2. The Quantum Mechanical Tool-Box

Quantum Computing

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The postulates

1. *The state of a quantum physical system is completely specified by its state vector of unit norm, indicated by the ket $|\psi\rangle \in \mathcal{H}$ (Hilbert space).*

Since $\mathcal{H}$ is a linear vector space, given two normalized vectors $|\psi_1\rangle, |\psi_2\rangle \in \mathcal{H}$

$$|\psi\rangle = \alpha|\psi_1\rangle + \beta|\psi_2\rangle \quad (\text{with } |\alpha|^2 + |\beta|^2 = 1)$$

still belongs to $\mathcal{H}$ and is a possible state vector of the system.

An equivalent representation is given in terms of the bra

$$\langle\psi| = \alpha^*\langle\psi_1| + \beta^*\langle\psi_2|$$

The postulates

2. *Let $|\psi\rangle$ be the state vector of a micro-system and $|\phi\rangle$ another state within the same Hilbert space. Then the probability amplitude to find $|\psi\rangle$ in $|\phi\rangle$ is the complex number $\langle\phi|\psi\rangle$ and the relative probability is $|\langle\phi|\psi\rangle|^2$.*

Being all the states normalized, we find

$$0 \leq |\langle\phi|\psi\rangle|^2 \leq 1$$

The postulates

3. *We can associate to each observable $\mathcal{A}$ an Hermitian operator A acting on the Hilbert space $\mathcal{H}$. The spectrum of A constitutes the range of possible values of the observable.*

Spectral decomposition of A: $A = \sum_k a_k |k\rangle\langle k|$ with non-degenerate a_k eigenvalues

In a measurement of the observable $\mathcal{A}$ for a system described by state vector $|\psi\rangle$, we will find the result a_k with probability $p_k = |\langle k|\psi\rangle|^2$. That is, if we consider N copies of the physical system (always prepared in state $|\psi\rangle$) our measurement will give us the result a_k for a number of times close to $N|\langle k|\psi\rangle|^2$ in the limit $N \to \infty$.

In such limit, the **expectation value** of $\mathcal{A}$ on state $|\psi\rangle$ is given by

$$\langle A\rangle_\psi = \langle\psi|A|\psi\rangle = \sum_k a_k \langle\psi|k\rangle\langle k|\psi\rangle = \sum_k a_k p_k$$

Degenerate eigenvalues

If the observable $\mathcal{A}$ has degenerate eigenvalues, each eigenvalue a_k corresponds to a subspace spanned by (ortho-normalized) eigenvectors

$$|k, l\rangle, \qquad l = 1, 2, \ldots, g(k)$$

with $g(k)$ the degeneracy of eigenvalue a_k.

The probability $P(a_k) = \sum_{l=1}^{g(k)} |\langle\psi|k,l\rangle|^2 = \langle\psi|P_k|\psi\rangle$

$$P_k = \sum_{l=1}^{g(k)} |k, l\rangle\langle k, l|$$

$$P_\psi = |\psi\rangle\langle\psi| \qquad \langle A\rangle_\psi = \langle\psi|A|\psi\rangle = \mathrm{Tr}[AP_\psi] \qquad p(a_k) = \mathrm{Tr}[P_k P_\psi]$$

The postulates

4. *After a measurements of the observable $\mathcal{A}$ with outcome a_k the state of the system is projected onto the corresponding subspace.*

$$|\psi\rangle \longrightarrow \frac{P_k|\psi\rangle}{\|P_k|\psi\rangle\|}$$

Hence a repetition of the same measurement yields a_k with probability 1.

Compatible observables $\iff$ $[A,B]=0$ $\iff$ A, B have a common eigenbasis

Complete set of commuting observables (CSCO): set of hermitian operators characterized by a non-degenerate complete set of orthonormal eigenvectors

$$p(A=a_k, B=b_l) = \sum_{m=1}^{g(k,l)} |\langle k,l,m|\psi\rangle|^2 = \langle\psi|P_{k,l}|\psi\rangle \qquad P_{k,l} = \sum_m |k,l,m\rangle\langle k,l,m|$$

The eigenvectors of a non-degenerate set of eigenvalues of a CSCO form a basis of the Hilbert space

The postulates

5. *The time-evolution of a closed quantum system is described by a unitary transformation.*

$$|\psi(t)\rangle = U(t,t_0)|\psi(t_0)\rangle$$

5. *The time-evolution of a closed quantum system is described by the Schrödinger equation*

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

Hamiltonian of the closed system (hermitian operator).
It completely determines the dynamics of the system.

Dynamics

We can write an analogous differential equation for the time evolution operator:

$$i\hbar \frac{d}{dt} U(t,t_0) = H(t)U(t,t_0) \qquad\qquad U(t_0,t_0) = \mathbb{I}$$

For time-independent Hamiltonian $\quad \frac{\partial H}{\partial t} = 0 \Longrightarrow U(t,t_0) = e^{-\frac{iH(t-t_0)}{\hbar}} = U(t-t_0)$

$$|\psi(t)\rangle = U\,|\psi(t_0)\rangle \Longrightarrow$$

$$\langle A(t)\rangle_\psi = \langle\psi(t)|A|\psi(t)\rangle = \big(\langle\psi(t_0)|U^\dagger\big)A\big(U|\psi(t_0)\rangle\big)$$

$$= \big\langle\psi(t_0)\big|U^\dagger A U\big|\psi(t_0)\big\rangle$$

Operator fixed,
Evolution of the ket (Schrödinger picture)

Evolution of the operator,
Ket fixed (Heisenberg picture)

A is a **constant** of motion if

$$\frac{d}{dt}\langle\psi(t)|A|\psi(t)\rangle = 0 \quad \forall|\psi(t_0)\rangle \quad \Longrightarrow \quad [A,H] + i\hbar\frac{\partial A(t)}{\partial t} = 0$$

In that case, its eigenvalues and probability distributions are independent of time.

Time evolution, time independent Hamiltonian

$$H = \sum_k E_k |\phi_k\rangle\langle\phi_k|$$ Spectral decomposition of the Hamiltonian

$$|\psi(0)\rangle = \sum_k |\phi_k\rangle\langle\phi_k|\psi(0)\rangle \Rightarrow \sum_k \alpha_k |\phi_k\rangle$$ $$\alpha_k = \langle\phi_k|\psi(0)\rangle$$

$$|\psi(t)\rangle = e^{-\frac{iHt}{\hbar}}|\psi(0)\rangle = \sum_k \alpha_k e^{-\frac{iE_k t}{\hbar}}|\phi_k\rangle = \sum_k \boxed{c_k(t)}|\phi_k\rangle$$

$$c_k(t) = \langle\phi_k|\psi(0)\rangle e^{-\frac{iE_k t}{\hbar}}$$

$$|\psi(0)\rangle = |\phi_k\rangle \;\Rightarrow\; |\psi(t)\rangle = e^{-\frac{iE_k t}{\hbar}}|\phi_k\rangle \;\Rightarrow\; |\langle\psi(0)|\psi(t)\rangle|^2 = 1$$

Eigenstates of H are stationary (overall phase is irrelevant)

Exercise

Given the Hamiltonian and three observables of a physical system

$$H = w\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad A = a\begin{pmatrix} -1 & 1 \\ 1 & 1 \end{pmatrix} \qquad B = b\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \qquad C = c\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

1. Determine which observables are constant of motion
2. A measurement of C at time $t = 0$ gives the result 0. Which is the result of a measurement of A at time $t > 0$?
3. Determine three different CSCO.

Exercise: spin precession

$$H = \frac{\Delta}{2}\sigma_z = \begin{pmatrix} \frac{\Delta}{2} & 0 \\ 0 & -\frac{\Delta}{2} \end{pmatrix} = \frac{\Delta}{2}|0\rangle\langle 0| - \frac{\Delta}{2}|1\rangle\langle 1| \qquad |\psi(0)\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$$

$$|\psi(t)\rangle = e^{-iHt/\hbar}|\psi(0)\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} e^{-i\Delta t/2\hbar} \\ e^{i\Delta t/2\hbar} \end{pmatrix} = \frac{1}{\sqrt{2}}\left(e^{-i\Delta t/2\hbar}|0\rangle + e^{i\Delta t/2\hbar}|1\rangle\right)$$

$$S_z = (|0\rangle\langle 0| - |1\rangle\langle 1|)/2 \qquad \Rightarrow \langle\psi(t)|S_z|\psi(t)\rangle = 0$$

$$S_x = (|0\rangle\langle 1| + |1\rangle\langle 0|)/2 \qquad \Rightarrow \langle\psi(t)|S_x|\psi(t)\rangle = \frac{1}{2}\cos\omega t$$

Check that $\langle\psi(t)|S_y|\psi(t)\rangle = \frac{1}{2}\sin\omega t$

The spin (prepared along x) precedes about the magnetic field (z axis) with $\omega = \Delta/\hbar$

Exercise: paramagnetic resonance (Rabi problem)

$$H = \frac{1}{2}\begin{pmatrix} -\Delta & g\, e^{i\omega t} \\ g\, e^{-i\omega t} & \Delta \end{pmatrix} = -\frac{\Delta}{2}\sigma_z + \frac{g}{2}\left(|0\rangle\langle 1|\, e^{i\omega t} + |1\rangle\langle 0|\, e^{-i\omega t}\right)$$

Pulse at frequency $\omega \neq \Delta/\hbar$

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

We look for a solution of the form

$$|\psi(t)\rangle = \begin{pmatrix} a(t) \\ b(t) \end{pmatrix} = \begin{pmatrix} \alpha(t)\, e^{i\omega t/2} \\ \beta(t)\, e^{-i\omega t/2} \end{pmatrix}$$

$$\frac{d}{dt}|\psi(t)\rangle = \begin{pmatrix} \dot{a}(t) \\ \dot{b}(t) \end{pmatrix} = \begin{pmatrix} [\dot{\alpha}\,(t) + \frac{i\omega}{2}]\, e^{\frac{i\omega t}{2}} \\ [\dot{\beta}(t) - \frac{i\omega}{2}]\, e^{-i\omega t/2} \end{pmatrix}$$

$$H|\psi(t)\rangle = \begin{pmatrix} [-\alpha(t)\Delta + \beta(t)g]/2\, e^{i\omega t/2} \\ [\alpha(t)g + \beta(t)\Delta]/2\, e^{-i\omega t/2} \end{pmatrix}$$

The Schrödinger equation $\quad i\hbar\frac{d}{dt}|\psi(t)\rangle = H|\psi(t)\rangle \quad$ becomes $\quad i\hbar\frac{d}{dt}|\tilde{\psi}\,(t)\rangle = \tilde{H}|\psi(t)\rangle$

$$\tilde{H} = \frac{1}{2}\begin{pmatrix} \hbar\omega - \Delta & g \\ g & -\hbar\omega + \Delta \end{pmatrix} \qquad |\tilde{\psi}\,(t)\rangle = \begin{pmatrix} \alpha(t) \\ \beta(t) \end{pmatrix}$$

Effective time-independent Hamiltonian

Exercise: paramagnetic resonance (Rabi problem)

$$\tilde{H} = \frac{1}{2}\begin{pmatrix} \hbar\omega - \Delta & g \\ g & -\hbar\omega + \Delta \end{pmatrix}$$

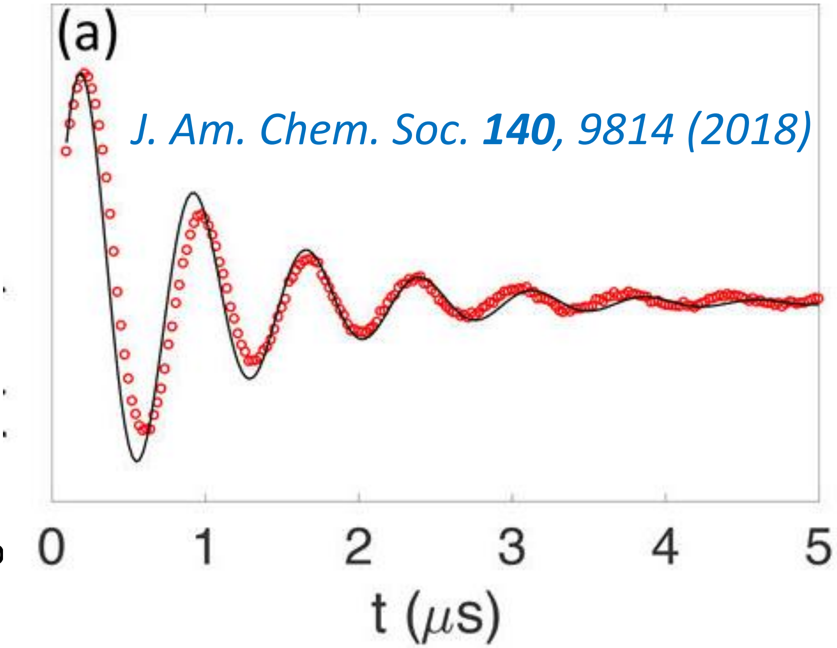
On resonance ($\hbar\omega = \Delta$) this implements a **rotation** about x

$$\tilde{H} = \frac{1}{2}\begin{pmatrix} 0 & g \\ g & 0 \end{pmatrix} \qquad U = e^{i\tilde{H}t} = \begin{pmatrix} \cos\Omega t & -i\sin\Omega t \\ -i\sin\Omega t & \cos\Omega t \end{pmatrix} \qquad \Omega = g/2\hbar$$

Out of resonance $\quad |\beta(t)|^2 = \frac{g^2/4\hbar^2}{\Omega^2}\sin^2\Omega\, t$

$$\Omega = \sqrt{\frac{g^2}{4\hbar^2} + \frac{(\omega - \Delta/\hbar)^2}{4}}$$

Rabi frequency



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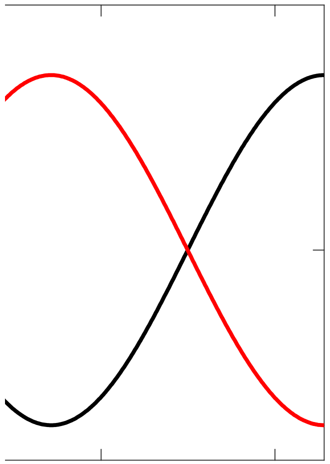

relativistica, 7.15

Additional problems

C. Alabiso, A. Chiesa, *Problemi di meccanica quantistica non relativistica*, Springer-Verlag (Milano, 2013)

Es.: 7.3, 9.4, 9.29, 9.30, 11.4, 11.38, 11.49

Uncertainty principle

$$\Delta A^2 = \langle\psi|(A - \langle A\rangle)^2|\psi\rangle = \langle\psi|A^2|\psi\rangle - \langle\psi|A|\psi\rangle^2 \qquad \Delta A = \sqrt{\Delta A^2} \qquad \text{uncertainty}$$

$$\Delta A\, \Delta B \geq \frac{1}{2}|\langle[A, B]\rangle|$$

Heisenberg principle*: if we prepare a large number of quantum systems in identical states and then we perform measurements of A on some systems and of B on some others, there is a lower bound on the product of the standard deviations of A and B. This limits our possible simultaneous knowledge of incompatible observables.*

Let's consider two incompatible observables A, B such that $[A, B] = iC \neq 0$ ($C^\dagger = \mathrm{C}$)

$$|\psi\rangle = |0\rangle \qquad [X, Y] = 2iZ \Longrightarrow \Delta X\, \Delta Y \geq |\langle Z\rangle| = 1 \Longrightarrow \qquad \Delta X, \Delta Y > 0$$

(We can easily check that $\Delta X^2 = \Delta Y^2 = 1$)