Introduction

January 14, 2020

1 Why Learn Computational Physics?

Physics is a fundamentally experimental science.

To understand the universe around us, experimental physicists design and set up experiments to measure physical properties as function of temperature, time, and external fields.

For example, experimentalists may set up an experiment to measure the resistivity of a material at low temperatures. They might then discover that the resistivity decreases slowly at first, plunges at a critical temperature, and thereafter remains zero as temperature is lowered. You might know that such a phenomenon is called superconductivity.

After the experimental physicists have collected enough high-quality data on how physical properties vary with the control quantity, theoretical physicists take over to develop models or theories, so that they can explain the phenomenon.

In physics, these models and theories are frequently in the form of equations like $m\vec{a} = \vec{F}$ (Newton's Second Law), or $\nabla \cdot \vec{E} = -\rho(\vec{r})/\epsilon_0$ (Poisson's equation). To test whether the models or theories indeed explain the experiments we need to solve these equations, to understand how physical properties depend on the control variables.

Naturally, exact solutions to these equations are the best, because we can summarize the physics of the problem in closed form. If exact solution is not possible, then approximate solutions are not bad too.

Why is this so?

For example, we find from Bohr's model of the hydrogen atom that in the ground state of the system, the electron orbits the nucleus at the Bohr radius

$$a_0 = \frac{4\pi\epsilon_0\hbar^2}{m_e e^2}. \tag{1}$$

In this solution, $\hbar = h/2\pi$ (the reduced Planck's constant), π, and e (the charge of the electron) are constants of nature, but ϵ_0 (permittivity of free space) and m_e (mass of the electron) are parameters that depend on the problem.

For example, an electron and a positron can form an atom-like bound state called a positronium. For the positronium, we have the same ϵ_0, but instead of m_e, we need to use the reduced mass μ of the electron and positron. Using

$$\frac{1}{\mu} = \frac{1}{m_e} + \frac{1}{m_p}, \tag{2}$$

and the fact that the positron has the same mass $m_p = m_e$ as the electron, we find that $\mu = m_e/2$. Therefore, the Bohr radius of the positronium is twice as large as that of the hydrogen atom!

More interestingly, in the compound semiconductor GaAs, we have a permittivity of $\epsilon = 12.9\epsilon_0$. From quantum mechanics and condensed matter physics, we also know that the electron wave packet (and also the hole wave packet) in a solid behaves as if it has a different mass from the bare electron. For GaAs, the effective mass of the electron in the conduction band is $m_e^* = 0.067 m_e$, whereas the effective mass of the hole in the valence band is $m_h^* = 0.082 m_e$.

In a GaAs quantum heterostructure, we can create conditions for the formation of a bound state between an electron (in the conduction band) and a hole (in the valence band). Such an entity is called an exciton. It is very similar to a positronium, except that its effective mass μ is

$$\frac{1}{\mu} = \frac{1}{m_e^*} + \frac{1}{m_h^*}, \tag{3}$$

giving us $\mu = 0.037 m_e$. Therefore, the Bohr radius

$$a_{\mathrm{GaAs}} = \frac{12.9}{0.037} a_0 = 349 a_0 \tag{4}$$

is two orders of magnitude larger than that of the hydrogen atom.

Seeing how powerful exact solutions are, why then do we even attempt computational solutions?

The reason is exact solutions are very rare. For most problems, we cannot find exact solutions. Even if we resort to approximate solutions, which are still analytical (i.e. in mathematical form), we still find more intractable problems than those whose solutions we can find.

For example, we do not understand the properties of steel well, when it is exposed to external loading. However, we still have to build a steel bridge that would not fail when cars, buses, and lorries are driven over it. To achieve this, we have to solve for stresses and strains of the steel bridge numerically, to find out where in the structure we might want to make improvements.