

Lecture 23 (Nov. 29, 2017)

23.1 Consequences of Time Reversal Symmetry

23.1.1 Spinless Particles

Theorem 5. *Consider a system of spinless particles. Suppose that H is time-reversal invariant, and that there exists a non-degenerate energy eigenket $|n\rangle$. The corresponding energy eigenfunction can be chosen to be real.*

Proof. Because $|n\rangle$ is an energy eigenket, we have

$$H|n\rangle = E_n|n\rangle. \quad (23.1)$$

Because time reversal is a symmetry, we then have

$$H(\theta|n\rangle) = \theta H|n\rangle = E_n(\theta|n\rangle), \quad (23.2)$$

which implies

$$|n\rangle = \eta\theta|n\rangle \quad (23.3)$$

for some phase η , because $|n\rangle$ is non-degenerate. The corresponding wavefunction is then

$$\psi_n(x) = \langle x|n\rangle = \eta\langle x|\theta|n\rangle = \eta\psi_n^*(x). \quad (23.4)$$

We can then make the redefinition $\tilde{\psi}_n(x) = \eta^{-1/2}\psi_n(x)$ in order to get a real wavefunction. This completes the proof. \square

23.1.2 No Conservation Law

There is no conservation law associated with time reversal. Even though $[\theta, H] = 0$, there is no concept of a time reversal quantum number. Despite the fact that θ commutes with the Hamiltonian, we find that

$$\theta U(t, t_0) \neq U(t, t_0)\theta, \quad (23.5)$$

where $U(t, t_0)$ is the time-evolution operator. For example, suppose that we consider an energy eigenstate,

$$H|\psi\rangle = E|\psi\rangle. \quad (23.6)$$

Then,

$$|\psi(t)\rangle = e^{-iEt/\hbar}|\psi(0)\rangle, \quad (23.7)$$

while

$$\theta|\psi(t)\rangle = e^{iEt/\hbar}|\psi(0)\rangle \neq |\psi(t)\rangle. \quad (23.8)$$

Thus, $\theta|\psi\rangle = |\psi\rangle$ is not preserved under time evolution.

23.1.3 Kramer's Rule for Half-Integer Spin

Theorem 6 (Kramer's Rule). *Time-reversal symmetry implies a two-fold degeneracy all energy eigenstates.*

Proof. Suppose we have an energy eigenket $|n\rangle$,

$$H|n\rangle = E_n|n\rangle. \quad (23.9)$$

If time-reversal is a symmetry, then $\theta|n\rangle$ has the same energy E_n . Suppose that

$$\theta|n\rangle = e^{i\delta}|n\rangle. \quad (23.10)$$

Then,

$$\begin{aligned} \theta^2|n\rangle &= \theta\left(e^{i\delta}|n\rangle\right) \\ &= e^{-i\delta}\theta|n\rangle \\ &= e^{-i\delta}e^{i\delta}|n\rangle \\ &= |n\rangle. \end{aligned} \quad (23.11)$$

However, for half-integer spin, we have seen that $\theta^2 = -\mathbb{1}$, so this is a contradiction. Thus, $\theta|n\rangle$ must be a distinct state from $|n\rangle$. Thus, we get a two-fold degeneracy for all energy eigenstates. There may be additional degeneracy, but all states will come in pairs in this way. \square

23.2 Uses of Symmetry in Solving the Schrödinger Equation

23.2.1 Symmetric Double-Well Potential

Consider some symmetric double-well potential $V(x)$ and Hamiltonian

$$H = \frac{p^2}{2m} + V(x). \quad (23.12)$$

By definition, we have $V(x) = V(-x)$, because the potential is symmetric.

This Hamiltonian is invariant under both Π and θ . The eigenfunctions can thus be chosen to be real (from time-reversal invariance) and either even or odd under $x \rightarrow -x$ (from parity invariance). We can argue that the ground state $\psi_0(x)$ must be symmetric under $x \rightarrow -x$ (specifically, it has no nodes); furthermore, it is physically apparent that the ground state should be peaked near the bottom of each well. To see the first point, imagine that the ground state were antisymmetric; in this case, we must have $\psi(0) = 0$. The squared slope of the wavefunction gives the contribution to the kinetic energy. We can then cut the ground state apart at $x = 0$, negate one side, and then glue the halves back together to give a symmetric function (with a small amount of smoothing at the origin to make the new wavefunction continuously differentiable). The resulting wavefunction has the same potential energy as the supposed ground state wavefunction, but has a smaller slope at the origin, meaning it has lower energy than the ground state, which is a contradiction. Using this approach repeatedly, we can argue that the ground state has no nodes.

What can we say about the first excited state $\psi_1(x)$? Note that if we try to construct another wavefunction with zero nodes, it will not be orthogonal to the ground state. The next-lowest energy state will have the fewest nodes possible, from the argument above, and so we thus expect the first excited state to be antisymmetric with a single node.

Classically, a particle moving in such a potential will oscillate around the bottom of one of the two wells; it must choose a particular well to reside in. This is a classical example of what is called a *spontaneously broken symmetry*.

23.2.2 3D Particle in a Spherically Symmetric Potential

Consider a 3D Hamiltonian

$$H = -\frac{\hbar^2}{2m}\nabla^2 + V(r). \quad (23.13)$$

The spin decouples from the orbital angular momentum, and so we will ignore spin for now. We see that $[\mathbf{L}, H] = 0$, because $[\mathbf{J}, H] = 0$ and $[\mathbf{S}, H] = 0$. We can then choose the energy eigenstates to be eigenstates of \mathbf{L}^2 and L_z . We then label the energy eigenstates by $|n, \ell, m\rangle$, where ℓ and m specify the eigenvalues of \mathbf{L}^2 and L_z , respectively. The wavefunction can then be written in the form

$$\psi_{n,\ell,m}(\mathbf{x}) = \langle \mathbf{x} | n, \ell, m \rangle = R_{n,\ell}(r)Y_{\ell,m}(\theta, \phi). \quad (23.14)$$

That is, the radial and angular parts of the wavefunction factorize. We will see the details of this in a moment.

In polar coordinates, we can write

$$\begin{aligned} -\nabla^2 &= -\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{\mathbf{L}^2}{r^2} \\ &= -\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} \right) + \frac{\mathbf{L}^2}{r^2}. \end{aligned} \quad (23.15)$$

Thus, the Hamiltonian acts as

$$\begin{aligned} HR_{n,\ell}(r)Y_{\ell,m}(\theta, \phi) &= \left[-\frac{\hbar^2}{2m} \frac{d}{dr} \left(r^2 \frac{dR_{n,\ell}}{dr} \right) + \frac{\hbar^2 \ell(\ell+1)}{2mr^2} R_{n,\ell} + V(r)R_{n,\ell} \right] Y_{\ell,m} \\ &= E_n R_{n,\ell} Y_{\ell,m}. \end{aligned} \quad (23.16)$$

We can cancel $Y_{\ell,m}$ from both sides of this equation, and it becomes an ordinary differential equation for $R_{n,\ell}(r)$.

From the requirement that $\langle n, \ell, m | n, \ell, m \rangle = 1$, we have

$$\int_0^\infty dr r^2 R_{n,\ell}^*(r) R_{n,\ell}(r) \underbrace{\int d\Omega Y_{\ell,m}^*(\theta, \phi) Y_{\ell,m}(\theta, \phi)}_1 = 1, \quad (23.17)$$

giving

$$\int_0^\infty dr r^2 R_{n,\ell}^*(r) R_{n,\ell}(r) = 1. \quad (23.18)$$

We can understand this ODE more easily by making the change of variables

$$R_{n,\ell}(r) = \frac{u_{n,\ell}(r)}{r}. \quad (23.19)$$

The radial equation then becomes

$$-\frac{\hbar^2}{2m} \frac{d^2 u_{n,\ell}}{dr^2} + V_{\text{eff}}(r) u_{n,\ell} = E_n u_{n,\ell}, \quad (23.20)$$

where

$$V_{\text{eff}}(r) = V(r) + \frac{\hbar^2 \ell(\ell+1)}{2mr^2} \quad (23.21)$$

and

$$\int_0^\infty dr |u_{n,\ell}(r)|^2 = 1. \quad (23.22)$$

This effective potential has a local minimum (for sufficiently non-singular potentials $V(r)$), which serves to localize the energy eigenfunctions.

23.3 Approximation Methods

23.3.1 Time-Independent Perturbation Theory

Suppose that we have a Hamiltonian of the form

$$H = H_0 + V, \quad (23.23)$$

where H_0 is a Hamiltonian with known spectrum and V is small. We can try to find the energy eigenstates and corresponding energy eigenvalues of the full Hamiltonian by treating V as a perturbation, and writing these quantities as a systematic power series in V .

As a formal bookkeeping device, let's introduce a parameter λ , and write

$$H = H_0 + \lambda V. \quad (23.24)$$

We will then expand in powers of λ (ultimately, we are interested in $\lambda = 1$, so we will set it to be so at the end). Choose an orthonormal energy eigenbasis of H_0 ,

$$H_0|n_0\rangle = E_{n,0}|n_0\rangle, \quad \langle m_0|n_0\rangle = \delta_{m_0,n_0}. \quad (23.25)$$

We then assume we can expand the energy eigenstates of H in the form

$$|n\rangle = |n_0\rangle + \lambda|n_1\rangle + \lambda^2|n_2\rangle + \dots, \quad (23.26)$$

and the corresponding energy eigenvalues in the form

$$E_n = E_{n,0} + \lambda E_{n,1} + \lambda^2 E_{n,2} + \dots. \quad (23.27)$$

If we plug these expansions into the Schrödinger equation, $H|n\rangle = E_n|n\rangle$, we will get an infinite number of equations from matching the two sides order by order in λ . Explicitly, we have

$$(H_0 + \lambda V)(|n_0\rangle + \lambda|n_1\rangle + \dots) = (E_{n,0} + \lambda E_{n,1} + \dots)(|n_0\rangle + \lambda|n_1\rangle + \dots). \quad (23.28)$$

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