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Advanced Quantum Theory

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Chapter 1

Formal Methods

1.1 Postulate 1: States and State Space

Every isolated physical system has associated with it a complex inner-product space (or Hilbert Space). This is known as its state space. A complete description of the system is given by its state vector, $|\Psi\rangle$, a unit-normalised vector in the state space.

1.1.1 Dirac Notation

Notation	Description
$ \Psi\rangle$	Vector in a state space (a “ket”)
$\langle\Psi $	Dual vector to $ \Psi\rangle$ (a “bra”)
$\langle\Phi \Psi\rangle$	Inner product between $ \Phi\rangle$ and $ \Psi\rangle$
$ \Psi\rangle\langle\Phi $	Outer product between $ \Psi\rangle$ and $ \Phi\rangle$

1.1.2 Column Vector Representation

Any state in an n -dimensional space may be represented by an n -element complex column vector. Given an orthonormal basis $\{|\phi_j\rangle\}$, we can write any state $|\Psi\rangle$ as:

$$|\Psi\rangle = \sum_{j=1}^n c_j |\phi_j\rangle$$

This corresponds to a column vector of coefficients:

$$\vec{c} = \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \end{pmatrix}$$

The norm of $|\Psi\rangle$ is:

$$\begin{aligned} |||\Psi\rangle|| &= \sqrt{\langle\Psi|\Psi\rangle} \\ &= \sqrt{\sum_{j,k} (c_j^* \langle\phi_j|)(c_k |\phi_k\rangle)} \\ &= \sqrt{\sum_{j,k} c_j^* c_k \delta_{j,k}} \\ &= \sqrt{\sum_j c_j^* c_j} = ||\vec{c}|| \end{aligned}$$

More generally, the inner product between $|\Psi\rangle = \sum c_j |\phi_j\rangle$ and $|\chi\rangle = \sum b_k |\phi_k\rangle$ is:

$$\begin{aligned} \langle\Psi|\chi\rangle &= \sum_{j,k} (c_j^* \langle\phi_j|)(b_k |\phi_k\rangle) \\ &= \sum_{j,k} c_j^* b_k \delta_{j,k} \\ &= \sum_j c_j^* b_j = (\vec{c}, \vec{b}) \end{aligned}$$

This is the inner product between column vectors \vec{c} and \vec{b} . For a normalized state vector, $(\vec{c}, \vec{c}) = 1$.

The dual vector $\langle\Psi|$ is represented by the row vector:

$$[\vec{c}]^\dagger = [c_1^* \quad c_2^* \quad \cdots \quad c_n^*]$$

1.1.3 Spin-Half Particles

The state space for a spin-half particle is 2-dimensional, with basis states $|1/2, +1/2\rangle = |\uparrow\rangle$ and $|1/2, -1/2\rangle = |\downarrow\rangle$. An arbitrary state can be written:

$$|\Psi\rangle = c_1 |\uparrow\rangle + c_2 |\downarrow\rangle = \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$$

with unit-normalization $|c_1|^2 + |c_2|^2 = 1$.

1.1.4 Change of Basis

A state can be represented using different sets of basis states. $|\Psi\rangle$ can be represented in $\{|\phi_k\rangle\}$ or $\{|\chi_j\rangle\}$ basis:

$$|\Psi\rangle = \sum_k c_k |\phi_k\rangle = \sum_j d_j |\chi_j\rangle \quad (1.1)$$

where $d_j = \langle\chi_j|\Psi\rangle$ and $c_k = \langle\phi_k|\Psi\rangle$.

We can expand the basis states in terms of each other. They form complete sets:

$$|\phi_n\rangle = \sum_m \langle\chi_m|\phi_n\rangle |\chi_m\rangle = \sum_m S_{mn} |\chi_m\rangle$$

$$|\chi_m\rangle = \sum_n \langle\phi_n|\chi_m\rangle |\phi_n\rangle = \sum_n S_{mn}^* |\phi_n\rangle$$

From above:

$$\begin{aligned} d_m &= \langle \chi_m | \Psi \rangle = \langle \chi_m | \sum_n c_n | \phi_n \rangle \\ &= \sum_n \langle \chi_m | \phi_n \rangle c_n = \sum_n S_{mn} c_n \end{aligned}$$

In matrix form:

$$\vec{d} = S \vec{c} \quad (1.2)$$

where $S_{mn} = \langle \chi_m | \phi_n \rangle$.

Explicit form of Eq. 1.2:

$$\begin{pmatrix} d_1 \\ d_2 \end{pmatrix} = \begin{pmatrix} \langle \chi_1 | \phi_1 \rangle & \langle \chi_1 | \phi_2 \rangle \\ \langle \chi_2 | \phi_1 \rangle & \langle \chi_2 | \phi_2 \rangle \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$$

S is the matrix that transforms between the two representations.

We can start from $|\phi_n\rangle = \sum_m \langle \chi_m | \phi_n \rangle |\chi_m\rangle$ to obtain the inverse transformation:

$$\begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} \langle \phi_1 | \chi_1 \rangle & \langle \phi_1 | \chi_2 \rangle \\ \langle \phi_2 | \chi_1 \rangle & \langle \phi_2 | \chi_2 \rangle \end{pmatrix} \begin{pmatrix} d_1 \\ d_2 \end{pmatrix}$$

Thus $\vec{c} = S^\dagger \vec{d}$.

Multiplying both sides by S :

$$S \vec{c} = S S^\dagger \vec{d}$$

Since $S \vec{c} = \vec{d}$, we must have:

$$S S^\dagger = I_n$$

Hence S is unitary. S is called a similarity transformation.

Example

Basis Change Example

Let $|\Psi\rangle = \sqrt{\frac{2}{3}} |\phi_1\rangle + i\sqrt{\frac{1}{3}} |\phi_2\rangle$. Let a new basis be:

$$|\chi_1\rangle = \frac{1}{\sqrt{2}} (|\phi_1\rangle + i|\phi_2\rangle)$$

$$|\chi_2\rangle = \frac{1}{\sqrt{2}} (|\phi_1\rangle - i|\phi_2\rangle)$$

This basis is orthonormal, $\langle \chi_i | \chi_j \rangle = \delta_{ij}$. Inverting for $|\phi_i\rangle$:

$$|\phi_1\rangle = \frac{1}{\sqrt{2}} (|\chi_1\rangle + |\chi_2\rangle)$$

$$|\phi_2\rangle = \frac{1}{i\sqrt{2}} (|\chi_1\rangle - |\chi_2\rangle)$$

The transformation matrix S has elements $S_{mn} = \langle \chi_m | \phi_n \rangle$:

$$\begin{aligned} S &= \begin{pmatrix} \langle \chi_1 | \phi_1 \rangle & \langle \chi_1 | \phi_2 \rangle \\ \langle \chi_2 | \phi_1 \rangle & \langle \chi_2 | \phi_2 \rangle \end{pmatrix} \\ &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i \\ 1 & -i \end{pmatrix} \end{aligned}$$

1.1.5 Subspaces

Given a vector space V , a sub-space W is a space containing some of the vectors of V and satisfying all properties of a vector space. Vectors in a subspace must be closed under addition and scalar multiplication, i.e., given any 2 vectors in W , v_1 and v_2 , we know that $\alpha v_1 + \beta v_2$ is also in W .

1.2 Postulate 2: Operators

Linear operators are the mathematical objects which capture the transformations undergone by states as they evolve and are measured.

1.2.1 Linear Operator

\hat{A} is a linear operator if the following holds:

$$\hat{A}(a_1 |\Psi_1\rangle + a_2 |\Psi_2\rangle) = \hat{A}a_1 |\Psi_1\rangle + \hat{A}a_2 |\Psi_2\rangle$$

1.2.2 Outer Product

$|\Psi\rangle\langle\phi|$ is a linear operator which transforms a state $|\chi\rangle$ into state $|\chi'\rangle$:

$$|\chi'\rangle = (|\Psi\rangle\langle\phi|) |\chi\rangle = \langle\phi|\chi\rangle |\Psi\rangle$$

$\hat{O} = |\Psi\rangle\langle\phi|$ has converted $|\chi\rangle$ into $|\Psi\rangle$.

1.2.3 Closure Relation

This represents the identity operator:

$$\hat{I} = \sum_j |\phi_j\rangle\langle\phi_j|$$

This acting on a state $|\Psi\rangle = \sum_k c_k |\phi_k\rangle$:

$$\begin{aligned} \left(\sum_j |\phi_j\rangle\langle\phi_j| \right) |\Psi\rangle &= \sum_j |\phi_j\rangle\langle\phi_j| \sum_k c_k |\phi_k\rangle \\ &= \sum_{j,k} c_k \langle\phi_j|\phi_k\rangle |\phi_j\rangle \\ &= \sum_{j,k} c_k \delta_{jk} |\phi_j\rangle \\ &= \sum_k c_k |\phi_k\rangle = |\Psi\rangle \end{aligned}$$

Sometimes referred to as the resolution of the identity.

1.2.4 Basis Transformation as an Outer Product Operator

We can re-examine the change of basis using the resolution of the identity $\mathbb{I} = \sum_j |\chi_j\rangle\langle\chi_j|$.

$$\begin{aligned} |\Psi\rangle &= \sum_k c_k |\phi_k\rangle = \mathbb{I} \cdot \sum_k c_k |\phi_k\rangle \\ &= \left(\sum_j |\chi_j\rangle\langle\chi_j| \right) \sum_k c_k |\phi_k\rangle \\ &= \sum_{j,k} c_k |\chi_j\rangle \langle\chi_j|\phi_k\rangle \\ &= \sum_j \left(\sum_k \langle\chi_j|\phi_k\rangle c_k \right) |\chi_j\rangle \\ &= \sum_j d_j |\chi_j\rangle \end{aligned}$$

where $d_j = \sum_k c_k \langle\chi_j|\phi_k\rangle$.

1.2.5 Matrix Representations of Linear Operators

Find matrix representation of operator \hat{A} :

$$\hat{A} = \mathbb{I} \cdot \hat{A} \cdot \mathbb{I} = \sum_{j,k} |\phi_j\rangle\langle\phi_j| \hat{A} |\phi_k\rangle\langle\phi_k| = \sum_{j,k} A_{jk} |\phi_j\rangle\langle\phi_k| \quad (1.3)$$

Matrix element of \hat{A} : $A_{jk} = \langle\phi_j|\hat{A}|\phi_k\rangle$.

Consider \hat{A} acting on general state $|\Psi\rangle$:

$$\begin{aligned} \hat{A}|\Psi\rangle &= \sum_{j,k} A_{jk} |\phi_j\rangle\langle\phi_k| \sum_m c_m |\phi_m\rangle \\ &= \sum_{j,k,m} A_{jk} c_m |\phi_j\rangle \langle\phi_k|\phi_m\rangle \\ &= \sum_{j,k,m} A_{jk} c_m |\phi_j\rangle \delta_{km} \\ &= \sum_{j,m} A_{jm} c_m |\phi_j\rangle \\ &= \sum_j \beta_j |\phi_j\rangle \end{aligned}$$

where $\beta_j = \sum_m A_{jm} c_m$, giving $\vec{\beta} = \hat{A}\vec{c}$.

1.2.6 Change of Basis for Operators

From Eq. 1.3, \hat{A} in $|\phi\rangle$ basis:

$$\hat{A}_\phi = \sum_{j,k} A_{jk}^{(\phi)} |\phi_j\rangle\langle\phi_k|$$

where $A_{jk}^{(\phi)} = \langle\phi_j|\hat{A}|\phi_k\rangle$, elements of matrix \hat{A}_ϕ .

Represent the same operator using basis χ_j :

$$\hat{A}_\chi = \sum_{l,m} A_{lm}^{(\chi)} |\chi_l\rangle\langle\chi_m|$$

Use 2 resolutions of the identity into the $\{|\chi_k\rangle\}$ basis:

$$\begin{aligned} \hat{A}_\phi &= \sum_{j,k} A_{jk}^{(\phi)} \hat{I} \cdot |\phi_j\rangle\langle\phi_k| \cdot \hat{I} \\ &= \sum_{j,k} A_{jk}^{(\phi)} \left(\sum_l |\chi_l\rangle\langle\chi_l| \right) |\phi_j\rangle\langle\phi_k| \left(\sum_m |\chi_m\rangle\langle\chi_m| \right) \\ &= \sum_{j,k,l,m} A_{jk}^{(\phi)} \langle\chi_l|\phi_j\rangle \langle\phi_k|\chi_m\rangle |\chi_l\rangle\langle\chi_m| \\ &= \sum_{l,m} A_{lm}^{(\chi)} |\chi_l\rangle\langle\chi_m| \end{aligned}$$

where:

$$\begin{aligned} A_{lm}^{(\chi)} &= \sum_{j,k} \langle\chi_l|\phi_j\rangle A_{jk}^{(\phi)} \langle\phi_k|\chi_m\rangle \\ &= \sum_{j,k} S_{lj} A_{jk}^{(\phi)} S_{mk}^* \end{aligned}$$

In vector notation:

$$A_\chi = S A_\phi S^\dagger$$

Using $SS^\dagger = \mathbb{I}$ we get:

$$S^\dagger A_\chi S = S^\dagger S A_\phi S^\dagger S$$

Thus:

$$A_\phi = S^\dagger A_\chi S$$

1.2.7 Hermitian Conjugate or Adjoints

Hermitian conjugate of operator \hat{A} , denoted \hat{A}^\dagger , is defined:

- Inner product notation: $(\hat{A}^\dagger |\Psi\rangle, |\phi\rangle) = (|\Psi\rangle, \hat{A} |\phi\rangle)$
- Dirac notation: $(\langle\phi|\hat{A}^\dagger|\Psi\rangle)^* = \langle\Psi|\hat{A}|\phi\rangle$

Using axiom 1 for inner products $\langle\Psi|\phi\rangle = \langle\phi|\Psi\rangle^*$.

Property:

$$(\langle\phi|\hat{A}\hat{B}|\Psi\rangle)^\dagger = \langle\Psi|\hat{B}^\dagger\hat{A}^\dagger|\phi\rangle$$

1.2.8 Hermitian Operator

\hat{A} is called Hermitian (or self-adjoint) if:

$$A^\dagger = A$$

Hermitian operators have real eigenvalues.

1.2.9 Spectral Decomposition of a Hermitian Operator

Consider $\hat{A}|\chi_j\rangle = \lambda_j|\chi_j\rangle$.

$\hat{A} = \sum_{j,k} A_{jk} |\phi_j\rangle \times |\phi_k\rangle$ takes the form of a diagonal matrix if \hat{A} is represented in $|\chi_j\rangle$ basis:

$$A_\chi = S A_\phi S^\dagger = A_D$$

where $A_D = \begin{pmatrix} \lambda_1 & & \\ & \lambda_2 & \\ & & \ddots \end{pmatrix}$.

Theorem then states that any Hermitian operator can be written as:

$$\hat{A} = \sum_{j,k} A_{jk} |\phi_j\rangle \times |\phi_k\rangle \equiv \sum_{j=1}^d \lambda_j |\chi_j\rangle \langle \chi_j|$$

where d is the dimension of the space on which \hat{A} acts. The above is called the spectral decomposition. Spectrum \Rightarrow set of eigenvalues.

For an Hamiltonian:

$$\hat{H} = \sum_j E_j |\chi_j\rangle \langle \chi_j| \quad (1.4)$$

where E_j are energy eigenvalues and $|\chi_j\rangle$ are energy eigenstates.

1.2.10 Projector

Def: Projector is any linear operator \hat{P} which satisfies:

$$\hat{P}^2 = \hat{P}$$

We can construct a projector from any normalized state $|\Psi\rangle$:

$$\hat{P}_{|\Psi\rangle} = |\Psi\rangle \langle \Psi|$$

Proof that this satisfies the above definition:

$$\begin{aligned} \hat{P}_{|\Psi\rangle}^2 &= |\Psi\rangle \langle \Psi| |\Psi\rangle \langle \Psi| \\ &= |\Psi\rangle \langle \Psi| \Psi \rangle \langle \Psi| = \hat{P}_{|\Psi\rangle} \end{aligned}$$

Generally projectors include sums of operators of the form:

$$\hat{P} = \sum_{j=1}^r |\phi_j\rangle \langle \phi_j|$$

r = projector rank (dimension of sub-space onto which \hat{P} is projecting). Action of a projector is to “project” a vector onto a sub-space by removing the components of the vector which causes it to lie outside the sub-space.

Example

Projector Example

Consider the matrix operator on \mathcal{R}^3 :

$$\hat{P} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

The action of this operator is to project a general vector onto its component in the x - y plane,

which is a subspace:

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} a \\ b \\ 0 \end{pmatrix}$$

1.2.11 Degenerate Eigenvalues

When two or more eigenvalues in the spectral decomposition coincide, they are degenerate. Consider a 3D example:

$$H = \lambda_1 |\phi_1\rangle \langle \phi_1| + \lambda_2 |\phi_2\rangle \langle \phi_2| + \lambda_2 |\phi_3\rangle \langle \phi_3|$$

We can rewrite this as:

$$\begin{aligned} H &= \lambda_1 |\phi_1\rangle \langle \phi_1| + \lambda_2 (|\phi_2\rangle \langle \phi_2| + |\phi_3\rangle \langle \phi_3|) \\ &= \lambda_1 \hat{P}_1 + \lambda_2 \hat{P}_2 \end{aligned}$$

The subspace spanned by $\{|\phi_2\rangle, |\phi_3\rangle\}$ is the eigenspace associated with λ_2 . Any vector in this subspace is an eigenvector of H with eigenvalue λ_2 :

$$\begin{aligned} H(\alpha |\phi_2\rangle + \beta |\phi_3\rangle) &= \alpha \lambda_2 |\phi_2\rangle + \beta \lambda_2 |\phi_3\rangle \\ &= \lambda_2 (\alpha |\phi_2\rangle + \beta |\phi_3\rangle) \end{aligned}$$

In general, the spectral decomposition can always be written in terms of projectors:

$$H = \sum_j \lambda_j \hat{P}_j$$

1.2.12 Operator Multiplication and the Commutator

Operators may be applied sequentially. $\hat{O}_3 \hat{O}_2 \hat{O}_1 |\psi\rangle$ means apply \hat{O}_1 first, then \hat{O}_2 , then \hat{O}_3 (read right-to-left). The commutator is defined as:

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$$

When the commutator is zero, the operators commute.

1.3 Postulate 3: Time-Evolution

The evolution of an isolated system is described by the (time-dependent) Schrödinger equation:

$$i\hbar \frac{\partial |\Psi\rangle}{\partial t} = \hat{H} |\Psi\rangle$$

where \hat{H} is the Hamiltonian, a Hermitian operator.

1.3.1 Time Evolution and Unitarity

Evolution under the Schrödinger equation is always unitary. The state at time t_1 evolves to the state at t_2 via a unitary evolution operator $\hat{U}(t_2, t_1)$:

$$|\psi(t_2)\rangle = \hat{U}(t_2, t_1) |\psi(t_1)\rangle$$

An operator \hat{U} is unitary if its Hermitian conjugate is its inverse:

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

Properties of unitary operators:

- They are norm-preserving: $\|\hat{U}|\psi\rangle\| = \||\psi\rangle\|$.
- They preserve the inner product: $(\hat{U}|\phi\rangle, \hat{U}|\psi\rangle) = \langle\phi|\psi\rangle$.
- They have eigenvalues of the form $e^{i\theta}$.

Unitary operators are a generalization of rotation operators. For time-independent Hamiltonians, the time-evolution operator takes the form:

$$\hat{U}_\chi(t) = \sum_{j=1}^d e^{-iE_j t/\hbar} |\chi_j\rangle\langle\chi_j|$$

1.4 Postulate 4: Measurement

This postulate is for discrete systems. Associated with every observable quantity is a Hermitian operator \hat{M} with a spectral decomposition $\hat{M} = \sum_j \lambda_j \hat{P}_j$. The eigenvalues λ_j label the possible outcomes of the measurement. When the measurement is performed on a system in state $|\Psi\rangle$, the probability that eigenvalue λ_j is returned is:

$$P(\lambda_j) = \langle\Psi|\hat{P}_j|\Psi\rangle$$

After a measurement which has returned eigenvalue λ_j , the state of the system becomes:

$$|\Psi'\rangle = \frac{\hat{P}_j|\Psi\rangle}{\sqrt{\langle\Psi|\hat{P}_j|\Psi\rangle}}$$

1.4.1 Pauli Matrices

The Pauli matrices are:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Properties for $k = x, y, z$:

- Self-inverse: $\sigma_k^2 = \mathbb{I}$.
- Hermitian: $\sigma_k^\dagger = \sigma_k$.
- Unitary: $\sigma_k \sigma_k^\dagger = \mathbb{I}$.
- Anti-commute (for $j \neq k$): $\sigma_j \sigma_k = -\sigma_k \sigma_j$.

1.4.2 Spin-Half Operator Matrix Representations

Using the \hat{S}_z eigenbasis $|\uparrow\rangle \cong \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, $|\downarrow\rangle \cong \begin{pmatrix} 0 \\ 1 \end{pmatrix}$, the spin operators are:

$$\begin{aligned} \hat{S}_x &\cong \frac{\hbar}{2} \sigma_x = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\ \hat{S}_y &\cong \frac{\hbar}{2} \sigma_y = \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \\ \hat{S}_z &\cong \frac{\hbar}{2} \sigma_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \end{aligned}$$

The eigenvectors of σ_x are $|x\pm\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle \pm |\downarrow\rangle)$ with eigenvalues ± 1 . The eigenvectors of σ_y are $|y\pm\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle \pm i|\downarrow\rangle)$ with eigenvalues ± 1 .

1.4.3 Spin Measurement Example

Consider measurement of spin in the x -direction. The outcomes are $\pm\hbar/2$. The operator is:

$$\hat{S}_x = \frac{+\hbar}{2} |x_+\rangle\langle x_+| + \frac{-\hbar}{2} |x_-\rangle\langle x_-|$$

The outcome $+\hbar/2$ is associated with the projector $\hat{P}_+ = |x_+\rangle\langle x_+|$. For a general state $|\Psi\rangle = \alpha|\uparrow\rangle + \beta|\downarrow\rangle$, the probability of getting $+\hbar/2$ is:

$$\begin{aligned} P(+\hbar/2) &= \langle\Psi|\hat{P}_+|\Psi\rangle \\ &= |\langle x_+|\Psi\rangle|^2 \\ &= \left| \left(\frac{1}{\sqrt{2}}(\langle\uparrow| + \langle\downarrow|) \right) (\alpha|\uparrow\rangle + \beta|\downarrow\rangle) \right|^2 \\ &= \frac{1}{2} |\alpha + \beta|^2 \end{aligned}$$

After the measurement, the state transforms to:

$$\begin{aligned} |\Psi'\rangle &= \frac{\hat{P}_+|\Psi\rangle}{\sqrt{P(+\hbar/2)}} \\ &= \frac{(\langle x_+|\Psi\rangle)|x_+\rangle}{|\langle x_+|\Psi\rangle|} = |x_+\rangle \end{aligned}$$

Example

Degenerate Measurement

Consider the degenerate Hamiltonian from earlier:

$$H = \lambda_1 |\phi_1\rangle\langle\phi_1| + \lambda_2 (|\phi_2\rangle\langle\phi_2| + |\phi_3\rangle\langle\phi_3|)$$

For a general state $|\Psi\rangle = \alpha|\phi_1\rangle + \beta|\phi_2\rangle + \gamma|\phi_3\rangle$ (with $|\alpha|^2 + |\beta|^2 + |\gamma|^2 = 1$). The projector corresponding to outcome λ_2 is $\hat{P}_2 = |\phi_2\rangle\langle\phi_2| +$

$|\phi_3\rangle\langle\phi_3|$. The probability of this outcome is:

$$\begin{aligned} P(\lambda_2) &= \langle\Psi|\hat{P}_2|\Psi\rangle \\ &= \langle\Psi|(|\phi_2\rangle\langle\phi_2| + |\phi_3\rangle\langle\phi_3|)|\Psi\rangle \\ &= |\langle\phi_2|\Psi\rangle|^2 + |\langle\phi_3|\Psi\rangle|^2 \\ &= |\beta|^2 + |\gamma|^2 \end{aligned}$$

The state transforms to:

$$|\Psi'\rangle = \frac{\hat{P}_2|\Psi\rangle}{\sqrt{P(\lambda_2)}} = \frac{\beta|\phi_2\rangle + \gamma|\phi_3\rangle}{\sqrt{|\beta|^2 + |\gamma|^2}}$$

1.4.4 Expectation Value

The expectation value is the average value of a measurement outcome for an observable \hat{X} .

$$\langle\hat{X}\rangle = \langle\Psi|\hat{X}|\Psi\rangle$$

Using the spectral decomposition $\hat{X} = \sum_j \lambda_j \hat{P}_j$ (or $\sum_j \lambda_j |\phi_j\rangle\langle\phi_j|$ for non-degenerate):

$$\begin{aligned} \langle\hat{X}\rangle &= \langle\Psi|(\sum_j \lambda_j |\phi_j\rangle\langle\phi_j|)|\Psi\rangle \\ &= \sum_j \lambda_j |\langle\phi_j|\Psi\rangle|^2 \\ &= \sum_j \lambda_j p_j \end{aligned}$$

where p_j is the probability of outcome λ_j .

1.4.5 Global Phase

Two states which differ only by a global phase, e.g., $|\Psi\rangle$ and $|\phi\rangle = e^{i\theta}|\Psi\rangle$, have no measurable difference in quantum mechanics. This is because all expectation values are the same:

$$\begin{aligned} \langle\hat{X}\rangle_\phi &= \langle\phi|\hat{X}|\phi\rangle \\ &= (e^{-i\theta}\langle\Psi|)\hat{X}(e^{i\theta}|\Psi\rangle) \\ &= e^{-i\theta}e^{i\theta}\langle\Psi|\hat{X}|\Psi\rangle = \langle\hat{X}\rangle_\Psi \end{aligned}$$

1.5 Density Operator and Density Matrix

The state vector description is not the most general. Some experiments have additional “classical” randomness, such as an imperfect device or entanglement with an environment. This requires a new formalism: the density matrix or density operator.

1.5.1 Adding Classical Uncertainty

Measurements in quantum mechanics are intrinsically non-deterministic. We can also have “classical randomness” (e.g., a coin toss) which arises from a lack of detailed information. We need a formalism to combine both types of randomness.

Toy Example

An experiment prepares state $|\Psi_1\rangle$ with probability p_1 and state $|\Psi_2\rangle$ with probability $p_2 = 1 - p_1$. The expectation value for an observable \hat{O} is the average-of-averages:

$$\begin{aligned} \langle\hat{O}\rangle_1 &= \langle\Psi_1|\hat{O}|\Psi_1\rangle \\ \langle\hat{O}\rangle_2 &= \langle\Psi_2|\hat{O}|\Psi_2\rangle \\ \langle\hat{O}\rangle_{\text{total}} &= p_1 \langle\hat{O}\rangle_1 + p_2 \langle\hat{O}\rangle_2 \\ &= p_1 \langle\Psi_1|\hat{O}|\Psi_1\rangle + p_2 \langle\Psi_2|\hat{O}|\Psi_2\rangle \end{aligned}$$

The states $|\Psi_1\rangle$ and $|\Psi_2\rangle$ do not need to be orthogonal.

- **Pure States:** States described by a single state vector $|\Psi\rangle$.
- **Mixed States:** States that require a probabilistic (classical) mixture of wavefunctions.

1.5.2 Pure States

Any state whose density matrix consists of a single projector:

$$\hat{\rho} = |\Psi\rangle\langle\Psi|$$

Calculations can be made in either the $\hat{\rho}$ picture or the state vector picture.

1.5.3 Mixed States

Its density matrix cannot be written as a single projector. Constructed from the sum of a set of projectors:

$$\hat{\rho} = \sum_j p_j |\Psi_j\rangle\langle\Psi_j| \quad (1.5)$$

where p_j are probabilities. $|\Psi_j\rangle$ don't have to be orthonormal to each other.

1.5.4 Properties of the Density Operator

- Can be represented as a matrix: $\hat{\rho} = \sum_{j,k} \rho_{jk} |\phi_j\rangle\langle\phi_k|$ where $\rho_{jk} = \langle\phi_j|\hat{\rho}|\phi_k\rangle$.
- $\hat{\rho}$ is Hermitian linear operator: $\hat{\rho} = \hat{\rho}^\dagger$.
- $\hat{\rho}$ has unit trace, to ensure probability for outcomes is summed to 1.

- $\hat{\rho}$ is a positive operator, ensures that any measurement is given by +ve probability.

$$\begin{aligned}\langle \hat{\rho} | &= \langle \phi | \left(\sum_j p_j |\Psi_j\rangle\langle\Psi_j| \right) | \phi \rangle \\ &= \sum_j p_j |\langle \Psi_j | \phi \rangle|^2 \geq 0\end{aligned}$$

Additional properties:

Trace

For operator \hat{A} :

$$\text{Tr}(\hat{A}) = \sum_j A_{jj} = \sum_j \langle \phi_j | \hat{A} | \phi_j \rangle$$

where $|\phi_j\rangle$ are orthonormal basis.

Linearity of Trace: Linear in its argument:

$$\text{Tr}(\lambda_1 \hat{A}_1 + \lambda_2 \hat{A}_2) = \lambda_1 \text{Tr}(\hat{A}_1) + \lambda_2 \text{Tr}(\hat{A}_2)$$

Cyclic Invariance of Trace:

$$\text{Tr}(\hat{A}\hat{B}) = \sum_j \langle \phi_j | \hat{A}\hat{B} | \phi_j \rangle$$

Use $\hat{I} = \sum_k |\phi_k\rangle\langle\phi_k|$:

$$\begin{aligned}&= \sum_{j,k} \langle \phi_j | \hat{A} | \phi_k \rangle \langle \phi_k | \hat{B} | \phi_j \rangle \\ &= \sum_{j,k} \langle \phi_k | \hat{B} | \phi_j \rangle \langle \phi_j | \hat{A} | \phi_k \rangle \\ &= \sum_k \langle \phi_k | \hat{B}\hat{A} | \phi_k \rangle = \text{Tr}(\hat{B}\hat{A})\end{aligned}$$

Permuted cyclically: $\text{Tr}(ABC) = \text{Tr}(CAB) = \text{Tr}(BCA)$.

Basis Independence of Trace: Consider 2 orthonormal bases $|\phi_j\rangle$ and $|\Psi_j\rangle = \hat{S} |\phi_j\rangle$. Defined with respect to 1st basis, $\text{Tr} \hat{A}$ is:

$$\text{Tr}_\phi(\hat{A}) = \sum_j \langle \phi_j | \hat{A} | \phi_j \rangle$$

Defined with respect to 2nd basis:

$$\text{Tr}_\Psi(\hat{A}) = \sum_j \langle \Psi_j | \hat{A} | \Psi_j \rangle$$

Since $|\Psi_j\rangle = \hat{S} |\phi_j\rangle$:

$$\begin{aligned}\text{Tr}_\Psi(\hat{A}) &= \sum_j \langle \phi_j | \hat{S}^\dagger \hat{A} \hat{S} | \phi_j \rangle \\ &= \text{Tr}_\phi(\hat{S}^\dagger \hat{A} \hat{S})\end{aligned}$$

Use the cyclic invariance of Trace:

$$\text{Tr}_\phi(\hat{S}^\dagger \hat{A} \hat{S}) = \text{Tr}_\phi(\hat{A} \hat{S} \hat{S}^\dagger) = \text{Tr}_\phi(\hat{A})$$

Hence: $\text{Tr}_\Psi(\hat{A}) = \text{Tr}_\phi(\hat{A})$. Trace of \hat{A} is independent of the basis chosen for the matrix representation.

1.5.5 Measurements and the Density Operator

Expectation value of an operator can be written as:

$$\langle \hat{O} \rangle = \text{Tr}(\hat{\rho} \hat{O}) \quad (1.6)$$

Expectation value averaged over a statistical mixture of states (from p.4 toy example):

$$\langle \hat{O} \rangle = \sum_n p_n \langle \Psi_n | \hat{O} | \Psi_n \rangle$$

Trace of $\hat{\rho} \hat{O}$:

$$\begin{aligned}\text{Tr}(\hat{\rho} \hat{O}) &= \sum_k \langle \phi_k | \hat{\rho} \hat{O} | \phi_k \rangle \\ &= \sum_k \langle \phi_k | \sum_n p_n |\Psi_n\rangle\langle\Psi_n| \hat{O} | \phi_k \rangle \\ &= \sum_n p_n \sum_k \langle \phi_k | \Psi_n \rangle \langle \Psi_n | \hat{O} | \phi_k \rangle \\ &= \sum_n p_n \sum_k \langle \Psi_n | \hat{O} | \phi_k \rangle \langle \phi_k | \Psi_n \rangle \\ &= \sum_n p_n \langle \Psi_n | \hat{O} \left(\sum_k |\phi_k\rangle\langle\phi_k| \right) | \Psi_n \rangle \\ &= \text{Tr}(\hat{\rho} \hat{O}) = \sum_n p_n \langle \Psi_n | \hat{O} | \Psi_n \rangle \quad (1.7)\end{aligned}$$

Eq. 1.6 \equiv Eq. 1.7.

1.5.6 Purity

For a pure state $\hat{\rho} = \hat{\rho}^2$, $\text{Tr}(\hat{\rho}^2) = 1$.

For mixed state (Eq. 1.5):

$$\hat{\rho} = \sum_j p_j |\phi_j\rangle\langle\phi_j|$$

$$\begin{aligned}\hat{\rho}^2 &= \sum_{j,k} p_j p_k |\phi_j\rangle\langle\phi_j| |\phi_k\rangle\langle\phi_k| \\ &= \sum_{j,k} p_j p_k |\phi_j\rangle\langle\phi_j| \langle\phi_j|\phi_k\rangle \langle\phi_k| \delta_{jk} \\ &= \sum_k p_k^2 |\phi_k\rangle\langle\phi_k|\end{aligned}$$

\neq Eq. 1.5 $= \sum_k p_k |\phi_k\rangle\langle\phi_k|$.

Hence for mixed state $\hat{\rho} \neq \hat{\rho}^2$.

$$\begin{aligned}\text{Tr}(\hat{\rho}^2) &= \sum_l \langle \phi_l | \left(\sum_k p_k^2 |\phi_k\rangle\langle\phi_k| \right) | \phi_l \rangle \\ &= \sum_{k,l} p_k p_l |\langle \phi_k | \phi_l \rangle|^2 \delta_{kl} \\ &= \sum_l p_l^2\end{aligned}$$

Since $p_l < 1$, $p_l^2 < p_l$ so $\sum_l p_l^2 < \sum_l p_l = 1$.

Define purity of a state as:

$$\mathcal{P} = \text{Tr}(\hat{\rho}^2)$$

- Pure state: $\mathcal{P} = 1$.
- Mixed state: $\mathcal{P} < 1$.

1.5.7 Examples

Example

Spin system (pure case)

Consider spin 1/2 particle:

$$|+\rangle_x = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)$$

Density operator: $\hat{\rho} = |+\rangle_x \langle +|_x$

$$= \frac{1}{2}(|\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow| + |\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow|)$$

Matrix representation:

$$\rho = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$$

Example

Spin system (mixed case)

Assume mixture of probability 1/4 of being 'up' and 3/4 of being 'down'.

$$\hat{\rho} = \sum_n p_n |\phi_n\rangle\langle\phi_n| = \frac{1}{4} |\uparrow\rangle\langle\uparrow| + \frac{3}{4} |\downarrow\rangle\langle\downarrow|$$

Matrix representation:

$$\rho = \begin{pmatrix} 1/4 & 0 \\ 0 & 3/4 \end{pmatrix} \text{ in } |\uparrow\rangle, |\downarrow\rangle \text{ basis}$$

Purity: $\mathcal{P} = \text{Tr}(\rho^2) = 1/16 + 9/16 = 5/8$.

Max mixing: $\rho = \begin{pmatrix} 1/N & & \\ & \ddots & \\ & & 1/N \end{pmatrix}$, $N =$

dimension.

In this case 2D: $\rho = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}$.

Example

Systems in Thermal Equilibrium

Probability that the system (at temp T) is in state $|\Psi_n\rangle$ is given by the Boltzmann factor. At non-zero T , the system is given by mixed state:

$$\hat{\rho} = \frac{\sum_n e^{-\beta E_n} |\Psi_n\rangle\langle\Psi_n|}{\sum_m e^{-\beta E_m}}$$

For nuclear spins, MRI machines are close to max. mixed state (50% spin-up, 50% spin-down). Preparing nuclear spins in pure states is very challenging.

Example

Different Representations of $\hat{\rho}$

Consider we want to prepare a $|+\rangle_x$ state. Experiment went wrong; the state is 50% $|+\rangle_x$, 25% $|-\rangle_x$ and 12.5% $|+\rangle_z$ and 12.5% $|-\rangle_z$.

a) Write directly $\hat{\rho} = \sum_j p_j |\phi_j\rangle\langle\phi_j|$:

$$\hat{\rho} = \frac{1}{2} |+\rangle_x \langle +|_x + \frac{1}{4} |-\rangle_x \langle -|_x + \frac{1}{8} |+\rangle_z \langle +|_z + \frac{1}{8} |-\rangle_z \langle -|_z$$

$|\pm\rangle_x$ and $|\pm\rangle_z$ are not orthogonal.

b) Represent $\hat{\rho}$ using $|\pm\rangle_z$ basis. Use: $\hat{\rho} = \sum_{jk} \rho_{jk} |\phi_j\rangle\langle\phi_k|$

Remember $|+\rangle_z = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, $|-\rangle_z = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$.

z -Basis projectors: $|+\rangle_x \langle +|_x = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$,

$$|-\rangle_x \langle -|_x = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}.$$

x -Basis projectors: By definition $|+\rangle_x = \frac{1}{\sqrt{2}}(|+\rangle_z + |-\rangle_z)$, $|-\rangle_x = \frac{1}{\sqrt{2}}(|+\rangle_z - |-\rangle_z)$.

This gives: $|+\rangle_x \langle +|_x = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$, $|-\rangle_x \langle -|_x =$

$$\frac{1}{2} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}.$$

Put all together:

$$\begin{aligned}\rho &= \frac{1}{2} \left(\frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \right) + \frac{1}{4} \left(\frac{1}{2} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} \right) + \frac{1}{8} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \frac{1}{8} \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \\ &= \begin{pmatrix} 1/2 & 1/8 \\ 1/8 & 1/2 \end{pmatrix}\end{aligned}$$

c) $\hat{\rho}$ as a spectral decomposition. Write in the form: $\hat{\rho} = \sum_k \lambda_k |\phi_k\rangle\langle\phi_k|$.

Solve characteristic equation of the above matrix: $\lambda_1 = 3/8, \lambda_2 = 5/8$.
 Eigenvectors $|1\rangle, |2\rangle$: $\hat{\rho} = \frac{3}{8}|1\rangle\langle 1| + \frac{5}{8}|2\rangle\langle 2|$.
 Traces of all the representations are unchanged:
 $\sum \lambda = \sum p = 1$.

1.6 Composite Systems

Consider 2 systems A and B, each has orthonormal basis:

$$|a_1\rangle, |a_2\rangle, \dots, |a_{d_a}\rangle \quad |b_1\rangle, |b_2\rangle, \dots, |b_{d_b}\rangle$$

We are interested in finding a joint description of these 2 systems.

Properties required:

- Closed under vector addition and scalar multiplication \Rightarrow Superposition must apply to joint state.

Example

Two Spin Half Particles

Consider particle A and B: Basis states labeled as $|\uparrow\rangle_A, |\downarrow\rangle_A$ and $|\uparrow\rangle_B, |\downarrow\rangle_B$. Full basis of joint system:

$$\begin{aligned} |1\rangle &\leftarrow |\uparrow\rangle_A |\uparrow\rangle_B \\ |2\rangle &\leftarrow |\uparrow\rangle_A |\downarrow\rangle_B \\ |3\rangle &\leftarrow |\downarrow\rangle_A |\uparrow\rangle_B \\ |4\rangle &\leftarrow |\downarrow\rangle_A |\downarrow\rangle_B \end{aligned}$$

Note: ordering is arbitrary. General state for 2-spin system:

$$\begin{aligned} |\Psi\rangle &= \sum_n \alpha_n |n\rangle \\ &= \alpha_1 |\uparrow\rangle_A |\uparrow\rangle_B + \alpha_2 |\uparrow\rangle_A |\downarrow\rangle_B \\ &\quad + \alpha_3 |\downarrow\rangle_A |\uparrow\rangle_B + \alpha_4 |\downarrow\rangle_A |\downarrow\rangle_B \end{aligned}$$

1.6.1 Tensor Products for Composite Systems

Given d_a dimensional space \mathcal{A} with basis states $\{|a_j\rangle\}$, $j = 1, 2, \dots, d_a$ and d_b dimensional space \mathcal{B} with basis states $\{|b_k\rangle\}$, $k = 1, 2, \dots, d_b$.

The tensor product is: $\mathcal{A} \otimes \mathcal{B}$.

$|a_1\rangle \otimes |b_1\rangle$ corresponds to system A being in state $|a_1\rangle$ and system B being in state $|b_1\rangle$.

Full basis for $\mathcal{A} \otimes \mathcal{B}$ is constructed by including all $d_a \times d_b$ pairings of basis vectors from the two spaces,

in such way:

$$|\Psi\rangle = \sum_{j,k} c_{jk} |a_j\rangle \otimes |b_k\rangle$$

Dimension of new space is $d_a \times d_b$.

Notation

Drop \otimes : $|a_1, b_1\rangle \equiv |a_1\rangle \otimes |b_1\rangle$.

Example - when combining orbital and spin angular momenta:

$$|\Psi\rangle = \sum C_{m_l m_s} |l m_l\rangle |s m_s\rangle \equiv \sum C_{m_l m_s} |s m_s\rangle |l m_l\rangle$$

Tensor Products of Operators

Given operator \hat{P} acting on \mathcal{A} and operator \hat{Q} acting on \mathcal{B} , $\hat{P} \otimes \hat{Q}$ is:

$$\hat{P} \otimes \hat{Q} |\Psi\rangle = \sum_{j,k} c_{jk} (\hat{P} |a_j\rangle) \otimes (\hat{Q} |b_k\rangle)$$

Operators of the form $\hat{P} \otimes \mathbb{I}$ or $\mathbb{I} \otimes \hat{Q}$ which acts only on subspace 1 or A in this case are written as \hat{P}_1 or \hat{P}_A .

1.6.2 Product States vs Entangled States

Product state: if $\mathcal{A} \otimes \mathcal{B}$ can be written as a tensor product over individual states.

Consider 2 level systems. The following are product states:

$$\begin{aligned} |\psi_1\rangle &= |\uparrow\rangle_A |\uparrow\rangle_B \\ |\psi_2\rangle &= |\downarrow\rangle_A |\uparrow\rangle_B \\ |\psi_3\rangle &= \frac{1}{2} (|\uparrow\rangle_A |\uparrow\rangle_B + |\uparrow\rangle_A |\downarrow\rangle_B + |\downarrow\rangle_A |\uparrow\rangle_B + |\downarrow\rangle_A |\downarrow\rangle_B) \\ &= \frac{1}{2} (|\uparrow\rangle_A + |\downarrow\rangle_A) (|\uparrow\rangle_B + |\downarrow\rangle_B) \end{aligned}$$

\Rightarrow Each particle has its own well defined state, independent of each other.

Entangled state: a state which is impossible to write in product state. They exhibit strong correlation between outcomes. Bell state is entangled:

$$|\psi_4\rangle = \frac{1}{\sqrt{2}} (|\uparrow\rangle_A \otimes |\uparrow\rangle_B + |\downarrow\rangle_A \otimes |\downarrow\rangle_B) \quad (1.8)$$

The above, there is no way to write it as a separate "state vector for system A" and "state vector for system B".

Extra clarification:

State $|\psi_3\rangle$: if system A is in $|\uparrow\rangle$ state then system B can be $|\uparrow\rangle$ or $|\downarrow\rangle$.

State $|\psi_4\rangle$ (Eq. 1.8): if system A is in $|\uparrow\rangle$ state then system B must be in $|\uparrow\rangle$ state.

If a measurement on A yield $|\uparrow\rangle$, a measurement on B will also yield $|\uparrow\rangle$ no matter the distance between the two.

This does not violate relativity. Observer at B without classical communication about the result at A, cannot know that a measurement has occurred. Observer at B can describe state of B using reduced state of B:

$$\rho_B^{\text{reduced}} = \frac{1}{2}(|\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow|)$$

This comes from: $\rho_B = \sum_{i,j} \rho_{ij} |\phi_i\rangle\langle\phi_j|$.

This reduced state for B will remain the same regardless of the measurement basis chosen in A. \Rightarrow Ensures no faster than light signaling is possible.

1.6.3 Entanglement and Independent Degrees of Freedom

Tensor product are applied between spaces corresponding independent degrees of freedom. For a free particle in a box:

$$|\Psi\rangle = \sum_{n_x, n_y, n_z} c_{n_x n_y n_z} |n_x\rangle \otimes |n_y\rangle \otimes |n_z\rangle$$

Total angular momentum and it's eigenstates are not independent:

$$|jm\rangle \neq |j\rangle \otimes |m\rangle$$

Example: H atom with $n = 2$, $l = 0, 1$, $m = -1, 0, 1$. One would expect $d_l \times d_m = 6$. However we have 4: $(0, 0), (1, -1), (1, 0), (1, 1)$ since $l \geq |m|$.

1.6.4 Density Matrix for Composite Systems

We construct $\hat{\rho}$ for composite system the same way we do it for isolated systems.

General $\hat{\rho}$ on systems A and B with orthonormal basis $|a_j\rangle$ and $|b_k\rangle$:

$$\hat{\rho} = \sum_{j,k,j',k'} \rho_{jk,j'k'} |a_j, b_k\rangle\langle a_{j'}, b_{k'}|$$

where $\rho_{jk,j'k'} = \langle a_j, b_k | \hat{\rho} | a_{j'}, b_{k'} \rangle$.

1.6.5 Reduced States

Reduced state for system A is the state which allows one to calculate the value of any observable which acts solely on system A, ignoring system B.

Reduced state is obtained by an operation called partial trace.

Partial Trace

Use definition of trace:

$$\text{Tr}(\hat{\rho}) = \sum_{j,k} \rho_{jk,jk}$$

where $\rho_{jk,jk} = \langle a_j, b_k | \hat{\rho} | a_{j'}, b_{k'} \rangle \delta_{jj'} \delta_{kk'}$.

Partial trace is an operation which allows us to “delete” a system from our tensor product composite system, and gives us a reduced state of remaining system.

Example: To delete system A, perform partial trace over system A.

$$\text{Tr}_A(\hat{\rho}) = \sum_j \sum_{k,k'} \rho_{jk,jk'} |b_k\rangle\langle b_{k'}| \quad (1.9)$$

Note: sum over j only and not j' . We say that system A is “traced out” of the state description.

Eq. 1.9 is equal to:

$$\text{Tr}_A(\hat{\rho}) = \sum_{k,k'} \rho_{kk'}^{(B)} |b_k\rangle\langle b_{k'}| = \hat{\rho}_B \quad (1.10)$$

This state is constructed from B basis alone. Notation: Trace of A: Tr_A . Reduced state of B: $\hat{\rho}_B$.

Now we can use Eq. 1.10 to calculate observables which act only on B:

$$\langle \hat{O} \rangle = \text{Tr}(\hat{O} \hat{\rho}_B) = \text{Tr} \left(\hat{O} \sum_{k,k'} \rho_{kk'}^{(B)} |b_k\rangle\langle b_{k'}| \right)$$

Similarly, the reduced state for A is $\hat{\rho}_A = \text{Tr}_B(\hat{\rho})$.

The reduced state of an entangled system is **always** a mixed state.

Example

Spontaneous Decay

Excited state $|e\rangle$ can decay spontaneously to a lower energy ground state $|g\rangle$.

Vacuum state $|0\rangle$, state where 1 photon is present $|1\rangle$.

Spontaneous emission described via the following time-varying state. At $t = 0$:

$$|\Psi(t=0)\rangle = |e\rangle |0\rangle \Rightarrow \text{Pure state}$$

$$|\Psi(t)\rangle = e^{-\kappa t} |e\rangle |0\rangle + \sqrt{1 - e^{-2\kappa t}} |g\rangle |1\rangle \Rightarrow \text{Pure entangled state}$$

Rewrite as $= c_0 |e, 0\rangle + c_1 |g, 1\rangle$.

Density matrix $\hat{\rho} = \sum_{i,j} \rho_{ij} |\phi_i\rangle\langle\phi_j|$:

$$|\Psi\rangle\langle\Psi| = |c_0|^2 |e, 0\rangle\langle e, 0| + |c_1|^2 |g, 1\rangle\langle g, 1| + c_0 c_1^* |e, 0\rangle\langle g, 1| + c_1 c_0^* |g, 1\rangle\langle e, 0|$$

Take partial trace over the γ mode:

$$\begin{aligned}\hat{\rho}_{\text{atom}} &= \text{Tr}_{\text{light}}(|\Psi\rangle\langle\Psi|) \\ &= |c_0|^2 |e\rangle\langle e| + |c_1|^2 |g\rangle\langle g|\end{aligned}$$

\Rightarrow Mixed state.

Restoring the j_1 label:

$$\hat{\rho}_1 = \sum_{m_1} |\mathcal{C}_{m_1, M-m_1}^{(M)}|^2 |j_1 m_1\rangle\langle j_1 m_1|$$

The reduced density matrix of system 1 is a mixed state and is diagonal in the $|j_1 m_1\rangle$ basis.

Example

Total Angular Momentum States

Two systems with momentum eigenstates $|j_1 m_1\rangle$ and $|j_2 m_2\rangle$ can form a total momentum eigenstate $|JM\rangle$:

$$|JM; j_1 j_2\rangle = \sum_{m_1, m_2} \mathcal{C}_{m_1, m_2}^{(M)} |j_1 m_1\rangle \otimes |j_2 m_2\rangle$$

The j_1 , j_2 subsystems may be considered to be fully entangled. The coefficients are called Clebsch-Gordan coefficients.

Since $M = m_1 + m_2$, a measurement of any value of m_1 fully determines m_2 . Hence we may write:

$$|JM; j_1 j_2\rangle = \sum_{m_1} C_{m_1} |m_1\rangle |M - m_1\rangle$$

A simple case is the spin singlet state ($j_1 = j_2 = 1/2$, $J = 0$, $M = 0$):

$$|S = 0, M = 0\rangle = \frac{1}{\sqrt{2}}(|\frac{1}{2}\rangle_1 |-\frac{1}{2}\rangle_2 - |-\frac{1}{2}\rangle_1 |\frac{1}{2}\rangle_2)$$

The general density operator for the joint pure state is:

$$\begin{aligned}\hat{\rho} &= |JM\rangle\langle JM| \\ &= \sum_{m_1, m'_1} C_{m_1} C_{m'_1}^* |m_1, M - m_1\rangle\langle m'_1, M - m'_1|\end{aligned}$$

We trace over subsystem 2 to find the reduced state of system 1:

$$\begin{aligned}\hat{\rho}_1 &= \text{Tr}_2(\hat{\rho}) = \sum_{n_2} \langle n_2 | \hat{\rho} | n_2 \rangle \\ &= \sum_{n_2} \sum_{m_1, m'_1} C_{m_1} C_{m'_1}^* |m_1\rangle\langle m'_1| \langle n_2 | M - m_1 \rangle \langle M - m'_1 | n_2 \rangle \\ &= \sum_{n_2} \sum_{m_1, m'_1} C_{m_1} C_{m'_1}^* |m_1\rangle\langle m'_1| \delta_{n_2, M - m_1} \delta_{M - m'_1, n_2}\end{aligned}$$

The Kronecker deltas imply $n_2 = M - m_1$ and $n_2 = M - m'_1$, which means $m_1 = m'_1$.

$$\hat{\rho}_1 = \sum_{m_1} |C_{m_1}|^2 |m_1\rangle\langle m_1|$$

Chapter 2

Time Dependent Perturbation Theory

2.1 Intro

Consider the following system:

$$\hat{H}(t) = \hat{H}_0 + \lambda \hat{V}(t)$$

\hat{H}_0 is a time-independent Hamiltonian. $\hat{V}(t)$ is a Hamiltonian, and λ is a real parameter.

Perturbation theory is effective when the perturbation $\hat{V}(t)$ is weak: Matrix elements of $\hat{V}(t)$ are $\ll E_j - E_k$.

If no perturbation is present ($\hat{V}(t) = 0$), solving TDSE gets:

$$|\Psi(t)\rangle = \sum_k e^{\frac{-iE_k t}{\hbar}} c_k |\phi_k\rangle$$

Coefficients c_k are constant in time, and depend on initial state:

$$|\Psi(0)\rangle = \sum_k c_k |\phi_k\rangle$$

2.2 Dirac's method of variation of constants

Consider eigenstates of \hat{H}_0 :

$$|\Psi(t)\rangle = \sum_j c_j(t) e^{(-iE_j t/\hbar)} |\phi_j\rangle$$

Now probability amplitudes $c_j(t)$ vary in time.

Sub into TDSE:

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} \sum_j c_j(t) e^{\frac{-iE_j t}{\hbar}} |\phi_j\rangle \\ = (\hat{H}_0 + \lambda \hat{V}(t)) |\Psi(t)\rangle \end{aligned}$$

LHS:

$$\begin{aligned} \sum_j c_j(t) E_j e^{\frac{-iE_j t}{\hbar}} |\phi_j\rangle \\ + i\hbar \sum_j \dot{c}_j(t) e^{\frac{-iE_j t}{\hbar}} |\phi_j\rangle \end{aligned}$$

The \hat{H}_0 terms cancel, leaving:

$$\begin{aligned} i\hbar \sum_j \dot{c}_j(t) e^{\frac{-iE_j t}{\hbar}} |\phi_j\rangle \\ = \lambda \hat{V}(t) \sum_j c_j(t) e^{\frac{-iE_j t}{\hbar}} |\phi_j\rangle \end{aligned} \quad (2.1)$$

Multiply with $\langle \phi_m |$ and use $V_{mj}(t) = \langle \phi_m | \hat{V}(t) | \phi_j \rangle$:

$$\dot{c}_m(t) e^{\frac{-iE_m t}{\hbar}} = \frac{\lambda}{i\hbar} \sum_j V_{mj}(t) c_j(t) e^{\frac{-iE_j t}{\hbar}}$$

Let $\omega_{mk} = (E_m - E_k)/\hbar$ (Bohr angular frequency).

$$\dot{c}_m(t) = \frac{\lambda}{i\hbar} \sum_k c_k(t) e^{i\omega_{mk} t} V_{mk}(t) \quad (2.2)$$

2.3 Perturbation Expansion

Express $c_m(t)$ as a power series of λ :

$$\begin{aligned} c_m(t) &= c_m^{(0)}(t) + \lambda c_m^{(1)}(t) + \lambda^2 c_m^{(2)}(t) + \dots \\ &= \sum_j \lambda^j c_m^{(j)}(t) \end{aligned}$$

Sub into Eq. 2.2:

$$\begin{aligned} \frac{\partial}{\partial t} \left(\sum_j \lambda^j c_m^{(j)}(t) \right) = \\ \frac{\lambda}{i\hbar} \sum_k e^{i\omega_{mk} t} V_{mk}(t) \left(\sum_n \lambda^n c_k^{(n)}(t) \right) \end{aligned}$$

Powers of λ on LHS = powers of λ on RHS.

Equating powers of λ :

0th-order: No term on RHS satisfies for $j = 0$:

$$\dot{c}_m^{(0)}(t) = 0$$

0th order coefficients are equal to the unperturbed solution.

1st-order ($j = 1, n = 0$):

$$\dot{c}_m^{(1)}(t) = \frac{1}{i\hbar} \sum_k e^{i\omega_{mk}t} V_{mk}(t) c_k^{(0)}(t) \quad (2.3)$$

2nd-order ($j = 2, n = 1$):

$$\dot{c}_m^{(2)}(t) = \frac{1}{i\hbar} \sum_k e^{i\omega_{mk}t} V_{mk}(t) c_k^{(1)}(t) \quad (2.4)$$

n-th-order:

$$\dot{c}_m^{(n)}(t) = \frac{1}{i\hbar} \sum_k e^{i\omega_{mk}t} V_{mk}(t) c_k^{(n-1)}(t)$$

2.4 First-order term

Assume perturbation is only "switched on" at a certain time $t = 0$. Prior to that moment, the system is in an eigenstate $|\Psi(t)\rangle = |\phi_j\rangle$, which is a state of \hat{H}_0 with energy E_j .

At time $t = 0$, evolution will still satisfy the unperturbed Hamiltonian:

$$c_m^{(0)}(t) = \delta_{mj}$$

Consider 1st order term, sub the above into Eq. 4.2:

$$\dot{c}_m^{(1)}(t) = \frac{1}{i\hbar} e^{i\omega_{mj}t} V_{mj}(t)$$

Integrate between $t = 0$ and $t = \tau$:

- For $m = j$ (phase vanishes since $\omega_{jj} = 0$):

$$c_j^{(1)}(\tau) = \frac{1}{i\hbar} \int_0^\tau V_{jj}(t) dt$$

- For $m \neq j$:

$$c_m^{(1)}(\tau) = \frac{1}{i\hbar} \int_0^\tau V_{mj}(t) e^{i\omega_{mj}t} dt \quad (2.5)$$

When perturbation is sufficiently weak, 1st order solutions are a good approximation:

$$c_m(\tau) \approx \delta_{jm} + c_m^{(1)}(\tau)$$

For $m \neq j$, $c_m^{(1)}(\tau)$ is non-zero, hence there is a probability (P) that at time τ the system is in $|\phi_m\rangle$. This P is called the transition probability:

$$P_{j \rightarrow m}^{(1)}(\tau) = |c_m^{(1)}(\tau)|^2$$

$|1 + c_j^{(1)}(\tau)|^2$ is the P that the system remains in the initial state $|\phi_j\rangle$.

$c_j(\tau)$ to 1st order:

$$\begin{aligned} c_j(\tau) &\approx 1 + c_j^{(1)} \\ &= 1 + \frac{1}{i\hbar} \int_0^\tau V_{jj}(t) dt \end{aligned} \quad (2.6)$$

This can be written as an expansion of an exponent:

$$\begin{aligned} \exp\left(-\frac{i}{\hbar} \int_0^\tau dt V_{jj}(t)\right) &\approx \\ 1 - \frac{i}{\hbar} \int_0^\tau dt V_{jj}(t) & \end{aligned}$$

Eq. 4.5 becomes $c_j(\tau) \approx e^{i\phi} c_j(0)$ where:

$$\phi = -\frac{1}{\hbar} \int_0^\tau dt V_{jj}(t)$$

2.5 Second order correction

For stronger perturbation 2nd order terms are required. Once 1st order terms (e.g., Eq. 4.3) have been derived, sub it into Eq. 4.4 and integrate:

$$\begin{aligned} c_m^{(2)}(\tau) &= -\frac{1}{\hbar^2} \int_0^\tau dt' \int_0^{t'} dt \times \\ &\sum_k e^{i\omega_{mk}t'} e^{i\omega_{kj}t} V_{mk}(t') V_{kj}(t) \end{aligned}$$

An n-th order correction term will contain an n-fold time integral. $V_{mk}(t') V_{kj}$ can be written as $\langle \phi_m | \hat{V} | \phi_k \rangle \langle \phi_k | \hat{V} | \phi_j \rangle$. This is associated with:

- Transition $|\phi_j\rangle \rightarrow |\phi_k\rangle$
- Transition $|\phi_k\rangle \rightarrow |\phi_m\rangle$

Even if 1st order transition V_{mj} is 0 (forbidden), the transition may be made via an intermediate state: $\phi_j \rightarrow \phi_k \rightarrow \phi_m$ (Termed 2nd order coupling).

Example

Constant Perturbation

Assume perturbation is switched on at $t = 0$.

$$\hat{H} = \begin{cases} \hat{H}_0 & t < 0 \\ \hat{H}_0 + \hat{V} & 0 \leq t < \tau \end{cases}$$

Operator \hat{V} is constant in time. We want to find coefficients $c_m(\tau)$. Assume 1st order is enough, from Eq. 4.3:

$$c_m^{(1)}(\tau) = \frac{1}{i\hbar} \int_0^\tau dt V_{mj} e^{i\omega_{mj}t}$$

Integrate:

$$\begin{aligned} c_m^{(1)}(\tau) &= \frac{V_{mj}}{i\hbar} \int_0^\tau e^{i\omega_{mj}t} dt \\ &= \frac{V_{mj}}{\hbar\omega_{mj}} (1 - e^{i\omega_{mj}\tau}) \end{aligned}$$

Notice it's proportional to $V_{mj}/\hbar\omega_{mj} = V_{mj}/(E_m - E_j)$. Higher order corrections will be proportional to powers of this. Hence perturbation theory is applicable only when energy scales of the perturbations are much smaller than the energy scales associated with \hat{H}_0 .

Calculate first order transition probability:

$$\begin{aligned} P_{j \rightarrow m}^{(1)}(\tau) &= |c_m^{(1)}(\tau)|^2 \\ &= \frac{|V_{mj}|^2}{\hbar^2 \omega_{mj}^2} |1 - e^{i\omega_{mj}\tau}|^2 \\ &= \frac{|V_{mj}|^2}{\hbar^2 \omega_{mj}^2} (2 - 2\cos(\omega_{mj}\tau)) \\ &= \frac{4|V_{mj}|^2}{\hbar^2} \frac{\sin^2(\omega_{mj}\tau/2)}{\omega_{mj}^2} \\ P_{j \rightarrow m}^{(1)}(\tau) &= \frac{2|V_{mj}|^2}{\hbar^2} F(\tau, \omega_{mj}) \quad (2.7) \end{aligned}$$

where we defined

$$\begin{aligned} F(\tau, \omega) &= \frac{2\sin^2(\omega\tau/2)}{\omega^2} \\ &= \frac{\tau^2 \sin^2(\omega\tau/2)}{2(\omega\tau/2)^2} \\ &= \frac{\tau^2}{2} \text{sinc}^2(\omega\tau/2) \end{aligned}$$

Use $\text{sinc}(x) = \sin(x)/x$.

Plot of $F(\tau, \omega)$: Sinc-shape has 1 dominant broad peak. Height of the central peak is $\tau^2/2$ and full-width at half max is $2\pi/\tau$. As τ increases (duration of perturbation increases) the peak gets narrower and taller.

Aside: Dirac delta function Integral definition:

$$f(x) = \int_{-\infty}^{\infty} f(x') \delta(x - x') dx'$$

Properties:

1. For $x \neq 0$ it takes the value $\delta(x) = 0$. For $x = 0$ the value of $\delta(x)$ is undefined ("infinite").
2. Satisfies: $\int_{-\infty}^{\infty} \delta(x) dx = 1$
3. Satisfies: $\delta(ax) = \frac{1}{|a|} \delta(x)$

$F(\tau, \omega)$ in the limit $\tau \rightarrow \infty$ can be written in terms of $\delta(\omega)$:

$$\lim_{\tau \rightarrow \infty} F(\tau, \omega) = \pi\tau\delta(\omega) \quad (2.8)$$

Its integral over ω :

$$\begin{aligned} \int_{-\infty}^{\infty} \frac{F(\tau, \omega)}{\pi\tau} d\omega &= \frac{\tau}{2\pi} \int_{-\infty}^{\infty} \text{sinc}^2\left(\frac{\omega\tau}{2}\right) d\omega \\ &= \frac{1}{\pi} \int_{-\infty}^{\infty} \text{sinc}^2(x) dx \end{aligned}$$

Using the standard integral $\int_{-\infty}^{\infty} \text{sinc}^2(x) dx = \pi$:

$$= \frac{1}{\pi} (\pi) = 1$$

Hence satisfies the same property (2) as the δ -function.

Perturbation Time-Scales and Fermi's Golden Rule From Eq. 4.8:

$$P_{j \rightarrow m}^{(1)}(\tau) = \frac{2|V_{mj}|^2}{\hbar^2} F(\tau, \omega_{mj})$$

Limits:

- **Long perturbations** ($\tau \rightarrow \infty$): Use Eq. 4.9:

$$P_{j \rightarrow m}^{(1)}(\tau) = \frac{2|V_{mj}|^2}{\hbar^2} \pi\tau\delta(\omega_{mj})$$

Recall $\hbar\omega_{mj} = E_m - E_j$ is the energy difference. In this limit $P_{j \rightarrow m}$ is zero unless $E_m - E_j = 0$. Hence regardless of the form of \hat{V} , 1st order transitions can only occur between states of identical energy. This is a natural consequence of the conservation of energy.

- **Short perturbations** (small τ): $F(\tau, \omega_{mj})$ has a broad central peak, thus transitions are allowed to states with a significant range of energies around E_j . Let $\Delta\omega \approx 1/\tau$ be the width of the central peak and $\Delta t = \tau$ be the length of the perturbation. Writing $\Delta E = \hbar\Delta\omega$ to represent the uncertainty in energy of the final state, we get the relation:

$$\Delta E \Delta t \approx \hbar$$

This reflects the time-energy uncertainty relation.

Differentiating $P_{j \rightarrow m}^{(1)}(\tau)$ w.r.t τ we derive the transition rate:

$$\begin{aligned} \Gamma_{j \rightarrow m}^{(1)} &= \frac{dP_{j \rightarrow m}^{(1)}}{d\tau} \\ &= \frac{2\pi}{\hbar^2} |V_{mj}|^2 \delta(\omega_{mj}) \\ &= \frac{2\pi}{\hbar} |V_{mj}|^2 \delta(E_m - E_j) \quad (2.9) \end{aligned}$$

This equation is called **Fermi's Golden Rule**.

2.6 Harmonic Perturbation

Consider a perturbation varying sinusoidally in time. This describes, to a first approximation, how atoms interact with light. An electric dipole in an electric field \vec{E} has the potential energy:

$$V = -\vec{E} \cdot \vec{D}$$

where \vec{D} is the dipole moment. Consider an atom interacting with a monochromatic laser. The E-field will be: $\vec{E}(t) = \vec{E}_0 \cos(\omega t)$, where ω is the angular frequency of the radiation. The Hamiltonian will have the form:

$$\hat{V} = \hat{H}_I \cos(\omega t)$$

Consider a more generic family of harmonic Hamiltonians:

$$\hat{V}(t) = \hat{A}e^{i\omega t} + \hat{A}^\dagger e^{-i\omega t} \quad (2.10)$$

As before, assume perturbation is "switched on" at $t = 0$ and the system is prepared in state $|\phi_j\rangle$. For $t \geq 0$, the Hamiltonian will be:

$$\hat{H} = \hat{H}_0 + \hat{A}e^{i\omega t} + \hat{A}^\dagger e^{-i\omega t}$$

Calculate coefficients to first order: $c_m(t) \approx c_m^{(0)} + c_m^{(1)}(t)$. 0th order terms are $c_m^{(0)} = \delta_{mj}$. 1st order term, use Eq. 4.3 and Eq. 4.10:

$$\begin{aligned} c_m^{(1)}(\tau) &= \frac{1}{i\hbar} \int_0^\tau dt V_{mj}(t) e^{i\omega_{mj}t} \\ &= \frac{1}{i\hbar} \int_0^\tau dt (A_{mj}e^{i\omega t} + A_{mj}^\dagger e^{-i\omega t}) e^{i\omega_{mj}t} \\ &= \frac{1}{i\hbar} \left[A_{mj} \int_0^\tau dt e^{i(\omega_{mj}+\omega)t} + A_{mj}^\dagger \int_0^\tau dt e^{i(\omega_{mj}-\omega)t} \right] \\ &= \frac{A_{mj}}{\hbar} \frac{1 - e^{i(\omega_{mj}+\omega)\tau}}{\omega_{mj} + \omega} + \frac{A_{mj}^*}{\hbar} \frac{1 - e^{i(\omega_{mj}-\omega)\tau}}{\omega_{mj} - \omega} \end{aligned}$$

In the limit $\tau \gg 0$, the sinc functions become Dirac delta functions. $c_m^{(1)}(\tau)$ will only be non-zero if one of two conditions is fulfilled:

1. $\omega_{mj} = \omega \implies E_m = E_j + \hbar\omega$
(Energy of state $|\phi_m\rangle$ is one unit $\hbar\omega$ higher than E_j).
2. $\omega_{mj} = -\omega \implies E_m = E_j - \hbar\omega$
(Energy of state $|\phi_m\rangle$ is one unit $\hbar\omega$ lower than E_j).

This predicts that light energy can only be absorbed or emitted by an atom in units of $\hbar\omega$, i.e., single photons.

2.6.1 Fermi's Golden Rules for Harmonic Perturbation

Absorption rate ($E_k = E_j + \hbar\omega$):

$$\Gamma_{j \rightarrow k}^{(1)} = \frac{2\pi}{\hbar} |A_{kj}|^2 \delta(E_k - E_j - \hbar\omega) \quad (2.11)$$

Emission rate ($E_k = E_j - \hbar\omega$):

$$\Gamma_{j \rightarrow k}^{(1)} = \frac{2\pi}{\hbar} |A_{jk}^*|^2 \delta(E_k - E_j + \hbar\omega) \quad (2.12)$$

Note that by swapping the labels j and k in the emission rate Eq. 2.12 we get the absorption rate from k to j :

$$\begin{aligned} \Gamma_{k \rightarrow j}^{(1)} &= \frac{2\pi}{\hbar} |A_{kj}^*|^2 \delta(E_j - E_k + \hbar\omega) \\ &= \frac{2\pi}{\hbar} |A_{kj}|^2 \delta(E_k - E_j - \hbar\omega) \end{aligned}$$

where we used $\delta(x) = \delta(-x)$ and $|A_{kj}^*|^2 = |A_{kj}|^2$.

This means the rate of stimulated emission from k to j is equal to the rate of absorption from j to k . This is an example of "detailed balance".

Chapter 3

Unitary Time Evolution

3.1 Intro

According to postulate 2, we can study the dynamics of isolated systems by solving the Schrödinger equation:

$$i\hbar \frac{\partial |\Psi(t)\rangle}{\partial t} = H |\Psi(t)\rangle \quad (3.1)$$

3.2 Evolution Operator

Given $|\Psi(0)\rangle$, the Schrödinger equation allows us to calculate the state of the system at any other time t , $|\Psi(t)\rangle$. This evolution is a map from a state to the other, and can be described in terms of an evolution operator $U(t)$:

$$|\Psi(t)\rangle = U(t) |\Psi(0)\rangle \quad (3.2)$$

$U(t)$ it is always unitary, regardless of the form of H and whether or not H is time-dependent. When H is time-independent, $U(t)$ has the form:

$$U(t) = e^{-i\frac{H}{\hbar}t} \quad (3.3)$$

Aside: Exponential Operators

Exponentiated operators or matrices are defined using the power-series definition of e^x :

$$e^x = \sum_j \frac{x^j}{j!}$$

For operators (or square matrix):

$$e^{\hat{A}} = \sum_j \frac{\hat{A}^j}{j!}$$

where powers of \hat{A} are: $\hat{A}^0 = \mathbb{I}$, $\hat{A}^1 = \hat{A}$, $\hat{A}^2 = \hat{A}\hat{A}$, etc.

Example

Diagonal Matrix

Consider diagonal matrix B :

$$B = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix}$$

Take powers of diagonal elements:

$$B^j = \begin{pmatrix} \lambda_1^j & 0 \\ 0 & \lambda_2^j \end{pmatrix}$$

Hence:

$$\begin{aligned} e^B &= \sum_j \begin{pmatrix} \lambda_1^j/j! & 0 \\ 0 & \lambda_2^j/j! \end{pmatrix} \\ &= \begin{pmatrix} e^{\lambda_1} & 0 \\ 0 & e^{\lambda_2} \end{pmatrix} \end{aligned}$$

In general (non-diagonal matrices):

$$e \begin{pmatrix} a & b \\ c & d \end{pmatrix} \neq \begin{pmatrix} e^a & e^b \\ e^c & e^d \end{pmatrix}$$

In general the following does not hold for operators and matrices:

$$e^{\hat{A}+\hat{B}} \neq e^{\hat{A}}e^{\hat{B}}$$

If operators commute then it holds.

Time-independent H

As before, for time-independent H , the evolution operator is:

$$U(t) = e^{-i\frac{H}{\hbar}t}$$

Verify that $|\Psi(t)\rangle = U(t) |\Psi(0)\rangle$ is the solution of Schrödinger eq. Compute:

$$\frac{\partial}{\partial t} |\Psi(t)\rangle = \frac{\partial}{\partial t} (U(t) |\Psi(0)\rangle) \quad (3.4)$$

$|\Psi(0)\rangle$ is time invariant:

$$\frac{\partial}{\partial t}(U(t)) = \frac{\partial}{\partial t} \exp\left(-i\frac{H}{\hbar}t\right)$$

Use power-series definition:

$$\begin{aligned} &= \frac{\partial}{\partial t} \sum_{j=0}^{\infty} \left(\frac{-iH}{\hbar}\right)^j \frac{t^j}{j!} \\ &= \sum_{j=1}^{\infty} \left(\frac{-iH}{\hbar}\right)^j \frac{j t^{j-1}}{j!} \\ &= \frac{-iH}{\hbar} \sum_{j=1}^{\infty} \left(\frac{-iH}{\hbar}\right)^{j-1} \frac{t^{j-1}}{(j-1)!} \end{aligned}$$

Reuse definition of power series:

$$= \frac{-iH}{\hbar} \exp\left(-i\frac{H}{\hbar}t\right)$$

So Eq. 3.4 becomes:

$$\begin{aligned} \frac{\partial}{\partial t} |\Psi(t)\rangle &= \frac{-iH}{\hbar} \exp\left(-i\frac{H}{\hbar}t\right) |\Psi(0)\rangle \\ &= \frac{-iH}{\hbar} U(t) |\Psi(0)\rangle \end{aligned}$$

Use Eq. 3.2:

$$= \frac{-iH}{\hbar} |\Psi(t)\rangle$$

Sub. into Schrödinger eq:

$$i\hbar \left(\frac{-iH}{\hbar}\right) |\Psi(t)\rangle = H |\Psi(t)\rangle$$

LHS = RHS hence $|\Psi(t)\rangle = U(t) |\Psi(0)\rangle$ is a solution.

Unitary

Take Hermitian conjugate of Eq. 3.3:

$$U(t)^\dagger = \exp\left(i\frac{H}{\hbar}t\right)$$

$$\begin{aligned} U(t)U(t)^\dagger &= \exp\left[-i\frac{H}{\hbar}t\right] \exp\left[i\frac{H}{\hbar}t\right] \\ &= \mathbb{I} \end{aligned}$$

In the above we are allowed to combine the exponents since H and $-H$ commute. Note $U(t)^\dagger$ is inverse of $U(t)$, which is also equal to $U(-t)$.

The Physics

There is no time arrow direction. We can introduce time arrow by introducing some type of dissipation.

Tracking evolution from other times

We can derive evolution operators which track evolution from states at other times.

$$|\Psi(t_1)\rangle = U(t_1) |\Psi(0)\rangle$$

Hence, rearranging:

$$|\Psi(0)\rangle = U(t_1)^\dagger |\Psi(t_1)\rangle = U(-t_1) |\Psi(t_1)\rangle$$

So we can write the state at any time t in terms of $|\Psi(t_1)\rangle$:

$$|\Psi(t)\rangle = U(t) |\Psi(0)\rangle = U(t)U(-t_1) |\Psi(t_1)\rangle$$

Use $U(x)U(y) = U(x+y)$:

$$|\Psi(t)\rangle = U(t-t_1) |\Psi(t_1)\rangle$$

Step-wise changing Hamiltonian

We can use evolution operators to solve the Schrödinger eq for a Hamiltonian which evolves step-wise.

Example

Step-wise Hamiltonian

Consider H which between time $0 < t < t_1$ the H is H_1 and between $t_1 < t < t_2$ the H is H_2 . Define:

$$U_1(t) = e^{-i\frac{H_1}{\hbar}t}$$

$$U_2(t) = e^{-i\frac{H_2}{\hbar}t}$$

So evolution for time $0 < t < t_1$ will be $U_1(t)$ and for time $t_1 < t < t_2$: $U_2(t-t_1)U_1(t_1)$. i.e. the first operator applies for the segment of time t_1 and the second applies for the segment of length $t-t_1$.

Continuously changing Hamiltonian

Consider a $H(t)$ which varies constantly in time. Approx. it by a series of n discrete slices, each applied for time $\delta t = t/n$. Approx. evolution operator:

$$U(t) \approx \prod_{j=1}^n e^{-i\frac{H(jt/n)}{\hbar}t}$$

This operator is still unitary. We obtain an exact representation in the limit $n \rightarrow \infty$:

$$U_{\text{exact}}(t) = \lim_{n \rightarrow \infty} \prod_{j=1}^n e^{-i\frac{H(jt/n)}{\hbar}t}$$

Notation

The above limit is also known in literature as a time-ordered integral:

$$\lim_{n \rightarrow \infty} \prod_{j=1}^n e^{-i \frac{H(jt/n)}{\hbar} t} = \mathcal{T} \exp \left(-i \int_0^t dt' \frac{H(t')}{\hbar} \right)$$

3.3 Suzuki-Trotter Decomposition

Often H has the form:

$$H = H_1 + H_2$$

where operators H_1 and H_2 do not commute, for example when:

$$H_i = \frac{\hat{p}_i^2}{2m} + V_i(\hat{x})$$

Often individual terms can be solved individually, but the full H cannot be solved exactly (Unless $V(x)$ has a very special form).

In such case we can use the Suzuki-Trotter decomposition. For any operator (or square matrix), the following holds:

$$e^{\hat{A} + \hat{B}} = \lim_{n \rightarrow \infty} \left(e^{\hat{A}/n} e^{\hat{B}/n} \right)^n = \lim_{n \rightarrow \infty} \left(e^{\hat{B}/n} e^{\hat{A}/n} \right)^n$$

For Quantum evolution operators, implies:

$$U(t) = e^{-\frac{it}{\hbar} (H_1 + H_2)} = \lim_{n \rightarrow \infty} [U_1(t/n) U_2(t/n)]^n$$

Suzuki-Trotter approx. (ST)

Expression for exact operator (neglect i/\hbar from calculations). Expand the following as a power series:

$$\begin{aligned} e^{(\hat{A} + \hat{B})t} &= \sum_j \frac{(\hat{A} + \hat{B})^j t^j}{j!} \\ &= \mathbb{I} + (\hat{A} + \hat{B})t + \frac{(\hat{A} + \hat{B})^2 t^2}{2} + \dots \\ &= \mathbb{I} + (\hat{A} + \hat{B})t + \frac{(\hat{A}^2 + \hat{B}^2 + \hat{A}\hat{B} + \hat{B}\hat{A})t^2}{2} + \dots \end{aligned}$$

$n = 1$ ST approximation

There are two possible decompositions: $e^{\hat{A}t} e^{\hat{B}t}$ or $e^{\hat{B}t} e^{\hat{A}t}$. If \hat{A}, \hat{B} do not commute, these decompositions are not equal. Choose the first:

$$e^{\hat{A}t} e^{\hat{B}t} = \sum_j \frac{\hat{A}^j t^j}{j!} \sum_k \frac{\hat{B}^k t^k}{k!}$$

Collecting same powers of t :

$$= \mathbb{I} + (\hat{A} + \hat{B})t + \left(\frac{\hat{A}^2}{2} + \frac{\hat{B}^2}{2} + \hat{A}\hat{B} \right) t^2 + \dots$$

Comparing with the exact expression, we see that the $n = 1$ ST approx. has the correct t^0 and t^1 terms, but error in the t^2 term.

Hence for $n = 1$ we have 1st order in t accuracy and error is order t^2 .

$n = 2$ ST approx.

There are 4 possible decompositions as operators can be applied in any order (e.g., $ABAB, BABA, BAAB, ABBA$). The latter 2 can be reduced to 3 operators as $e^{\hat{B}t/2} e^{\hat{B}t/2} = e^{\hat{B}t}$. Hence study the last:

$$\begin{aligned} e^{\hat{A}t/2} e^{\hat{B}t} e^{\hat{A}t/2} &= \sum_j \frac{\hat{A}^j (t/2)^j}{j!} \sum_k \frac{\hat{B}^k t^k}{k!} \sum_l \frac{\hat{A}^l (t/2)^l}{l!} \\ &= \mathbb{I} + (A + B)t + \frac{(\hat{A}^2 + \hat{B}^2 + \hat{A}\hat{B} + \hat{B}\hat{A})t^2}{2} + \dots \end{aligned}$$

Comparing this with the exact expression, we get that this expression is exact to 2nd order in t .

In general, for a given n the approx. is valid to n th order in t and the error is of order t^{n+1} .

3.4 Schrödinger and Heisenberg Pictures

For operators \hat{O} the time-evolving expectation value is:

$$\langle \hat{O}(t) \rangle = \langle \Psi(t) | \hat{O} | \Psi(t) \rangle$$

Rewrite expression as:

$$\langle \hat{O}(t) \rangle = \langle \Psi(0) | U(t)^\dagger \hat{O} U(t) | \Psi(0) \rangle$$

Schrödinger interpretation

$$\langle \hat{O}(t) \rangle = \underbrace{\langle \Psi(0) | U(t)^\dagger}_{\text{State evolves in time}} \hat{O} \underbrace{U(t) | \Psi(0) \rangle}_{\text{State evolves in time}}$$

Schrödinger picture: State vectors evolve in time $|\Psi(t)\rangle = U(t) |\Psi(0)\rangle$ and observables remain constant in time.

Notation: Schrödinger picture use subscript S: $|\Psi(t)\rangle_S$ and \hat{O}_S .

Heisenberg interpretation

$$\langle \hat{O}(t) \rangle = \langle \Psi(0) | \underbrace{U(t)^\dagger \hat{O} U(t)}_{\text{Operator evolves in time}} | \Psi(0) \rangle$$

Heisenberg picture use subscript H.

Heisenberg picture: At time $t = 0$ the two approaches are equivalent. In Heisenberg picture time evolution is carried by the operators, which evolve as:

$$\hat{O}_H(t) = U(t)^\dagger \hat{O}(0) U(t)$$

where $\hat{O}(0) = \hat{O}_S$.

Reasons for using it:

1. Simplify calculation.
2. Time dependence is closer in a way to classical physics, where observable quantities $x(t)$, $p(t)$ do vary in time.
3. Equations of motion are very similar to classical equations.

If $[H_H, \hat{O}_H(t)] = 0$ the $\hat{O}_H(t)$ is constant in time. So expectation value of $\hat{O}_H(t)$ is a constant of motion.

There exist an intermediate picture of time-evolution called Interaction picture. Discussed at end of Chapter 4.

Evolution equation in the Heisenberg picture

In the Schrödinger picture the Schrödinger's equation allows us to compute $|\Psi(t)\rangle_S$ given H_S and $|\Psi(0)\rangle$. Equivalently there is a Heisenberg eq. which allows us to compute $\hat{O}_H(t)$ given H and $\hat{O}_H(0)$.

Derivation:

Consider the derivative of $\hat{O}_H(t)$:

$$\frac{\partial}{\partial t} \hat{O}_H(t) = \frac{\partial}{\partial t} [U(t)^\dagger \hat{O}_H(0) U(t)]$$

Apply product rule:

$$\begin{aligned} \frac{\partial}{\partial t} \hat{O}_H(t) &= \frac{\partial}{\partial t} (U(t)^\dagger) \hat{O}_H(0) U(t) \\ &\quad + U(t)^\dagger \frac{\partial}{\partial t} (\hat{O}_H(0)) U(t) \\ &\quad + U(t)^\dagger \hat{O}_H(0) \frac{\partial}{\partial t} (U(t)) \end{aligned}$$

Middle term is zero, since $\hat{O}_H(0)$ is constant.

Sub in:

$$\begin{aligned} \frac{\partial}{\partial t} U(t) &= -\frac{i}{\hbar} H_S(t) U(t) \\ \frac{\partial}{\partial t} U(t)^\dagger &= \frac{i}{\hbar} U(t)^\dagger H_S(t) \\ &= \frac{i}{\hbar} \left(U(t)^\dagger H(t) U(t) U(t)^\dagger \hat{O}_H(0) U(t) - U(t)^\dagger \hat{O}_H(0) U(t) U(t)^\dagger H(t) U(t) \right) \end{aligned}$$

Add identity where H are placed:

$$= \frac{i}{\hbar} \left[U(t)^\dagger H(t) U(t) U(t)^\dagger \hat{O}_H(0) U(t) - U(t)^\dagger \hat{O}_H(0) U(t) U(t)^\dagger H(t) U(t) \right]$$

Since operator evolves as $\hat{O}(t) = U(t)^\dagger \hat{O}_H(0) U(t)$ and $H_H(t) = U(t)^\dagger H(t) U(t)$ in Heisenberg picture:

$$= \frac{i}{\hbar} \left(H_H(t) \hat{O}_H(t) - \hat{O}_H(t) H_H(t) \right)$$

Heisenberg equation:

$$\frac{\partial}{\partial t} \hat{O}_H(t) = \frac{i}{\hbar} [H_H(t), \hat{O}_H(t)]$$

Chapter 4

Quantum Light, Atoms and the Interaction Picture

4.1 Quantum Harmonic Oscillator

Revision

A Quantum Harmonic Oscillator (QHO) has the Hamiltonian:

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2$$

Eigenstates of the Hamiltonian are a set of energy levels labelled $|n\rangle$ where n is an integer, with equally spaced energies:

$$E_n = \left(n + \frac{1}{2}\right) \hbar\omega$$

QHO using ladder operators:

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}(\hat{x} + i\hat{p}), \quad \hat{a}^\dagger = (\hat{a})^\dagger \quad (4.1)$$

where \hat{a} is lowering (annihilation) and \hat{a}^\dagger is raising (creation) operator, which act on $|n\rangle$ as:

$$\begin{aligned} \hat{a} |n\rangle &= \sqrt{n} |n-1\rangle \\ \hat{a}^\dagger |n\rangle &= \sqrt{n+1} |n+1\rangle \end{aligned}$$

They satisfy $[\hat{a}, \hat{a}^\dagger] = 1$.

The operator $\hat{a}^\dagger \hat{a}$ is called the number operator since its eigenvalue is n , the number of excitations in state $|n\rangle$:

$$\hat{a}^\dagger \hat{a} |n\rangle = n |n\rangle$$

Rearranging definition in 4.1:

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a}^\dagger + \hat{a}), \quad \hat{p} = \sqrt{\frac{\hbar}{2m\omega}}i(\hat{a}^\dagger - \hat{a})$$

Hamiltonian in ladder operator form:

$$H = \hbar\omega(\hat{a}^\dagger \hat{a} + 1/2)$$

4.2 Quantum Light

Quantum description of light may be obtained using Maxwell equations, which can be combined to derive the electric field wave-equation:

$$\left(\nabla^2 - \frac{1}{c^2} \frac{\partial^2}{\partial t^2}\right) E = 0$$

where $1/c^2 = \mu_0\epsilon_0$.

Solve this equation using separation of variable technique, using $E(r, t) = u(r)T(t)$:

$$\nabla^2 E = \frac{1}{c^2} \frac{\partial^2 E}{\partial t^2}$$

Sub. in E and divide by E :

$$\begin{aligned} \frac{(\nabla^2 u(r))T(t)}{u(r)T(t)} &= \frac{u(r)}{c^2} \frac{\partial^2 T}{\partial t^2} \frac{1}{u(r)T(t)} \\ \frac{\nabla^2 u(r)}{u(r)} &= \frac{1}{c^2} \frac{\partial^2 T}{\partial t^2} \frac{1}{T(t)} = -\frac{\omega^2}{c^2} \end{aligned}$$

where $-\omega^2/c^2$ is chosen to be the separation constant for convenience. This gives us two equations:

- **Spatial equation** (called Helmholtz equation):

$$\nabla^2 u(r) = -\frac{\omega^2}{c^2} u(r)$$

- **Temporal equation** (HO equation):

$$\frac{\partial^2 T}{\partial t^2} = -\omega^2 T(t)$$

Solutions to this have the form $\exp(\pm i\omega t)$.

Label solutions as $T_j(t)$ and $u_j(r)$. Obtain a general solution by combining them linearly:

$$E(r, t) = \sum_j \alpha_j u_j(r) T_j(t)$$

where α_j coeff. depend on the initial condition; they contain E_{0j} which are vectors representing the polarization of the mode and their amplitudes.

The quantization of the EM-field proceeds by replacing each of the classical oscillators with a quantum oscillator. Energy eigenstate of each oscillator $|n\rangle$ represents a state of n photons in the mode.

4.3 Quantum Light Modes

Label the states and operators for mode j with subscript j ($|n\rangle_j$, a_j , etc.). Thus each mode has a Hamiltonian:

$$H_j = \hbar\omega_j(\hat{a}_j^\dagger\hat{a}_j + 1/2)$$

The Hamiltonian for the full field is $H = \sum_j H_j$. The E field is now represented by quantum operators as:

$$\hat{E} = \sum_j u_j(r)E_{0j}(a_j + a_j^\dagger)$$

Optical Cavities

It is possible to trap light inside a set of mirrors, called a cavity. In this, interactions with atoms can be enhanced or suppressed. It is possible to cause the atom to interact with a single mode alone.

For the interaction between an atom and a single cavity mode, the Hamiltonian is:

$$H = \hbar\omega(a^\dagger a + 1/2)$$

The electric field operator is:

$$\hat{E} = u(r)E_0(\hat{a} + \hat{a}^\dagger) \quad (4.2)$$

4.4 Interaction between light and an atom

We approximate the atom as a dipole where the outer electron has charge $-e$ and the remainder of the atom has charge $+e$. A classical dipole in an electric field has interaction energy:

$$U = -\vec{D} \cdot \vec{E}$$

The dipole operator \hat{D} for a two-level system can only have 4 matrix elements. Classically $\vec{D} = -e\vec{r}$, so:

$$\begin{aligned} \langle g|\hat{D}|g\rangle &= -e\langle g|\hat{r}|g\rangle \\ \langle e|\hat{D}|e\rangle &= -e\langle e|\hat{r}|e\rangle \end{aligned}$$

These elements are zero since the electron wavefunction is symmetric about the nucleus (mean displacement is zero). So we assume $\langle g|\hat{D}|g\rangle = \langle e|\hat{D}|e\rangle = 0$.

We also assume off-diagonals are real: $\langle g|\hat{D}|e\rangle = \langle e|\hat{D}|g\rangle$. The dipole moment is a 3D vector, so the matrix elements have 3 components:

$$\langle g|\hat{D}|e\rangle = \langle e|\hat{D}|g\rangle = \vec{d}$$

So \hat{D} has the form:

$$\hat{D} = \vec{d}(|g\rangle\langle e| + |e\rangle\langle g|) \quad (4.3)$$

Two-level atom

We make a further approximation, a "toy model" of an atom, the 2-level atom where the atom has only 2 levels:

- Ground state $|g\rangle$ with zero energy.
- Excited state $|e\rangle$ with $\hbar\omega_a$ energy.

The Hamiltonian for this atom is:

$$H = 0|g\rangle\langle g| + \hbar\omega_a|e\rangle\langle e| = \hbar\omega_a|e\rangle\langle e| \quad (4.4)$$

This model is a good approximation for an atom that is interacting with a light mode at resonance, e.g., atomic transition energy $\hbar\omega_a$ is equal to energy of photon in mode $\hbar\omega_j$, hence $\omega_j = \omega_a$.

Dipole interaction Hamiltonian

Using classical $U = -\vec{E} \cdot \vec{D}$ with dipole quantum quantities 4.2 and 4.3:

$$\begin{aligned} H_{int} &= [-\vec{d} \cdot u(r)E_0](\hat{a} + \hat{a}^\dagger)[|g\rangle\langle e| + |e\rangle\langle g|] \\ &= \hbar g(r)(\hat{a} + \hat{a}^\dagger)[|g\rangle\langle e| + |e\rangle\langle g|] \end{aligned} \quad (4.5)$$

where $\hbar g(r) = -\vec{d} \cdot u(r)E_0$ is the strength of the coupling between light and atom.

Notation

In the above we implicitly combined the state space of the atom with the state space of light. The joint state has basis:

$$|g, n\rangle = |g\rangle \otimes |n\rangle, \quad |e, n\rangle = |e\rangle \otimes |n\rangle$$

We use notation abbreviation (e.g., $1 \otimes \hat{a} \rightarrow \hat{a}$, $|g\rangle\langle e| \otimes 1 \rightarrow |g\rangle\langle e|$). Operators act on the joint state as follows:

$$\begin{aligned} \hat{a}|g, n\rangle &= \sqrt{n}|g, n-1\rangle \\ \hat{a}^\dagger|g, n\rangle &= \sqrt{n+1}|g, n+1\rangle \\ |g\rangle\langle e||e, n\rangle &= |g, n\rangle \\ |g\rangle\langle e||g, n\rangle &= 0 \end{aligned}$$

Full Hamiltonian

Full Hamiltonian for atom and light $H = H_0^{LIGHT} + H_0^{ATOM} + H_{INT}$:

$$H = \text{Eq.2} + \text{Eq.4} + \text{Eq.6}$$

$$H = \hbar\omega_j(\hat{a}^\dagger\hat{a} + 1/2) + \hbar\omega_a|e\rangle\langle e| + \hbar g(r)(\hat{a} + \hat{a}^\dagger)(|g\rangle\langle e| + |e\rangle\langle g|)$$

This can be solved in Heisenberg or Schrödinger pictures, but it can be simplified by adopting the Interaction Picture.

4.5 Interaction Picture (IP)

If we know the eigenstates $|\phi_j\rangle$ of a constant Hamiltonian H , we can compute the evolution of the system via:

$$|\Psi(t)\rangle = \sum_j \alpha_j e^{-iE_j t/\hbar} |\phi_j\rangle$$

where constants α_j are determined by initial conditions.

For interactive systems, the H has the form:

$$H = H_0 + V$$

where H_0 is the solvable non-interacting Hamiltonian, and V is the term due to the interaction.

Hamiltonian derived above has this form:

$$H_0 = \hbar\omega_j(\hat{a}^\dagger\hat{a} + 1/2) + \hbar\omega_a|e\rangle\langle e|$$

$$V = \hbar g(r)(\hat{a} + \hat{a}^\dagger)(|g\rangle\langle e| + |e\rangle\langle g|)$$

Eigenstates of H_0 are known ($|g, n\rangle, |e, n\rangle$).

In Interaction picture, map the dynamics associated with the solved part of the Hamiltonian (H_0) onto operators, and thus the evolution of the states reflects the interaction alone.

Define the evolution operator $U_0(t)$, also called free-evolution operator:

$$U_0(t) = e^{-iH_0 t/\hbar}$$

represents the dynamics we would see if no interaction were present.

Let $|\Psi(t)\rangle_S$ be the time-evolving state in Schrödinger picture. "Remove" from the $|\Psi(t)\rangle_S$ state the dynamics due to H_0 , by defining $|\Psi(t)\rangle_I$:

$$|\Psi(t)\rangle_I = U_0^\dagger(t) |\Psi(t)\rangle_S \quad (4.6)$$

Expectation values must be the same in all pictures, hence observables $\hat{O}_I(t)$ must evolve as:

$$\hat{O}_I(t) = U_0^\dagger(t) \hat{O}_S U_0(t)$$

Note that they evolve under $U_0(t)$, not the full evolution operator $U(t)$.

Summary of the Methods:

Picture	Observables	States
Schrödinger	\hat{O}_S	$ \psi(t)\rangle_S = U(t) \psi(0)\rangle_S$
Heisenberg	$\hat{O}_H = U^\dagger(t) \hat{O}_S U(t)$	$ \psi\rangle_H = \psi(0)\rangle_S$
Interaction	$\hat{O}_I = U_0^\dagger(t) \hat{O}_S U_0(t)$	$ \Psi(t)\rangle_I = U_0^\dagger(t) \Psi(t)\rangle_S$

All 3 pictures coincide at $t = 0$.

Interaction Picture Schrödinger Equation

From Schr. eq:

$$i\hbar \frac{\partial}{\partial t} |\psi_S(t)\rangle = H |\psi_S(t)\rangle \quad (4.7)$$

Rearrange Eq. 4.6: $|\psi(t)\rangle_S = U_0(t) |\psi(t)\rangle_I$. Sub into LHS of above eq:

$$i\hbar \frac{\partial}{\partial t} (U_0(t) |\psi(t)\rangle_I) = i\hbar \left(U_0(t) \frac{\partial |\psi(t)\rangle_I}{\partial t} + \frac{\partial U_0(t)}{\partial t} |\psi(t)\rangle_I \right)$$

$$= i\hbar \left(U_0(t) \frac{\partial |\psi(t)\rangle_I}{\partial t} - \frac{iH_0}{\hbar} U_0(t) |\psi(t)\rangle_I \right)$$

Eq. 4.7 becomes:

$$i\hbar U_0(t) \frac{\partial |\psi(t)\rangle_I}{\partial t} + H_0 U_0(t) |\psi(t)\rangle_I = H U_0(t) |\psi(t)\rangle_I$$

Multiply from the left by $U_0^\dagger(t)$:

$$i\hbar \frac{\partial |\Psi(t)\rangle_I}{\partial t} = U_0^\dagger(t) (H - H_0) U_0(t) |\psi(t)\rangle_I$$

Use $H = H_0 + V$:

$$= U_0^\dagger(t) V U_0(t) |\Psi(t)\rangle_I$$

Define Interaction Picture Hamiltonian:

$$H_I = U_0^\dagger(t) V U_0(t)$$

The above equation becomes the Interaction Picture Schrödinger equation:

$$i\hbar \frac{\partial |\Psi(t)\rangle_I}{\partial t} = H_I |\Psi(t)\rangle_I$$

Example

Atom - Cavity coupling with Interaction Picture

In section 4.3 we derived the \hat{H} for the interaction between an atom and a single mode of light - inside an optical cavity. It was of the form $H = H_0 + V$ with:

$$H_0 = \hbar\omega_j(\hat{a}^\dagger\hat{a} + 1/2) + \hbar\omega_a |e\rangle\langle e| \quad (4.8)$$

and

$$V = \hbar g(r)(\hat{a} + \hat{a}^\dagger)(|g\rangle\langle e| + |e\rangle\langle g|) \quad (4.9)$$

Compute $H_I = U_0^\dagger(t)VU_0(t)$: Box derivation
 $U_0(t) = e^{-iH_0t/\hbar}$. Sub Eq. 4.8:

$$U_0(t) = \exp[-i\omega_j(\hat{a}^\dagger\hat{a} + 1/2)t] \exp[-i\omega_a |e\rangle\langle e| t]$$

Recall that \hat{a} , \hat{a}^\dagger commute with $|g\rangle\langle e|$.

$$H_I = U_0^\dagger(t)VU_0(t)$$

Group the 2 types of operators in H_I :

$$= \hbar g(r)e^{+i\omega_j(\hat{a}^\dagger\hat{a}+1/2)t}(\hat{a}+\hat{a}^\dagger)e^{-i\omega_j(\hat{a}^\dagger\hat{a}+1/2)t} \times \dots$$

Copy steps use in lecture notes.

Important proof:

$$\hat{a} = \sum_n \sqrt{n+1} |n\rangle \langle n+1|$$

Take $\hat{a} |m\rangle$:

$$\begin{aligned} &= \sum_{nm} \sqrt{n+1} |n\rangle \langle n+1|m\rangle \\ &= \sum_{nm} \sqrt{n+1} |n\rangle \delta_{n+1,m} \end{aligned}$$

Sub. $n = m - 1$:

$$= \sqrt{m} |m-1\rangle$$

as required by lowering operator.

So the Interaction Picture (IP) Hamiltonian is:
 $H_I =$ Copy Eq. 4.51 and previous step
 Atom and cavity mode have a strong interaction when they are at resonance, i.e., transition energy $\hbar\omega_a$ is close to photon energy $\hbar\omega_j$. At exact resonance $\omega_a = \omega_j = \omega$, the IP Hamiltonian is:

$$\begin{aligned} H_I &= \hbar g(r)(\hat{a} |e\rangle\langle g| + \hat{a}^\dagger |g\rangle\langle e|) \\ &+ \exp[-i2\omega t]\hat{a} |g\rangle\langle e| + \exp[i2\omega t]\hat{a}^\dagger |e\rangle\langle g| \end{aligned} \quad (4.10)$$

Rotating Wave Approximation - RWA

In Eq. 4.10, 2 terms are time independent, while 2 terms are oscillating at angular frequency 2ω .

In RWA we neglect those fast oscillating terms. This is justified when the period of oscillation is much shorter than the time-scales of the most significant physical process.

So the new H_I is:

$$H_I = \hbar g(\hat{a} |e\rangle\langle g| + \hat{a}^\dagger |g\rangle\langle e|) \quad (4.11)$$

These terms correspond to energy conservation processes.

Meaning of the terms:

- 1st - absorption of a photon + excitation of atom.
- 2nd - emission of photon + de-excitation of atom.

The dropped terms from Eq. 4.10 describe non-energy conserving processes, i.e. photon absorbed + atom excited.

Example

Single photon in a cavity

Solve IP Schrödinger equation for a system that initially has only a single photon in the cavity and the atom is in GS:

$$|\psi(0)\rangle_I = |g, 1\rangle$$

Note using 4.11:

$$H_I |g, 1\rangle = \hbar g |e, 0\rangle, \quad H_I |e, 0\rangle = \hbar g |g, 1\rangle$$

So general solution is a linear combination of these allowed states:

$$|\Psi(t)\rangle_I = \alpha(t) |g, 1\rangle + \beta(t) |e, 0\rangle \quad (4.12)$$

Compute $\alpha(t), \beta(t)$. Use 4.12 with the IP Schrödinger Eq. Multiply from the left with $\langle g, 1|$ or $\langle e, 0|$ to get coupled differential equations:

$$\begin{aligned} \frac{\partial \alpha(t)}{\partial t} &= -ig\beta(t) \\ \frac{\partial \beta(t)}{\partial t} &= -ig\alpha(t) \end{aligned}$$

Since we started the state as $|\psi(0)\rangle_I = |g, 1\rangle$, the boundary condition is $\alpha(0) = 1, \beta(0) = 0$.

Solution:

$$\begin{aligned} \alpha(t) &= \cos(gt) \\ \beta(t) &= -i \sin(gt) \end{aligned}$$

So general solution:

$$|\Psi(t)\rangle_I = \cos(gt) |g, 1\rangle - i \sin(gt) |e, 0\rangle$$

So the system oscillates between these two states. Signature of strong atom cavity coupling. Called **Rabi oscillation**.

To transform this state back to Schrödinger picture apply $U_0(t)$:

$$|\psi(t)\rangle_S = U_0(t) |\psi(t)\rangle_I$$

From 4.8 (with $\omega_a = \omega_j$), $H_0 |g, 1\rangle = 3\hbar\omega/2 |g, 1\rangle$, $H_0 |e, 0\rangle = 3\hbar\omega/2 |e, 0\rangle$. Thus $E_0 = 3\hbar\omega/2$.

$$|\psi(t)\rangle_S = e^{-i3\omega t/2} (\cos(gt) |g, 1\rangle - i \sin(gt) |e, 0\rangle)$$

Rabi oscillation occurs when the cavity is prepared in any Fock state $|n\rangle$. Similar oscillation occurs when the system is prepared in $|g, n\rangle$:

$$|\Psi(t)\rangle_I = \cos(\sqrt{n}gt) |g, n\rangle - i \sin(\sqrt{n}gt) |e, n-1\rangle$$

Chapter 5

Dynamics of open quantum systems

5.1 Introduction

Postulate 2 - any isolated quantum system is governed by the Schrödinger equation.

$$i\hbar \frac{\partial |\psi(t)\rangle}{\partial t} = H|\psi(t)\rangle$$

However, in nature most quantum systems are not isolated. They are constantly interacting with all the other systems around them, which we call their environment.

Systems interacting with an environment are called open quantum systems. We want the evolution of the systems we are interested in without having to solve the Schrödinger equation for the whole environment.

System and environment tend to become entangled. This means that the global state no longer factorises, and we cannot assign a state vector to the system or environment individually.

5.2 Density Matrices

5.2.1 Recap of chapter 1

This subsection can be skipped, as it's a revision from chapter 1.

Density matrix (operator) is a Hermitian operator which represents the state of a system. The density matrix for a pure state $|\psi\rangle$ is $|\psi\rangle\langle\psi|$

For an ensemble of states $|\psi_j\rangle$, each prepared with probability p_j is:

$$\rho = \sum_j p_j |\psi_j\rangle\langle\psi_j|$$

where $|\psi_j\rangle\langle\psi_j|$ are the projectors.

Expectation value for any operator \hat{O} :

$$\langle\hat{O}\rangle = \text{Tr}[\rho\hat{O}]$$

physical density operator must satisfy:

- Unit Trace: $\text{Tr}[\rho] = 1$.
- Hermiticity: $\rho = \rho^\dagger$.
- Positive semi-definiteness: ρ has no negative eigenvalues.

It can be written in terms of orthonormal basis $|\phi_j\rangle$

$$\rho = \sum_{j,k} \rho_{j,k} |\phi_j\rangle\langle\phi_k|$$

where $\rho_{j,k} = \langle\phi_j|\rho|\phi_k\rangle$.

Joint systems:

A joint system composed of system A with basis $|\alpha_j\rangle$ and system B with basis $|\beta_j\rangle$, we may write a general density matrix for the joint system with respect to tensor product basis $|\alpha_j\rangle|\beta_k\rangle$

$$\rho = \sum_{j,k,l,m} \rho_{j,k,l,m} |\alpha_j\rangle|\beta_k\rangle\langle\alpha_l|\langle\beta_m|$$

where $\rho_{j,k,l,m} = \langle\alpha_j|\langle\beta_k|\rho|\alpha_l\rangle|\beta_m\rangle$.

A reduced state of a system is a density matrix which specifies all the local properties of system A or B alone. It may be obtained using the partial trace operation

$$\rho_A = \text{Tr}_B \rho = \sum_l \rho_{j,l,k,l} |\alpha_j\rangle\langle\alpha_k|$$

or similarly

$$\rho_B = \text{Tr}_A \rho = \sum_l \rho_{l,j,l,k} |\beta_j\rangle\langle\beta_k|$$

Unitary evolution of density matrices

In a closed system, a pure state, described as a state vector, $|\psi(t)\rangle$ evolves under the Schrödinger equation via a unitary evolution operator $|\psi(t)\rangle = U(t)|\psi(0)\rangle$ where $U(t) = \exp[-i\hat{H}t/\hbar]$.

Consider a closed system prepared in a mixed state at time $t = 0$

$$\rho(0) = \sum_j p_j |\psi_j\rangle\langle\psi_j|$$

If the system evolves under Hamiltonian H , then each of the state vectors $|\psi_j\rangle$ will evolve to $U(t)|\psi_j\rangle$ and the full mixed state ρ will evolve as follows:

$$\begin{aligned}\rho(t) &= \sum_j p_j U(t)|\psi_j\rangle\langle\psi_j|U^\dagger(t) \\ &= U(t)\rho(0)U^\dagger(t)\end{aligned}$$

Derive a version of the Schrödinger equation for mixed states:

$$\begin{aligned}\frac{\partial}{\partial t}\rho(t) &= \frac{\partial}{\partial t}(U(t)\rho(0)U^\dagger(t)) \\ &= \dot{U}(t)\rho(0)U^\dagger(t) + U(t)\rho(0)\dot{U}^\dagger(t) \\ &= -\frac{i}{\hbar}\hat{H}U(t)\rho(0)U^\dagger(t) + \frac{i}{\hbar}U(t)\rho(0)U^\dagger(t)\hat{H} \\ &= -\frac{i}{\hbar}[\hat{H}, \rho(t)]\end{aligned}\quad (5.1)$$

where we used $\dot{U}(t) = \partial U(t)/\partial t = -(i\hat{H}/\hbar)U(t)$.

This compact equation is a density matrix formulation of the Schrödinger equation, and is called the **von Neumann** equation.

5.2.2 Purity: Pure states vs mixed states

- pure state is any state which can be expressed as a single projector, e.g. in the form: 2

$$\rho = |\psi\rangle\langle\psi|$$

Purity: Pure states versus mixed states Recall that a pure state is any state which can be expressed as a single projector, e.g. in the form:

$$\rho = |\psi\rangle\langle\psi|$$

Pure states are the states which can be equally described in the state vector picture by state vector $|\psi\rangle$.

- A mixed state is one written as a sum of projectors

$$\rho = \sum_j p_j |\psi_j\rangle\langle\psi_j|$$

where $\sum_j p_j = 1$.

Purity measures of "how pure" a state is. It is equal to $\text{Tr}[\rho^2]$. For any pure state $\text{Tr}[\rho^2] = \text{Tr}[|\psi\rangle\langle\psi|] = 1$ whereas for all mixed states $\text{Tr}[\rho^2] < 1$. Unitary evolution does not change the purity of a state.

$$\begin{aligned}\text{Tr}[\rho(t)^2] &= \text{Tr}[U(t)\rho(0)U^\dagger(t)U(t)\rho(0)U^\dagger(t)] \\ &= \text{Tr}[U(t)\rho(0)^2U^\dagger(t)] \\ &= \text{Tr}[\rho(0)^2]\end{aligned}$$

where in the last step we used $\text{Tr}[ABC] = \text{Tr}[BCA]$ Any closed system which starts in a pure (or mixed) state will remain as a pure (mixed) state for the whole of its evolution.

5.3 Super-operators and non-unitary evolution

mixed states arise in two contexts. Firstly, when classical randomness is employed in the creation of a state. Secondly, when a system becomes entangled with another system.

Example

Consider classical randomness.

Start with a system in pure state $\rho = |\psi\rangle\langle\psi|$ and we wish to construct a mixed state.

Implement a set of unitary transformations U_j for $j = 1, 2, \dots, n$ on the system (by implementing certain Hamiltonians for a certain time). Each of these will transform the state of the system to $U_j\rho U_j^\dagger$

Introduce classical randomness by randomly generating probabilities p_j . density matrix for the state ρ' which will be created

$$\rho' = \sum_j p_j U_j \rho U_j^\dagger$$

Overall evolution is not unitary, due to the classical randomness. This evolution can transform a state from a pure state to a mixed state.

Example

Imagine we start in a pure spin-half state $|\uparrow\rangle$, and apply unitaries \mathbb{I} and σ_X with equal probability. The state which results in the mixed state $(1/2)(|\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow|)$.

5.3.1 Superoperator

An operator \hat{O} was defined as a mathematical object which transformed one vector to another

$$|\psi'\rangle = \hat{O}|\psi\rangle$$

A superoperator $S[\]$ is a mathematical object which transforms one operator to another.

$$\rho' = S[\rho]$$

in the previous example

$$\rho' = S[\rho] = \sum_j p_j U_j \rho U_j^\dagger$$

All superoperators which occur in quantum mechanics may be written in the form:

$$S[\rho] = \sum_j K_j \rho K_j^\dagger$$

where K_j are linear operators which satisfy,

$$\sum_j K_j^\dagger K_j = \mathbb{I}$$

This is called the "operator-sum", the operators K_j are called Kraus operators. In the above example, the Kraus operators are $K_j = \sqrt{p_j} U_j$.

operators K_j do not have to be unitary.

Any super-operator which can be expressed as a Kraus decomposition has the following properties.

- If ρ is Hermitian, has trace 1 and no negative eigenvalues then $\rho' = S[\rho]$ is Hermitian, trace 1 and has no negative eigenvalues.

Proof of the Hermiticity of $S[\rho]$

$$(\rho')^\dagger = \left(\sum_j K_j \rho K_j^\dagger \right)^\dagger$$

Use $(ABC)^\dagger = C^\dagger B^\dagger A^\dagger$

$$(\rho')^\dagger = \sum_j K_j^\dagger \rho K_j = \rho'$$

and therefore ρ' is Hermitian.

Proof that trace of ρ' is 1:

$$\begin{aligned} \text{Tr}[\rho'] &= \text{Tr}\left[\sum_j K_j \rho K_j^\dagger\right] \\ &= \sum_j \text{Tr}[K_j^\dagger K_j \rho] \\ &= \text{Tr}\left[\sum_j K_j^\dagger K_j \rho\right] = \text{Tr}[\rho] \end{aligned}$$

Kraus form superoperators transform physical density matrices to physical density matrices.

Open quantum systems

5.4 Open Quantum Systems

the system plus the environment constitute a closed system, (this assumes that the environment includes everything which may affect the system we are studying). Closed systems evolve unitarily under the Schrödinger equation.

We are interested into deriving an evolution equation for the reduced state of the system ρ alone without having to compute the reduced states from the system + environment. In other words, we would like to find an equation of the form

$$\dot{\rho}(t) = \frac{\partial \rho(t)}{\partial t} = S[\rho(t)] \quad (5.2)$$

This analogous to the Schrödinger equation, which has the form

$$\frac{\partial |\psi(t)\rangle}{\partial t} = \hat{O} |\psi(t)\rangle$$

where operator $\hat{O} = -i\hat{H}/\hbar$. Via the definition of the derivative, $\dot{\rho}(t)$ can be written

$$\dot{\rho}(t) = \lim_{\delta t \rightarrow 0} \frac{\rho(t + \delta t) - \rho(t)}{\delta t}$$

rewrite as the $\delta t \rightarrow 0$ limit of

$$\rho(t + \delta t) = \rho(t) + \dot{\rho}(t) \delta t$$

to achieve an evolution equation of the form of equation above (Eq. 5.2), $\rho(t + \delta t)$ must only depend on the state of the system immediately before, i.e. $\rho(t)$. This means that the evolution cannot depend on:

- state of the environment
- the state $\rho(t')$ for some earlier time $t' < t$

Evolution of this type is called Markovian. Markovian evolution means that the way the system will change depends only on its state now.

Markovian evolution

Most forms of evolution for interacting quantum systems are not Markovian.

When the evolution of an open quantum system is Markovian it is possible to write down an evolution equation in the form of equation 5.2. This type of equation is called a **master equation**.

Example

Non-Markovian evolution

The weather. The probability that it rains today is influenced by the weather yesterday.

Example

Markovian evolution

The board-game Snakes and Ladders. The probability that you land on a ladder or a snake depends only on your current position, not on the history of the game previously.

5.5 The Markovian master equation

For an open quantum system interacting with its environment in a Markovian manner, we would like to

derive an evolution equation of the form,

$$\dot{\rho}(t) = \frac{\partial \rho(t)}{\partial t} = S[\rho(t)]$$

There are a number of ways we could proceed:

- Write down a Hamiltonian for the full system and environment, than compute a partial trace over the environment to derive a master equation.
- Derive a general form in which all Markovian master equations can be expressed (used method).

Start with

$$\rho(t + \delta t) = \rho(t) + \delta t \dot{\rho}(t)$$

which is exact in the limit δt goes to zero.

We are going to derive a general form for $\dot{\rho}(t)$ based on just two assumptions:

- Evolution is Markovian
- There is a physical superoperator which transforms $\rho(t)$ to $\rho(t + \delta t)$ which can therefore be expressed as a Kraus decomposition.

To simplify notation, consider $\rho(0)$ and $\rho(\delta t)$ instead of $\rho(t)$ and $\rho(t + \delta t)$. The assumption that the transformation from $\rho(0)$ to $\rho(\delta t)$ has a Kraus decomposition means we can write

$$\rho(\delta t) = S[\rho(0)] = \sum_j K_j(\delta t) \rho(0) K_j^\dagger(\delta t) \quad (5.3)$$

Rewrite eq 5.5

$$\rho(\delta t) = \rho(0) + \delta t \dot{\rho}(0) \quad (5.4)$$

For these two equations to be equal, there must be one Kraus operator (label K_0) which is given by

$$K_0 = \mathbb{I} + \delta t A$$

where A is a linear operator, and the remaining Kraus operators (which we label K_j) must have the form

$$K_j = \sqrt{\delta t} L_j$$

where L_j are linear operators. Sub these Kraus operators into eq. 5.3:

$$\begin{aligned} \rho(\delta t) &= K_0 \rho(0) K_0^\dagger + \sum_{j=1}^{\infty} K_j(\delta t) \rho(0) K_j^\dagger(\delta t) \\ &= (\mathbb{I} + \delta t A) \rho(0) (\mathbb{I} + \delta t A^\dagger) + \delta t \sum_{j=1}^{\infty} L_j \rho(0) L_j^\dagger \\ &= \rho(0) + \delta t A \rho(0) + \delta t \rho(0) A^\dagger + \\ &\quad O((\delta t)^2) + \delta t \sum_{j=1}^{\infty} L_j \rho(0) L_j^\dagger \end{aligned}$$

neglect the terms of order $(\delta t)^2$ to write:

$$\rho(\delta t) = \rho(0) + \delta t (A \rho(0) + \rho(0) A^\dagger) + \sum_{j=1}^{\infty} L_j \rho(0) L_j^\dagger$$

comparing this equation with eq. 5.4, we can simply read off an expression for $\dot{\rho}(0)$:

$$\dot{\rho}(0) = A \rho(0) + \rho(0) A^\dagger + \sum_{j=1}^{\infty} L_j \rho(0) L_j^\dagger$$

If the evolution is constant in time, this derivation does not depend on the value of t, and the following holds:

$$\dot{\rho}(t) = A \rho(t) + \rho(t) A^\dagger + \sum_{j=1}^{\infty} L_j \rho(t) L_j^\dagger \quad (5.5)$$

Any linear operator A can be decomposed as $A = B + iC$ where B and C are Hermitian operators. This is equivalent to decomposing a complex number $z = x + iy$. it will be convenient to express operator A as follows

$$A = -\frac{i}{\hbar} H + M$$

where H and M are Hermitian. Hence

$$K_0 = \mathbb{I} + \delta t \left(-\frac{i}{\hbar} H + M \right)$$

Recall that Kraus operators satisfy a condition $\sum_j K_j^\dagger K_j = \mathbb{I}$

$$\begin{aligned} \mathbb{I} &= \sum_j K_j^\dagger K_j \\ &= (\mathbb{I} + \delta t \left(-\frac{i}{\hbar} H + M \right)) (\mathbb{I} + \delta t \left(-\frac{i}{\hbar} H + M \right)) \\ &\quad + \delta t \sum_{j=1}^{\infty} L_j^\dagger L_j \\ &= \mathbb{I} + \delta t \left(-\frac{i}{\hbar} H + M \right) + \delta t \left(-\frac{i}{\hbar} H + M \right) \\ &\quad + O((\delta t)^2) + \delta t \sum_{j=1}^{\infty} L_j^\dagger L_j \end{aligned}$$

Neglecting the term of order $(\delta t)^2$ and cancelling terms:

$$\begin{aligned} \delta t \ 2M &= -\delta t \sum_{j=1}^{\infty} L_j^\dagger L_j \\ M &= -\frac{1}{2} \sum_{j=1}^{\infty} L_j^\dagger L_j \end{aligned}$$

So the master equation (eq. 5.5) becomes:

$$\begin{aligned} \dot{\rho}(t) &= \left(-\frac{iH}{\hbar} - \frac{1}{2} \sum_{j=1}^{\infty} L_j^\dagger L_j \right) \rho(t) + \\ &\quad \rho(t) \left(+\frac{iH}{\hbar} - \frac{1}{2} \sum_{j=1}^{\infty} L_j^\dagger L_j \right) + \sum_{j=1}^{\infty} L_j \rho(t) L_j^\dagger \end{aligned}$$

Simplify this by defining an operator called the effective Hamiltonian

$$H_{eff} = H - i\frac{\hbar}{2} \sum_{j=1}^{\infty} L_j^\dagger L_j$$

This is not a proper Hamiltonian, since it is not a Hermitian operator, but it plays a similar role to the Hamiltonian in the master equation. The master equation becomes:

$$\dot{\rho}(t) = -\frac{i}{\hbar}(H_{eff}\rho(t) - \rho(t)H_{eff}^\dagger) + \sum_{j=1}^{\infty} L_j\rho(t)L_j^\dagger \quad (5.6)$$

This is called the Lindblad equation, or the Lindblad form of the master equation. All Markovian open systems will evolve according to an equation of this form.

Physical meaning

Set all the L_j operators to zero. H_{eff} becomes equal to H , and the evolution equation reduces to

$$\dot{\rho}(t) = -\frac{i}{\hbar}(H\rho(t) - \rho(t)H) = -\frac{i}{\hbar}[H, \rho(t)]$$

This is identical to eq. 5.1, the Von Neumann equation, which is the evolution equation.

The operator H represents the Hamiltonian of the system we are studying, if interactions with the environment are not taken into account, and the L_j operators, called **jump operators** represent processes associated with the interaction with the environment.

Example

Spontaneous Emission

Consider a two-level atom, its ground state $|g\rangle$ and its excited state $|e\rangle$ with energy $\hbar\omega$. The Hamiltonian for the atom is $H = \hbar\omega|e\rangle\langle e|$. Spontaneous emission occurs due to the interaction between the atom and all the modes of the electromagnetic field surrounding it. An atom may interact with an empty mode by decaying from excited to ground state via the emission of a photon. Photons emitted into free-space are not likely to be reabsorbed by the atom, and the system's evolution is therefore Markovian. In this scenario we have a single jump operator $L = \gamma|g\rangle\langle e|$. The jump operator transforms state $|e\rangle$ to the ground state $|g\rangle$, the constant γ is related to the rate at which spontaneous emission occurs. Hamiltonian of the system is $H = \hbar\omega|e\rangle\langle e|$.

Insert these operators in the master equation (eq. 5.6) gives us the master equation derived in

Wigner-Weisskopf theory. First consider the effective Hamiltonian in this evolution:

$$\begin{aligned} H_{eff} &= \hbar\omega|e\rangle\langle e| - \frac{i\hbar}{2}|\gamma|^2|e\rangle\langle g|g\rangle\langle e| \\ &= \hbar\omega|e\rangle\langle e| - \frac{i\hbar}{2}|\gamma|^2|e\rangle\langle e| \\ &= (\hbar\omega - \frac{i\hbar}{2}|\gamma|^2)|e\rangle\langle e| \end{aligned}$$

The master equation for the problem is then

$$\dot{\rho}(t) = -\frac{i}{\hbar}(H_{eff}\rho(t) - \rho(t)H_{eff}^\dagger) + L\rho(t)L^\dagger$$

Assume that the initial state of the atom is the excited state $\rho(0) = |e\rangle\langle e|$. To simplify the calculation, we will consider a time-evolving state of the form

$$\rho(t) = \rho_{ee}(t)|e\rangle\langle e| + \rho_{gg}(t)|g\rangle\langle g| \quad (5.7)$$

For a full treatment we should also have included terms $\rho_{eg}(t)|e\rangle\langle g|$ and $\rho_{ge}(t)|g\rangle\langle e|$, neglect these terms here to simplify the calculation.

Using eq. 5.7:

$$\begin{aligned} H_{eff}\rho(t) &= \hbar(\omega - i|\gamma|^2/2)\rho_{ee}(t)|e\rangle\langle e| \\ \rho(t)H_{eff}^\dagger &= \hbar(\omega + i|\gamma|^2/2)\rho_{ee}(t)|e\rangle\langle e| \\ L\rho(t)L^\dagger &= |\gamma|^2\rho_{ee}(t)|g\rangle\langle g| \end{aligned}$$

Take the time derivative of 5.7 and equate with RHS of master equation:

$$\begin{aligned} \dot{\rho}(t) &= \dot{\rho}_{ee}(t)|e\rangle\langle e| + \dot{\rho}_{gg}(t)|g\rangle\langle g| \\ &= -\frac{i}{\hbar}(\hbar(\omega - i|\gamma|^2/2) - \hbar(\omega + i|\gamma|^2/2)) \\ &\quad \times \rho_{ee}(t)|e\rangle\langle e| + |\gamma|^2\rho_{ee}(t)|g\rangle\langle g| \\ &= -|\gamma|^2\rho_{ee}(t)|e\rangle\langle e| + |\gamma|^2\rho_{ee}(t)|g\rangle\langle g| \end{aligned}$$

Multiplying $\langle e|$ from the left and $|e\rangle$ from the right we obtain:

$$\dot{\rho}_{ee}(t) = -|\gamma|^2\rho_{ee}(t)$$

Multiplying $\langle g|$ from the left and $|g\rangle$ from the right we obtain:

$$\dot{\rho}_{gg}(t) = |\gamma|^2\rho_{ee}(t)$$

Integrating these, we get:

$$\rho_{ee}(t) = \exp[-|\gamma|^2 t]\rho_{ee}(0)$$

$$\rho_{gg}(t) = 1 - \exp[-|\gamma|^2 t]\rho_{ee}(0)$$

This equation tells us that the probability of measuring that the state of the atom in the excited state $|e\rangle$ will decay exponentially in time with rate $|\gamma|^2$.

5.5.1 Phenomenological master equations

The **Main Idea**: "Smart Guessing" Instead of deriving the Master Equation from complex first principles every time, we can build it using "intelligent guesswork" based on what we see happening in the experiment.

The **Recipe**: To build the equation, you just need to identify two things:

- The **Hamiltonian** (H): The standard energy description of the system.
- The **Jump Operator** (L): An operator that literally mimics the physical decay or noise you observe (e.g., if an atom drops from excited $|e\rangle$ to ground $|g\rangle$, you pick an operator that mathematically does exactly that).

Pros and Cons

- **Pro**: It is a powerful, fast way to model open systems like quantum computers or biological molecules.
- **Con**: It cannot tell you the rate of the decay (how fast it happens). You cannot calculate the constants (like $|\gamma|^2$), you have to measure them or calculate them separately.

Example

Random magnetic field

If a spin encounters a randomly varying magnetic field it will shift the energies of the spin energy levels. This leads to random phase shifts.

Quantum state of the spin becomes mixed. A jump operator which implements this dephasing behaviour is $L = \gamma(|1\rangle\langle 1| - |\downarrow\rangle\langle \downarrow|) = \gamma\sigma_z$, where $|\gamma|^2$ is a rate in the evolution equations.

Example

Damped quantum oscillator (leaking cavity)

In a physical optical cavity, photons are leaked over time from the cavity and are lost. This process is mathematically equivalent to a damped Harmonic oscillator and is described by a jump operator $L = \gamma\hat{a}$.

This jump operator has a literal interpretation, it is proportional to the lowering operator, which annihilates photons.

Chapter 6

WKB Approximation

6.1 Preloge

Previously, we studied tunnelling in an idealised setting, where the potential is modelled by a step function (see figure 6.1). In this case, the time-independent Schrödinger equation (TISE)

$$\left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x)\right]\psi(x) = E\psi(x)$$

(6.1) can be separately integrated for each distinct region of constant potential.

Solutions:

- Classically allowed region where $E > V_0$, where $p = \sqrt{2m(E - V_0)}$;

$$\psi(x) = Ae^{ipx/\hbar} + Be^{-ipx/\hbar}$$

- classically forbidden" region where $E < V_0$, where $q = \sqrt{2m(V_0 - E)}$;

$$\psi(x) = Ce^{+qx/\hbar} + De^{-qx/\hbar}$$

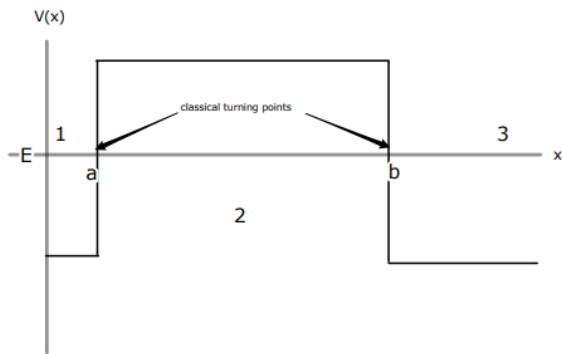


Figure 6.1: Idealised potential illustrating quantum tunnelling. Diagram taken from professors' notes.

6.2 Introduction

Solving the TISE exactly for an arbitrary smooth $V(x)$ can be very hard and often impossible with known

techniques. The Wentzel-Kramers-Brillouin or WKB approximation solves the TISE under the condition that the potential $V(x)$ is varying sufficiently slowly.

Recall that, in a constant potential in a classically allowed region, the eigenfunctions of the TISE are plane-waves, eigenstates of momentum with momentum $p = \sqrt{2m(E - V)}$ and which have a de Broglie wave-length $\lambda = \frac{h}{p}$. If $V(x)$ is varying slowly, in particular, slowly with respect to λ , it can still be meaningful to define a local momentum

$$p(x) = \sqrt{2m(E - V(x))}$$

and corresponding local wavelength $\lambda(x) = \frac{h}{p(x)}$

6.3 WKB approximation

Assume that, if $V(x)$ is varying sufficiently slowly, the wave-function has a form similar to the idealised case where $V(x)$ is constant, such as in equation 6.1; start with a trial solution (Ansatz) of the form:

$$\psi(x) = Ae^{\frac{i}{\hbar}S(x)} \quad (6.1)$$

Substitute this expression into the TISE: Using

$$\begin{aligned} \frac{\partial^2 \psi(x)}{\partial x^2} &= \frac{\partial}{\partial x} \left(\frac{i}{\hbar} S'(x) Ae^{\frac{i}{\hbar}S(x)} \right) \\ &= \left(\frac{i}{\hbar} S''(x) - \frac{S'(x)^2}{\hbar^2} \right) Ae^{\frac{i}{\hbar}S(x)} \end{aligned}$$

to obtain,

$$-\frac{i\hbar}{2m} S''(x) + \frac{1}{2m} (S'(x))^2 + V(x) - E = 0. \quad (6.2)$$

This equation is exact but non-linear. Neglecting the term proportional to \hbar recovers the plane-wave solution $S(x) = \int p(x)dx$. Motivated by this semi-classical limit ($\hbar \rightarrow 0$), we treat \hbar as a variable and expand $S(x)$ as a power series.

$$S(x) = S_0(x) + \hbar S_1(x) + \hbar^2 S_2(x) + \dots = \sum_{j=0}^{\infty} \hbar^j S_j(x)$$

Substitute this power series into equation 6.2 to obtain

$$\frac{-i\hbar}{2m} \sum_j \hbar^j S_j''(x) + \frac{1}{2m} \left(\sum_j \hbar^j S_j'(x) \right)^2 + V(x) - E = 0.$$

Match powers of \hbar (these terms must independently sum to zero); this will give a set of simultaneous equations.

- 0th order (\hbar^0)

$$\frac{1}{2m} (S_0'(x))^2 + V(x) - E = 0$$

Rearrange and integrate

$$\begin{aligned} \frac{\partial S_0(x)}{\partial x} &= \pm \sqrt{2m(E - V(x))} \\ S_0(x) &= \pm \int^x dx' p(x') + c \end{aligned} \quad (6.3)$$

Hence neglecting c we get

$$S_0'(x) = \pm p(x) \quad (6.4)$$

- 1st order (\hbar^1)

$$\frac{-i}{2m} S_0''(x) + \frac{2}{2m} S_1'(x) S_0'(x) = 0$$

Rearrange

$$\frac{S_0''(x)}{S_0'(x)} = -i2S_1'(x)$$

Use $\int f'(x)/f(x)dx = \ln(f(x)) + c$ to get

$$\ln(S_0'(x)) = -i2S_1(x) + c$$

Sub in 6.4

$$\begin{aligned} -2iS_1(x) &= \ln(\pm p(x)) - c \\ iS_1(x) &= -\ln(\pm \sqrt{p(x)}) + \frac{c}{2} \end{aligned} \quad (6.5)$$

- 2nd order (\hbar^2) Integrating the second-order equation gives:

$$S_2(x) = \frac{1}{2} \frac{m}{p(x)^3} \frac{\partial V(x)}{\partial x} - \frac{1}{4} m^2 \int \frac{1}{p(x')^5} \left(\frac{\partial V(x')}{\partial x'} \right)^2 dx'$$

So provided $\frac{\partial V(x)}{\partial x}$ is sufficiently small S_2 will vanish. This justifies taking only the first two terms in the expansion provided these conditions hold.

Thus approximate $S(x)$ to first order in \hbar :

$$S(x) \approx S_0(x) + \hbar S_1(x)$$

Substituting into equation 6.1 we obtain:

$$\begin{aligned} \psi(x) &= A e^{\frac{i}{\hbar} S(x)} \\ &= A e^{\frac{i}{\hbar} S_0(x)} e^{i S_1(x)} \end{aligned}$$

Substituting eqs 6.4 and 6.5:

$$\begin{aligned} &= A e^{\pm \frac{i}{\hbar} \int^x dx' p(x')} e^{-\ln \sqrt{p(x)} + c} \\ &= \frac{A'}{\sqrt{p(x)}} e^{\pm \frac{i}{\hbar} \int^x dx' p(x')} \\ \psi(x) &= \frac{A}{\sqrt{p(x)}} e^{+ \frac{i}{\hbar} \int^x p(x') dx'} + \frac{B}{\sqrt{p(x)}} e^{- \frac{i}{\hbar} \int^x p(x') dx'} \end{aligned} \quad (6.6)$$

In the last step, the constant of integration c was absorbed into A and B .

The WKB wavefunction mirrors classical mechanics in two key ways:

- Amplitude: The probability density $|\psi(x)|^2 \propto 1/p(x)$ is inversely proportional to velocity, matching the classical expectation that a particle is less likely to be found where it moves faster (spending less time there).
- Phase: The integral term $e^{i \int p(x') dx' / \hbar}$ generalizes plane-wave behavior to systems with spatially varying momentum.

Classically forbidden region

In the forbidden region: $E < V(x)$, hence $p(x) = \sqrt{2m(E - V(x))}$ becomes imaginary.

Define $q(x)$ such that:

$$q(x) = ip(x) = \sqrt{2m(V(x) - E)}$$

The wave-function in the forbidden region becomes:

$$\psi(x) = \frac{C}{\sqrt{q(x)}} e^{+ \int^x q(x') dx' / \hbar} + \frac{D}{\sqrt{q(x)}} e^{- \int^x q(x') dx' / \hbar} \quad (6.7)$$

Classical Turning Point - CTP

To fully solve the TISE, apply boundary conditions at the classical turning points (CTPs), which mark the transition between allowed and forbidden regions.

At the CTP, $E = V(x)$, $p(x) = 0$, the WKB solutions $\propto 1/\sqrt{p(x)}$ diverge to infinity. Hence the **WKB solutions** in equations 6.6 and 6.7 **cannot be valid close to the CTP**. We need to find an additional family of wave-functions which while valid at the CTP, converge to the WKB solutions away from the CTP.

6.4 Connection Formulae

Label $x = a$ as being very close to the classical turning point, expanding $V(x)$ as a Taylor expansion around $V(a)$:

$$V(x) = V(a) + \left. \frac{\partial V}{\partial x} \right|_{x=a} (x - a) + \dots$$

and since $V(a) = E$ and defining the slope $A = \left. \frac{\partial V}{\partial x} \right|_{x=a}$:

$$V(x) - E = A(x - a)$$

Substituting this into the TISE:

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} + A(x - a)\psi(x) = 0$$

Perform a change of variables $z = (2mA/\hbar^2)^{1/3}(x - a)$ so that the TISE takes the form

$$\frac{\partial^2 \psi(z)}{\partial z^2} - z\psi(z) = 0$$

This equation is called the **Airy equation**. Label its solutions $Ai(z)$ and $Bi(z)$; plotted, they look like this:

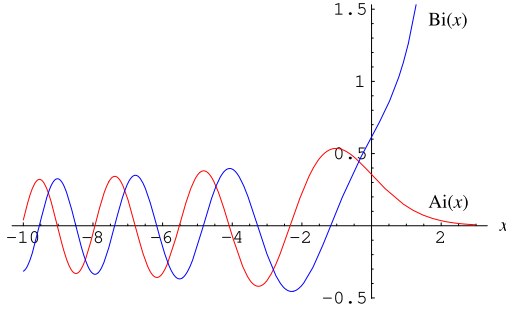


Figure 6.2: Airy functions $Ai(z)$ and $Bi(z)$. Taken from <https://mathworld.wolfram.com/AiryFunctions.html>

A general solution will be a linear combination of these functions. $Ai(z)$ and $Bi(z)$ are illustrated in figure 6.2.

Asymptotic forms

Large positive z

$$Ai(z) \approx \frac{1}{2\sqrt{\pi}} \frac{\exp[-\frac{2}{3}|z|^{3/2}]}{|z|^{1/4}}$$

$$Bi(z) \approx \frac{1}{\sqrt{\pi}} \frac{\exp[+\frac{2}{3}|z|^{3/2}]}{|z|^{1/4}}$$

Large negative z

$$Ai(z) \approx \frac{1}{\sqrt{\pi}} \frac{\cos[\frac{2}{3}|z|^{3/2} - \frac{\pi}{4}]}{|z|^{1/4}}$$

$$Bi(z) \approx \frac{-1}{\sqrt{\pi}} \frac{\sin[\frac{2}{3}|z|^{3/2} - \frac{\pi}{4}]}{|z|^{1/4}}$$

These solutions have most of the behaviour we need, they are continuous across the CTP, and they converge

to exponential growth and decay, and oscillatory behaviour on the appropriate sides of the CTP. However, the Airy function alone cannot be our full solution. It was derived for a linear potential, not a smooth curve $V(x)$, so one would not expect it to.

Far from the turning point, the Airy functions converge to standard WKB forms with specific phase factors:

- Allowed region:

$$\psi_A(x) = \frac{1}{2\sqrt{\pi}} \frac{1}{\sqrt{p(x)}} \cos\left(\int_x^a p(x')dx'/\hbar - \frac{\pi}{4}\right)$$

$$\psi_B(x) = \frac{-1}{\sqrt{\pi}} \frac{1}{\sqrt{p(x)}} \sin\left(\int_x^a p(x')dx'/\hbar - \frac{\pi}{4}\right)$$

- Forbidden region:

$$\psi_A(x) = \frac{1}{\sqrt{\pi}} \frac{1}{\sqrt{q(x)}} \exp\left(-\int_a^x q(x')dx'/\hbar\right)$$

$$\psi_B(x) = \frac{1}{\sqrt{\pi}} \frac{1}{\sqrt{q(x)}} \exp\left(+\int_a^x q(x')dx'/\hbar\right)$$

Connection Formulae

Equate the allowed and forbidden side of each wave function together to obtain the connection formulae in Table 6.1.

The arrows represent the "safe" direction for calculation to prevent information loss.

The Problem (Forbidden Region): The wavefunction here is a superposition of an exponentially growing term ($e^{+\lambda}$) and a decaying term ($e^{-\lambda}$). The growing term mathematically "swamps" the decaying term, rendering its coefficient numerically invisible.

The Consequence (Allowed Region): In the allowed region, these terms become sine and cosine waves of equal amplitude. The "invisible" decaying term from the forbidden region is responsible for the specific phase of the oscillation here. If you lost that term in the forbidden region, your phase in the allowed region will be wrong.

The Rule: You cannot connect from a region where a term is hidden (swamped) to a region where it is visible.

- **Safe:** Decay (Forbidden) \rightarrow Oscillating (Allowed). (You are tracking the pure, unique subdominant term).
- **Unsafe:** Growth (Forbidden) \rightarrow Oscillating (Allowed). (You cannot know if a tiny decaying term was hidden under the growth).

Exception: If you possess an exact analytic solution (e.g., knowing the growing coefficient is exactly zero at infinity), you may ignore the arrows.

Table 6.1: WKB Connection Formulas at Turning Points. The arrows represent the "safe" direction for calculation to prevent information loss. Note the right-hand barrier is actually on the left on the diagram.

Barrier	Relation	
Right-hand	$\psi_A^{\text{allowed}} = \psi_A^{\text{forb.}}$	$\frac{2}{\sqrt{p(x)}} \cos \left(\int_x^a p(x') dx' / \hbar - \frac{\pi}{4} \right) \longleftarrow \frac{1}{\sqrt{q(x)}} \exp \left[- \int_a^x q(x') dx' / \hbar \right]$
	$\psi_B^{\text{allowed}} = \psi_B^{\text{forb.}}$	$-\frac{1}{\sqrt{p(x)}} \sin \left(\int_x^a p(x') dx' / \hbar - \frac{\pi}{4} \right) \longrightarrow \frac{1}{\sqrt{q(x)}} \exp \left[+ \int_a^x q(x') dx' / \hbar \right]$
Left-hand	$\psi_A^{\text{forb.}} = \psi_A^{\text{allowed}}$	$\frac{1}{\sqrt{q(x)}} \exp \left[- \int_x^a q(x') dx' / \hbar \right] \longrightarrow \frac{2}{\sqrt{p(x)}} \cos \left(\int_a^x p(x') dx' / \hbar - \frac{\pi}{4} \right)$
	$\psi_B^{\text{forb.}} = \psi_B^{\text{allowed}}$	$\frac{1}{\sqrt{q(x)}} \exp \left[+ \int_x^a q(x') dx' / \hbar \right] \longleftarrow -\frac{1}{\sqrt{p(x)}} \sin \left(\int_a^x p(x') dx' / \hbar - \frac{\pi}{4} \right)$

6.5 Example 1: Bound states in a quantum well

A quantum well is illustrated in fig. 6.3. Consider a particle of energy E less than the highest potential on both sides of the well, which therefore has classical turning points (where $V(x) = E$) at points $x = a$ and $x = b$. The classical turning points divide the space into three regions.

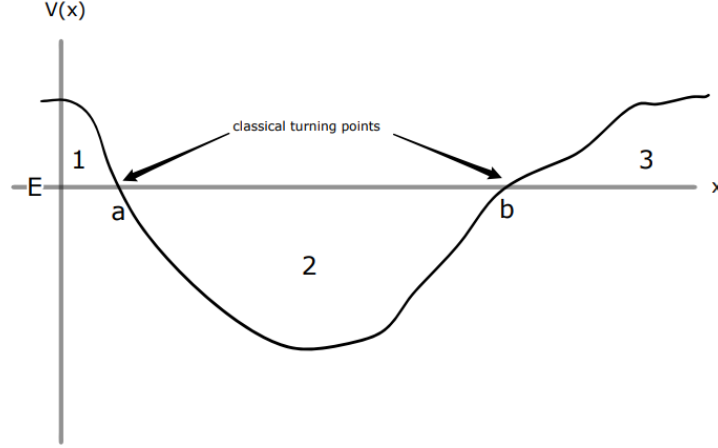


Figure 6.3: Potential for a one-dimensional smooth well. Diagram taken from professor's notes.

Region 1: is a classically forbidden region, and hence the WKB wavefunction will have the form of eq. 6.7. Assume that there are no more classical turning points between $x = a$ and $x = -\infty$. Neglect the term which will "blow up" at minus infinity (1st):

$$\psi_1(x) = \frac{A_1}{\sqrt{q(x)}} \exp \left[- \int_x^a q(x') dx' / \hbar \right]$$

where $q(x) = \sqrt{2m(V(x) - E)}$.

Region 3: Similarly to region 1, the WKB wave-function must take the form (neglect 2nd term):

$$\psi_3(x) = \frac{A_3}{\sqrt{q(x)}} \exp \left[- \int_b^x q(x') dx' / \hbar \right]$$

Region 2: From region 1 to 2:

- left-hand barrier
- Forbidden \rightarrow Allowed

By looking at the table of connection formulas (Table 6.1) using the 3rd one to get:

$$\psi_2^{\text{left}}(x) = \frac{2A_1}{\sqrt{p(x)}} \cos \left(\int_a^x p(x') dx' / \hbar - \frac{\pi}{4} \right) \quad (6.8)$$

From region 3 to 2:

- right-hand barrier
- Allowed \rightarrow Forbidden

By looking at the same table (use the 1st eq):

$$\psi_2^{\text{right}}(x) = \frac{2A_3}{\sqrt{p(x)}} \cos \left(\int_x^b p(x') dx' / \hbar - \frac{\pi}{4} \right) \quad (6.9)$$

These two must be equal (they are both representing the same region of space). By using $\int_x^b dx = \int_a^b dx - \int_a^x dx$, eq 6.8 becomes:

$$\psi_2^{\text{right}}(x) = \frac{2A_3}{\sqrt{p(x)}} \cos \left(\underbrace{\int_a^b p(x')dx'/\hbar}_P - \underbrace{\int_a^x p(x')dx'/\hbar}_Q - \frac{\pi}{4} \right) \quad (6.10)$$

where we have labelled the integrals within the cosine P and Q, for easier manipulation.

Consider the following trigonometric identities:

$$\cos(P - (Q + \pi/4)) = \sin(P - (Q - \pi/4)) \quad (6.11)$$

$$= \sin(P) \cos(Q - \pi/4) - \cos(P) \sin(Q - \pi/4) \quad (6.12)$$

Eq. 6.10 becomes:

$$\psi_2^{\text{right}}(x) = \frac{2A_3}{\sqrt{p(x)}} [\sin(P) \cos(Q - \pi/4) - \cos(P) \sin(Q - \pi/4)] \quad (6.13)$$

Eq 6.8 is proportional to $\cos(Q - \pi/4)$; this implies that in the above equation the following must be satisfied:

$$\cos(P) \sin(Q - \pi/4) = 0$$

This is satisfied if:

- $\sin(Q - \pi/4) = 0$. This is true if $\cos(Q - \pi/4)$ is always equal to 1, which we know is not the case.
- $\cos(P) = 0$

This requirement implies that $P = (n + 1/2)\pi$, and gives us the WKB quantum well quantisation condition:

$$P = \int_a^b p(x')dx'/\hbar = \left(n + \frac{1}{2}\right)\pi \quad (6.14)$$

where $n = 0, 1, 2, \dots$

This implies that the bound particle can only have energies which satisfy this equation. Eq. 6.14 implies that $\sin(P) = (-1)^n$, 6.13 becomes

$$\psi_2(x) = \frac{2A_3(-1)^n}{\sqrt{p(x)}} \cos \left(\int_a^x p(x')dx'/\hbar - \frac{\pi}{4} \right)$$

By comparison with equation 6.8 we see that $A_1 = A_3(-1)^n$.

6.6 Example 2: Tunnelling

Assume that the particle is incident from the left with energy less than the height of the barrier.

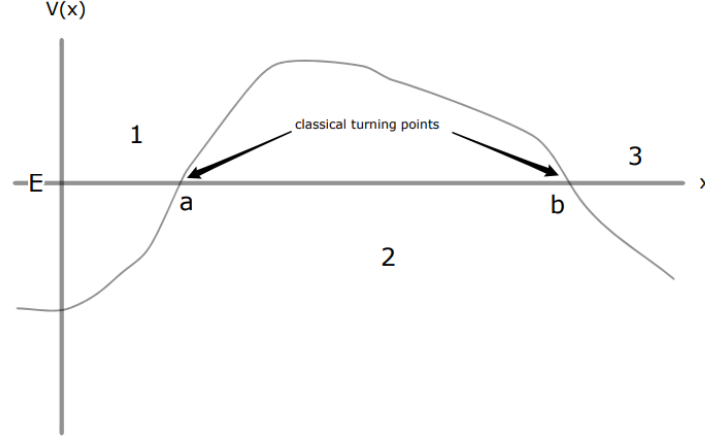


Figure 6.4: Potential for a one-dimensional smooth barrier. Diagram taken from professor's notes.

Region 3 This will consist solely of a WKB wave-function travelling from left to right direction, of the form (from eq. 6.6)

$$\psi_3(x) = \frac{A'}{\sqrt{p(x)}} \exp \left[i \int_b^x p(x') dx' / \hbar \right]$$

To make it easier to apply the connection formulae, introduce the new constant $A = A' e^{i\pi/4}$ and write

$$\psi_3(x) = \frac{A}{\sqrt{p(x)}} \exp \left[i \int_b^x p(x') dx' / \hbar - i \frac{\pi}{4} \right]$$

Expand

$$\psi_3(x) = \frac{A}{\sqrt{p(x)}} \left(\cos \left[\int_b^x p(x') dx' / \hbar - \frac{\pi}{4} \right] + i \sin \left[\int_b^x p(x') dx' / \hbar - \frac{\pi}{4} \right] \right) \quad (6.15)$$

Region 2 Apply the connection formulae for a left-hand barrier to get region 2 (table 6.1); for 1st terms use 3rd eq, and for 2nd term use 4th eq.

$$\psi(x)_2 = \frac{A}{\sqrt{q(x)}} \left(\frac{1}{2} \exp \left[- \int_x^b q(x') dx' / \hbar \right] - i \exp \left[\int_x^b q(x') dx' / \hbar \right] \right) \quad (6.16)$$

Note: we have used the connection formulae against the direction of its arrow. The arrows in the connection formulae are there to prevent small errors in the wave-function on one side of the classical turning point, being amplified by the exponential terms on the other side of the turning point.

However, we know that the wave-function in region 3 has to be a travelling wave of WKB form; this implies that cosine and sine components of eq 6.15 have to have exactly equal amplitudes so we may safely apply connection formulae in the opposite direction to its arrow.

Region 1 To derive the form of the wave-function in region 1, we need to rewrite eq. 6.16 such that the limits in the integrals are in the correct form for application of connection

formulae, use

$$\begin{aligned}\exp\left[\int_x^b q(x')dx'/\hbar\right] &= \exp\left[\int_a^b q(x')dx'/\hbar\right] \exp\left[-\int_a^x q(x')dx'/\hbar\right] \\ &= r \exp\left[-\int_a^x q(x')dx'/\hbar\right]\end{aligned}$$

where we define $r = \exp\left[\int_a^b q(x')dx'/\hbar\right]$ Substitute this into 6.16 for the a turning point:

$$\psi_2(x) = \frac{A}{\sqrt{q(x)}} \left(\frac{1}{2r} \exp\left[\int_a^x q(x')dx'/\hbar\right] - ir \exp\left[-\int_a^x q(x')dx'/\hbar\right] \right)$$

Apply connection formulae across a right-hand barrier

$$\psi_1(x) = \frac{A}{\sqrt{p(x)}} \left(-\frac{1}{2r} \sin\left[\int_x^a p(x')dx'/\hbar - \frac{\pi}{4}\right] - 2ir \cos\left[\int_x^a p(x')dx'/\hbar - \frac{\pi}{4}\right] \right)$$

Define $\phi(x) = \left[\int_x^a p(x')dx'/\hbar - \frac{\pi}{4}\right]$

$$\psi_1(x) = \frac{A}{\sqrt{p(x)}} \left(-\frac{1}{2r} \sin \phi(x) - 2ir \cos \phi(x) \right) \quad (6.17)$$

$$= \frac{iA}{\sqrt{p(x)}} \left[\left(\frac{1}{4r} - r \right) e^{i\phi(x)} - \left(\frac{1}{4r} + r \right) e^{-i\phi(x)} \right] \quad (6.18)$$

Counterintuitively, $e^{-i\phi(x)}$ is the incident wave and $e^{i\phi(x)}$ is the reflected wave. To see why consider the limit of $e^{i\phi(x)}$ as $x \rightarrow -\infty$.

Find the Transmission coefficient

Assume that the potential $V(x)$ tends to a constant V_0 in the $x \rightarrow -\infty$ limit, and that there is a value $x = x_0$ beyond which $V(x) \approx V_0$. In this region $p(x)$ is also approximately constant with value $p_0 = \sqrt{2m(E - V_0)}$

Year 3 reminder

The wavefunctions of particles that tunnel through a square barrier are given by:

$$\psi_1(x) = e^{ipx/\hbar} + Re^{-ipx/\hbar}$$

$$\psi_2(x) = Ce^{qx/\hbar} + De^{-qx/\hbar}$$

$$\psi_3(x) = Te^{ipx/\hbar}$$

where $p = \sqrt{2mE}$ and $q = \sqrt{2m(V - E)}$.

The probability flux for the tunnelling particles, in 1-D:

$$J = \frac{\hbar}{2im} \left(\psi(x)^* \frac{\partial \psi(x)}{\partial x} - \psi(x) \frac{\partial \psi(x)^*}{\partial x} \right) \quad (6.19)$$

Substituting the solutions into this gives the following probability currents:

- Incident: $J_I = p/m$
- Reflected: $J_R = |R|^2 p/m$
- Transmitted: $J_T = |T|^2 p/m$

The tunnelling transmission coefficient is: $T = J_T/J_I = |T|^2$.

Consider the part of the wave that is going backwards:

$$\begin{aligned}
e^{i\phi(x)} &= e^{-i\pi/4} \exp \left[i \int_x^a p(x') dx' / \hbar \right] \\
&= e^{-i\pi/4} \exp \left[i \int_x^{x_0} p(x') dx' / \hbar \right] \exp \left[i \int_{x_0}^a p(x') dx' / \hbar \right]
\end{aligned}$$

Use the fact that for $x \rightarrow -\infty$, $p(x) \approx p_0$

$$\begin{aligned}
&\approx e^{-i\pi/4} \exp \left[i \int_{x_0}^a p(x') dx' / \hbar \right] \exp [i(p_0(x_0 - x)/\hbar)] \\
&\propto \exp [-ip_0x/\hbar]
\end{aligned}$$

wave-function for region 1 as

$$\psi(x)_1 = \psi_I(x) + \psi_R(x)$$

$\psi_I(x)$ represents incident flux, travelling towards the barrier, and $\psi_R(x)$ is associated with reflected flux. In the region $x \ll x_0$ far away from the barrier, $\psi_I(x)$ takes the form

$$\psi_I(x) \approx \frac{-iA}{\sqrt{p_0}} e^{i\alpha} \left(\frac{1}{4r} + r \right) e^{ip_0x/\hbar}$$

where $e^{i\alpha} = e^{i\pi/4} \exp \left[-i \int_{x_0}^a p(x') dx' / \hbar \right] \exp [-ip_0x_0/\hbar]$ is a constant phase.

Assume that the potential also converges to the constant value $V(x) \rightarrow V_0$ as $x \rightarrow \infty$. Wave function in region 3

$$\psi_3(x) \approx \frac{A}{\sqrt{p_0}} e^{i\alpha'} e^{ip_0x/\hbar}$$

where $e^{i\alpha'}$ are constant phases which are unimportant for the following calculation. Using the probability flux equation (eq. 6.19) we get the probability currents for the incident and transmitted (region 3) waves

$$\begin{aligned}
J_I &= \frac{|A|^2}{m} \left| \frac{1}{4r} + r \right|^2 \\
J_T &= \frac{|A|^2}{m}
\end{aligned}$$

The transmission coefficient is therefore

$$\frac{J_T}{J_I} = \frac{1}{\left| \frac{1}{4r} + r \right|^2}$$

Important:

- WKB approximation is valid only if:
- turning points are well-separated
 - barrier is significantly higher than the particle's energy

In such a domain

$$r = \exp \left[\int_a^b q(x') dx' / \hbar \right] \gg 1$$

In this limit, for $r \gg 1$, the transmission coefficient simplifies to (in 2nd step use definition of r)

$$\frac{J_T}{J_I} \approx \frac{1}{r^2} = e^{-2 \int_a^b q(x') dx' / \hbar} = e^{-2\lambda}$$

where $\lambda = \int_a^b q(x') dx' / \hbar$. Hence in the WKB approximation, the tunnelling coefficient is related to the integral over $q(x)$ across the barrier.