PHYS 487: Lecture # 2

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Lecture Span

- Symmetries; invariance under transformations
- transformations in space
- generators
- translational invariance

What is a symmetry?

A symmetry exists if applying a transformation to an object will not change anything observable of the object. There exists discrete symmetries (flipping, rotating by $\pi/2$) and continuous symmetries (circle).

Describing transformations

Suppose

$$A|\psi\rangle = |\psi'\rangle \tag{1}$$

Where A is some operator that acts on the wave function. If A acts on a symmetry of the wave function, then its expectation value shouldn't change. That is

$$\langle O\rangle = \langle\psi|O|\psi\rangle = \langle\psi|A^\dagger O A|\psi\rangle \tag{2}$$

If this is true, then we say that $\langle O\rangle$ is unchanged under the transformation of A. This formalism is equivalent to a relative transformation, either transforming $|\psi\rangle$ or $\hat{O}$. Eitherway, they are equivalent. We call a transformation of the wavefunction an "active transformation" and the transformation of the observable as a "passive transformation".

Symmetries + Hamiltonian

A wavefunction is translationally invariant if its Hamiltonian is also translationally invariant.

$$\text{Invariance: } A^\dagger H A = H' = H$$

We first define "unitarity", that is $A^\dagger A = AA^\dagger = \mathbb{I}$. That is $A^\dagger = A^{-1}$.

$$\begin{aligned} A^\dagger H A &= H \\ AA^\dagger H A &= AH \text{ (assume } A \text{ is unitary)} \\ HA &= AH \\ [\hat{H}, \hat{A}] &= 0 \end{aligned}$$

This proof is saying what (by default A is unitary), that if $\hat{H}$ is invariant under A, then $[\hat{H}, \hat{A}] = 0$.
A unitary is reversible and energy conserving. They also preserve inner product:

$$\langle\psi|A^\dagger A|\psi\rangle = \langle\psi|\psi\rangle \tag{3}$$

Transformations in space

1. Translation
$$\hat{T}(a)\psi(x) = \psi'(x) = \psi(x-a) \tag{4}$$
2. Rotation
$$R_z(\varphi)\psi(r,\theta,\phi) = \psi(r,\theta,\phi-\varphi) \tag{5}$$
3. Parity: reflection about the origin
$$\hat{\Pi}\psi(r) = \psi(-r) \tag{6}$$

Translation operator

$$T(a)\psi(x) = \psi(x-a) \tag{7}$$

Maybe momentum? Recall, momentum: $\hat{p} = -i\hbar\partial_x$. Let's try to taylor expand $T\psi$ by expanding $\psi(x-a)$. Recall that a taylor expansion about a is

$$f(x) \approx \sum_n \frac{f'(a)}{n!}(x-a)^n \tag{8}$$

Then let $h = x-a$, then we obtain

$$f(a+h) \approx \sum_n \frac{f'(a)}{n!}(h)^n \tag{9}$$

Note that a can be x.

$$\begin{aligned}
&\sum_{n=0}^{\infty} \frac{1}{n!}\frac{d^n}{dx^n}\psi(x)((-a)^n) \\
&= \sum_n \frac{1}{n!}\left(-\frac{ia}{\hbar}\hat{p}\right)^n \psi \\
&= T(a) = \exp\left(-\frac{ia}{\hbar}\hat{p}\right)
\end{aligned}$$

We then call $\hat{p}$ a generator.

Properties

1. Unitarity: $T^{-1}(a) = T(-a) = T(a)^\dagger$

if $\hat{Q}$ is hermitian, then $u = \exp(iQ)$ is unitary.

2. Action on $\hat{x}$

$$\begin{aligned}
T^\dagger(a)\hat{x}T(a) &= \hat{x} + a = \hat{x}' && (10) \\
\hat{x}'\psi(x) &= T^\dagger(a)\hat{x}T(a)\psi(x) && (11) \\
&= T(-a)x\psi(x-a) && (12) \\
&= (x+a)\psi(x) \text{ (assuming that } \psi \text{ is invariant under } T) && (13)
\end{aligned}$$

In general, $T^\dagger Q(x,p)T = Q(x+a,p)$. Note, in more dimensions, stepping Δx_i in any dimension wouldn't change the observable of the object. If $[A,B] = 0$, then $\exp(A+B) = \exp(A)\exp(B)$. But if $[A,B] \neq 0$, then there is a geometric phase acquired when stepping Δx_i.

Translational Symmetry

1. Continuous: free particle
2. Periodic (and infinite)

Consider a infinitely periodic potential with a period. Then consider

$$H' = T^\dagger(a) H T(a) = T^\dagger(a)\left(\frac{p^2}{2m} + V(x)\right)T(a) \tag{14}$$

$$= \frac{p^2}{2m} + T^\dagger(a)V(x)T(a) = \frac{p^2}{2m}V(x+a) \tag{15}$$

Bloch's Theorem

Know: $[\hat{H}, \hat{T}] = 0$. And assume,

$$H\psi(x) = E\psi(x) \tag{16}$$

Then because H and T commute, they share a simulatenous set of eigenvalues. Therefore, assume

$$T(a)\psi(x) = \lambda\psi(x) \quad \lambda \in \mathbb{C} \tag{17}$$

But since T preserves the inner product,

$$\langle\psi|T^\dagger T|\psi\rangle = \langle\psi|\psi\rangle \tag{18}$$

$$\lambda^2 = \langle\psi|\psi\rangle \implies \lambda = \exp(i\phi) \quad \phi \in \mathbb{R} \tag{19}$$

Let $\phi = qa$, then

$$\psi(x-a) = e^{-iqa}\psi(x) \tag{20}$$

We can call $\hbar q$ the "crystal momentum". Then let $\psi(x) = e^{iqx}u(x)$

$$e^{-iqa}e^{iqx}u(x) = e^{iq(x-a)}u(x) \tag{21}$$

Then shift by a

$$\psi(x) = e^{iqx}u(x+a) \tag{22}$$

Thus, we obtain

$$e^{iqx}u(x) = e^{iqx}u(x+a) \tag{23}$$

This means that u is periodic in a.