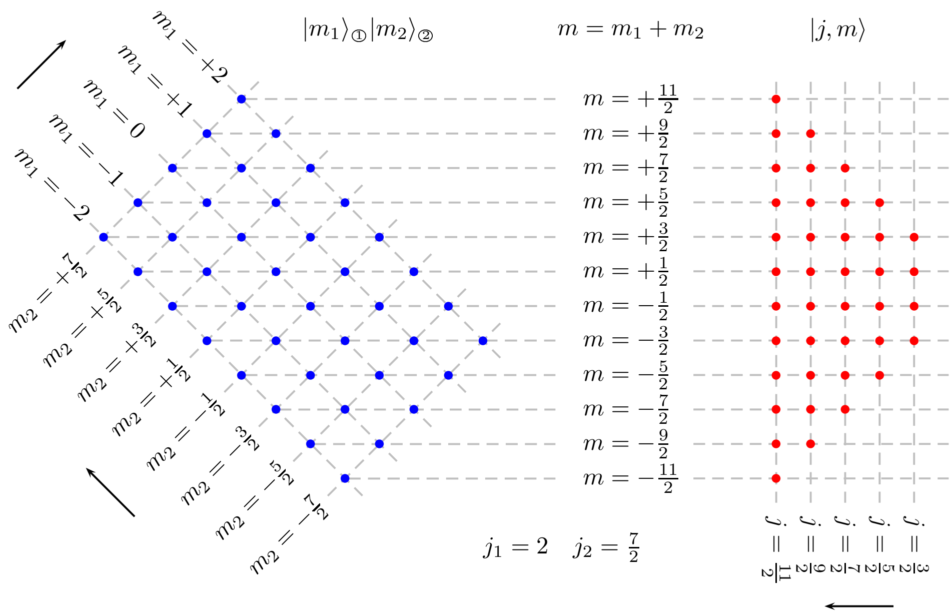

Figure 10.1: Product of individual angular momentum states $|m_1\rangle_{①}|m_2\rangle_{②}$ (in blue) versus sum of total angular momentum states $|j, m\rangle$ (in red) for $j_1 = 2$ and $j_2 = \frac{7}{2}$. The states on the same horizontal line in the figure satisfy $m = m_1 + m_2$. Each of the pruduct states in blue can be written as a linear combination of the sum states in red on the same horizontal line.

2. (**20 points.**) We constructed the total angular momentum states of two spin-$\frac{1}{2}$ systems, $j_1 = \frac{1}{2}$, $j_2 = \frac{1}{2}$, by beginning with the total angular momentum state

$$|1, 1\rangle = \left|\frac{1}{2}, \frac{1}{2}\right\rangle_{①} \left|\frac{1}{2}, \frac{1}{2}\right\rangle_{②} \tag{10.8}$$

and using the lowering operator to construct the $|1, 0\rangle$ and $|1, -1\rangle$ states. The state $|0, 0\rangle$ was then constructed (to within a phase factor) as the state orthogonal to $|1, 0\rangle$.

(a) Repeat this exercise by beginning with the total angular momentum state $|1, -1\rangle$ and using the raising operator to construct $|1, 0\rangle$ and $|1, 1\rangle$ states.

(b) Investigate the property of the total angular momentum states under the interchange ①↔②. In particular, find out if each of the total angular momentum states are symmetrical (do not change sign) or antisymmetrical (change sign).

3. (**40 points.**) Let us construct the total angular momentum states for the composite system built out of two angular momenta $j_1 = 2, j_2 = \frac{1}{2}$.

(a) Determine the total number of states by counting the individual states,

$$\left(\sum_{m_1=-j_1}^{j_1}\right)\left(\sum_{m_2=-j_2}^{j_2}\right). \tag{10.9}$$

Repeat this by counting the number of total angular momentum states,

$$\sum_{j=|j_1-j_2|}^{j_1+j_2} \sum_{m=-j}^{j}. \tag{10.10}$$

Particle	$\|T, T_3\rangle$	Q
proton	$\|\frac{1}{2}, \frac{1}{2}\rangle$	1
neutron	$\|\frac{1}{2}, -\frac{1}{2}\rangle$	0
$\boldsymbol{\pi}^+$	$\|1, 1\rangle$	1
$\boldsymbol{\pi}^0$	$\|1, 0\rangle$	0
$\boldsymbol{\pi}^-$	$\|1, -1\rangle$	-1

Table 10.1: Isospin assignments for particles.

(b) Beginning with $|5/2, 5/2\rangle$ use the lowering operator to build five other states with $j = 5/2$.

(c) Construct $|3/2, 3/2\rangle$ state by requiring it to be orthogonal to $|5/2, 3/2\rangle$, and be normalized.

(d) Beginning with $|3/2, 3/2\rangle$ use the lowering operator to build three other states with $j = 3/2$.

4. (**20 points.**) Construct the total angular momentum state $|3, 3\rangle$ for the composite system built out of two angular momenta $j_1 = 3, j_2 = 1$.

5. (**20 points.**) Construct the total angular momentum state $|N, N\rangle$ for the composite system built out of two angular momenta $j_1 = N$ and $j_2 = 1$.

6. (**60 points.**) Construct the total angular momentum state $|1, 1\rangle$ for the composite system built out of two angular momenta $j_1 = 2, j_2 = 1$. Investigate the property of this state under the interchange ①↔②.

7. (**20 points.**) Construct the total angular momentum state $|68, -67\rangle$ for the composite system built out of two angular momenta $j_1 = 31, j_2 = 37$.

8. (**20 points.**) (Schwinger's QM book, Prob. 3-4a.) Iso(topic) spin T: The nucleon is a particle of isospin $T = \frac{1}{2}$; the state with $T_3 = \frac{1}{2}$ is the proton (p), the state with $T_3 = -\frac{1}{2}$ is the neutron (n). Electric charge of a nucleon is given by $Q = \frac{1}{2} + T_3$. The $\boldsymbol{\pi}$ meson, or pion, has isospin $T = 1$, and electric charge $Q = T_3$, so there are three kinds of pions with different electric charge: $T_3 = 1$ ($\boldsymbol{\pi}^+$), $T_3 = 0$ ($\boldsymbol{\pi}^0$), $T_3 = -1$ ($\boldsymbol{\pi}^-$). (Refer Table 10.1.)

   Consider the system of a nucleon and a pion. The electric charge of this system is $Q = \frac{1}{2} + T_3$. Check that a system of charge 2, $T_3 = \frac{3}{2}$, is p+$\boldsymbol{\pi}^+$, according to the isospin assignments. Now, if the system is in the state $T = \frac{3}{2}$, $T_3 = \frac{1}{2}$, what is the probability of finding a proton? What is the accompanying $\boldsymbol{\pi}$-meson?

Chapter 11

Perturbation theory

11.1 Solutions to algebraic equations

1. (**30 points.**) Find the two roots of the quadratic equation

$$\varepsilon x^2 - x + 1 = 0. \tag{11.1}$$

Show that the series expansion of the roots in the variable ε are

$$x = \begin{cases} 1 + \varepsilon + \mathcal{O}(\varepsilon)^2, \\ \dfrac{1}{\varepsilon} - 1 + \mathcal{O}(\varepsilon). \end{cases} \tag{11.2}$$

Let us treat the quadratic equation in Eq. (11.1) as a perturbation to the trivial equation

$$x_0 = 1, \tag{11.3}$$

obtained by setting $\varepsilon = 0$ in Eq. (11.1). To find the roots to the leading order in the perturbation parameter ε we use the ansatz

$$x = x_0 + a_1\varepsilon + \mathcal{O}(\varepsilon)^2. \tag{11.4}$$

Substitute Eq. (11.4) in Eq. (11.1) to show that $a_1 = 1$. Thus, we learn that

$$x = 1 + \varepsilon + \mathcal{O}(\varepsilon)^2, \tag{11.5}$$

which is indeed one of the root, to the leading order in ε. What about the other root? To this end, let us make the change of variables using the substitution

$$x = \frac{y}{\varepsilon}. \tag{11.6}$$

Show that this leads to the quadratic equation

$$y^2 - y + \varepsilon = 0. \tag{11.7}$$

The unperturbed equation, obtained by setting $\varepsilon = 0$, is

$$y_0^2 - y_0 = 0, \tag{11.8}$$

whose roots are $y_0 = 0, 1$. Use the ansatz

$$y = y_0 + b_1\varepsilon + b_2\varepsilon^2 + \mathcal{O}(\varepsilon)^3 \tag{11.9}$$

to derive

$$b_1 = \frac{1}{1 - 2y_0}, \quad b_2 = \frac{b_1^2}{1 - 2y_0}. \tag{11.10}$$

Thus, reproduce the results in Eq. (11.2), this time using the techniques of perturbation theory.

(a) Using the ideas described above find the three roots of the cubic equation

$$\varepsilon x^3 - x + 1 = 0, \tag{11.11}$$

to the leading order in ε.
Solution:

$$x = \begin{cases} 1 + \varepsilon + \mathcal{O}(\sqrt{\varepsilon})^3, \\ \pm\dfrac{1}{\sqrt{\varepsilon}} - \dfrac{1}{2} + \mathcal{O}(\sqrt{\varepsilon}). \end{cases} \tag{11.12}$$

(b) Using the ideas described above find the five roots of the quintic equation

$$\varepsilon x^5 - x + 1 = 0, \tag{11.13}$$

to the leading order in ε. Abel's impossibility theorem rules out algebraic solutions to general quintic equations. Verify your solutions for $\varepsilon = 0.01, 0.001, 0.0001$, say using Mathematica. Most often, when a system is disturbed by a small perturbation (parameter ε) the solutions converge to the unperturbed solutions for smaller ε's. Is that the case here?
Solution:

$$y_0 = 0, \pm 1, \pm i, \quad b_1 = \frac{1}{1 - 5y_0^4}, \quad x = \begin{cases} 1 + \varepsilon + \mathcal{O}(\sqrt{\varepsilon})^{\frac{5}{4}}, \\ \pm\dfrac{1}{\varepsilon^{\frac{1}{4}}} - \dfrac{1}{4} + \mathcal{O}(\varepsilon)^{\frac{1}{4}}, \\ \pm\dfrac{i}{\varepsilon^{\frac{1}{4}}} - \dfrac{1}{4} + \mathcal{O}(\varepsilon)^{\frac{1}{4}}. \end{cases} \tag{11.14}$$

2. (**20 points.**) Consider the eigenvalue problem for a Hermitian matrix A,

$$A|A'\rangle = A'|A'\rangle, \tag{11.15}$$

where $|A'\rangle$ form an orthonormal set of eigenfunctions. Variation, with respect to an arbitrary parameter, δA in the operator leads to the relation

$$\delta A|A'\rangle + A\delta|A'\rangle = \delta A'|A'\rangle + A'\delta|A'\rangle. \tag{11.16}$$

(a) Thus, derive the variation in the eigenvalue $\delta A'$ to be given by

$$\delta A' = \langle A'|\delta A|A'\rangle, \tag{11.17}$$

(b) and the variation in the eigenfunction $\delta|A'\rangle$, given in terms of its projection on the original eigenfunctions, to be

$$\langle A''|\delta\left(|A'\rangle\right) = \frac{\langle A''|\delta A|A'\rangle}{A' - A''}, \qquad A' \neq A''. \tag{11.18}$$

In particular, we can express the variation in the eigenfunction in terms of the original eigenfunctions as

$$\delta|A'\rangle = \sum_{A''} |A''\rangle\langle A''| \left(\delta|A'\rangle\right). \tag{11.19}$$

Further, since

$$\delta\langle A'|A'\rangle = 0, \tag{11.20}$$

one chooses

$$\langle A'|\delta\left(|A'\rangle\right) = 0. \tag{11.21}$$

3. (**20 points.**) Show that the matrix

$$A = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \tag{11.22}$$

has eigenvalues $A'_1 = e^{+i\theta}$ and $A'_2 = e^{-i\theta}$, and the corresponding eigenfunctions

$$|A'_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix} \quad \text{and} \quad |A'_2\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \end{pmatrix}. \tag{11.23}$$

Consider the perturbation

$$A + \delta A = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} + \alpha \begin{pmatrix} -\sin\theta & \cos\theta \\ -\cos\theta & -\sin\theta \end{pmatrix}. \tag{11.24}$$

Determine the eigenvalues and eigenfunctions of $A + \delta A$ to the leading order in α.
Solution: Eigenvalues:

$$A'_1 + \delta A'_1 = (1 + i\alpha)e^{+i\theta}, \qquad A'_2 + \delta A'_2 = (1 - i\alpha)e^{+i\theta}. \tag{11.25}$$

Eigenfunctions: $\delta|A'_1\rangle = \delta|A'_2\rangle = 0$.

4. (**20 points.**) Consider the unperturbed Hamiltonian to be

$$H = \omega J_z, \tag{11.26}$$

where $\mathbf{J}$ is the angular momentum. Let $j = 1/2$. Further, choose units such that $\omega = 1$. Consider the perturbation

$$H + \delta H = J_z + \alpha J_x. \tag{11.27}$$

Determine the eigenvalues and eigenfunctions of $H + \delta H$ to the leading order in α. Further, verify that the eigenfunctions are orthonormal upto the leading order in α.
Solution: Eigenvalues: $\delta H'_1 = \delta H'_2 = 0$. Eigenfunctions:

$$|+\rangle + \delta|+\rangle = |+\rangle + \frac{\alpha}{2}|-\rangle, \tag{11.28}$$

$$|-\rangle + \delta|-\rangle = |-\rangle - \frac{\alpha}{2}|+\rangle. \tag{11.29}$$

5. (**20 points.**) Consider the operator

$$\gamma = \sigma_x, \tag{11.30}$$

and the same operator with a perturbation

$$\bar{\gamma} = \gamma + \delta\gamma = \sigma_x + \epsilon\,\sigma_z. \tag{11.31}$$

(a) Find the eigenvalues of the operator γ to be $\gamma' = \pm 1$, and the respective eigenvectors to be

$$|\gamma' = +\rangle = |\sigma'_x = +\rangle = \frac{1}{\sqrt{2}}|\sigma'_z = +\rangle + \frac{1}{\sqrt{2}}|\sigma'_z = -\rangle, \tag{11.32a}$$

$$|\gamma' = -\rangle = |\sigma'_x = -\rangle = -\frac{1}{\sqrt{2}}|\sigma'_z = +\rangle + \frac{1}{\sqrt{2}}|\sigma'_z = -\rangle. \tag{11.32b}$$

(b) Determine the eigenvalues of $\bar{\gamma}$ to be

$$\bar{\gamma}' = \pm\sqrt{1 + \epsilon^2}, \tag{11.33}$$

and the respective eigenvectors to be

$$|\bar{\gamma}' = +\rangle = +\cos\frac{\alpha}{2}|\sigma'_z = +\rangle + \sin\frac{\alpha}{2}|\sigma'_z = -\rangle, \tag{11.34a}$$

$$|\bar{\gamma}' = -\rangle = -\sin\frac{\alpha}{2}|\sigma'_z = +\rangle + \cos\frac{\alpha}{2}|\sigma'_z = -\rangle, \tag{11.34b}$$

where

$$\tan\alpha = \frac{1}{\epsilon}. \tag{11.35}$$

(c) Determine the eigenvalues to order ϵ to be

$$\bar{\gamma}' = \pm 1 + \mathcal{O}(\epsilon)^2, \tag{11.36}$$

and eigenvectors of $\bar{\gamma}$ to order ϵ to be

$$|\bar{\gamma}' = +\rangle = |\gamma' = +\rangle - \frac{\epsilon}{2}|\gamma' = -\rangle + \mathcal{O}(\epsilon)^2, \tag{11.37a}$$

$$|\bar{\gamma}' = -\rangle = |\gamma' = -\rangle + \frac{\epsilon}{2}|\gamma' = +\rangle + \mathcal{O}(\epsilon)^2. \tag{11.37b}$$

Hint: Show that

$$\cos\frac{\alpha}{2} = \sqrt{\frac{\sqrt{1+\epsilon^2}+\epsilon}{2\sqrt{1+\epsilon^2}}} \approx \frac{1}{\sqrt{2}}\left(1+\frac{\epsilon}{2}\right), \tag{11.38a}$$

$$\sin\frac{\alpha}{2} = \sqrt{\frac{\sqrt{1+\epsilon^2}-\epsilon}{2\sqrt{1+\epsilon^2}}} \approx \frac{1}{\sqrt{2}}\left(1-\frac{\epsilon}{2}\right). \tag{11.38b}$$

(d) Show that

$$\sigma_z|\gamma' = +\rangle = -|\gamma' = -\rangle, \tag{11.39a}$$

$$\sigma_z|\gamma' = -\rangle = -|\gamma' = +\rangle. \tag{11.39b}$$

(e) Determine the eigenvalues and eigenvectors of $\bar{\gamma}$ to order ϵ using perturbation theory. Compare your results with the results above.

Chapter 12

Hydrogen atom

12.1 Classical hydrogen atom

Problems

1. (**20 points.**) An ellipse is defined as the locus of all points whose distance from a line (the directrix) and distance from a point (the focus) are such that the ratio of the distance to the focus to the distance to the directrix is a constant (the eccentricity). Let us choose the focus to be on the x-axis with coordinates $(-f, 0)$. Let us choose the directrix to be parallel to the y-axis and passing through the point $(-d, 0)$.

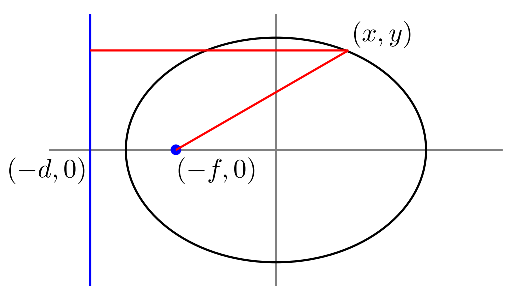

Figure 12.1: Ellipse

(a) Show that the definition of ellipse corresponds to the equation

$$(x + f)^2 + y^2 = \varepsilon^2 (x + d)^2, \tag{12.1}$$

where ε is the eccentricity.

(b) Identify the points $(\pm a, 0)$, and $(0, b)$, on the ellipse, in terms of the semi-major axis a and semi-minor axis b of the ellipse. These points correspond to the relations

$$(a + f)^2 = \varepsilon^2 (a + d)^2, \tag{12.2a}$$

$$(-a + f)^2 = \varepsilon^2 (-a + d)^2, \tag{12.2b}$$

$$f^2 + b^2 = \varepsilon^2 d^2. \tag{12.2c}$$

Thus, derive the defining relations for the focus f, the directrix d, and the eccentricity ε, in terms of

a and b to be

$$f = \sqrt{a^2 - b^2}, \tag{12.3a}$$

$$d = \frac{a^2}{f} = \frac{a^2}{\sqrt{a^2 - b^2}}, \tag{12.3b}$$

$$\varepsilon = \frac{f}{a} = \frac{\sqrt{a^2 - b^2}}{a}. \tag{12.3c}$$

(c) Rewrite the equation of an ellipse as

$$\frac{x^2}{a^2} + \frac{y^2}{b^2} = 1. \tag{12.4}$$

2. (**20 points.**) The equation of an ellipse in Cartesian coordinates, when the center of the ellipse is chosen as origin, is given by the equation

$$\frac{x^2}{a^2} + \frac{y^2}{b^2} = 1, \tag{12.5}$$

where a is the semi-major axis and b is the semi-minor axis. The equation of an ellipse in polar coordinates, when the one of the foci is chosen as the origin, is given by the equation

$$r(\theta) = \frac{r_0}{1 - \varepsilon \cos\theta}, \tag{12.6}$$

where r_0 is the semi-latus rectum and ε is the eccentricity of the ellipse.

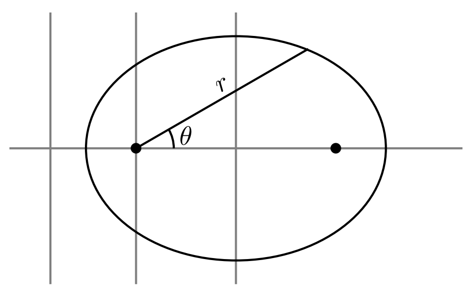

Figure 12.2: Ellipse

(a) Show that

$$a = \frac{r(0) + r(\pi)}{2} = \frac{r_0}{1 - \varepsilon^2}. \tag{12.7}$$

(b) Observe that for the point on the ellise representing the semi-minor axis we have $r \cos\theta|_{\theta=\theta_b} = f$ and $r(\theta_b) = a$. Thus, show that

$$b = \frac{r_0}{\sqrt{1 - \varepsilon^2}}. \tag{12.8}$$

(c) Further, show that

$$f = r(0) - a = \frac{r_0 \varepsilon}{1 - \varepsilon^2}, \tag{12.9a}$$

$$d = \frac{a^2}{f} = \frac{1}{\varepsilon} \frac{r_0}{(1 - \varepsilon^2)}. \tag{12.9b}$$

3. (**20 points.**) Verify that

$$\mathbf{L}\times\mathbf{L} = \begin{cases} 0 & \text{in classical mechanics,} \\ i\hbar\,\mathbf{L} & \text{in quantum mechanics.} \end{cases} \tag{12.10}$$

What about $\mathbf{p}\times\mathbf{p}$? In general, if

$$\frac{1}{i\hbar}\big[\mathbf{A},\mathbf{B}\big] = \mathbf{C}, \tag{12.11}$$

where $\mathbf{A}$ and $\mathbf{B}$ are vectors and $\mathbf{C}$ is a tensor, express

$$\mathbf{V} = \mathbf{A}\times\mathbf{B} + \mathbf{B}\times\mathbf{A} \tag{12.12}$$

in terms of $\mathbf{C}$.
Hint: Use index notation.

4. (**20 points.**) Show that, if $\mathbf{r}$ and $\mathbf{p}$ are Hermitian, the operator construction for angular momentum

$$\mathbf{L} = \mathbf{r}\times\mathbf{p} \tag{12.13}$$

is also Hermitian. Show that the symmetric construction

$$\mathbf{L} = \frac{1}{2}\Big[(\mathbf{r}\times\mathbf{p}) + (\mathbf{r}\times\mathbf{p})^\dagger\Big] \tag{12.14}$$

is also Hermitian. Evaluate the measure of non-commutativity of the angular momentum operator by evaluating

$$\frac{1}{2}\Big[(\mathbf{r}\times\mathbf{p}) - (\mathbf{r}\times\mathbf{p})^\dagger\Big]. \tag{12.15}$$

5. (**20 points.**) The components of the position and momentum operator, $\mathbf{r}$ and $\mathbf{p}$, respectively, satisfy the commutation relations $[r_i, p_j] = i\hbar\delta_{ij}$. Verify the following:

   (a) $\mathbf{r}\times\mathbf{p} + \mathbf{p}\times\mathbf{r} = 0$.

   (b) $\mathbf{r}\cdot\mathbf{p} - \mathbf{p}\cdot\mathbf{r} = 3i\hbar$.

   (c) $(\mathbf{a}\cdot\mathbf{r})(\mathbf{b}\cdot\mathbf{p}) - (\mathbf{b}\cdot\mathbf{p})(\mathbf{a}\cdot\mathbf{r}) = i\hbar(\mathbf{a}\cdot\mathbf{b})$, where $\mathbf{a}$ and $\mathbf{b}$ and numerical.

   (d) $\mathbf{r}\times(\mathbf{r}\times\mathbf{p}) = \mathbf{r}\,\mathbf{p}\cdot\mathbf{r} - \mathbf{p}r^2 + i\hbar\mathbf{r}$.

6. (**10 points.**) The components of the position and momentum operator, $\mathbf{r}$ and $\mathbf{p}$, respectively, satisfy the commutation relations $[r_i, p_j] = i\hbar\delta_{ij}$. Evaluate

$$r^2\,\mathbf{p} - \mathbf{p}\,r^2. \tag{12.16}$$

7. (**20 points.**) Evaluate the commutation relation between $1/r$, the inverse of the magnitude of the position operator $\mathbf{r}$, and the angular momentum operator $\mathbf{L}$,

$$\Big[\frac{1}{r},\mathbf{L}\Big], \tag{12.17}$$

which is encountered, for example, in the analysis of hydrogen atom.

8. (**20 points.**) Using commutation relations between $\mathbf{r}$, $\mathbf{p}$, and $\mathbf{L}$, verify the following:

   (a) $\mathbf{L}\times\mathbf{L} = i\hbar\mathbf{L}$.

   (b) $\mathbf{p}\times\mathbf{L} + \mathbf{L}\times\mathbf{p} = 2i\hbar\mathbf{p}$.

   (c) $-\mathbf{L}\times\mathbf{p}\cdot\dfrac{\mathbf{r}}{r} = L^2\dfrac{1}{r} = \dfrac{1}{r}L^2$.

   (d) $\mathbf{p}\times\mathbf{L}\cdot\mathbf{p} = 2i\hbar\,p^2$.

9. (**20 points.**) Verify the following equation of motion for the hydrogen atom,

$$\frac{1}{i\hbar}[\mathbf{p}, H] = -\frac{Ze^2\mathbf{r}}{r^3}, \tag{12.18}$$

where the Hamiltonian is

$$H = \frac{p^2}{2\mu} - \frac{Ze^2}{r}. \tag{12.19}$$

10. (**20 points.**) Verify that the axial vector,

$$\mathbf{A} = \frac{\mathbf{r}}{r} - \frac{1}{\mu Ze^2}\frac{1}{2}(\mathbf{p}\times\mathbf{L} - \mathbf{L}\times\mathbf{p}), \tag{12.20}$$

satisfies

$$\mathbf{A}\cdot\mathbf{L} = 0 \qquad \text{and} \qquad \mathbf{L}\cdot\mathbf{A} = 0. \tag{12.21}$$

11. (**10 points.**) Using commutation relations between position **r** momentum **p**, verify the relation

$$\mathbf{r}\cdot\mathbf{p} \,-\, \mathbf{p}\cdot\mathbf{r} = c\, i\hbar, \tag{12.22}$$

where c is a number. Determine c.

12. (**30 points.**) Using commutation relations between position **r**, linear momentum **p**, and angular momentum **L**, verify the relation

$$\mathbf{p}\times\mathbf{L}\cdot\mathbf{p} = c\, i\hbar\, p^2, \tag{12.23}$$

where c is a number. Determine c.

13. (**30 points.**) Using commutation relations between **r**, **p**, and **L**, verify the relation

$$\mathbf{p}\times\mathbf{L}\cdot\mathbf{p} = 2i\hbar\, p^2. \tag{12.24}$$

Thus, verify that either of the three equalities for

$$\mathbf{M} = -\frac{1}{2}\,(\mathbf{p}\times\mathbf{L} - \mathbf{L}\times\mathbf{p}) = -\mathbf{p}\times\mathbf{L} + i\hbar\mathbf{p} = \mathbf{L}\times\mathbf{p} - i\hbar\mathbf{p} \tag{12.25}$$

leads to

$$M^2 = (L^2 + \hbar^2)p^2. \tag{12.26}$$

This ensures that either of the following three expressions for the Axial vector

$$\mathbf{A} \;=\; \hat{\mathbf{r}} - \frac{1}{\mu Ze^2}\frac{1}{2}\,(\mathbf{p}\times\mathbf{L} - \mathbf{L}\times\mathbf{p}) \tag{12.27a}$$

$$= \hat{\mathbf{r}} - \frac{1}{\mu Ze^2}\mathbf{p}\times\mathbf{L} + \frac{i\hbar}{\mu Ze^2}\mathbf{p} \tag{12.27b}$$

$$= \hat{\mathbf{r}} + \frac{1}{\mu Ze^2}\mathbf{L}\times\mathbf{p} - \frac{i\hbar}{\mu Ze^2}\mathbf{p} \tag{12.27c}$$

leads to

$$A^2 = 1 + \frac{2(L^2+\hbar^2)H}{\mu Z^2e^4}. \tag{12.28}$$

After using the Bohr quantization condition $L = n'\,\hbar$, where $n' = 0, 1, 2, \ldots$, and presuming that the orbit is a circle that has eccentricity $A = 0$, Eq. (12.28) leads to the energy levels predicted by the Bohr model,

$$H = -\frac{\mu Z^2 e^4}{\hbar^2}\frac{1}{2n^2}, \qquad n = 1, 2, 3, \ldots. \tag{12.29}$$

Show that the (classical) analysis of hydrogen atom, (that does not accommodate the Heisenberg uncertainty relation contained in the commutation relations between **r** and **p**,) in addition, admits the $n = 0$ energy state which permits orbits of vanishing radius.

14. (**20 points.**) Consider the Hamiltonian

$$H = \frac{p^2}{2\mu} + V(\mathbf{r}). \tag{12.30}$$

Under what conditions is $r = |\mathbf{r}|$ a conserved quantity? Describe the path of motion when r is a conserved quantity.

15. (**50 points.**) (Let $\hbar = 0$. That is, we are discussing a classical hydrogenic atom.) The Hamiltonian for a hydrogenic atom is

$$H(\mathbf{r}, \mathbf{p}) = \frac{p^2}{2\mu} - \frac{Ze^2}{r}. \tag{12.31}$$

The Hamiltonian H, the angular momentum $\mathbf{L} = \mathbf{r} \times \mathbf{p}$, and the axial vector $\mathbf{A}$, are conserved quantities for a hydrogenic atom.

(a) Show that

$$\mathbf{W} = \frac{\mu Z e^2}{L^2} \mathbf{A} \times \mathbf{L} \tag{12.32}$$

is also a conserved quantity. That is, show that $d\mathbf{W}/dt = 0$. Thus, together, the vectors $\mathbf{L}$, $\mathbf{A}$, and $\mathbf{W}$, form an orthogonal set that remain fixed in time. Show that the vector $\mathbf{W}$ can be expressed in the form

$$\mathbf{W} = \mathbf{p} + \frac{\mu Z e^2}{L^2} \hat{\mathbf{r}} \times \mathbf{L}. \tag{12.33}$$

Further, show that

$$W = \mu Z e^2 \frac{A}{L}. \tag{12.34}$$

(b) Determine the components of the momentum $\mathbf{p}$ along these orthogonal vectors by evaluating $(\mathbf{p} \cdot \hat{\mathbf{L}})$, $(\mathbf{p} \cdot \hat{\mathbf{A}})$, and $(\mathbf{p} \cdot \hat{\mathbf{W}})$. Thus, construct the momentum $\mathbf{p}$ in the form

$$\mathbf{p} = (\mathbf{p} \cdot \hat{\mathbf{L}})\, \hat{\mathbf{L}} + (\mathbf{p} \cdot \hat{\mathbf{A}})\, \hat{\mathbf{A}} + (\mathbf{p} \cdot \hat{\mathbf{W}})\, \hat{\mathbf{W}}. \tag{12.35}$$

Hint: Show that

$$\mathbf{p} \cdot \mathbf{L} = 0, \qquad \mathbf{p} \cdot \mathbf{A} = \mathbf{p} \cdot \hat{\mathbf{r}}, \qquad \mathbf{p} \cdot \mathbf{W} = \frac{p^2}{2} + \mu H. \tag{12.36}$$

(c) It is well known that the position $\mathbf{r}$ traverses an ellipse about the origin. This is the content of Kepler's first law of motion. Show that the momentum $\mathbf{p}$ traverses a circle about a fixed point $\mathbf{p}_0$. That is, show that the momentum $\mathbf{p}$ satisfies the equation of a circle,

$$|\mathbf{p} - \mathbf{p}_0| = q. \tag{12.37}$$

Hint: Rewrite the expression for $(\mathbf{p} \cdot \hat{\mathbf{W}})$ in the form $\mathbf{p} \cdot \mathbf{p} - 2\mathbf{p} \cdot \mathbf{W} + \mathbf{W} \cdot \mathbf{W} = W^2 - 2\mu H$.

(d) Determine the vector $\mathbf{p}_0$ representing the center of this circle, and find the radius q of this circle. Verify that the center $\mathbf{p}_0$ is a conserved quantity.
Solution: $\mathbf{p}_0 = \mathbf{W}$ and $q = \mu Z e^2/L$.

(e) Show that when the position $\mathbf{r}$ traverses a circle ($A = 0$) the center of the circle traversed by momentum $\mathbf{p}$ is the origin.

16. (**110 points.**) The Hamiltonian for an hydrogenic atom is

$$H = \frac{p^2}{2\mu} - \frac{Ze^2}{r}. \tag{12.38}$$

(a) The eigenvalue equation for the hydrogenic atom is

$$H|E_n\rangle = E_n|E_n\rangle, \tag{12.39}$$

where $H' = E_n$ are the eigenvalues of the Hamiltonian H. Projecting the above eigenvalue equation on to the position basis we obtain

$$\langle \mathbf{r}|H|E_n\rangle = E_n\langle \mathbf{r}|E_n\rangle. \tag{12.40}$$

The projection of the energy eigenfunctions $|E_n\rangle$ on to the position basis

$$\psi_n(\mathbf{r}) = \langle \mathbf{r}|E_n\rangle. \tag{12.41}$$

are defined as the hydrogenic wavefunctions. Starting from Eq. (12.40) show that the hydrogenic wavefunction satisfies the 'time-independent Schrödinger equation'

$$\left(-\frac{\hbar^2}{2\mu}\nabla^2 - \frac{Ze^2}{r}\right)\psi_n(\mathbf{r}) = E_n\psi_n(\mathbf{r}). \tag{12.42}$$

The effectively involves the substitution

$$\mathbf{p} = \frac{\hbar}{i}\boldsymbol{\nabla} \tag{12.43}$$

in the Hamiltonian.

(b) We shall confine our discussion to bound states ($E_n < 0$). Define

$$E_n = -\frac{\mu Z^2 e^4}{2\hbar^2}\frac{1}{n^2} \qquad \text{and} \qquad a_0 = \frac{\hbar^2}{\mu e^2}, \tag{12.44}$$

later being the (first) Bohr radius. Thus, derive

$$\left(\nabla^2 + \frac{2Z}{a_0 r}\right)\psi_n(\mathbf{r}) = \frac{Z^2}{a_0^2}\frac{1}{n^2}\psi_n(\mathbf{r}). \tag{12.45}$$

(c) The Laplacian in spherical polar coordinates is

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} + \frac{1}{r^2}\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right). \tag{12.46}$$

Since angular momentum is a constant of motion we can expand the wavefunctions in the form

$$\psi_n(\mathbf{r}) = \sum_{l=0}^{n-1}\sum_{m=-l}^{l} R_{nl}(r)Y_{lm}(\theta,\phi), \tag{12.47}$$

where the spherical harmonics satisfy

$$L^2 Y_{lm}(\theta,\phi) = -\hbar^2\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right) = \hbar^2 l(l+1)Y_{lm}(\theta,\phi). \tag{12.48}$$

Thus, derive the differential equation for the radial part of the wavefunction as

$$\left[\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr} - \frac{l(l+1)}{r^2} + \frac{2Z}{a_0 r} - \frac{Z^2}{a_0^2 n^2}\right]R_{nl}(r) = 0. \tag{12.49}$$

(d) In terms of the dimensionless variable

$$x = \frac{2Zr}{a_0} \tag{12.50}$$

derive

$$\left[\frac{d^2}{dx^2} + \frac{2}{x}\frac{d}{dx} - \frac{l(l+1)}{x^2} + \frac{1}{x} - \frac{1}{(2n)^2}\right]R_{nl}(x) = 0. \tag{12.51}$$

(e) For $x \gg 1$ argue that we have

$$\left[\frac{d^2}{dx^2} - \frac{1}{(2n)^2}\right] R_{nl}(x) = 0. \tag{12.52}$$

Solve this equation to learn the asymptotic behaviour of the radial wavefunction to be

$$R_{nl}(x) \sim e^{-\frac{x}{2n}} \qquad \text{for} \qquad x \gg 1. \tag{12.53}$$

(f) For $x \ll 1$ argue that we have

$$\left[\frac{1}{x^2}\frac{d}{dx}x^2\frac{d}{dx} - \frac{l(l+1)}{x^2}\right] R_{nl}(x) = 0. \tag{12.54}$$

Solve this equation to learn the limiting behaviour of the radial wavefunction to be

$$R_{nl}(x) \sim x^l \qquad \text{for} \qquad x \ll 1. \tag{12.55}$$

(g) Use the above limiting forms to define

$$R_{nl}(x) = x^l e^{-\frac{x}{2n}} L(x), \tag{12.56}$$

and derive, in terms of

$$y = \frac{x}{n}, \tag{12.57}$$

$$\left[y\frac{d^2}{dy^2} + \{(2l+1) + 1 - y\}\frac{d}{dy} + (n - l - 1)\right] L(y) = 0. \tag{12.58}$$

Compare this to the differential equation satisfied by the Laguerre polynomials, $L_n^{(\alpha)}(y)$, the Laguerre equation,

$$\left[y\frac{d^2}{dy^2} + \{\alpha + 1 - y\}\frac{d}{dy} + n\right] L_n^{(\alpha)}(y) = 0. \tag{12.59}$$

Thus, derive

$$R_{nl}(r) = N\left(\frac{2Zr}{na_0}\right)^l e^{-\frac{Zr}{na_0}} L_{n-l-1}^{(2l+1)}\left(\frac{2Zr}{na_0}\right), \tag{12.60}$$

where N is a normalization constant.

(h) The normalization constant N is, in principle, determined using

$$\int_0^\infty r^2 dr |R_{nl}(r)|^2 = 1. \tag{12.61}$$

Verify that, the above statement does not, immediately, lead to the orthogonality relation for Laguerre polynomials,

$$\int_0^\infty dx\, x^\alpha e^{-x} L_n^{(\alpha)}(x) L_{n'}^{(\alpha)}(x) = \delta_{nn'} \frac{(n+\alpha)!}{n!}. \tag{12.62}$$

(i) Let us derive the Hellmann-Feynman theorem. Consider the energy eigenvalue equation

$$[H(\lambda) - E(\lambda)]|E,\lambda\rangle = 0 \tag{12.63}$$

and its adjoint

$$\langle E,\lambda|[H(\lambda) - E(\lambda)] = 0. \tag{12.64}$$

Differentiate with respect to λ:

$$\left(\frac{\partial E}{\partial \lambda} - \frac{\partial H}{\partial \lambda}\right)|E,\lambda\rangle + (E - H)|E,\lambda\rangle = 0, \tag{12.65}$$

and multiply with $\langle E,\lambda|$ to obtain

$$\left\langle \frac{\partial H}{\partial \lambda} \right\rangle = \langle E,\lambda|\frac{\partial H}{\partial \lambda}|E,\lambda\rangle = \frac{\partial E}{\partial \lambda}, \tag{12.66}$$

which is the statement of the Hellmann-Feynman theorem.

(j) Use the Hellmann-Feynman theorem, by regarding λ as Z, in the hydrogenic atom to evaluate

$$\left\langle \frac{1}{r} \right\rangle_n = \int_0^\infty r^2 dr\, \frac{1}{r}\, |R_{nl}(r)|^2 = \frac{Z}{a_0 n^2}. \tag{12.67}$$

(k) Use the orthogonality relation of Laguerre polynomials in Eq. (12.62) in Eq. (12.67) to derive the normalization constant N as

$$N = \frac{2}{n^2}\left(\frac{Z}{a_0}\right)^{\frac{3}{2}} \sqrt{\frac{(n-l-1)!}{(n+l)!}}. \tag{12.68}$$

Thus, derive the radial part of the hydrogenic wavefunction

$$R_{nl}(r) = \frac{2}{n^2}\left(\frac{Z}{a_0}\right)^{\frac{3}{2}} \sqrt{\frac{(n-l-1)!}{(n+l)!}} \left(\frac{2Zr}{na_0}\right)^l e^{-\frac{Zr}{na_0}} L_{n-l-1}^{(2l+1)}\left(\frac{2Zr}{na_0}\right). \tag{12.69}$$

17. (**50 points.**) In this problem we shall construct the ground state of a hydrogenic atom, $|100\rangle$. For the ground state, $n=1$, we have $j_1=0$, $j_2=0$, which corresponds to $l=0$, $m=0$. Thus, we conclude

$$\mathbf{J}^{(1)}|100\rangle = 0 \qquad \text{and} \qquad \mathbf{J}^{(2)}|100\rangle = 0, \tag{12.70}$$

which implies

$$\mathbf{L}|100\rangle = 0 \qquad \text{and} \qquad \mathbf{A}|100\rangle = 0. \tag{12.71}$$

Show that, in conjunction, these equations imply

$$\left(\frac{\mathbf{r}}{r} + \frac{i\hbar\,\mathbf{p}}{\mu Z e^2}\right)|100\rangle = 0. \tag{12.72}$$

(a) With the goal of finding the projection of the ground state in the position basis, the wavefunction

$$\langle \mathbf{r}|100\rangle = \psi_{100}(\mathbf{r}), \tag{12.73}$$

we identify the Bohr radius

$$a_0 = \frac{\hbar^2}{\mu e^2}, \tag{12.74}$$

to rewrite Eq. (12.72) in the form

$$\left(\frac{\mathbf{r}}{r} + \frac{a_0}{Z}\frac{i}{\hbar}\mathbf{p}\right)|100\rangle = 0. \tag{12.75}$$

Show that the projection on the position basis leads to the differential equation for the wavefunction

$$\left(\frac{\mathbf{r}}{r} + \frac{a_0}{Z}\boldsymbol{\nabla}\right)\psi_{100}(\mathbf{r}) = 0. \tag{12.76}$$

Thus, determine the normalized ground state wavefunction to be

$$\psi_{100}(\mathbf{r}) = \frac{1}{\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{\frac{3}{2}} e^{-Z\frac{r}{a_0}}. \tag{12.77}$$

(b) With the goal of finding the projection of the ground state in the momentum basis,

$$\langle \mathbf{p}|100\rangle = \psi_{100}(\mathbf{p}), \tag{12.78}$$

we identify the wavevector corresponding to the Bohr radius, $k_0 = 2\pi/a_0$, and the related Bohr momentum

$$p_0 = \frac{\hbar}{a_0}, \tag{12.79}$$

to rewrite Eq. (12.72) in the form

$$\left(\frac{\mathbf{r}}{r} + \frac{i}{Z}\frac{\mathbf{p}}{p_0}\right)|100\rangle = 0. \tag{12.80}$$

Use the Hamiltonian to interpret

$$\frac{1}{r}|100\rangle = \frac{(p^2 + Z^2 p_0^2)}{2\mu Z e^2}|100\rangle, \tag{12.81}$$

and show that

$$\Big[\mathbf{r}(p^2 + Z^2 p_0^2) + 2i\hbar\mathbf{p}\Big]|100\rangle = 0. \tag{12.82}$$

Show that the projection on the momentum basis leads to the differential equation

$$\left(\frac{\partial}{\partial \mathbf{p}} + \frac{4\mathbf{p}}{(p^2 + Z^2 p_0^2)}\right)\psi_{100}(\mathbf{p}) = 0. \tag{12.83}$$

Thus, determine the solution

$$\psi_{100}(\mathbf{p}) = \frac{2}{\pi}\frac{\sqrt{2Z^5 p_0^5}}{(p^2 + Z^2 p_0^2)^2}. \tag{12.84}$$

(c) Evaluate the Fourier transformation

$$\psi_{100}(\mathbf{p}) = (2\pi\hbar)^{-\frac{3}{2}}\int d^3\mathbf{r}\, e^{-\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{r}}\,\psi_{100}(\mathbf{r}), \tag{12.85}$$

and verify that this is indeed equal to the result in Eq. (12.84).

(d) Evaluate the inverse Fourier transformation

$$\psi_{100}(\mathbf{r}) = (2\pi\hbar)^{-\frac{3}{2}}\int d^3\mathbf{p}\, e^{\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{r}}\,\psi_{100}(\mathbf{p}) \tag{12.86}$$

and verify that this is indeed equal to the result in Eq. (12.77).
Hint: Use the integral

$$\int_0^\infty \frac{x\,dx}{(x^2+1)^2}\sin ax = \frac{\pi a}{4}e^{-a}. \tag{12.87}$$

18. (**50 points.**) In this problem we shall construct the eigenfunction $\psi_{n,n-1,n-1}(\mathbf{r})$, known as circular Rydberg states.

(a) Since $|n, n-1, n-1\rangle$ is in the highest possible l and m, we have

$$J_+^{(1)}|n, n-1, n-1\rangle = 0 \qquad \text{and} \qquad J_+^{(2)}|n, n-1, n-1\rangle = 0. \tag{12.88}$$

Thus, conclude that

$$L_+|n, n-1, n-1\rangle = 0 \qquad \text{and} \qquad \hbar n\, A_+|n, n-1, n-1\rangle = 0. \tag{12.89}$$

(b) Show that

$$(\mathbf{p}\times\mathbf{L})_+ = -ip_+L_z + ip_zL_+. \tag{12.90}$$

Use this in the equation for A_+, in conjunction with the equation for L_+, and $L_z|n,n-1,n-1\rangle = (n-1)|n,n-1,n-1\rangle$, to obtain

$$\left(\frac{r_+}{r} + \frac{i\hbar n}{\mu Z e^2}p_+\right)|n,n-1,n-1\rangle = 0. \tag{12.91}$$

Project this into the position basis to obtain the corresponding differential equation

$$\left[\left(\frac{x+iy}{r}\right) + \frac{na_0}{Z}\left(\frac{\partial}{\partial x} + i\frac{\partial}{\partial y}\right)\right]\psi_{n,n-1,n-1}(r,\theta,\phi) = 0. \tag{12.92}$$

(c) Since the state $|n,n-1,n-1\rangle$ is an eigenstate of L^2 we can write the wavefunction in the form

$$\psi_{n,n-1,n-1}(r,\theta,\phi) = R_n(r)Y_{n-1,n-1}(\theta,\phi). \tag{12.93}$$

Using the definition of spherical harmonics,

$$Y_{lm}(\theta,\phi) = e^{im\phi}\sqrt{\frac{2l+1}{4\pi}}\sqrt{\frac{(l+m)!}{(l-m)!}}\frac{1}{(\sin\theta)^m}\left(\frac{d}{d\cos\theta}\right)^{l-m}\frac{(\cos^2\theta-1)^l}{2^l l!}, \tag{12.94}$$

show that

$$Y_{n-1,n-1}(\theta,\phi) \sim \left(\frac{x+iy}{r}\right)^{n-1}. \tag{12.95}$$

Thus, construct the eigenfunction to have the form

$$\psi_{n,n-1,n-1}(r,\theta,\phi) = (x+iy)^{n-1}f_n(r). \tag{12.96}$$

(d) Show that $[r_+,p_+]=0$, and using this derive

$$\left(1 + \frac{na_0}{Z}\frac{\partial}{\partial r}\right)f_n(r) = 0. \tag{12.97}$$

Show that

$$f_n(r) = Ce^{-\frac{Zr}{na_0}}, \tag{12.98}$$

where C is a normalization constant. Thus, derive

$$\psi_{n,n-1,n-1}(r,\theta,\phi) = C(r\sin\theta e^{i\phi})^{n-1}e^{-\frac{Zr}{na_0}}. \tag{12.99}$$

(e) Requiring

$$\int d^3r|\psi_{n,n-1,n-1}(r,\theta,\phi)|^2 = 1, \tag{12.100}$$

which involves the integral

$$I_l = \frac{1}{2}\int_{-1}^{1} dt(1-t^2)^l, \tag{12.101}$$

determine the normalization constant (upto a phase) to be

$$|C| = \frac{2}{n^2}\left(\frac{Z}{a_0}\right)^{\frac{3}{2}}\left(\frac{2Z}{na_0}\right)^{n-1}\frac{1}{\sqrt{4\pi}}\frac{1}{2^{n-1}(n-1)!}. \tag{12.102}$$

Hint: Evaluate I_l using integration by parts to notice

$$I_l = \frac{2l}{2l+1}I_{l-1}, \tag{12.103}$$

and iterate this relation to yield

$$I_l = \frac{(2^l l!)^2}{(2l+1)!}. \tag{12.104}$$

(f) Verify that the solution is indeed

$$\psi_{n,n-1,n-1}(r,\theta,\phi) = R_{n,n-1}(r) Y_{n-1,n-1}(\theta,\phi). \tag{12.105}$$

19. (**20 points.**) Derive the relation

$$\mathbf{r}\, H_0 = -\frac{3Ze^2}{4}\mathbf{A} + \frac{d\mathbf{X}}{dt}, \tag{12.106}$$

where

$$\mathbf{X} = -\frac{1}{8}(\mathbf{r}\times\mathbf{L} - \mathbf{L}\times\mathbf{r}) + \frac{3}{4} i\hbar\, \mathbf{r}. \tag{12.107}$$

Take the time average and give the physical interpretation of this equation in classical mechanics.

20. (**20 points.**) A mass m oscillates about an equilibrium point with angular frequency ω. This motion, the harmonic oscillator, is described by the Hamiltonian

$$H_0(x,p) = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2, \tag{12.108}$$

in conjunction with the Heisenberg relation $[x,p] = i\hbar$. Let us chose our units such that m=1 and $\omega = 1$. The above Hamiltonian takes the form

$$H_0 = \left(y^\dagger y + \frac{1}{2} \right) \hbar \tag{12.109}$$

in terms of the operators

$$x + ip = \sqrt{2\hbar}\, y, \tag{12.110a}$$
$$x - ip = \sqrt{2\hbar}\, y^\dagger. \tag{12.110b}$$

The harmonic oscillator is characterized by the algebra $[y, y^\dagger] = 1$. The eigen basis set $|n'\rangle$ of the harmonic oscillator satisfies the eigenvalue equation

$$y^\dagger y |n'\rangle = n' |n'\rangle, \qquad n' = 0, 1, 2, \ldots. \tag{12.111}$$

Let us place a charge q on the mass m, such that it interacts with a weak electric field $\mathbf{E}$. We choose the direction of the electric field $\mathbf{E}$ to be in the direction of the oscillations of the mass. The Hamiltonian of the oscillator in the presence of the electric field is described by

$$H = H_0 - qEx. \tag{12.112}$$

In the presence of the electric field the oscillator ceases to stay in a stationary state $|n'\rangle$, and makes transitions to another state. These transitions are described by the matrix elements

$$\langle n''|H|n'\rangle. \tag{12.113}$$

Find a selection rule that states which elements in the above transitions are not zero.
Hint: Use equations of motion

$$\frac{dF}{dt} = \frac{1}{i\hbar}[F, H_0]. \tag{12.114}$$

Solution:

$$\frac{dx}{dt} = \frac{1}{i\hbar}[x, H_0] = p \quad \Longrightarrow \quad (n' - n'')\langle n''|x|n'\rangle = i\langle n''|p|n'\rangle, \tag{12.115a}$$
$$\frac{dp}{dt} = \frac{1}{i\hbar}[p, H_0] = -x \quad \Longrightarrow \quad (n' - n'')\langle n''|p|n'\rangle = -i\langle n''|x|n'\rangle, \tag{12.115b}$$

which, together, implies the selection rule

$$n' - n'' = \pm 1. \tag{12.116}$$

Comment: Students tend to do this the brute foce way, which is okay.

Chapter 13

Scattering in quantum mechanics

13.1 Problems

1. (**20 points.**) Verify, by substitution, that

$$G_0(\mathbf{r},\mathbf{r}') = -\frac{1}{4\pi}\left[A\frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} + B\frac{e^{-ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}\right] \tag{13.1}$$

with the constraint $A + B = 1$ is a particular solution to the Green's function equation

$$\left[\nabla^2 + k^2\right] G_0(\mathbf{r},\mathbf{r}') = \delta^{(3)}(\mathbf{r}-\mathbf{r}'). \tag{13.2}$$

Hint: Prove that

$$-\nabla^2 \frac{1}{4\pi}\frac{1}{|\mathbf{r}-\mathbf{r}'|} = \delta^{(3)}(\mathbf{r}-\mathbf{r}'). \tag{13.3}$$

2. (**20 points.**) Verify, by substitution, that

$$G(\mathbf{r}) = -\frac{e^{ikr}}{4\pi r} \tag{13.4}$$

is a particular solution to the Green's function equation

$$\left[\nabla^2 + k^2\right] G(\mathbf{r}) = \delta^{(3)}(\mathbf{r}). \tag{13.5}$$

3. (**20 points.**) Consider the Schrödinger equation

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r},t)\right]\psi(\mathbf{r},t) = i\hbar\frac{\partial}{\partial t}\psi(\mathbf{r},t). \tag{13.6}$$

(a) Derive the statement of probability conservation (continuity equation),

$$\frac{\partial}{\partial t}\rho(\mathbf{r},t) + \boldsymbol{\nabla}\cdot\mathbf{j}(\mathbf{r},t) = s(\mathbf{r},t), \tag{13.7}$$

where

$$\rho(\mathbf{r},t) = |\psi(\mathbf{r},t)|^2, \tag{13.8}$$

$$\mathbf{j}(\mathbf{r},t) = \frac{\hbar}{2im}\left[\psi^*(\mathbf{r},t)\boldsymbol{\nabla}\psi(\mathbf{r},t) - \psi(\mathbf{r},t)\boldsymbol{\nabla}\psi^*(\mathbf{r},t)\right], \tag{13.9}$$

$$s(\mathbf{r},t) = \frac{2}{\hbar}\left[\text{Im}\, V(\mathbf{r},t)\right]|\psi(\mathbf{r},t)|^2. \tag{13.10}$$

(b) For a time-independent potential the scattering wavefunction can be expressed in the form, after replacing $\psi(\mathbf{r},t) \to e^{-iEt/\hbar}\psi(\mathbf{r})$,

$$\psi_{r\to\infty}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} + f(\theta,\phi)\frac{e^{ikr}}{r}. \tag{13.11}$$

Construct the continuity equation for the above scattering wavefuntion. Then, after integrating over a large sphere ($r \to \infty$), derive

$$\lim_{r\to\infty} \oint d\mathbf{S}\cdot\mathbf{j}(\mathbf{r}) = \lim_{r\to\infty} \int d^3r\, s(\mathbf{r}). \tag{13.12}$$

(c) Show that

$$\lim_{r\to\infty} \oint d\mathbf{S}\cdot\mathbf{j}(\mathbf{r}) = \frac{\hbar k}{m}\int_0^\pi \sin\theta d\theta \int_0^{2\pi} d\phi\,|f(\theta,\phi)|^2 - \frac{4\pi\hbar}{m}\left[\text{Im}\, f(0)\right]. \tag{13.13}$$

(d) Thus, derive the optical theorem,

$$\sigma_{\text{scatt.}} + \sigma_{\text{abs.}} = \frac{4\pi}{k}\left[\text{Im}\, f(0)\right], \tag{13.14}$$

where

$$\sigma_{\text{scatt.}} = \int_0^\pi \sin\theta d\theta \int_0^{2\pi} d\phi\,|f(\theta,\phi)|^2, \tag{13.15}$$

$$\sigma_{\text{abs.}} = -\lim_{r\to\infty}\frac{2m}{\hbar^2 k}\int d^3r\,[\text{Im}\, V(\mathbf{r})]\,|\psi(\mathbf{r})|^2. \tag{13.16}$$

4. (**20 points.**) Consider a scattering process that involves an incident plane wave of energy $E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$, moving in the positive z direction, interacting with the potential of an inverted finite spherical well of radius a

$$V(\mathbf{r}') = \begin{cases} V, & r' < a, \\ 0, & r' > a. \end{cases} \tag{13.17}$$

The leading order contribution to the scattering amplitude, for this process, in the eikonal approximation (small angle large momentum) is

$$f^{(0)}(\theta) = \frac{k}{i}\int_0^\infty b db\, J_0(kb\theta)\left[e^{i\chi(b)} - 1\right], \tag{13.18}$$

where

$$\chi(b) = -\frac{k}{2E}\int_{-\infty}^\infty dz'\, V(b,z'). \tag{13.19}$$

Here b is the magnitude of the coordinate $\mathbf{r}'$ in the plane perpendicular to the direction of z,

$$\mathbf{r}' = b\cos\phi'\hat{\mathbf{i}} + b\sin\phi'\hat{\mathbf{j}} + z'\hat{\mathbf{k}}, \tag{13.20}$$

and the coordinate $\hat{\mathbf{r}}$ represents the position of the detector,

$$\hat{\mathbf{r}} = \sin\theta\cos\phi\hat{\mathbf{i}} + \sin\theta\sin\phi\hat{\mathbf{j}} + \cos\theta\hat{\mathbf{k}}. \tag{13.21}$$

The process is independent of ϕ and ϕ' because of the azimuthal symmetry in the potential. Evaluate $\chi(b)$ for the process.

5. (**20 points.**) For potentials that are independent of ϕ the axial symmetry allows us to write the leading order contribution to scattering amplitude in the eikonal approximation (small angle large momentum) as

$$f^{(0)}(\theta) = \frac{k}{i} \int_0^\infty bdb\, J_0(kb\theta) \left[e^{i\chi(b)} - 1 \right], \tag{13.22}$$

where

$$\chi(b) = -\frac{k}{2E} \int_{-\infty}^{\infty} dz\, V(b, z). \tag{13.23}$$

(a) For potentials that have no imaginary parts show that the optcal theorem takes the form

$$\sigma_{\text{scatt.}} = \int_0^\pi \sin\theta d\theta \int_0^{2\pi} d\phi \left| f(\theta, \phi) \right|^2 = \frac{4\pi}{k} \left[\text{Im}\, f(0) \right]. \tag{13.24}$$

(b) Using the second equality in Eq. (13.24) verify that

$$\sigma_{\text{scatt.}} = 8\pi \int_0^\infty bdb\, \sin^2 \left[\frac{\chi(b)}{2} \right]. \tag{13.25}$$

(c) Using the first equality in Eq. (13.24) and arguing that small angle approximation is represented by the range of integration $0 \le \theta < V/E$ show that

$$\sigma_{\text{scatt.}} = 2\pi k^2 \int_0^\infty bdb \int_0^\infty b'db' \left[e^{i\chi(b)} - 1 \right] \left[e^{-i\chi(b')} - 1 \right] \int_0^{\frac{V}{E}} \theta d\theta J_0(kb\theta) J_0(kb'\theta). \tag{13.26}$$

(d) Show that in the limit

$$ka\frac{V}{E} \to \infty \tag{13.27}$$

the optical theorem, which is the statement of probability conservation, is satisfied. Hint: Use

$$\int_0^\infty xdxJ_0(tx)J_0(t'x) = \frac{\delta(x - x')}{x}. \tag{13.28}$$

Chapter 14

Dirac equation

14.1 Clifford-Dirac algebra

1. (**20 points.**) An arbitrary 2×2 matrix M with complex numbers as elements can be expressed as a linear combination of Pauli matrices $\boldsymbol{\sigma}$ and the identity matrix in the form

$$M = a_0 + \mathbf{a}\cdot\boldsymbol{\sigma}. \tag{14.1}$$

Show that the coefficients a_0 and $\mathbf{a}$ satisfy the relations

$$\mathrm{tr}(M) = 2a_0, \tag{14.2a}$$
$$\mathrm{tr}(M\boldsymbol{\sigma}) = 2\mathbf{a}. \tag{14.2b}$$

As an illustration, write

$$\sigma^i\sigma^j\sigma^k = A^{ijk} + B^{ijk}{}_m\sigma^m, \tag{14.3}$$

and determine the coefficients A^{ijk} and $B^{ijk}{}_m$.

2. Quaternions are extensions of complex numbers, like complex numbers are extensions of real numbers. A quaternion P can be expressed in terms of Pauli matrices as

$$P = a_0 - i\mathbf{a}\cdot\boldsymbol{\sigma}. \tag{14.4}$$

(a) Show that the (Hamilton) product of two quaternions,

$$P = a_0 - i\mathbf{a}\cdot\boldsymbol{\sigma}, \tag{14.5a}$$
$$Q = b_0 - i\mathbf{b}\cdot\boldsymbol{\sigma}, \tag{14.5b}$$

is given by

$$PQ = (a_0b_0 - \mathbf{a}\cdot\mathbf{b}) - i(a_0\mathbf{b} + b_0\mathbf{a} + \mathbf{a}\times\mathbf{b})\cdot\boldsymbol{\sigma}. \tag{14.6}$$

(b) Verify that the Hamilton product is non-commutative. Determine $\big[P,Q\big]$.
Solution:

$$\big[P,Q\big] = -2i(\mathbf{a}\times\mathbf{b})\cdot\boldsymbol{\sigma}. \tag{14.7}$$

3. Clifford-Dirac algebra

(a) Let β and α^i, where $i = 1,2,3$, be four matrices that obey the algebra

$$\beta^2 = 1, \qquad \frac{1}{2}\big\{\alpha^i,\alpha^j\big\} = \delta^{ij}, \qquad \big\{\beta,\alpha^i\big\} = 0. \tag{14.8}$$

Deduce the trace identities

$$\operatorname{tr}(\beta) = 0, \tag{14.9a}$$
$$\operatorname{tr}(\alpha^i) = 0, \tag{14.9b}$$
$$\operatorname{tr}(\beta\alpha^i) = 0. \tag{14.9c}$$

(b) Define the Dirac matrices γ^μ, where $\mu = 0, 1, 2, 3$, using the definitions

$$\gamma^0 = \beta, \qquad \gamma^i = \beta\alpha^i. \tag{14.10}$$

i. Using Eq. (14.8), show that the algebra of the Dirac matrices is given by

$$\frac{1}{2}\{\gamma^\mu, \gamma^\nu\} = -g^{\mu\nu} \tag{14.11}$$

ii. and the corresponding trace identities are contained in the relation

$$\operatorname{tr}(\gamma^\mu\gamma^\nu) = -4g^{\mu\nu}. \tag{14.12}$$

(c) Define the matrix

$$\gamma_5 = \gamma^0\gamma^1\gamma^2\gamma^3. \tag{14.13}$$

i. Deduce the following algebraic properties

$$\gamma_5^2 = -1, \qquad \{\gamma^\mu, \gamma_5\} = 0 \tag{14.14}$$

ii. and the corresponding trace identities

$$\operatorname{tr}(\gamma_5) = 0, \tag{14.15a}$$
$$\operatorname{tr}(\gamma_5\gamma^\mu) = 0, \tag{14.15b}$$
$$\operatorname{tr}(\gamma_5^2) = -4. \tag{14.15c}$$

iii. Further, verify the trace identity

$$\operatorname{tr}(\gamma^\mu\gamma^\nu\gamma_5) = 0. \tag{14.16}$$

(d) i. Show that

$$\operatorname{tr}(\gamma^\mu\gamma^\nu\gamma^\alpha) = 0. \tag{14.17}$$

Hint: Introduce $\gamma_5^2 = -1$ inside the trace, and use the cyclic property of trace.

ii. Show that the trace of odd number of γ^μ matrices vanishes.

iii. Show that

$$\operatorname{tr}(\gamma^\mu\gamma^\nu\gamma^\alpha\gamma^\beta) = 4(g^{\mu\nu}g^{\alpha\beta} - g^{\mu\alpha}g^{\nu\beta} + g^{\mu\beta}g^{\nu\alpha}). \tag{14.18}$$

(e) Define the matrices

$$\sigma^{\mu\nu} = \frac{i}{2}[\gamma^\mu, \gamma^\nu]. \tag{14.19}$$

The components of $\sigma^{\mu\nu}$ comprise the six ways of multiplying together two different γ^μ matrices.

i. Verify that $\sigma^{\mu\nu}$ is antisymmetric under the interchange of indices μ and ν.

ii. Show that

$$\sigma^{0k} = i\alpha^k. \tag{14.20}$$

iii. Show that

$$\sigma^{ij} = -\frac{i}{2}[\alpha^i, \alpha^j] = \varepsilon^{ijk}\Sigma^k, \tag{14.21}$$

with the last equality serving as the definition of Σ^k.

iv. Combining the commutation and anti-commutation relations for γ^μ matrices, deduce the relation

$$\gamma^\mu \gamma^\nu = -g^{\mu\nu} - i\sigma^{\mu\nu}, \tag{14.22}$$

which is the generalization of the corresponding relation for Pauli matrices

$$\sigma^i \sigma^j = \delta^{ij} + i\varepsilon^{ijk}\sigma^k. \tag{14.23}$$

v. Derive the algebraic properties

$$\left\{\gamma^\mu, \sigma^{\mu\nu}\right\} = \tag{14.24a}$$

$$\left\{\gamma_5, \sigma^{\mu\nu}\right\} = \tag{14.24b}$$

$$\left\{\sigma^{\alpha\beta}, \sigma^{\mu\nu}\right\} = \tag{14.24c}$$

vi. Derive the trace identities

$$\mathrm{tr}(\sigma^{\mu\nu}) = 0, \tag{14.25a}$$

$$\mathrm{tr}(\sigma^{\mu\nu}\gamma^\alpha) = 0, \tag{14.25b}$$

$$\mathrm{tr}(\sigma^{\mu\nu}\gamma_5) = 0, \tag{14.25c}$$

$$\mathrm{tr}(\sigma^{\mu\nu}\sigma^{\alpha\beta}) = 4(g^{\mu\alpha}g^{\nu\beta} - g^{\mu\beta}g^{\nu\alpha}). \tag{14.25d}$$

(f) Define the matrices

$$(i\gamma^\mu\gamma_5). \tag{14.26}$$

The components of $(i\gamma^\mu\gamma_5)$ comprise the four ways of multiplying together three different γ^μ matrices.

i. Derive the algebraic properties

$$\left\{\gamma^\alpha, (i\gamma^\nu\gamma_5)\right\} = \tag{14.27a}$$

$$\left\{\gamma_5, (i\gamma^\nu\gamma_5)\right\} = 0 \tag{14.27b}$$

$$\left\{\sigma^{\alpha\beta}, (i\gamma^\nu\gamma_5)\right\} = \tag{14.27c}$$

$$\left\{(i\gamma^\mu\gamma_5), (i\gamma^\nu\gamma_5)\right\} = 2g^{\mu\nu}. \tag{14.27d}$$

ii. Derive the trace identities

$$\mathrm{tr}(i\gamma^\mu\gamma_5) = 0, \tag{14.28a}$$

$$\mathrm{tr}((i\gamma^\mu\gamma_5)\gamma^\alpha) = 0, \tag{14.28b}$$

$$\mathrm{tr}((i\gamma^\mu\gamma_5)\gamma_5) = 0, \tag{14.28c}$$

$$\mathrm{tr}((i\gamma^\mu\gamma_5)\sigma^{\alpha\beta}) = 0, \tag{14.28d}$$

$$\mathrm{tr}((i\gamma^\mu\gamma_5)(i\gamma^\nu\gamma_5)) = 4g^{\mu\nu}. \tag{14.28e}$$

iii. Further, in the trace identity

$$\mathrm{tr}(\gamma_5\gamma^\mu\gamma^\nu\gamma^\alpha\gamma^\beta) = c\,\varepsilon^{\mu\nu\alpha\beta} \tag{14.29}$$

find c.

(g) An arbitrary 4×4 matrix M with complex elements can be expressed in terms of the 16 independent matrices above

$$M = a + b_\mu\gamma^\mu + c\gamma_5 + d_\mu i\gamma^\mu\gamma_5 + \frac{1}{2}e_{\mu\nu}\sigma^{\mu\nu}. \tag{14.30}$$

Using the trace identities show the coefficients are given by

$$\mathrm{tr}(M) = 4a, \tag{14.31a}$$

$$\mathrm{tr}(M\gamma^\alpha) = -4b^\alpha, \tag{14.31b}$$

$$\mathrm{tr}(M\gamma_5) = -4c, \tag{14.31c}$$

$$\mathrm{tr}(Mi\gamma^\alpha\gamma_5) = 4d^\alpha, \tag{14.31d}$$

$$\mathrm{tr}(M\sigma^{\alpha\beta}) = 4e^{\alpha\beta}. \tag{14.31e}$$

4. Express the matrix
$$\gamma^\mu \gamma^\nu \gamma^\alpha \tag{14.32}$$
in terms of the 16 independent matrices above.
Solution:
$$\gamma^\mu \gamma^\nu \gamma^\alpha = -g^{\mu\nu}\gamma^\alpha + g^{\mu\alpha}\gamma^\nu - g^{\nu\alpha}\gamma^\mu - \frac{i}{4}\varepsilon^{\mu\nu\alpha}{}_\beta i\gamma^\beta\gamma_5. \tag{14.33}$$

14.2 Free particle

1. (**20 points.**) A free particle is described by the Hamiltonian
$$H = \boldsymbol{\alpha}\cdot\mathbf{p}c + \beta mc^2. \tag{14.34}$$
Starting from the above equation derive the Lorentz covariant form of Dirac equation
$$\boldsymbol{\gamma}^\mu p_\mu + mc = 0, \tag{14.35}$$
where $\gamma^\mu = (\gamma^0, \boldsymbol{\gamma}) = (\beta, \beta\boldsymbol{\alpha})$ and $p^\mu = (E/c, \mathbf{p})$.

2. (**40 points.**) A free particle is described by the Hamiltonian
$$H = \boldsymbol{\alpha}\cdot\mathbf{p}c + \beta mc^2. \tag{14.36}$$
Derive the following equations of motion:
$$\frac{d\mathbf{r}}{dt} = \boldsymbol{\alpha}c, \tag{14.37a}$$
$$\frac{d\mathbf{p}}{dt} = 0, \tag{14.37b}$$
$$\frac{i\hbar}{2}\frac{d\boldsymbol{\alpha}}{dt} = -i\boldsymbol{\Sigma}\times\mathbf{p}c + \boldsymbol{\alpha}\beta mc^2, \tag{14.37c}$$
$$\frac{i\hbar}{2}\frac{d\beta}{dt} = \beta\boldsymbol{\alpha}\cdot\mathbf{p}c. \tag{14.37d}$$
Derive the relations
$$\frac{d\mathbf{L}}{dt} = \boldsymbol{\alpha}\times\mathbf{p}c, \qquad \text{where} \qquad \mathbf{L} = \mathbf{r}\times\mathbf{p}, \tag{14.38a}$$
$$\frac{d}{dt}\left(\frac{\hbar}{2}\boldsymbol{\Sigma}\right) = -\boldsymbol{\alpha}\times\mathbf{p}c, \qquad \text{where} \qquad \boldsymbol{\Sigma} = -\frac{i}{2}\boldsymbol{\alpha}\times\boldsymbol{\alpha}, \tag{14.38b}$$
$$\frac{d\mathbf{J}}{dt} = 0, \qquad \text{where} \qquad \mathbf{J} = \mathbf{L} + \frac{\hbar}{2}\boldsymbol{\Sigma}, \tag{14.38c}$$
which unambiguously indicates the existance of the Spin. Further, deduce
$$\frac{d}{dt}(\boldsymbol{\Sigma}\cdot\mathbf{p}) = 0, \tag{14.39a}$$
$$\frac{d}{dt}\left(\frac{\hbar}{2}\boldsymbol{\Sigma}\cdot\mathbf{L}\right) = -c\boldsymbol{\alpha}\cdot(\mathbf{p}\times\mathbf{L}) + i\hbar c\boldsymbol{\alpha}\cdot\mathbf{p}, \tag{14.39b}$$
$$\frac{d\mathbf{K}}{dt} = 0, \qquad \text{where} \qquad K = \beta(\boldsymbol{\Sigma}\cdot\mathbf{L} + \hbar). \tag{14.39c}$$

3. (**40 points.**)

   (a) The momentum of a non-relativistic classical (non-quantum) free particle of mass m is related to it's velocity by the relation
$$\mathbf{v} = \frac{\mathbf{p}}{m}. \tag{14.40}$$

(b) Show that the momentum of a relativistic classical (non-quantum) free particle of mass m is related to it's velocity by the relation

$$\mathbf{v} = \frac{\mathbf{p}c}{E/c}, \tag{14.41}$$

where $E^2 = p^2c^2 + m^2c^4$.

(c) Let us denote a time derivative with a dot over the respective variable. The 'velocity' of relativistic quantum free particle of mass m is $\boldsymbol{\alpha}c$, as per the equation of motion

$$\dot{\mathbf{r}} = \boldsymbol{\alpha}c. \tag{14.42}$$

Derive the equation of motion

$$i\hbar\dot{\boldsymbol{\alpha}} = 2\mathbf{p}c - 2H\boldsymbol{\alpha} = -2\mathbf{p}c + 2\boldsymbol{\alpha}H. \tag{14.43}$$

(d) Derive the equation of motion

$$i\hbar\ddot{\boldsymbol{\alpha}} = -2H\dot{\boldsymbol{\alpha}} = 2\dot{\boldsymbol{\alpha}}H. \tag{14.44}$$

The ordering of H matters because the Hamiltonian does not commute with $\dot{\boldsymbol{\alpha}}(t)$.

(e) Integrate to yield

$$\dot{\boldsymbol{\alpha}}(t) = e^{i\frac{2H}{\hbar}t}\dot{\boldsymbol{\alpha}}(0) = \dot{\boldsymbol{\alpha}}(0)e^{-i\frac{2H}{\hbar}t}, \tag{14.45}$$

where $\dot{\boldsymbol{\alpha}}(0)$ is a constant and thus commutes with the Hamiltonian. Verify this solution by differentiating it with time.

(f) Integrate again to derive the relation between momentum and 'velocity',

$$c\boldsymbol{\alpha}(t) = \frac{\mathbf{p}c}{H/c} + \frac{i\hbar c}{2}\dot{\boldsymbol{\alpha}}(0)e^{-i\frac{2H}{\hbar}t}H^{-1} \tag{14.46a}$$

$$= \frac{\mathbf{p}c}{H/c} - \frac{i\hbar c}{2}H^{-1}\dot{\boldsymbol{\alpha}}(0)e^{i\frac{2H}{\hbar}t}. \tag{14.46b}$$

The frist term relates to the classical relativistic formula. The second term oscillates with a frequency of $2H/\hbar$, which is at least $2mc^2/\hbar$. Evaluate this frequency, for an electron, in units of radian/second. This oscillatory part of the motion is called Zitterbewegung. For comparison, the plasma frequency associated with oscillations in electron density inside a conductor is about 10^{16} radian/second.

Chapter 15

Graphene

15.1 Number density for thin films (electron gas model)

To describe the electrons (in the electron gas) in a slab, we consider the energy states of a particle confined in a slab of thickness d and infinite in extent along the x-y directions using the Schrödinger equation

$$-\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right]\psi(x,y,z)=E\psi(x,y,z). \tag{15.1}$$

The confinement of the particle inside the slab requires the proability flux to be zero on the walls,

$$\frac{\partial}{\partial z}\psi^*\psi\bigg|_{z=0,d}=\left[\psi^*\left(\frac{\partial}{\partial z}\psi\right)+\left(\frac{\partial}{\partial z}\psi^*\right)\psi\right]\bigg|_{z=0,d}=0. \tag{15.2}$$

The above condition can be satisfied by either requiring Dirichlet boundary condition ($\psi = 0$), or requiring Neumann boundary condition ($\partial\psi/\partial z = 0$) on the wavefunction at the walls. But, Dirichlet boundary conditions are over-imposing because it does not allow surface charges on the slabs. Thus, we rule out Dirichlet boundary condition and impose Neumann boundary condition on the particles. Fourier transforming in the x-y directions we have

$$E_n(k_x,k_y)=\frac{\hbar^2}{2m^*}\left[k_x^2+k_y^2+n^2\frac{\pi^2}{d^2}\right], \qquad n=0,1,2,\ldots. \tag{15.3}$$

Unlike Dirichlet condition $n = 0$ state is not excluded when Neumann boundary conditions are imposed.

The total number of electrons in the slab is equal to twice the sum of occupied energy levels. In terms of the maximum occupied energy level at zero temperature, termed Fermi energy E_F, we can thus write

$$n_f=\frac{n_{\text{tot}}(E_F)}{L_xL_yd}=2\,\frac{1}{d}\sum_{n=0}^{\infty}\int_{-\infty}^{\infty}\frac{dk_x}{2\pi}\int_{-\infty}^{\infty}\frac{dk_y}{2\pi}\,\theta(E_F-E_n(k_x,k_y)), \tag{15.4}$$

where the factor of 2 accomodates two electrons in each state. Observing the facorization

$$\theta(a-x-y)=\theta(a-x-y)\theta(a-x) \tag{15.5}$$

allows the separation of the variables in the form

$$\begin{aligned}
n_f=\frac{n_{\text{tot}}(E_F)}{L_xL_yd} &= 2\,\frac{1}{d}\sum_{n=0}^{\infty}\theta\left(E_F-n^2\frac{\hbar^2}{2m}\frac{\pi^2}{d^2}\right)\int_{-\infty}^{\infty}\frac{dk_x}{2\pi}\int_{-\infty}^{\infty}\frac{dk_y}{2\pi}\theta\left(E_F-\frac{\hbar^2}{2m}k^2-n^2\frac{\hbar^2}{2m}\frac{\pi^2}{d^2}\right) && (15.6)\\
&= \frac{1}{2\pi d}\sum_{n=0}^{\infty}\theta\left(E_F-n^2\frac{\hbar^2}{2m}\frac{\pi^2}{d^2}\right)\left[\frac{2mE_f}{\hbar^2}-n^2\frac{\pi^2}{d^2}\right] && (15.7)\\
&= \frac{\pi}{2d^3}\sum_{n=0}^{\infty}(N^2-n^2)\theta(N^2-n^2)=\frac{\pi}{2d^3}\sum_{n=0}^{[N]}(N^2-n^2), && (15.8)
\end{aligned}$$

where $[N]$ is the integer part of

$$N = \sqrt{\frac{2m^* E_F d^2}{\hbar^2 \pi^2}} = \frac{k_F d}{\pi} = \frac{2d}{\lambda_F}, \tag{15.9}$$

and expressed in terms of Fermi wave-vector, k_F, and Fermi wavelength, λ_F. Using the sums

$$\sum_{n=0}^{[N]} N^2 = N^2([N]+1), \qquad \sum_{n=0}^{[N]} n^2 = \frac{1}{6}[N]([N]+1)(2[N]+1), \tag{15.10}$$

we immediately have

$$n_f(N) = \frac{\pi}{2d^3}\left[\left([N]N^2 - \frac{1}{3}[N]^3\right) + \left(N^2 - \frac{1}{2}[N]^2\right) - \frac{1}{6}[N]\right], \tag{15.11}$$

For metals described by the DLS model the Fermi wavelength ranges between 0.3 nm - 1 nm. Notice that the limit $\hbar \to 0$ is equivalent to taking $k_F \to \infty$ ($N \to \infty$). The number density in the limit $N \to \infty$ is

$$n_f(\infty) = \frac{\pi}{2d^3}\frac{2}{3}N^3 = \frac{k_F^3}{3\pi^2}. \tag{15.12}$$

Using Eq. (15.12) in Eq. (15.11) we have

$$n_f(N) = n_f(\infty)\nu(x), \tag{15.13}$$

where

$$\nu(x) = \frac{3}{2}\left(x - \frac{1}{3}x^3\right) + \frac{3}{2N}\left(1 - \frac{1}{2}x^2\right) - \frac{1}{4N^2}x, \qquad x = \frac{[N]}{N}. \tag{15.14}$$

We note the limiting cases (see FIG. 15.1)

$$x = \frac{[N]}{N} \to \begin{cases} 0 & \text{if} \quad N < 1, \\ 1 & \text{if} \quad N \to \infty. \end{cases} \tag{15.15}$$

Convergence of x to unity is very slow. In particular we make an error of 1% in replacing $x \to 1$ even for N=100. The limiting cases for $\nu(x)$ in Eq. (15.14) are:

$$\nu(x) \to \begin{cases} \frac{3}{2N} & \text{if} \quad N < 1, \\ 1 & \text{if} \quad N \to \infty. \end{cases} \tag{15.16}$$

Using Eq. (15.16) we have the following limiting expressions for the number density in Eq. (15.13):

$$\frac{n_{\text{tot}}}{A\,d} = n_f(N) \to n_f(\infty)\left\{\begin{array}{c} \frac{3}{2N} \\ 1 \end{array}\right\} = \begin{cases} \frac{k_F^2}{2\pi d} & \text{if} \quad N < 1 \ (2d < \lambda_F), \\ \frac{k_F^3}{2\pi^2} & \text{if} \quad N \to \infty \ (2d \gg \lambda_F). \end{cases} \tag{15.17}$$

It is suggestive to explore the physical nature of the condition $N < 1$, which states $d^2 n_{\text{tot}}/A < \pi/2$. Introducing the packing fraction of a material defined as $\nu_0 = N_{\text{atoms}} A_{\text{atom}}/A$, in terms of the total number of atoms N_{atoms}, and area of an atom $A_{\text{atom}} = \pi a_0^2$ with a_0 being the radius of the atom, we recognize that the condition $N < 1$ corresponds to the window

$$1 \leq \frac{d}{2a_0} < \frac{\pi}{\sqrt{8}}\frac{1}{\sqrt{\nu_0 n_0}}, \tag{15.18}$$

where the inequality on the left is imposed because a thin sheet of material has to be at least one atomic layer thick. The total number of carrier charges per atom is defined to be n_0. The packing fraction is always less than unity, $\nu_0 < 1$. Thus, the condition $N < 1$ states that a one-atom-layer thick material behaves like a two-dimensional sheet unless the packing fraction is very low.

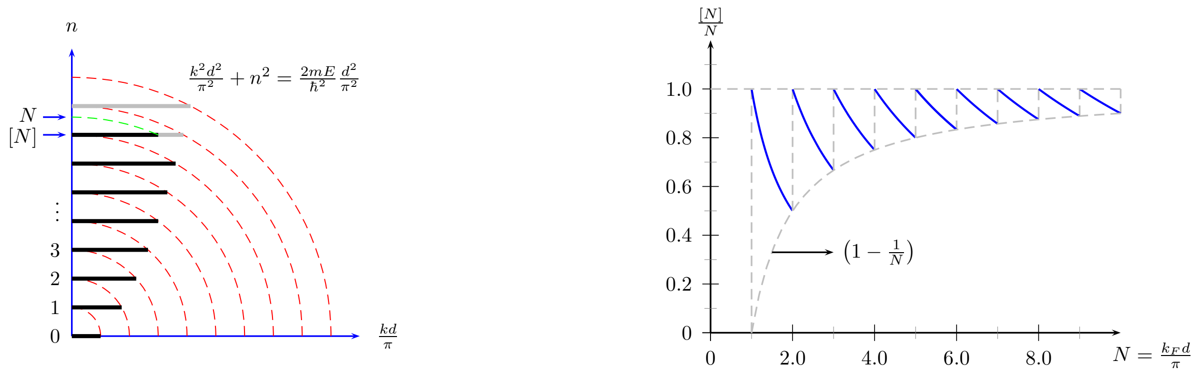

Figure 15.1: Left: Energy filling scheme and description of $[N]$ and N. Right: Fractional Floor function $\frac{[N]}{N}$ plotted with respect to N.

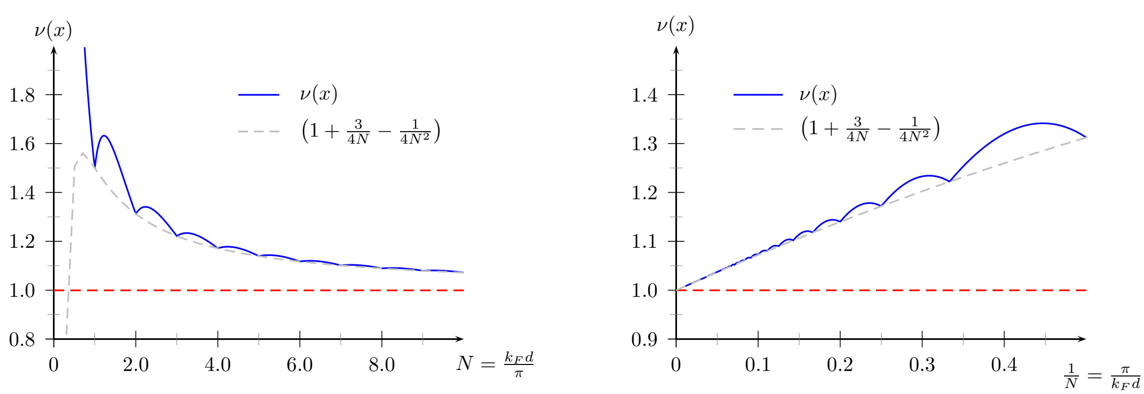

Figure 15.2: Plot of $\nu(x)$ versus N (on left) and versus $\frac{1}{N}$ (on right).

15.2 Graphene

Graphene is a single layer of graphite. The carbon atoms in graphene arrange to form a two-dimensional hexagonal lattice with each side of a hexagon measuring 0.142 nm. The interlayer separation between the layers in graphite is 0.337 nm.

15.2.1 Dielectric function for graphene

Our goal is to determine the dielectric model for graphene. To this end we note that conduction electrons in undoped graphene (a 2-dimensional structure) in the lowest Brillouin zone are decribed by a Diriac-like dispersion relation [2]

$$E = v_F|\mathbf{p}|, \tag{15.19}$$

where $\mathbf{p}$ is the momentum of the electrons in the plane of graphene, and $v_F = c/300$ is determined in terms of the lattice parameters. Introducing a mass which is loosely equivalent to considering doped graphene we have

$$E^2 = \frac{v_F^2}{c^2}p^2c^2 + m^2c^4, \tag{15.20}$$

which leads to the Dirac's dispersion relation for $v_F = c$. We introduced c in the expression for clarity. In terms of Diriac-like matrices we can write

$$E = \tilde{\gamma}_0\tilde{\boldsymbol{\gamma}}\cdot\mathbf{p} + m\tilde{\gamma}_0, \tag{15.21}$$

where the modified γ-matrices are defined as $\tilde{\gamma}^\mu = (\gamma, v_F\boldsymbol{\gamma})$ and satisfy the anti-commutation relations

$$\{\tilde{\gamma}^\mu,\tilde{\gamma}^\nu\} = -2\eta^\mu{}_\lambda\eta^\nu{}_\sigma g^{\lambda\sigma}, \qquad \{\gamma^\mu,\gamma^\nu\} = -2g^{\mu\nu}, \qquad \eta^\mu{}_\nu = \text{diag}(1,\mathbf{v}_F), \qquad \mu = 0,1,2,\ldots,D, \tag{15.22}$$

with D being the number space dimensions in a $(D+1)$-dimensional space-time. The conduction electrons in graphene are confined to be in a 2-dimensional sheet in (3+1)-dimensional space-time, thus $D = 2$. The interaction between conduction electrons and electromagnetic fields will be described by the action

$$W = i\int d^2x \int dt \left[-\frac{1}{4}\int dz\, F_{\mu\nu}F^{\mu\nu} - \int_0^d dz\, \psi^\dagger\tilde{\gamma}^0\left\{\tilde{\gamma}^\mu\left(\frac{1}{i}\partial_\mu - eA_\mu\right) + m\right\}\psi\right], \tag{15.23}$$

in which the electrons are confined to move in the graphene sheet. We shall assume that the Dirac fields have no knowledge of the thickness d. This probably needs to be taken care of more rigorously if one intends to compare our final results more precisely with experiments. But, as we mentioned earlier our goal will be simply to get the numbers in the right ballpark.

The dielectric permittivity in this model is given by

$$[\varepsilon^{ij}(\mathbf{k},\omega) - \delta^{ij}]\omega^2 = \Pi^{ij}(\mathbf{k},\omega;m), \tag{15.24}$$

where the right hand side is given in terms of the vacuum polarization contribution

$$i\Pi^{\mu\nu}(\mathbf{k},\omega;m) = -\frac{e^2}{d}\text{tr}\int\frac{d^{D+1}p}{(2\pi)^{D+1}}\,\tilde{\gamma}^\mu\frac{1}{[m+\tilde{\gamma}p]}\tilde{\gamma}^\nu\frac{1}{[m+\tilde{\gamma}(p-k)]}. \tag{15.25}$$

In terms of redefined momentums, $\tilde{p}^\mu = \eta^\mu{}_\nu p^\nu$, after evaluating the traces over the gamma indices we have

$$i\Pi^{\mu\nu}(\mathbf{k},\omega;m) = -\frac{e^2}{d}\frac{1}{v_F^D}\int\frac{d^{D+1}\tilde{p}}{(2\pi)^{D+1}}\,\frac{1}{[m^2+\tilde{p}^2]}\frac{1}{[m^2+(\tilde{p}-\tilde{k})^2]}T^{\mu\nu}, \tag{15.26}$$

where

$$T^{\mu\nu} = -4[m^2+\tilde{p}(\tilde{p}-\tilde{k})]\eta^\mu{}_\lambda\eta^\nu{}_\sigma g^{\lambda\sigma} + 4[\tilde{p}^\sigma(\tilde{p}-\tilde{k})^\lambda + \tilde{p}^\lambda(\tilde{p}-\tilde{k})^\sigma]\eta^\mu{}_\lambda\eta^\nu{}_\sigma. \tag{15.27}$$

Using the integral representation

$$\frac{1}{M} = \lim_{\delta\to 0}\frac{1}{M-i\delta} = \lim_{\delta\to 0} i\int_0^\infty ds\, e^{-is(M-i\delta)}, \tag{15.28}$$

where the parameter δ is a positive real number, to invert the denominators and then using the substitutions $s_1 = su$, $s_2 = s(1-u)$, we can write

$$i\Pi^{\mu\nu}(\mathbf{k},\omega;m) = -\frac{e^2}{d}\frac{1}{v_F^D}\int_0^\infty s ds\, e^{-ism^2}\int_0^1 du\, e^{-is\tilde{k}^2 u(1-u)}\int\frac{d^{D+1}\tilde{p}}{(2\pi)^{D+1}}\,(T_1^{\mu\nu}+T_2^{\mu\nu}+T_3^{\mu\nu})e^{-is(\tilde{p}-u\tilde{k})^2}, \tag{15.29}$$

where

$$T_1^{\mu\nu} = 4u(1-u)\left[\tilde{k}^2 g^{\lambda\sigma} - 2\tilde{k}^\lambda\tilde{k}^\sigma\right]\eta^\mu{}_\lambda\eta^\nu{}_\sigma, \tag{15.30}$$

$$T_2^{\mu\nu} = -4\left[\{m^2+(\tilde{p}-u\tilde{k})^2\}g^{\lambda\sigma} - 2(\tilde{p}-u\tilde{k})^\lambda(\tilde{p}-u\tilde{k})^\sigma\right]\eta^\mu{}_\lambda\eta^\nu{}_\sigma, \tag{15.31}$$

$$T_3^{\mu\nu} = -4(2u-1)\left[\tilde{k}\cdot(\tilde{p}-u\tilde{k})g^{\lambda\sigma} - \{\tilde{k}^\lambda(\tilde{p}-u\tilde{k})^\sigma + \tilde{k}^\sigma(\tilde{p}-u\tilde{k})^\lambda\}\right]\eta^\mu{}_\lambda\eta^\nu{}_\sigma. \tag{15.32}$$

After the Euclidean rotation, $\tilde{p}^0 \to i\tilde{p}^0$, we can evaluate

$$\int\frac{d^{D+1}\tilde{p}}{(2\pi)^{D+1}}\,e^{-is(\tilde{p}-u\tilde{k})^2} = \frac{i^{(1-D)/2}}{(4\pi s)^{(1+D)/2}}, \tag{15.33}$$

$$\int\frac{d^{D+1}\tilde{p}}{(2\pi)^{D+1}}\,e^{-is(\tilde{p}-u\tilde{k})^2}(\tilde{p}-u\tilde{k})^\mu = 0, \tag{15.34}$$

$$\int\frac{d^{D+1}\tilde{p}}{(2\pi)^{D+1}}\,(\tilde{p}-u\tilde{k})^2 e^{-is(\tilde{p}-u\tilde{k})^2} = \frac{(1+D)}{2}\frac{1}{is}\frac{i^{(1-D)/2}}{(4\pi s)^{(1+D)/2}}, \tag{15.35}$$

$$\int\frac{d^{D+1}\tilde{p}}{(2\pi)^{D+1}}\,(\tilde{p}-u\tilde{k})^\lambda(\tilde{p}-u\tilde{k})^\sigma e^{-is(\tilde{p}-u\tilde{k})^2} = \frac{g^{\lambda\sigma}}{2is}\frac{i^{(1-D)/2}}{(4\pi s)^{(1+D)/2}}, \tag{15.36}$$

which immediately impies that $T_3^{\mu\nu}$ does not contribute. Rest of the two contributions lets us write

$$\Pi^{\mu\nu}(\mathbf{k},\omega;m) = \Pi_1^{\mu\nu}(\mathbf{k},\omega;m) + \Pi_2^{\mu\nu}(\mathbf{k},\omega;m), \tag{15.37}$$

where

$$\Pi_1^{\mu\nu}(\mathbf{k},\omega;m) = \frac{1}{2}\frac{1}{v_F^D}\left[2\tilde{k}^\lambda\tilde{k}^\sigma - \tilde{k}^2 g^{\lambda\sigma}\right]\eta^\mu{}_\lambda\eta^\nu{}_\sigma\,\Pi_D(\mathbf{k},\omega;m), \tag{15.38}$$

where

$$\Pi_D(\mathbf{k},\omega;m) = -\frac{1}{d}\frac{8e^2}{(4\pi i)^{(1+D)/2}}\int_0^\infty\frac{ds}{s}s^{(3-D)/2}e^{-ism^2}\int_0^1 du\, u(1-u)\, e^{-is\tilde{k}^2 u(1-u)}. \tag{15.39}$$

Evaluation of $\Pi_2^{\mu\nu}(\mathbf{k},\omega;m)$ involves the integral

$$\int\frac{d^{D+1}p}{(2\pi)^{D+1}}\,T_2^{\mu\nu}e^{-is(\tilde{p}-u\tilde{k})^2} = -4\eta^\mu{}_\lambda\eta^\nu{}_\sigma g^{\lambda\sigma}\frac{1}{(4\pi is)^{(1+D)/2}}\left[im^2+\frac{(D-1)}{2s}\right], \tag{15.40}$$

and integrating by parts using

$$\frac{d}{ds}\left[\frac{1}{s^{(D-1)/2}}\,e^{-ism^2}\right] = -\frac{1}{s^{(D-1)/2}}\left[im^2+\frac{(D-1)}{2s}\right]e^{-ism^2}, \tag{15.41}$$

and throwing away the surface term we have

$$\Pi_2^{\mu\nu}(\mathbf{k},\omega;m) = \frac{1}{2}\frac{1}{v_F^D}\tilde{k}^2\eta^\mu{}_\lambda\eta^\nu{}_\sigma g^{\lambda\sigma}\,\Pi_D(\mathbf{k},\omega;m). \tag{15.42}$$

Using Eqs. (15.38) and (15.42) in Eq. (15.37) we have

$$\Pi^{\mu\nu}(\mathbf{k},\omega;m) = \frac{1}{v_F^D}\left[\tilde{k}^\lambda\tilde{k}^\sigma - \tilde{k}^2 g^{\lambda\sigma}\right]\eta^\mu{}_\lambda\eta^\nu{}_\sigma\,\Pi_D(\mathbf{k},\omega;m). \tag{15.43}$$

Substituting $u = (1+v)/2$ in Eq. (15.39) ans performing the s-integral after Euclidean rotation ($s \to -is$) lets us write

$$\Pi_D(\mathbf{k},\omega;m) = \frac{2e^2\Gamma\left(\frac{3-D}{2}\right)}{(4\pi)^{(1+D)/2}}\frac{1}{d}\int_0^1 dv \frac{(1-v^2)}{\left[m^2+\frac{1}{4}\tilde{k}^2(1-v^2)\right]^{(3-D)/2}}. \tag{15.44}$$

We can evaluate the limiting cases

$$\Pi_D(\mathbf{k},\omega;0) = \frac{1}{d}\frac{e^2\Gamma\left(\frac{3-D}{2}\right)\Gamma\left(\frac{1+D}{2}\right)}{\pi^{D/2}2^{(1+D)}\Gamma\left(1+\frac{D}{2}\right)}\left(\frac{2}{\tilde{k}}\right)^{3-D}, \qquad -1 < D < 3, \tag{15.45}$$

$$\Pi_D(0,0;m) = \frac{1}{d}\frac{4e^2\Gamma\left(\frac{3-D}{2}\right)}{3(4\pi)^{(1+D)/2}}\frac{1}{m^{3-D}}, \qquad D < 3. \tag{15.46}$$

For $D = 2$ which is the case of our interest we have

$$\Pi_2(\mathbf{k},\omega;0) = \frac{e^2}{8}\frac{1}{\tilde{k}d}, \tag{15.47}$$

$$\Pi_2(0,0;m) = \frac{e^2}{6\pi}\frac{1}{md}. \tag{15.48}$$

We note that in $D = 2$ the contribution from vacuum polarization at zero momentum vanishes in the limit $d \to \infty$ for non-zero mass. Thus, there is no (re)normalization necessary.

At this stage it is worth pointing out that a more satisfatory exercise would be to compute the above for a sheet of finite thickness and then take the limit $d \to 0$, which we shall complete elesewhere. We do not expect the qualitative behaviour of the results to change.

For an isotropic medium, taking the trace in Eq. (15.24) we have

$$\varepsilon(\mathbf{k},\omega) - 1 = -\left(1 - \frac{v_F^2}{2}\frac{\mathbf{k}^2}{\omega^2}\right)\Pi_2(\mathbf{k},\omega;0). \tag{15.49}$$

Setting $\mathbf{k} = 0$ ($\tilde{k} \to i\omega$) we have

$$\varepsilon(0,\omega) - 1 = -\Pi_2(0,\omega;0) = -\frac{\sigma}{i\omega}, \tag{15.50}$$

where we identified the conductivity

$$\sigma = \frac{e^2}{8d}. \tag{15.51}$$

For graphene we have 2 electron states (4 two-component spinor states) in the lowest Brillouin zone [2], thus

$$\sigma_g = 2\frac{e^2}{8d} = \frac{\pi\alpha}{d}. \tag{15.52}$$

Using Eq. (15.52) we have for graphene

$$\lambda_g = \pi\alpha\zeta. \tag{15.53}$$

15.3 Problems

1. The number density of electron in a thin film of thickness d

$$n_f = \frac{n_{\text{tot}}}{L_x L_y d} \tag{15.54}$$

as a function of the Fermi energy E_F is conveniently expressed in terms of the parameter

$$N = \sqrt{\frac{2m^* E_F d^2}{\hbar^2 \pi^2}} = \frac{k_F d}{\pi} = \frac{2d}{\lambda_F}, \tag{15.55}$$

where k_F is the Fermi wave-vector and λ_F is the Fermi wavelength, by the expression

$$n_f(N) = n_f(\infty)\nu(x), \tag{15.56}$$

where

$$n_f(\infty) = \frac{\pi}{2d^3}\frac{2}{3}N^3 = \frac{k_F^3}{3\pi^2} \tag{15.57}$$

and

$$\nu(x) = \frac{3}{2}\left(x - \frac{1}{3}x^3\right) + \frac{3}{2N}\left(1 - \frac{1}{2}x^2\right) - \frac{1}{4N^2}x, \qquad x = \frac{[N]}{N}. \tag{15.58}$$

Here $[N]$ is the integer part of N.

(a) Plot $x = [N]/N$ as a function of N, for $0 < N < 10$. In particular, consider regions $0 \leq x < 1.2$.

(b) Plot $\nu(x)$ as a function of N, for $0 < N < 10$. In particular, consider regions $0.8 \leq \nu(x) < 2.0$.

(c) Plot $\nu(x)$ as a function of $1/N$, for $0 < 1/N < 0.5$. In particular, consider regions $0.9 \leq \nu(x) < 1.5$.

2. The electronic structure of an isolated carbon atom is $1s^2 2s^2 2p^2$. In graphene the carbon atoms arrange themselves in a single two-dimensional hexagonal pattern. The carbon atoms are 0.142 nm apart. Each carbon atom in graphene shares three electrons with three closest neighbours in sp^2 hydrid orbitals. The excitations of the remaining electron, corresponding to the remaining p-orbital oriented out of the plane (π-bond), is described by the Hamiltonian

$$H = v_F \boldsymbol{\alpha} \cdot \mathbf{p}, \tag{15.59}$$

where $\mathbf{p}$ represents the momentum in two dimensions ($p_z = 0$) and $v_F/c \sim 300$. In terms of the rescaled momentum

$$\tilde{p}^\mu = \left(\frac{H}{c}, \frac{v_F}{c}\mathbf{p}\right), \qquad \mu = 0, 1, 2, \tag{15.60}$$

and Dirac's Gamma matrices $\gamma^\mu = (\beta, \beta\alpha)$, for $\mu = 0, 1, 2$, we have the (massless) Dirac equation

$$\gamma^\mu \tilde{p}_\mu = 0. \tag{15.61}$$

The dielectric permittivity in this (quantum field theoretical) model is given in terms of vacuum polarization effects using the relation

$$\Pi^{ij}(0, \omega) = \delta^{ij}\omega^2(\varepsilon - 1), \tag{15.62}$$

where the vacuum polarization tensor is given by

$$i\Pi^{\mu\nu}(\tilde{\mathbf{k}}, \omega) = -4\pi\alpha \,\mathrm{tr} \int \frac{d^3\tilde{p}}{(2\pi)^3}\, \gamma^\mu \frac{1}{\gamma \cdot \tilde{p}} \gamma^\nu \frac{1}{\gamma \cdot (\tilde{p} - \tilde{k})}, \tag{15.63}$$

$\alpha = e^2/4\pi\hbar c$ is the fine structure constant.

(a) Using the idea of rationalizing denominators show that

$$\frac{1}{\gamma \cdot \tilde{p}} = -\frac{\gamma \cdot \tilde{p}}{\tilde{p}^2}. \tag{15.64}$$

(b) Use Eq. (15.64) to move all the Gamma matrices to the numerator in the expression for vacuum polarization tensor in Eq. (15.63). Evaluate the trace

$$\mathrm{tr}(\gamma^\mu\gamma^\alpha\gamma^\nu\gamma^\beta) = 4(g^{\mu\alpha}g^{\nu\beta} - g^{\mu\nu}g^{\alpha\beta} + g^{\mu\beta}g^{\nu\alpha}) \tag{15.65}$$

and then show that

$$i\Pi^{\mu\nu}(\tilde{\mathbf{k}},\omega) = -16\pi\alpha\int\frac{d^3\tilde{p}}{(2\pi)^3}\frac{\left[\tilde{p}^\mu(\tilde{p}-\tilde{k})^\nu + \tilde{p}^\nu(\tilde{p}-\tilde{k})^\mu - g^{\mu\nu}\tilde{p}\cdot(\tilde{p}-\tilde{k})\right]}{\tilde{p}^2(\tilde{p}-\tilde{k})^2}, \tag{15.66}$$

(c) Show that the inverse of an operator has the integral representation

$$\frac{1}{M} = \lim_{\delta\to 0}\frac{1}{M-i\delta} = \lim_{\delta\to 0} i\int_0^\infty ds\, e^{-is(M-i\delta)}, \tag{15.67}$$

where the parameter δ is a positive real number. Thus, show that

$$\frac{1}{\tilde{p}^2(\tilde{p}-\tilde{k})^2} = \lim_{\delta\to 0}\int_0^\infty ds_1 e^{-is_1(\tilde{p}^2-i\delta)}\int_0^\infty ds_2 e^{-is_2[(\tilde{p}-\tilde{k})^2-i\delta]}. \tag{15.68}$$

Using substitutions

$$s_1 = s(1-u), \tag{15.69a}$$

$$s_2 = su, \tag{15.69b}$$

deduce $ds_1 ds_2 = s ds du$, where $0 \le s < \infty$, $0 \le u \le 1$, and show that

$$\frac{1}{\tilde{p}^2(\tilde{p}-\tilde{k})^2} = \lim_{\delta\to 0}\int_0^\infty s ds\, e^{-s\delta}\int_0^1 du\, e^{-is(1-u)\tilde{p}^2}e^{-isu(\tilde{p}-\tilde{k})^2} \tag{15.70a}$$

$$= \lim_{\delta\to 0}\int_0^\infty s ds\, e^{-s\delta}\int_0^1 du\, e^{-isu(1-u)\tilde{k}^2}e^{-is(\tilde{p}-u\tilde{k})^2}. \tag{15.70b}$$

Thus, show that

$$i\Pi^{\mu\nu}(\tilde{\mathbf{k}},\omega) = \frac{2\alpha}{\pi^2}\lim_{\delta\to 0}\int_0^\infty s ds\, e^{-s\delta}\int_0^1 du\, e^{-isu(1-u)\tilde{k}^2} \times\int d^3\tilde{p}\left[\tilde{p}^\mu(\tilde{p}-\tilde{k})^\nu + \tilde{p}^\nu(\tilde{p}-\tilde{k})^\mu - g^{\mu\nu}\tilde{p}\cdot(\tilde{p}-\tilde{k})\right]e^{-is(\tilde{p}-u\tilde{k})^2}. \tag{15.71}$$

(d) Show that, replacing $\tilde{p}-u\tilde{k}\to\tilde{p}$ leads to the integral

$$\int d^3\tilde{p}\left[(\tilde{p}+u\tilde{k})^\mu(\tilde{p}-(1-u)\tilde{k})^\nu + (\tilde{p}+u\tilde{k})^\nu(\tilde{p}-(1-u)\tilde{k})^\mu - g^{\mu\nu}(\tilde{p}+u\tilde{k})\cdot(\tilde{p}-(1-u)\tilde{k})\right]e^{-is\tilde{p}^2}. \tag{15.72}$$

Evaluate this integral by computing the following integrals, (in terms of the Gaussian integral,)

$$\int d^3\tilde{p}\, e^{-is\tilde{p}^2} = \frac{1}{i}\left(\frac{\pi}{is}\right)^{\frac{3}{2}}, \tag{15.73a}$$

$$\int d^3\tilde{p}\left[\tilde{p}^\mu\tilde{k}^\nu\right]e^{-is\tilde{p}^2} = 0, \tag{15.73b}$$

$$\int d^3\tilde{p}\left[\tilde{p}^\mu\tilde{p}^\nu\right]e^{-is\tilde{p}^2} = -g^{\mu\nu}\frac{1}{2s}\left(\frac{\pi}{is}\right)^{\frac{3}{2}}, \tag{15.73c}$$

$$\int d^3\tilde{p}\left[\tilde{p}^2\right]e^{-is\tilde{p}^2} = -\frac{3}{2s}\left(\frac{\pi}{is}\right)^{\frac{3}{2}}. \tag{15.73d}$$

Thus, show that

$$
\begin{aligned}
i\Pi^{\mu\nu}(\tilde{\mathbf{k}},\omega) &= (2\tilde{k}^\mu\tilde{k}^\nu - g^{\mu\nu}\tilde{k}^2)\frac{2\alpha}{\sqrt{i\pi}}\lim_{\delta\to 0}\int_0^1 du\, u(1-u)\int_0^\infty \frac{ds}{s}\sqrt{s}\, e^{-s[\delta+iu(1-u)\tilde{k}^2]} \\
&\quad + g^{\mu\nu}\frac{\alpha}{i\sqrt{i\pi}}\lim_{\delta\to 0}\int_0^1 du\int_0^\infty \frac{ds}{s}\frac{1}{\sqrt{s}}\, e^{-s[\delta+iu(1-u)\tilde{k}^2]} \qquad (15.74)
\end{aligned}
$$

(e) Evaluate the s-integrals using the integral representation for the gamma function

$$
\Gamma(z) = \int_0^\infty ds s^{z-1} e^{-s}, \qquad (15.75)
$$

and evaluate the following u-integrals using the integral representation for the beta function

$$
\mathrm{B}(x,y) = \int_0^1 du\, u^{x-1}(1-u)^{y-1}. \qquad (15.76)
$$

In particular, $-\frac{1}{2}\Gamma(-\frac{1}{2}) = \Gamma(\frac{1}{2}) = \sqrt{\pi}$ and $\mathrm{B}(\frac{3}{2},\frac{3}{2}) = \pi/8$. Thus, evaluate the vacuum polarization tensor

$$
\Pi^{\mu\nu}(\tilde{\mathbf{k}},\omega) = -\frac{\pi\alpha}{2\tilde{k}}(\tilde{k}^\mu\tilde{k}^\nu - g^{\mu\nu}\tilde{k}^2). \qquad (15.77)
$$

(f) Show that, using $\tilde{k}^2 = v_F^2\mathbf{k}\cdot\mathbf{k} - \omega^2$,

$$
\Pi^{00}(0,\omega) = 0, \qquad (15.78a)
$$

$$
\Pi^{ij}(0,\omega) = -\frac{\pi\alpha}{2i\omega}\delta^{ij}\omega^2. \qquad (15.78b)
$$

Read out the dielectric permittivity of graphene, using Eq. (15.62), as

$$
\varepsilon - 1 = -2\times\frac{\pi\alpha}{2i\omega} = -\frac{\pi\alpha}{i\omega}, \qquad (15.79)
$$

where we multiplied by a factor of 2 for the two independent excitations (representing the Dirac points K and K').

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