Supplment to Chapter 24: Energy Levels of a Free Particle in a Box

Section 24.1's derivation of the equation of state of a gas of free, spin-1/2 fermions assumed some elementary and standard facts about the energy levels of single quantum mechanical particle confined to a box. For completeness, we review those facts here, although they can be found in any standard quantum mechanics text.

We consider a single particle of mass *m* moving freely in one-dimension (*x*) and confined to a box which extends from x = 0 to $x = \mathcal{L}$. The quantum state of such a particle is described by a wave function $\Psi(x)$. The Schrödinger equation for the allowed values of the energy *E* is

$$\hat{H}\Psi = \frac{\hat{p}^2}{2m} = -\frac{\hbar^2}{2m}\frac{d^2\Psi}{dx^2} = E\Psi$$
(1)

where a hat denotes an operator. As a convenience we define p by

$$E \equiv \frac{p^2}{2m} \,. \tag{2}$$

The quantity p can be thought of as the magnitude of the momentum. Then (2) can be written in the form

$$\hat{p}^{2}\Psi(x) = -\hbar^{2}\frac{d^{2}\Psi(x)}{dx^{2}} = p^{2}\Psi(x)$$
(3)

The most general solution of (3) is

$$\Psi(x) = A\sin(px/\hbar) + B\cos(px/\hbar)$$
(4)

where *A* and *B* are constants. If the particle is confined to the box then the wave function must vanish outside it. Continuity of Ψ at the walls at x = 0 and $x = \mathcal{L}$ implies the boundary conditions:

$$\Psi(0) = \Psi(\mathcal{L}) = 0.$$
⁽⁵⁾

These require B = 0 in (4) and the discrete values of p

$$p_k \equiv \frac{k\pi\hbar}{\mathcal{L}}, \qquad k = 1, 2, \cdots.$$
 (6)

(The value k = 0 corresponds to $\Psi = 0$ everywhere.) This is (24.2). The corresponding discrete energy levels are given by (2) as

$$E_k = \frac{1}{2m} \left(\frac{k\pi\hbar}{\mathcal{L}}\right)^2 \equiv \frac{p_k^2}{2m}, \qquad k = 1, 2, \cdots$$
(7)

This is (24.1).

The energy levels of a *free* relativistic fermion can be understood in much the same way. *Interacting* relativistic particles can be created and destroyed — a process which is most efficiently described in terms of quantum field theory. But it is possible to think of a *free* relativistic particle like a non-relativistic one with the Hamiltonian

$$\hat{H} = [(mc^2)^2 + (\hat{p}c)^2]^{1/2} .$$
(8)

Here, $\hat{p} = -\hbar (d/dx)$ is the usual momentum operator. (Momentum is the infinitesimal generator of displacements in x and a displacement is a displacement no matter what the kinematics.) If you are worried about what the square root of an operator means, think of specifying \hat{H} by its matrix elements in a basis of definite momentum states. The content of (8) is that the diagonal elements are $[(mc^2)^2 + (pc)^2]^{1/2}$ Once specified in one basis the operator is defined in all.

The Schrodinger equation $\hat{H}\Psi = E\Psi$ for the energy eigenvalues E leads to

$$\hat{H}^2 \Psi = [(mc^2)^2 + (\hat{p}c)^2] \Psi = E^2 \Psi .$$
(9)

But if we define a quantity *p* by

$$E \equiv [(mc^2)^2 + (pc)^2]^{1/2} , \qquad (10)$$

then (9) becomes

$$\hat{p}^{2}\Psi(x) = -\hbar^{2}\frac{d^{2}\Psi(x)}{dx^{2}} = p^{2}\Psi(x) .$$
(11)

This is just the same as (3) and all of its consequences follow in particular (6). The allowed energy levels for a relativistic particle in a box are given by

$$E_k = [(mc^2)^2 + (p_k c)^2]^{1/2} \quad k = 1, 2 \cdots .$$
(12)