DS 14:
Spin and Symmetries

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1 Spinors

Consider a particle prepared in the spin state

$$\chi = A\begin{pmatrix} 1-2i \\ 2 \end{pmatrix}$$

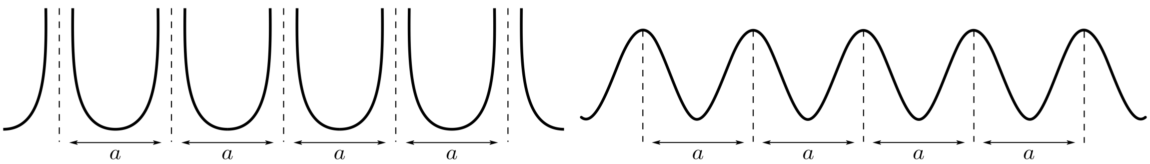
(a) If you measure S_z, what values could you get, and what is the probability of each? What is the expectation value of S_z?

(b) Answer the same question for S_x and S_y.

(c) Show that $\langle S_x\rangle^2 + \langle S_y\rangle^2 + \langle S_z\rangle^2 = (\hbar/2)^2$. What is $\langle S_x^2\rangle + \langle S_y^2\rangle + \langle S_z^2\rangle$?

2 Lattice Translations as a Discrete Symmetry

Consider a periodic potential in one dimension, where $V(x \pm a) = V(x)$, as shown in Figure (1a). This could be a model of electrons in a chain of regularly spaced positive ions.



(a) A periodic potential with infinite barriers. (b) A more realistic periodic potential.

Figure 1: Periodic potentials with discrete translation invariance.

A state in which the particle is completely localised in one of the lattice sites (say the nth site) is a good candidate for the ground state. Let us denote this state by $|n\rangle$, and say that this is an energy eigenstate with eigenvalue E_0, i.e. $H|n\rangle = E_0|n\rangle$.[1]

(a) Show that in general the Hamiltonian is *not* invariant under a translation represented by $T(l)$ for arbitrary l, where $T(l)$ has the property

[1] Of course, we could have chosen any one of these sites, and so there are an infinite number of ground states, all with energy E_0.

$$T^\dagger(l)\,x\,T(l) = x + l, \qquad T(l)\,|x\rangle = |x + l\rangle\,.$$

Show, however, that the Hamiltonian is invariant under translations when l coincides with the lattice spacing a:

$$T^\dagger(a)HT(a) = H \quad\Longrightarrow\quad [H, T(a)] = 0.$$

(b) Show that $|n\rangle$ is not an eigenstate of $T(a)$.

However, since H and $T(a)$ commute, we must be able to find a simultaneous eigenbasis for both of them. Consider the linear combination

$$|\theta\rangle \equiv \sum_{n=-\infty}^{\infty} e^{in\theta}\,|n\rangle$$

where θ is a real parameter $-\pi \le \theta \le \pi$.

(c) Show that $|\theta\rangle$ is a simultaneous eigenstate of H and $T(a)$, and find their eigenvalues.

Let us move to a slightly more physical potential, such as one depicted in Figure (1b) where the barrier between two adjacent sites is not infinitely high. Just as before, we can construct a localised ket $|n\rangle$, such that $T(a)\,|n\rangle = |n+1\rangle$, but we would now expect some *leakage* into neighbouring sites due to quantum mechanical tunnelling. In other words, the wavefunction is not *completely* localised to a site, but has a tail extending into neighbouring sites.

Since there is some coupling between the states $|n\rangle$ and $|n \pm 1\rangle$, we would expect some off-diagonal elements that connect immediate neighbours. We can thus say that

$$\langle n'|H|n\rangle \neq 0 \quad \text{only if } n' = n \quad \text{or} \quad n' = n \pm 1$$

This is called the **tight-binding approximation**: we ignore all interactions except for those between neighbouring sites. In particular, we choose

$$\begin{aligned}\langle n|H|n\rangle &= E_0\\ \langle n \pm 1|H|n\rangle &= -\Delta\\ \langle n'|H|n\rangle &= 0 \quad \text{otherwise.}\end{aligned}$$

(a) Show that $|n\rangle$ is no longer an eigenstate of the Hamiltonian.

(b) Show, however, that $|\theta\rangle$ is still an energy eigenstate which now depends on the (real) parameter θ.

(c) Show that when $\Delta = 0$ (the previous case), we have a degeneracy in energy eigenstates which is lifted as Δ becomes finite, forming a continuous energy *band* between $E_0 - 2\Delta$ and $E_0 + 2\Delta$.

(a) Show that

$$\langle x - a|\theta\rangle = \langle x|\theta\rangle\, e^{-i\theta}$$

(b) Show, by explicit substitution, that any wavefunction that satisfies this equation can be written as

$$\langle x|\theta\rangle = e^{ikx} u_k(x),$$

where we have written $\theta = ka$, and the only condition on $u_k(x)$ is that it is a *periodic* function of x with period a.

This is a very important condition known as **Bloch's theorem**: The wavefunction of $|\theta\rangle$, which is an eigenstate of $T(a)$, can be written as a plane wave e^{ikx} times a periodic function $u_k(x)$ with periodicity a.[2]

[2] It turns out that this theorem holds true even if the tight-binding approximation breaks down.