Dimensionless units for the h.o. basis

We wish to study the transition from regular units to dimensionless units for a two-particle harmonic oscillator system with Coulomb interaction. We also include a magnetic field in the discussion. Consider the Hamiltonian

$$H = \sum_{i=1}^{2} \left[\frac{1}{2m} \left(-i\hbar\nabla - e\vec{A} \right)^2 + \frac{1}{2} m\omega_0^2 r_i^2 + V(\vec{r}_i) \right] + C,$$

where V is a perturbation of the harmonic potential, and where C is the Coulomb interaction, viz.,

$$C = \frac{e^2}{4\pi\epsilon_0\epsilon} \frac{1}{r_{12}},$$

in which

$$\frac{e^2}{4\pi\epsilon_0} \approx 1.440 \text{ eVnm}.$$

The parameters to the model are thus

- Magnetic field strength γ. We intend to supply this in units of Tesla, i.e., $\gamma = \hat{\gamma}\ \mathrm{T} = \hat{\gamma}\ \mathrm{kg} \cdot \mathrm{s}^{-1} \cdot \mathrm{C}^{-1}$. The magnetic field is given as

  $$\vec{B} = \nabla \times \vec{A} = \gamma \vec{e}_z.$$

  We use the Coulomb gauge, in which the (otherwise nonunique) potential $\vec{A}$ is given by

  $$\vec{A} = \frac{\gamma}{2}(-y, x, 0).$$

- (Effective) mass m, in units of electron masses:

  $$m = \tilde{m} m_e, \quad m_e c^2 \approx 511000\,\mathrm{eV}.$$

- Harmonic potential confinement length a. This is the "trap size", i.e., the characteristic length of the harmonic oscillator potential, viz,

  $$a = \sqrt{\frac{\hbar}{m\omega_0}} \Leftrightarrow \omega_0 = \frac{\hbar}{ma^2}.$$

- Dielectric constant ϵ; a dimensionless parameter.

We know that introducing the length scale a and the energy unit $\hbar\omega_0$ in the harmonic oscillator with $\gamma = 0$ will render it dimensionless and on a particularly simple form. However, the magnetic field will alter the confinement length and hence the energy scale. In the following, we ignore the perturbation V. Its inclusion is easy once we have established the units.

Writing out the kinetic term in the Hamiltonian, we obtain

$$H = \sum_{i=1}^{2} \left[-\frac{\hbar^2}{2m}\nabla_i^2 + \frac{e^2\gamma^2}{8m} r_i^2 - 2\frac{\hbar e\gamma}{4m} \left(-\mathrm{i}\frac{\partial}{\partial\phi_i} \right) + \frac{1}{2} m\omega_0^2 r_i^2 \right] + C.$$

We observe that if we define

$$\Omega \equiv \sqrt{\omega_0^2 + \frac{e^2\gamma^2}{4m^2}},$$

we get

$$H = \sum_{i=1}^{2} \left[-\frac{\hbar^2}{2m}\nabla_i^2 + \frac{1}{2} m\Omega^2 r_i^2 - \frac{\hbar e\gamma}{2m} \left(-\mathrm{i}\frac{\partial}{\partial\phi_i} \right) \right] + C.$$

We now introduce the length and energy units:

$$H = \hbar\Omega\tilde{H}, \quad \vec{r}_i = \sqrt{\frac{\hbar}{m\Omega}}\vec{x}_i.$$

The dimensionless Hamiltonian becomes

$$\tilde{H} = \sum_{i=1}^{2}\left[-\frac{1}{2}\tilde{\nabla}_i^2 + \frac{1}{2}x_i^2 - \frac{e\gamma}{2m\Omega}\left(-\mathrm{i}\frac{\partial}{\partial\phi_i}\right)\right] + \tilde{C},$$

where

$$\tilde{C} = \frac{1}{\hbar\Omega}C = \frac{e^2}{4\pi\epsilon_0\epsilon}\sqrt{\frac{m}{\hbar^3\Omega}}\frac{1}{x_{12}}$$

is dimensionless. Note that a uniform scaling of $\vec{r}$ will not alter the angular momentum operator $\left(-\mathrm{i}\frac{\partial}{\partial\phi_i}\right)$.

Let ut introduce a proper scale for the magnetic field strength γ. A natural combination is

$$\gamma = \tilde{\gamma}\frac{\hbar\omega_0}{\mu_B} = \tilde{\gamma}\frac{2m_e\omega_0}{e},$$

where

$$\mu_B = \frac{e\hbar}{2m_e} \approx 5.7884\cdot 10^{-5}\ \mathrm{eV}\ \mathrm{T}^{-1}$$

is the Bohr magneton. Hence, $\tilde{\gamma}$ is dimensionless. We then obtain

$$\gamma = \frac{\tilde{\gamma}}{\tilde{m}}\frac{2\hbar}{ea^2} \approx \frac{\tilde{\gamma}}{\tilde{m}}1316.4\,\mathrm{T}\frac{\mathrm{nm}^2}{a^2}.$$

In other words, the chosen unit for magnetic field strength depends on the confinement strength and the mass. This is no surprise: The Lorentz force on a moving charge depends on the mass, and we introduced the length scale on this motion in the choice of units.

This also yields a particularly simple expression for Ω, viz,

$$\Omega = \omega_0\sqrt{1 + \frac{\tilde{\gamma}^2}{\tilde{m}^2}}.$$

Moreover, we obtain

$$\tilde{C} = \frac{e^2}{4\pi\epsilon_0}\frac{\tilde{m}a}{\epsilon}\frac{m_ec^2}{(\hbar c)^2}\frac{1}{\sqrt[4]{1+\tilde{\gamma}^2/\tilde{m}^2}}\frac{1}{x_{12}}.$$

For completeness, assume now that γ is given in units of Teslas, i.e., $\gamma = \hat{\gamma}\,\mathrm{T}$. We then obtain

$$\tilde{\gamma} = \frac{\hat{\gamma}}{1316.4}\tilde{m}\frac{a^2}{\mathrm{nm}^2}.$$

Inserting $\tilde{\gamma}$ into the Hamiltonian we obtain

$$\tilde{H} = \sum_{i=1}^{2}\left[-\frac{1}{2}\tilde{\nabla}_i^2 + \frac{1}{2}x_i^2 - \alpha\left(-\mathrm{i}\frac{\partial}{\partial\phi_i}\right)\right] + \lambda\frac{1}{x_{12}},$$

with

$$\alpha \equiv \frac{\tilde{\gamma}}{\tilde{m}}\frac{1}{\sqrt{1+\tilde{\gamma}^2/\tilde{m}^2}}$$

and

$$\lambda \equiv \frac{e^2}{4\pi\epsilon_0}\frac{\tilde{m}a}{\epsilon}\frac{m_ec^2}{(\hbar c)^2}\frac{1}{\sqrt[4]{1+\tilde{\gamma}^2/\tilde{m}^2}} \approx 18.903\frac{\tilde{m}a\,\mathrm{nm}^{-1}}{\epsilon}\frac{1}{\sqrt[4]{1+\tilde{\gamma}^2/\tilde{m}^2}}.$$

Remarks

Consider for the moment the case $\gamma = 0$, so that $\Omega = \omega_0$. Notice that C and $\tilde{C} = C/\hbar\omega_0$ scale differently with increasing confinement length a. Intuitively, with large a, the particles will spend more time away from each other, weakening the interaction on average. This agrees with $A \sim a^{-1}$. However, notice that the energy level spacing $\hbar\omega \sim a^{-2}$ gets smaller with larger a, i.e., the spectrum approaches a continuous one. This implies that the *scaled* interaction $\tilde{A}\tilde{\ }a$ becomes *stronger* with increasing a.

There is no way around this problem. Seemingly, we could use a basis of Hermite functions falling off faster, making the Coulomb matrix elements smaller. However, this will destroy the asymptotics of the wave function (it falls off too fast). Moreover, the h.o. part is no longer diagonal, implying the need of a bigger basis to obtain convergence.