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Lecture XIV

1.1.1 Time reversal

Time reversal is a tricky business. First consider a classical example. Suppose a planet is in orbit about the sun. At some time say $t = 0$ it has a velocity $\mathbf{v}(0)$. If we reverse the velocity so that $\mathbf{v}(0) \to -\mathbf{v}(0)$ then the planet will retrace it's trajectory so that $x_R(t) = x(-t)$ and $\mathbf{v}_R(t) = -\mathbf{v}(-t)$ where $x_R(t)$ is the position of the reversed planet at t and $\mathbf{v}_R(t)$ is the velocity of the reversed planet at time t. So we reverse the state and propagate by t and we should end up with exactly the same position and velocity as if we had propagated the original state by $-t$ and then reversed the velocity.

Now quantum mechanics. We have a state $|\,\psi\rangle$ and $|\,\psi^R\rangle$ the reversed state and suppose we have some operator that effects the reversal so that

$$I_t|\,\psi\rangle = |\,\psi^R\rangle$$

If $|\,\psi\rangle = |\,\mathbf{p}'\rangle$ represents a state with definite momentum then $|\,\psi^R\rangle = |\,-\mathbf{p}'\rangle$ and we expect that

$$\mathbf{p}|\,\psi^R\rangle = -\mathbf{p}'|\,\psi^R\rangle$$

and

$$\left\langle\psi^R \mid \mathbf{p} \mid \psi^R\right\rangle = -\left\langle\psi \mid \mathbf{p} \mid \psi\right\rangle \to I_t^{-1}\mathbf{p}I_t = -\mathbf{p}$$

So far so good. The reversed state at time t, $|\,\psi(t)^R\rangle$, should be the same as the original state at $-t$ and then reversed. So we have the state at $t = 0$ and we reverse it and propagate it by an infinitesimal time δt. Meanwhile we propagate the original state by $-\delta t$ and then reverse it and we should end up in the same place. That is

$$(1 - \frac{i}{\hbar}H\delta t)I_t|\,\psi\rangle = I_t(1 + \frac{i}{\hbar}H\delta)|\,\psi\rangle \to iHI_t = -I_t iH \tag{1.1}$$

Unitary and anti unitary operators

The parity operator π, like all of the others that we have discussed, is unitary. We found that $\pi^2|\,\alpha\rangle = |\,\alpha\rangle$ so we see that $\pi\pi = 1$. Therefore $\pi = \pi^{-1}$ and $\pi = \pi^\dagger$. Finally $\left\langle\alpha \mid \pi^{-1}\pi \mid \beta\right\rangle = \langle\alpha \mid \beta\rangle$. The parity operator preserves the inner product.

We like unitary operators so that the inner product is invariant. In particular, if U is unitary then $U|\,\alpha\rangle = |\,\alpha\rangle'$ and $U|\,\beta\rangle = |\,\beta\rangle'$ and

$$\langle\alpha' \mid \beta'\rangle = \left\langle\alpha \mid U^\dagger U \mid \beta\right\rangle = \langle\alpha \mid \beta\rangle$$

which is nice but perhaps not essential. What is essential is that

$$|\langle\alpha' \mid \beta'\rangle| = |\langle\alpha \mid \beta\rangle|.$$

It turns out that this transformation is necessarily unitary or anti-unitary. Those are the only possibilities. As we will see in a moment a unitary operator does not work for time reversal. We consider an anti-unitary operator I_t such that $I_t|\,\alpha\rangle = |\,\alpha'\rangle$ and $I_t|\,\beta\rangle = |\,\beta'\rangle$ but now

$$\langle\alpha' \mid \beta'\rangle = \langle\alpha \mid \beta\rangle^*$$

so we preserve length but perhaps not phase. In practice if

$$| \psi\rangle = a_1| 1\rangle + a_2| 2\rangle$$

then

$$I_t| \psi\rangle = a_1^* I_t| 1\rangle + a_2^* I_t| 2\rangle$$

In general we can write an anti-unitary operator as the product of a unitary operator and the complex conjugation operator. That is

$$I_t = UK, \qquad I_t^{-1} = KU^\dagger$$

where U is unitary and K takes the complex conjugate of the coefficients. The anti-unitary transformation is not useful as a member of a continuous group because applying I_t twice results in a unitary transformation and we like the composition rule where we can apply two transformations to get a third. The only candidates for an anti-unitary transformation are where T^2 gets you back where you started, namely parity and time reversal, charge conjugation, interchange.

Transformation of H under time reversal

Now back to the problem at hand. Referring back to Equation 1.1, if I_t is unitary then we conclude that $HI_t = -I_t H$ and for some eigenket of H

$$I_t H| n\rangle = I_t E_n| n\rangle = E_n I_t| n\rangle = -I_t H| n\rangle = -E_n I_t| n\rangle$$

which says that we have an eigenket of H with negative energy. That makes no sense. If we have a free particle and turn it around, we don't get negative energy since energy scales as p^2. The other choice is that I_t is anti-unitary. Then Equation 1.1 gives us

$$HI_t = I_t H \rightarrow [H, I_t] = 0$$

Anti-unitary transformation of expectation value

Suppose that

$$| \tilde{\alpha}\rangle = I_t| \alpha\rangle, \qquad | \tilde{\beta}\rangle = I_t| \beta\rangle$$

and I_t is anti-unitary. Then

$$\left\langle \tilde{\beta} \mid \tilde{\alpha} \right\rangle = \langle \alpha \mid \beta \rangle$$

and if $| \gamma\rangle = A^\dagger| \beta\rangle$ then

$$\langle \beta \mid A \mid \alpha \rangle = \langle \gamma \mid \alpha \rangle = \langle \tilde{\alpha} \mid \tilde{\gamma} \rangle = \left\langle \tilde{\alpha} \mid I_t A^\dagger \mid \beta \right\rangle = \left\langle \tilde{\alpha} \mid I_t A^\dagger I_t^{-1} I_t \mid \beta \right\rangle = \left\langle \tilde{\alpha} \mid I_t A^\dagger I_t^{-1} \mid \tilde{\beta} \right\rangle$$

So the rule for the anit-unitary operator I_t is that for any linear operator A,

$$\langle \beta \mid A \mid \alpha \rangle = \left\langle \tilde{\alpha} \mid I_t A^\dagger I_t^{-1} \mid \tilde{\beta} \right\rangle$$

If A is Hermitian then

$$\langle \beta \mid A \mid \alpha \rangle = \left\langle \tilde{\alpha} \mid I_t A I_t^{-1} \mid \tilde{\beta} \right\rangle$$

An observable is even or odd if

$$I_t A I_t^{-1} = \pm A.$$

Therefore

$$\langle \alpha \mid A \mid \alpha \rangle = \pm \left\langle \tilde{\alpha} \mid I_t A I_t^{-1} \mid \tilde{\alpha} \right\rangle$$

Transformation of position and angular momentum

The expectation value of position does not change under time reversal so

$$I_t^{-1}\mathbf{x}I_t = \mathbf{x}$$

In order that time reversal operation to effect no geometrical transformation it must be that angular momentum is odd. Then

$$I_t^{-1}\mathcal{D}I_t = I_t^{-1}e^{-\frac{i}{\hbar}\mathbf{J}\cdot\phi}I_t = e^{\frac{i}{\hbar}I_t^{-1}\mathbf{J}\cdot\phi I_t} = \mathcal{D}$$

as long as $I_t^{-1}\mathbf{J}I_t = -\mathbf{J}$ and this is also in agreement with the notion that x is even and p is odd.

Uncertainty principle

In view of the above

$$\begin{aligned}
[x_i, p_j] &= i\hbar\delta_{ij} \\
I_t[x_i, p_j]I_t^{-1} &= I_t i\hbar\delta_{ij}I_t^{-1} \\
[x_i, -p_j] &= -i\hbar\delta_{ij}
\end{aligned}$$

so the uncertainty principle hangs together. Note that $I_t\mathbf{J}I_t^{-1} = -\mathbf{J}$ is required so that

$$I_t[J_i, J_j]I_t^{-1} = I_t i\hbar\epsilon_{ijk}J_kI_t^{-1}$$

Scattering amplitude

Suppose we have a state in a basis of kets $\mid n\rangle$ and its time reversed counterparts $\mid n^R\rangle$ and $I_t\mid n\rangle = \mid n^R\rangle$. Then

$$\begin{aligned}
\mid \psi\rangle &= \sum_n \mid n\rangle\langle n \mid \psi\rangle \\
I_t\mid \psi\rangle &= \mid \psi^R\rangle = \sum_n \mid n^R\rangle\langle n \mid \psi\rangle^* = \sum_n U\mid n\rangle\langle n \mid \psi\rangle^*
\end{aligned}$$

Also

$$\begin{aligned}
\mid \phi\rangle &= \sum_m \mid m\rangle\langle n \mid \phi\rangle \\
I_t\mid \phi\rangle &= = \mid \phi^R\rangle = \sum_n U\mid m\rangle\langle m \mid \phi\rangle^*
\end{aligned}$$

Then

$$\left\langle \phi^R \mid \psi^R\right\rangle = \sum_{m,n} \langle m \mid \phi\rangle \left\langle m \mid U^\dagger U \mid n\right\rangle \langle n \mid \psi\rangle^* = \langle \psi \mid \phi\rangle$$

So suppose we have $\mid \psi\rangle$ as the initial state and $\mid \phi\rangle$ as the final state and we are interested in the amplitude

$$\langle \phi \mid A \mid \psi\rangle$$

where A is any operator. We showed that the forward and reversed amplitudes are related according to

$$\left\langle \psi^R \mid I_t A I_t^{-1} \mid \phi^R \right\rangle = \langle \phi \mid A \mid \psi \rangle$$

If A is Hermitian and invariant under time reversal

$$\left\langle \psi^R \mid A \mid \phi^R \right\rangle = \langle \phi \mid A \mid \psi \rangle$$

Wave function

How does the wave function transform? First let's note that if $\psi(t)$ is a solution to Schrodinger's equation then $\psi(-t)$ in general is not because of that first derivative. On the other hand $\psi^*(-t)$ is a solution as we can see by taking the complex conjugate of

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

where H is real. More generally,

$$\langle \mathbf{x} \mid \alpha, t\rangle = \left\langle \mathbf{x} \mid e^{-iHt/\hbar} \mid \alpha \right\rangle, \quad \left\langle \mathbf{x} \mid \alpha, t^R \right\rangle = \left\langle \mathbf{x} \mid e^{-iHt/\hbar} \mid \alpha^R \right\rangle$$

Now $\mid \mathbf{x}\rangle$ is invariant under time reversal so

$$\left\langle \mathbf{x} \mid e^{-iHt/\hbar} \mid \alpha^R \right\rangle = \left\langle \mathbf{x}^R \mid e^{-iHt/\hbar} \mid \alpha^R \right\rangle = \left\langle \alpha \mid I_t e^{iHt/\hbar} I_t^{-1} \mid \mathbf{x} \right\rangle = \left\langle \alpha \mid e^{-iHt/\hbar} \mid \mathbf{x} \right\rangle$$

$$\to \psi_R(x,t) = \psi^*(x,-t)$$

The angular part of the wave function written in terms of spherical harmonics will transform according to

$$Y_{lm} \to Y_{lm}^* = (-1)^m Y_{l,-m}$$

which suggests that

$$I_t \mid l, m\rangle = (-1)^m \mid l, -m\rangle$$

and

$$I_t^2 \mid l, m\rangle = \mid l, m\rangle \to I_t^2 = 1$$

Spin 1/2

We have established that $I_t \mathbf{J} I_t^{-1} = -\mathbf{J}$ so it stands to reason that for spin 1/2 that

$$I_t \sigma I_t^{-1} = UK\sigma K U^\dagger = U\sigma^* U^\dagger = -\sigma$$

which means that

$$U\sigma_x U^\dagger = -\sigma_x, \quad U\sigma_y U^\dagger = \sigma_y, \quad U\sigma_z U^\dagger = -\sigma_z$$

where we have used

$$\begin{aligned} \sigma_i\sigma_j + \sigma_j\sigma_i &= 2\delta_{ij} \\ \sigma_i\sigma_j &= 2\delta_{ij} - \sigma_j\sigma_i \\ \to \sigma_i\sigma_j\sigma_i^{-1} &= 2\delta_{ij}\sigma_i^{-1} - \sigma_j \\ \to U &= e^{i\delta}\sigma_y \end{aligned}$$

Then

$$I_t|+\rangle = e^{i\delta}\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} = ie^{i\delta}\begin{pmatrix}0\\1\end{pmatrix} = ie^{i\delta}|-\rangle$$

$$I_t|-\rangle = e^{i\delta}\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}\begin{pmatrix}0\\1\end{pmatrix} = -ie^{i\delta}\begin{pmatrix}1\\0\end{pmatrix} = -ie^{i\delta}|+\rangle$$

Also $I_t^2|+\rangle = e^{i\delta}\sigma_y K\left(ie^{i\delta}|-\rangle\right) = e^{i\delta}(-ie^{-i\delta})(-i)|+\rangle = -1$ In general

$$I_t^2 = e^{i\delta}\sigma_y K e^{i\delta}\sigma_y K = -\sigma_y^2 = -1$$

For integer spin $I_t^2 = 1$ and for half integer spin $I_t^2 = -1$. For half integer spin, $I_t^2 = (-1)^N$ where N is the number of half integer spin particles.

We can generalize to arbitrary spin by noting that an eigenket in the direction $\hat{\mathbf{n}}$ can be written

$$\begin{aligned}
|\,\hat{\mathbf{n}},+\rangle &= e^{-iJ_z\alpha/\hbar}e^{-iJ_y\beta/\hbar}|+\rangle \\
I_t|\,\hat{\mathbf{n}},+\rangle &= e^{-iJ_z\alpha/\hbar}e^{-iJ_y\beta/\hbar}I_t|+\rangle = \eta|\,\hat{\mathbf{n}},-\rangle
\end{aligned}$$

Meanwhile we might have written

$$|\,\hat{\mathbf{n}},-\rangle = e^{-iJ_z\alpha/\hbar}e^{-iJ_y(\pi+\beta)/\hbar}|+\rangle$$

Together we get

$$I_t = \eta e^{-iJ_y\pi/\hbar}K$$

It reduces to $I_t = e^{i\delta}\frac{2S_y}{\hbar}K$ when $j = \frac{1}{2}$. Now

$$I_t^2 = \eta e^{-iJ_y\pi/\hbar}K\eta e^{-iJ_y\pi/\hbar}K = \eta e^{-iJ_y\pi/\hbar}\eta^* e^{iJ_y^*\pi/\hbar} = |\eta|^2 e^{-i2\pi J_y/\hbar}$$

where we have used $J_y^* = -J_y$. It is evident that for half integer j, $I_t^2 = -1$.

1.2 Symmetry Properties of Scattering Amplitudes

If the interaction is rotationally invariant, the amplitude can depend only on $|\mathbf{k}|^2, |\mathbf{k}'|^2$ and $\mathbf{k}\cdot\mathbf{k}'$. Then the scattering amplitude depends only on k and the scattering angle θ.

$$f(\mathbf{k}',\mathbf{k}) = f(k,\theta)$$

If the interaction is reflection invariant

$$f(\mathbf{k}',\mathbf{k}) = f(-\mathbf{k}',-\mathbf{k})$$

What about time reversal. For any two states $\mid a\rangle$ and $\mid b\rangle$, operator A, and time reversal operator I_t

$$\langle a \mid A \mid b\rangle = \left\langle b^R \mid I_t A^\dagger I_t^{-1} \mid a^R\right\rangle .$$

If the scattering potential V is invariant with respect to time reversal then

$$\begin{aligned}
\mid \mathbf{k}^+\rangle &= \mid \mathbf{k}\rangle + \frac{1}{E-H_0+i\epsilon}V\mid \mathbf{k}^+\rangle \\
I_t\mid \mathbf{k}^+\rangle &= \mid -\mathbf{k}\rangle + \frac{1}{E-H_0-i\epsilon}V I_t\mid \mathbf{k}^+\rangle
\end{aligned}$$

Define

$$\mid \mathbf{k}^-\rangle = \mid \mathbf{k}\rangle + \frac{1}{E-H_0-i\epsilon}V\mid \mathbf{k}^-\rangle$$

as the state with incoming spherical wave that scatters into the momentum eigenstate $\mathbf{k}$. Then

$$I_t\mid \mathbf{k}^+\rangle = \mid -\mathbf{k}^-\rangle$$

Under time reversal incoming and outgoing states are reversed.

Another way to write an expression for the scattered state is to recognize that

$$\begin{aligned}
(E-H_0)\mid \mathbf{k}\rangle &= 0 \\
\to (E-H)\mid \mathbf{k}\rangle &= -V\mid \mathbf{k}\rangle \\
\to \mid \mathbf{k}\rangle &= \mid \mathbf{k}^\pm\rangle - \frac{1}{E-H\pm i\epsilon}V\mid \mathbf{k}\rangle \\
\to \mid \mathbf{k}^\pm\rangle &= \left(1+\frac{1}{E-H\pm i\epsilon}V\right)\mid \mathbf{k}\rangle
\end{aligned}$$

Next define:

$$T = V + V\frac{1}{E-H\pm \imath\epsilon}V$$

Then

$$\begin{aligned}
\left\langle \mathbf{p} \mid V \mid \mathbf{k}^+\right\rangle &= \langle \mathbf{p} \mid T(E) \mid \mathbf{k}\rangle \quad \text{iff } E_k = E_p = E, \\
&= \left\langle \mathbf{p}^- \mid V \mid \mathbf{k}\right\rangle \quad \text{iff } E_p = E_k .
\end{aligned}$$

Now the effect of time reversal is

$$\langle \mathbf{p} \mid T \mid \mathbf{k} \rangle = \left\langle -\mathbf{k} \mid I_t T^\dagger I_t^{-1} \mid -\mathbf{p} \right\rangle$$

because $\mid \mathbf{k}^R \rangle = \mid -\mathbf{k} \rangle$. If V is invariant under time reversal,

$$I_t T^\dagger I_t^{-1} = T$$

and

$$\left\langle -\mathbf{k} \mid I_t T^\dagger I_t^{-1} \mid -\mathbf{p} \right\rangle = \langle -\mathbf{k} \mid T \mid -\mathbf{p} \rangle$$

and

$$f(\mathbf{p}, \mathbf{k}) = f(-\mathbf{k}, -\mathbf{p}).$$