QUANTUM MECHANICS II
A Second Course in Quantum Theory
RUBIN H. LANDAU

APPENDIX A

NATURAL UNITS AND PLANE WAVES

A.1 Natural Units

It is common and useful to use natural units in derivations and problem solving. This serves to save time and make the equations more transparent by eliminating the physical constants which tend to clutter the equations. In contrast to the popular belief, once you have developed the knack of placing the constants back into the final answers, dimensional analysis is still possible. The basis of our natural units has Planck's constant $\hbar = 1$ and the speed of light $c = 1$.

To convert to natural units just take your formulas in conventional units and set $\hbar = 1$ and $c = 1$. The fine structure constant $\alpha = e^2/\hbar c \simeq 1/137.04$ becomes $\alpha = e^2 \simeq 1/137.04$. With these units, angular momenta are measured in $\hbar$'s, velocities in c's, and masses as rest energies $mc^2 = m$ (for example the electron has $mc^2 = m = 0.511\,\text{MeV}$). Thus the Compton wavelength $\hbar/mc = 1/m$ is in inverse mass (energy) units. In summary:

$$\hbar = c = 1, \tag{A.1}$$

$$\alpha = \frac{e^2}{\hbar c} = \frac{e^2}{4\pi\epsilon_0\hbar c} = e^2 \simeq \frac{1}{137.04}, \tag{A.2}$$

$$\frac{\hbar}{mc} = \frac{1}{m} = \frac{1}{0.511\,\text{MeV}}. \tag{A.3}$$

To convert from natural to conventional units, just insert the $\hbar$'s and c's. In practice, the author finds it simplest to:

- Change mass m to mc^2 so it has energy units.
- Change e^2 to $\alpha = e^2/\hbar c$ so it is dimensionless.
- Insert $\hbar c$, which has the dimensions of energy $\times$ length, in either numerator or denominator to get the dimensions in the desired form (or close to it as described next).

- If needed, insert c, which has the dimension of length $\div$ time, in either numerator or denominator to get the dimensions correct (for example to convert length to inverse time).
- To obtain actual numbers for your answers, substitute the explicit values for the constants:

$$\begin{aligned} \hbar c &= 197.329\,\text{MeV fm} &&= 1973.29\,\text{eV}A, \\ c &= 2.998\times 10^{8}\,\text{m/sec}, && \\ \hbar &= 6.582\times 10^{-22}\,\text{MeV sec} &&= 1.055\times 10^{-27}\,\text{erg sec}. \end{aligned} \tag{A.4}$$

For example, the Bohr radius of hydrogen (assuming an infinitely heavy proton) is $a_B = 1/me^2$ in natural units. In conventional units it is

$$a_B = \frac{1}{m_e e^2} = \frac{1}{m_e c^2}\frac{\hbar c}{e^2} = \frac{1}{0.511\,\text{MeV}} \times 137.04. \tag{A.5}$$

Yet because we know a_B is a length, we now multiply by $\hbar c$ which cancels the energy unit in the denominator and inserts a length into the numerator:

$$a_B = \frac{137.036}{0.511\,\text{MeV}} \times (\hbar c = 197.33\times 10^{-5}\,\text{MeV A}) = 0.529\,A = 5.29\times 10^{-9}\,\text{cm}. \tag{A.6}$$

A.2 Plane Waves in Little and Big Boxes

A plane wave is a mathematical abstraction, a solution to the wave equation which has constant phase along a 2D infinite plane. Although these may not be physically realizable, they are a convenient substitute for a wave packet of definite momentum and are the conventional basis for expanding the wave function of an interacting particle. The wave functions of quantum mechanics form a Hilbert space, that is, a linear vector space of infinite dimension.[1] Whereas the dynamical coordinates $\mathbf{r}$ and $\mathbf{p}$ of wave functions are continuous, the eigenvalues or parameters of these functions, such as the bound-state energies $E = -\kappa_i^2/2\mu$, are discrete. Any Hermitian Hamiltonian can be used to generate a complete, orthogonal set of wave functions. The free-particle Hamiltonian,

$$H_0 = \frac{\mathbf{p}^2}{2\mu} = -\frac{\nabla^2}{2\mu}, \tag{A.7}$$

is particularly convenient because it generates the plane waves:

$$\begin{aligned} \tilde{\mathbf{p}}\phi_{\mathbf{k}}(\mathbf{r}) &= \mathbf{k}\phi_{\mathbf{k}}(\mathbf{r}), & k &= |\mathbf{k}|, \\ H_0\phi_{\mathbf{k}}(\mathbf{r}) &= E_k\phi_{\mathbf{k}}(\mathbf{r}), & E_k &= k^2/2\mu, \\ \phi_{\mathbf{k}}(\mathbf{r}) &= Ne^{i\mathbf{k}\cdot\mathbf{r}}, & N &= \begin{cases} (2\pi)^{-3/2} & \text{infinite domain}, \\ V^{-1/2} & \text{finite domain}. \end{cases} \end{aligned} \tag{A.8}$$

For simplicity in developing the formalism (and a patina of mathematical rigor), it is useful to consider the plane waves as occupying a finite volume (a box). The box and the periodic boundary conditions we impose on the wave functions are just for convenience (scattered waves are certainly not periodic); eventually we go to the limit of an infinite domain.

[1] Jackson (1962); Gottfried (1966).

Little Boxes

To determine the allowed eigenenergies, we place the plane waves (A.8) in a box of volume V with sides (L_x, L_y, L_z), and demand that they satisfy periodic boundary conditions

$$\begin{aligned} \phi_{\mathbf{k}}(x+L_x, y+L_y, z+L_z) &= \phi_{\mathbf{k}}(x,y,z), \qquad \text{(A.9)} \\ \Rightarrow \quad (k_x L_x, k_y L_y, k_z L_z) &= 2\pi(i_x, i_y, i_z). \qquad \text{(A.10)} \end{aligned}$$

Here $(i_x, i_y, i_z) \equiv i$ is a set of three positive or negative integers which determine the allowed, discrete wave vectors and thus energies:

$$\mathbf{k}_i = 2\pi\left(\frac{i_x}{L_x}, \frac{i_y}{L_y}, \frac{i_z}{L_z}\right), \quad E_i = \frac{k_i^2}{2\mu}. \qquad \text{(A.11)}$$

With these boundary conditions, the plane waves for different values of i and j are *orthogonal.* By choosing the normalization constant N we make the plane waves *orthonormal*:

$$\begin{aligned} \phi_{\mathbf{k}_i}(\mathbf{r}) &\equiv \phi_i(\mathbf{r}) = \frac{e^{i\mathbf{k}_i \cdot \mathbf{r}}}{\sqrt{V}}, \qquad \text{(A.12)} \\ \Rightarrow \quad \int d^3r\, \phi_i^*(\mathbf{r})\phi_j(\mathbf{r}) &= \delta_{ij}, \quad \text{(orthonormality).} \qquad \text{(A.13)} \end{aligned}$$

Note that in the confined volume of the box, the variable $\mathbf{k}$ is discrete but the variable $\mathbf{r}$ is continuous (but limited). The discreteness of $\mathbf{k}_i$ leads to the *Kronecker delta function* in (A.13). Since the free Hamiltonian is Hermitian, plane waves form a *complete set* in which any solution of the Schrödinger equation $\psi(\mathbf{r})$ can be expanded:

$$\psi(\mathbf{r}) = \sum_i^{\infty} c_i \phi_i(\mathbf{r}). \qquad \text{(A.14)}$$

Orthonormality determines the c_i's [multiply (A.14) by ϕ_i^* and integrate over $\mathbf{r}$]:

$$c_i = \int d^3r' \phi_i^*(\mathbf{r}')\psi(\mathbf{r}'). \qquad \text{(A.15)}$$

If we substitute this back into (A.14) and interchange the order of integration and summation, we obtain

$$\psi(\mathbf{r}) = \int d^3r' \left[\sum_i^{\infty} \phi_i^*(\mathbf{r}')\phi_i(\mathbf{r})\right] \psi(\mathbf{r}'). \qquad \text{(A.16)}$$

Yet because (A.16) must be an identity, we identify the term in brackets as some kind of unit operator. This yields the *closure or completeness relation* for discrete states:

$$\sum_i^{\infty} \phi_i^*(\mathbf{r}')\phi_i(\mathbf{r}) = \delta(\mathbf{r}' - \mathbf{r}), \quad \text{(closure).} \qquad \text{(A.17)}$$

The Big Box

To obtain plane waves in an infinite domain, we let the box size approach infinity. In this limit of very large L and very large i, the index i is still an integer so $\Delta i \equiv 1$. The momenta

$\mathbf{k}_i$ in (A.11) remain finite but become continuous:

$$\frac{2\pi}{L_i}\Delta i \rightarrow dk_i, \quad \Delta i_x \rightarrow \frac{L_x}{2\pi}dk_x, \tag{A.18}$$

$$\sum \Delta i \rightarrow V\int \frac{d^3k}{(2\pi)^3}. \tag{A.19}$$

The relation (A.19) is the basis for the important result that the number of states in a volume V with momenta in the interval $\mathbf{k} \rightarrow \mathbf{k} + \Delta\mathbf{k}$ is:

$$dN = n_0 V \frac{d^3\mathbf{k}}{(2\pi)^3}. \tag{A.20}$$

Here n_0 is the number of states with the same momentum (for example, two for electrons with spins up and down in atoms, and four for nucleons with spins and isospins up and down in nuclei).

Equation (A.20) is often used to determine the Fermi momentum, $p_F = \hbar k_F = k_F$, for a gas of fermions confined to a box of volume V. If N electrons are placed in the box, they will progressively fill up all the levels until there are no particles left. The momentum at which all levels just get filled is $\mathbf{k}_F$. Since N equals the momentum-space density times the momentum-space volume, we have

$$N = n_0\frac{V}{(2\pi)^3}\int_0^{k_F} d^3k = \frac{n_0 V}{6\pi^2}k_F^3(r), \tag{A.21}$$

$$k_F^3 = \frac{6\pi^2 N/V}{n_0} = \frac{6\pi^2\rho}{n_0}, \tag{A.22}$$

$$k_F = \left(\frac{6\pi^2\rho(r)}{n_0}\right)^{1/3}. \tag{A.23}$$

Here $\rho = N/V$ is the number of particles per unit volume and, although the derivation assumes it to be a constant, it is sometimes taken to be a function of position r.

To generalize the closure relation (A.17) to a big box, we insert a $\Delta i \equiv 1$ into the sum in (A.17), and take the $L \rightarrow \infty$ limit:

$$\sum_i^{\infty} \Delta i\, \phi_i^*(\mathbf{r}')\phi_i(\mathbf{r}) = \delta(\mathbf{r}' - \mathbf{r}), \tag{A.24}$$

$$\Rightarrow V\int \frac{d^3k}{(2\pi)^3}\frac{e^{-i\mathbf{k}\cdot\mathbf{r}'}}{\sqrt{v}}\frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{\sqrt{v}} = \delta(\mathbf{r}' - \mathbf{r}), \quad \text{(closure)}. \tag{A.25}$$

This give : "s the form for plane waves in an infinite domain:

$$\phi_i(\mathbf{r}) = \frac{e^{i\mathbf{k}_i\cdot\mathbf{r}}}{\sqrt{V}} \Rightarrow \phi_{\mathbf{k}}(\mathbf{r}) = \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{(2\pi)^{3/2}}. \tag{A.26}$$

The orthogonality relation (A.13) for an infinite domain is now just the closure relation with a change of variable,

$$\delta_{ij} \rightarrow \int \frac{d^3r}{(2\pi)^3}e^{-i\mathbf{k}'\cdot\mathbf{r}}e^{i\mathbf{k}\cdot\mathbf{r}} = \delta(\mathbf{k}' - \mathbf{k}) \quad \text{(orthogonality)}. \tag{A.27}$$