Nondimensionalization

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The main idea of nondimensionalization is to separate the physics (units) from the mathematics (algebra and calculus). The units can be worked out quickly, and they give an idea of what order of magnitude the length scales and time scales will come out to be. This is useful especially if the mathematical equations are so complicated they need to be solved numerically. See the following article:

https://en.wikipedia.org/wiki/Natural_units#Systems_of_natural_units

1 Example: Hydrogen atom

Consider the Schrödinger equation for a hydrogen atom, together with the normalization condition for the wavefunction:

$$-\frac{\hbar^2}{2m} \nabla^2 \psi - \frac{e^2}{4\pi\varepsilon_0 r} \psi = E \psi$$
$$\int d^3 r \ |\psi|^2 = 1.$$

Atomic units

Write each independent and dependent *physical variable* as the product of a *dimensionless variable* (denoted by a tilde) and a *unit* (denoted by a subscript 0):

$$\psi = \tilde{\psi} \psi_0$$
 $\mathbf{r} = \tilde{\mathbf{r}} r_0$ $\nabla = r_0^{-1} \tilde{\nabla}$ $E = \tilde{E} E_0.$

The wavefunction normalization condition becomes $r_0^3 \psi_0^2 \int d^3 \tilde{r} |\tilde{\psi}|^2 = 1$. It will be convenient to choose $r_0^3 \psi_0^2 = 1$, so that $\int d^3 \tilde{r} |\tilde{\psi}|^2 = 1$. Thus we have $\psi_0 = r_0^{-3/2}$. The Schrödinger equation becomes

$$-\frac{\hbar^2 \psi_0}{2 m r_0^2} \tilde{\nabla}^2 \tilde{\psi} - \frac{e^2 \psi_0}{4 \pi \varepsilon_0 r_0} \frac{1}{\tilde{r}} \tilde{\psi} = E_0 \psi_0 \tilde{E} \tilde{\psi}$$

$$\therefore \qquad -\frac{\hbar^2}{2\,m\,r_0^{\,2}\,E_0}\,\tilde{\nabla}^{\,2}\tilde{\psi} - \frac{e^2}{4\,\pi\varepsilon_0\,r_0\,E_0}\,\frac{1}{\tilde{r}}\,\tilde{\psi} = \tilde{E}\,\tilde{\psi}.$$

Choose the length unit r_0 and the energy unit E_0 such that $\frac{\hbar^2}{m r_0^2 E_0} = \frac{e^2}{4 \pi \epsilon_0 r_0 E_0} = 1$. Solving for r_0 and E_0 , we find

$$r_0 = \frac{4\pi\varepsilon_0}{me^2} \frac{\hbar^2}{e^2} = a_0 \approx 5.29 \times 10^{-11} \,\mathrm{m}$$
 (the unit of length is the Bohr radius)
 $E_0 = \frac{me^4}{(4\pi\varepsilon_0)^2 \,\hbar^2} = 1 \,\mathrm{Hartree} = 1 \,\mathrm{Ha} \approx 27.2 \,\mathrm{eV}$ (the unit of energy is the Hartree).

With these units the Schrödinger equation for a hydrogen atom can be written in dimensionless form as

$$-\frac{1}{2}\tilde{\nabla}^2\tilde{\psi} - \frac{1}{\tilde{r}}\tilde{\psi} = \tilde{E}\tilde{\psi}.$$

Note that we left the factor of 2 in the Schrödinger equation but we incorporated the factor of 4π into the units.

If we had incorporated the factor of 2 into the units as well, we would have obtained

$$-\tilde{\mathbb{V}}^2 \tilde{\psi} - \frac{1}{\tilde{r}} \tilde{\psi} = \tilde{E} \tilde{\psi}$$
 and $E_0 = \frac{m e^4}{2 (4 \pi \epsilon_0)^2 \hbar^2} = 1 \text{ Rydberg} = 1 \text{ Ry} \approx 13.6 \text{ eV}.$

Example: ground state wavefunction

Solving the dimensionless Schrödinger equation using separation of variables, one obtains the associated Laguerre equation for the radial function and the associated Legendre equation for the angular function. One can show that the ground state wavefunction (of the 1s orbital) is

$$\tilde{\psi}_{100}(\tilde{r},\,\theta,\,\phi) = \pi^{-1/2}\,e^{-\tilde{r}/2}.$$

We can now convert this result back to conventional units using $\psi = \tilde{\psi} \psi_0$ and $r = \tilde{r} r_0$. This gives

$$\psi_{100}(\tilde{r}, \theta, \phi) = a_0^{-3/2} \pi^{-1/2} e^{-r/2a_0}.$$

2 Example: Maxwell's equations

Consider Maxwell's equations:

$$\nabla \cdot \mathbf{E} = \frac{\rho}{\varepsilon_0}$$

$$\nabla \cdot \mathbf{B} = 0$$

$$\nabla \times \mathbf{E} = -\partial_t \mathbf{B}$$

$$\nabla \times \mathbf{B} = \varepsilon_0 \,\mu_0 \,\partial_t \mathbf{E} + \mu_0 \,\mathbf{J}.$$

Natural units for electromagnetism

Write each independent and dependent *physical variable* as the product of a *dimensionless variable* and a *unit*:

$$\mathbf{E} = \tilde{\mathbf{E}} E_0 \qquad \rho = \tilde{\rho} \rho_0 \qquad t = \tilde{t} t_0 \qquad \partial_t = t_0^{-1} \partial_{\tilde{t}}$$

$$\mathbf{B} = \tilde{\mathbf{B}} B_0 \qquad \mathbf{J} = \tilde{\mathbf{J}} J_0 \qquad \mathbf{r} = \tilde{\mathbf{r}} r_0 \qquad \mathbb{\nabla} = r_0^{-1} \tilde{\mathbb{\nabla}}.$$

Then we obtain

$$\frac{1}{r_0} \tilde{\nabla} \cdot \tilde{\mathbf{E}} E_0 = \frac{\rho_0 \tilde{\rho}}{\varepsilon_0} \qquad \qquad \qquad \tilde{\nabla} \cdot \tilde{\mathbf{E}} = \frac{\rho_0 r_0}{\varepsilon_0 E_0} \tilde{\rho}$$

$$\frac{1}{r_0} \tilde{\nabla} \cdot \tilde{\mathbf{B}} B_0 = 0$$

$$\frac{1}{r_0} \tilde{\nabla} \times \tilde{\mathbf{E}} E_0 = -\frac{1}{t_0} \partial_{\tilde{t}} \tilde{\mathbf{B}} B_0 \qquad \qquad \vdots \qquad \tilde{\nabla} \times \tilde{\mathbf{E}} = -\frac{r_0 B_0}{t_0 E_0} \partial_{\tilde{t}} \tilde{\mathbf{B}}$$

$$\frac{B_0}{r_0} \tilde{\nabla} \times \tilde{\mathbf{B}} = \frac{E_0}{t_0} \, \varepsilon_0 \, \mu_0 \, \partial_{\tilde{t}} \tilde{\mathbf{E}} + J_0 \, \mu_0 \, \tilde{\mathbf{J}} \qquad \therefore \qquad \tilde{\nabla} \times \tilde{\mathbf{B}} = \frac{r_0 \, E_0 \, \varepsilon_0 \, \mu_0}{t_0 \, B_0} \, \partial_{\tilde{t}} \tilde{\mathbf{E}} + \frac{r_0 \, J_0 \, \mu_0}{B_0} \, \tilde{\mathbf{J}}.$$

We have six units $(E_0, B_0, \rho_0, J_0, r_0, t_0)$. Choose them to satisfy the four equations

$$\frac{\rho_0 r_0}{\varepsilon_0 E_0} = \frac{r_0 B_0}{t_0 E_0} = \frac{r_0 E_0 \varepsilon_0 \mu_0}{t_0 B_0} = \frac{r_0 J_0 \mu_0}{B_0} = 1.$$
 For now we will let r_0 and ρ_0 be arbitrary, and write $\rho_0 = q_0 / r_0^3$.

Then we find that

$$t_0 = \frac{r_0}{c_0}$$
 where $c_0 = \frac{1}{\sqrt{\varepsilon_0 \, \mu_0}}$

$$E_0 = \frac{q_0}{\varepsilon_0 r_0^2}$$

$$B_0 = \frac{E_0}{c_0}$$

$$\rho_0 = \frac{q_0}{r_0^3}$$
 by definition
$$J_0 = \frac{q_0}{r_0^2 t_0}.$$

With this system of units, Maxwell's equations can be written in dimensionless form in terms of the dimensionless fields and sources:

$$\begin{split} &\tilde{\mathbb{\nabla}} \cdot \tilde{\mathbf{E}} = \tilde{\rho} \\ &\tilde{\mathbb{\nabla}} \cdot \tilde{\mathbf{B}} = 0 \\ &\tilde{\mathbb{\nabla}} \times \tilde{\mathbf{E}} = -\partial_{\tilde{t}} \tilde{\mathbf{B}} \\ &\tilde{\mathbb{\nabla}} \times \tilde{\mathbf{B}} = \partial_{\tilde{t}} \tilde{\mathbf{E}} + \tilde{\mathbf{J}}. \end{split}$$

Example: waveguide

In H56 you found expressions for waveguide dispersion relations such as

"
$$\omega = \sqrt{\left(\frac{m\pi}{a}\right)^2 + \left(\frac{n\pi}{b}\right)^2 + k^2}.$$
"

This really means

$$\tilde{\omega} = \sqrt{\left(\frac{m\pi}{\tilde{a}}\right)^2 + \left(\frac{n\pi}{\tilde{b}}\right)^2 + \tilde{k}^2} \ .$$

Convert this back to conventional units using $\omega = \tilde{\omega} \omega_0$, $k = \tilde{k} k_0$, etc., where $\omega_0 = t_0^{-1}$, $k_0 = r_0^{-1}$. So

$$\omega = \frac{r_0}{t_0} \sqrt{\left(\frac{m\pi}{a}\right)^2 + \left(\frac{n\pi}{b}\right)^2 + k^2}$$

$$\therefore \qquad \omega = c_0 \sqrt{\left(\frac{m\pi}{a}\right)^2 + \left(\frac{n\pi}{b}\right)^2 + k^2} .$$

This tells us that we should restore a factor of c_0 in the expression.

Example: Hertzian dipole

In H57 we showed that for a Hertzian dipole of length a and current I the average Poynting vector is

$$\mathbf{S} = \frac{kIa^2\,\mathbf{\hat{r}}\sin^2\theta}{32\,\pi^2\,r^2}.$$

Since we were working in dimensionless units, we should really have written

$$\tilde{\mathbf{S}} = \frac{\tilde{k}^2 \tilde{I}^2 \tilde{a}^2 \hat{\mathbf{r}} \sin^2 \theta}{32 \pi^2 \tilde{r}^2}.$$

Convert this back to conventional units, using $S = \tilde{S} S_0$, $I = \tilde{I} I_0$, and so on. Using some common sense,

we have
$$S_0 = E_0 H_0 = \frac{E_0 B_0}{\mu_0} = \frac{E_0^2}{c_0 \mu_0} = \frac{1}{c_0 \mu_0} \left(\frac{q_0}{\varepsilon_0 r_0^2}\right)^2 = \frac{c_0 q_0^2}{\varepsilon_0 r_0^4}$$
 and $I_0 = \frac{q_0}{t_0}$. So

$$\frac{\mathbf{S}}{S_0} = \frac{1}{I_0^2} \, \frac{k I a^2 \, \hat{\mathbf{r}} \sin^2 \theta}{32 \, \pi^2 \, r^2}$$

$$\therefore \mathbf{S} = \frac{c_0 q_0^2}{\varepsilon_0 r_0^4} r_0^2 \left(\frac{t_0}{q_0}\right)^2 \frac{kIa^2 \,\hat{\mathbf{r}} \sin^2 \theta}{32 \,\pi^2 \,r^2} = \frac{1}{\varepsilon_0 c_0} \frac{kIa^2 \,\hat{\mathbf{r}} \sin^2 \theta}{32 \,\pi^2 \,r^2} = Z_0 \, \frac{kIa^2 \,\hat{\mathbf{r}} \sin^2 \theta}{32 \,\pi^2 \,r^2}.$$

So to convert from our "dimensionless" units to conventional units we multiply by $Z_0 = 377 \,\Omega$. Indeed it is easily seen that the units of the Poynting vector come out to be $[S] = \Omega \, A^2 \, m^{-2} = W \, m^{-2}$.