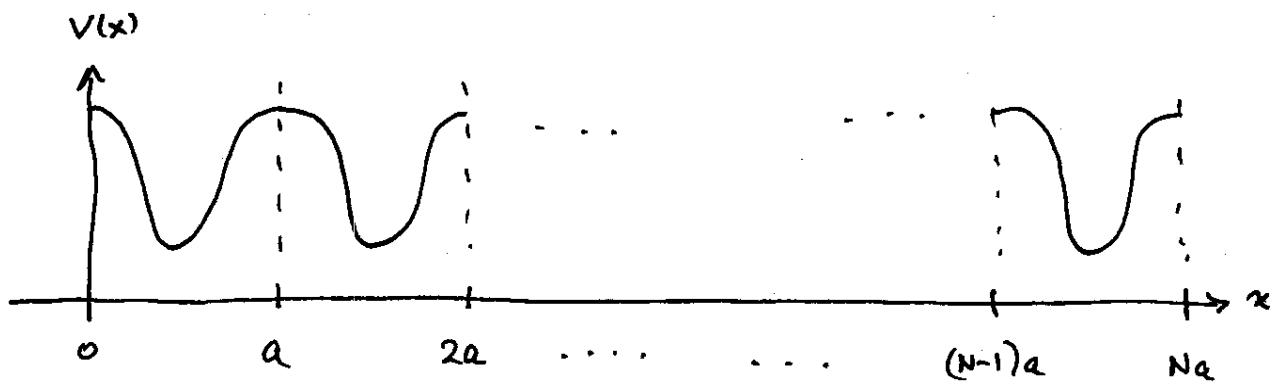


$$\left. \begin{array}{l} \Delta l = 0, \pm 1 \quad (\text{W.E. thm}) \\ \Delta l = \text{odd} \quad (\text{parity}) \end{array} \right\} \Rightarrow \boxed{\Delta l = \pm 1}$$

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The W.E. thm takes care of proper rotations, and parity means including improper ones, too. The case $\Delta l=0$, allowed by W-E thm., is excluded by parity.

Another example of a symmetry concerns lattice translations in systems with a periodic potential. Suppose $V(x)$ has period a , and suppose x itself is a periodic variable (an angle) with period Na . Think of the ethene molecule, with $Na = 2\pi$, $x = \theta$, and $N = 3$. General sketch:



The potential doesn't have to be a cosine wave, just periodic. So we have

$$V(x+a) = V(x).$$

Also, since Ψ is single-valued fn. of position,

$$\Psi(x+Na) = \Psi(x).$$

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Call $[0, a]$ the "small period", $[0, Na]$ the "big period".

Note that if $N \rightarrow \infty$, you get an infinite lattice, a common model for crystalline solids (in 1D here).

The Ham. is $H = \frac{p^2}{2m} + V(x)$. Introduce the translation operator $T(a)$,

$$T(a) = e^{-i\hat{p}a/\hbar} \quad \hat{p} = \text{momentum op.}$$

(this translates over a small period of the lattice). Note that

$$\begin{aligned} T(a) \hat{p} T(a)^+ &= \hat{p} \\ T(a) \hat{x} T(a)^+ &= \hat{x} + a \end{aligned} \quad (\text{hat} \equiv \text{operator}).$$

Thus,

$$T(a) H T(a)^+ = \frac{p^2}{2m} + V(x+a) = H \quad \text{if } V(x+a) = V(x).$$

So,

$$[T(a), H] = 0.$$

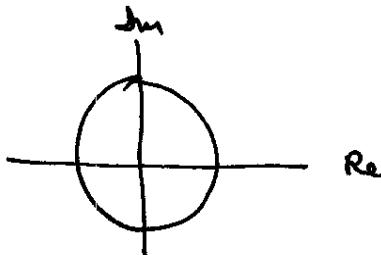
As with parity, we now seek to diagonalize $T(a)$ before worrying about H . It's usually easier to diagonalize symmetry operators than Hamiltonians. We will want eigenvalues, eigenfs, degeneracies, and symmetry adapted bases for $T(a)$.

Eigenvalue-fn. eqn:

$$(T(a)\psi)(x) = \psi(x-a) = \tau \psi(x)$$

where τ = eigenvalue. Since $T(a)$ is a unitary operator,

its eigenvalues τ are phase factors and lie on unit circle in
the complex plane:

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It's customary to write $\tau = e^{-ika}$, where a is the lattice spacing and k is a wave number that is equivalent to specifying τ . Can restrict k to interval $0 \leq k < 2\pi/a$, whereupon τ goes around unit circle. Many people prefer $-\pi/a < k \leq \pi/a$, which they call the first Brillouin zone. Anyways, the eigenvalue-fn. eqn is now

$$\psi(x-a) = e^{-ika} \psi(x)$$

or (by $x \rightarrow x+a$)

$$\psi(x+a) = e^{ika} \psi(x)$$

We need to find what values of $\tau = e^{-ika}$ are allowed (the eigenvalues). This comes from the bdry cond on ψ ,
 $\psi(x+Na) = \psi(x)$, or

$$\psi(x+Na) = e^{iNka} \psi(x) = \psi(x)$$

or $e^{iNka} = 1$, or

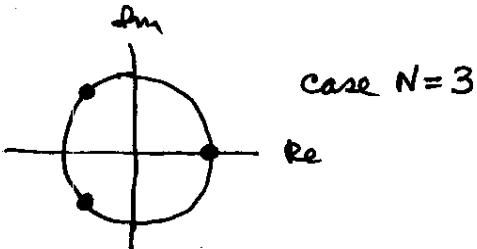
$$e^{ika} = e^{2\pi i n/N},$$

$$n=0, 1, \dots, N-1$$

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e^{ika} is one of the N -th roots of unity, for example



We can write k_n , $n=0, \dots, N-1$ if we want to emphasize that k takes on discrete values,

$$k_n = \frac{2\pi n}{Na}, \quad n=0, \dots, N-1.$$

In the limit $N \rightarrow \infty$, the eigenvalues on the unit circle become more and more dense, going to a continuum in the limit. For the ∞ lattice, any value of k (any phase factor) is allowed, and the spectrum of $T(a)$ becomes continuous.

As for the eigenfns, let's write $\psi_k(x)$ for them, to emphasize that they are eigenfns. of $T(a)$ with eigenvalue e^{-ika} , so that

$$\psi_k(x+a) = e^{ika} \psi_k(x).$$

This shows that if $\psi_k(x)$ is known on the (small) interval $[0, a]$, it becomes known everywhere. But no constraints are placed on what ψ does on $[0, a]$, so the eigenfns are ∞ -fold degenerate. A symmetry adapted basis must resolve this degeneracy (another index b besides k or k_n will be required).

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It's convenient to write

$$\psi_k(x) = e^{ikx} u_k(x),$$

which defines a fn. $u_k(x)$. The factor e^{ikx} smoothly interpolates the phase e^{ika} that ψ must acquire after a small period between $x=0$ and $x=a$, and $u_k(x)$ takes care of the rest.

Plugging ψ into $\psi_k(x+a) = e^{ika} \psi_k(x)$, we get

$$\psi_k(x+a) = e^{ik(\infty x+a)} u_k(x+a) = e^{ika} \psi_k(x) = e^{ika} e^{ikx} u_k(x),$$

or,

$$u_k(x) = u_k(x+a).$$

The fn. u_k is periodic on the small interval.

These facts are called Bloch's theorem. It's sometimes stated by saying that the Schrödinger eqn. for a periodic potential possesses solutions of the form $e^{ikx} u_k(x)$, where $u_k(x)$ is periodic. This misses the fact that solutions of this form are actually a complete set, that they are eigenfns of the $T(a)$ operator, and that k takes on only discrete values (for a finite lattice).

Specifying $\psi_k(x)$ on the small interval is equivalent to specifying $u_k(x)$ on the small interval, the latter of which is periodic. So we can choose a basis for periodic fns to

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resolve the degeneracy of the translation operator, of which the Fourier basis

$$\phi_m(x) = \frac{1}{\sqrt{a}} e^{2\pi i mx/a}$$

is an obvious choice. Then the symmetry adapted basis is

$$\langle x | k_n, m \rangle = e^{ik_n x} \cdot \frac{1}{\sqrt{a}} e^{2\pi i mx/a}.$$

It's easy to show that the ME's of H in the sym. adapt. basis have the form,

$$\langle k_n m | H | k_{n'} m' \rangle = \delta_{nn'} C_{mm'}^n.$$

H does not connect different symmetry classes (different n). The matrix for H is block diagonal; n labels the blocks (or k_n), and each block is a matrix in (m, m') . To diagonalize H you must diagonalize each block for different values of k_n .

This discussion has concentrated on the symmetry aspects only of periodic potentials. Another important topic is the band structure, which is covered in the notes.

The general idea in these examples is that if you have a symmetry δ that commutes with H , $[\delta, H] = 0$, you should

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diagonalize the symmetry operator first. If there is more than one symmetry S_1, \dots, S_n and they commute, then you should simultaneously diagonalize all of them. Commuting symmetry operators define an Abelian group ("Abelian" just means commutative).

If the symmetry operators don't commute, then you have a non-Abelian group. The only non-Abelian symmetry we will be interested in in 221A is the rotations ($SO(3)$), which we've covered in detail already. Let's just say that the analog of the symmetry adapted basis is the std. aug. norm. basis $|ajm\rangle$. According to the WE then, the matrix elements of a rotationally invariant (scalar H) wrt this basis are massively block-diagonal,

$$\langle ajm | H | a'j'm' \rangle = \delta_{jj'} \delta_{mm'} C_{aa'}^j$$

and there are repetitions (degeneracies) of the blocks since $C_{aa'}^j$ doesn't depend on m . That is, the energy eigenvalues come in $(2j+1)$ -fold degenerate multiplets.

Degeneracies like this are characteristic of non-Abelian symmetries. Abelian symmetries don't lead to degeneracies. If you have a system whose degeneracies go beyond the ones that can be explained by the obvious symmetries, then they probably indicate the existence

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of a larger symmetry group than the obvious one. This
happens in the H-atom (spinless-electrostatic model) with its
 n^2 -fold degeneracies (instead of just $(2l+1)$ -fold as in other
central force problems). This system has an $SO(4)$ symmetry,
not just $SO(3)$. 11/15/07

If you have not degenerate levels but close lying multiplets,
perhaps observed experimentally, then it's probably a sign of some
non-Abelian symmetry that is broken. That was the case of the
baryon octet (8 particles including the proton and neutron) that
turned out to be an $SU(3)$ multiplet. This was in the early '60's.
The theory led to the prediction of the Σ^- particle (last member of the
decuplet containing the Δ resonances), and (after 10 more years
or so) to the current theory of QCD.