NONDIMENSIONALIZATION TECHNIQUE FOR DIFFERENTIAL EQUATION IN PHYSICS

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DOI: 10.37550/tdmu.EJS/2024.02.558

Article Info

Volume: 6
Issue: 02
June 2024
Received: April 25th, 2024
Accepted: May 20th, 2024
Page No: 297-302

Abstract

In physics, the majority of natural events have been researched and described using differential equations, each having its own initial and boundary conditions. These differential equations contain a large number of fundamental constants as well as other model parameters. They add to the equation's complexity and rounding errors, making the problem more difficult to solve. In this work, we provide a method for transforming these physics differential equations into dimensionless equations, which are significantly simpler. Nondimensionalization, by suitably substituting variables, is the process of removing some or all of the physical dimensions from an equation that contains physical quantities. Some benefits of these dimensionless equations include that they are simpler to identify when using well-known mathematical methods, need less time to compute, and do not round off errors. Through several examples we discuss, this method is useful not just in quantum mechanics but also in classical physics.

Keywords: differential equation, dimensionless equation

1. Introduction

In the field of physics, the majority of natural phenomena have been studied and described using differential equations, each with unique initial and boundary conditions. Each term in those differential equations indicates a system attribute related to heat, mass, momentum transfer and etc. The same units are used for each term on both sides of the equations.

Solving these differential equations sometimes require specialist knowledge to handle sophisticated algorithms due to their complexity, which is often too great for existing computers to handle. In addition, these differential equations include many fundamental constants such as the electronic mass m_e and charge e, the Plank constant h, and other model parameters. The intricacy of the equation and the rounding errors are increased by these fundamental constants, making the problem difficult to solve (Conejo, 2021; Fernández, 2020).

If we can transform these differential equations into a dimensionless form, it will be much easier to solve them. By appropriately substituting variables, nondimensionalization refers to the partial or complete elimination of physical dimensions from an equation containing physical quantities. It is also understood in terms of meaning is the process of transforming an equation to a dimensionless form by rescaling its variables. When using this technique, problems involving measured units can be made simpler and more parameterized. It has a tight connection to dimensional analysis. Unlike SI units, these units relate to quantities that are inherent to the system. Nondimensionalization is not the same as converting extensive quantities in an equation to intensive quantities, since the latter procedure results in variables that still carry units. Characteristic properties of a system can also be recovered by nondimensionalization.

In the dimensionless forms, this has numerous advantages (Conejo, 2021, Fernández, 2020):

• It is easier to recognize when to apply familiar mathermatical techniques.

• The computation takes less time.

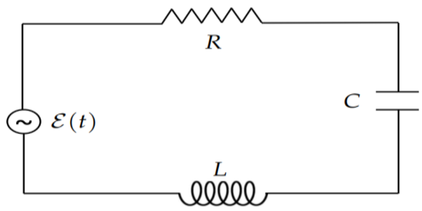
• Prevent rounding off errors.

We applied this technique for complex problems such as a two-dimensional exciton in a constant magnetic field (Hoang, 2016), a two-dimensional exciton screened by reduced dimensionality with the presence of a constant magnetic field (Nguyen, 2019), and orther problems (Le, 2017; Anh, 2018; Cao, 2019; Ly, 2023).

Because of this, we demonstrate the method's benefits in this work along with important details regarding the desired physical outcome, and we also demonstrate how to construct dimensionless equations.

In section 2 we discuss in the RLC circuit, hydrogen atom models and two-dimensional negatively charged exciton models are covered in sections 3 and 4, and we have utilized dimensionless forms to obtain numerically exact solutions for these models (Hoang, 2016; Nguyen; 2019, Ly; 2023). The main findings and conclusions are outlined in section 5.

2. RLC circuit



To illustrate how to convert differential equations into dimensionless differential equations we begin with a simple model, the RLC circuit. Consider a resistor R, an inductor L, and a capacitor C connected in series as shown in the above figure. An AC generator provides a time-varying electromotive force to the circuit, given by $\varepsilon(t) = \varepsilon_0 \cos \omega t$ (Chasnov, 2019). The equations for the voltage drop across a capacitor, a resistor, and an inductor are $V_C = \frac{q}{C}$, $V_R = iR$, $V_L = L\frac{di}{dt}$, where C is the capacitance, R is the resistance and L is the inductance. The charge q and the current i are related by $i = \frac{dq}{dt}$.

Kirchhoff's voltage law states that the electromotive force applied to any closed loop is equal to the sum of the voltage drops in that loop. Appying Kirchhoff's law, we have:

$$V_L + V_R + V_C = \varepsilon(t), \qquad (1)$$

or

$$L\frac{d^2q}{dt^2} + R\frac{dq}{dt} + \frac{1}{C}q = \varepsilon_0 \cos \omega t \qquad (2)$$

The equation (2) is a second-order linear inhomogeneous differential equation with constant coefficients. It has a lot of parameters in it, like R, L, C, ε, ω. To reduce the number of free parameters in the equation (2), we can nondimensionalize. We first define the natural frequency of oscillation of a system to be the frequency of oscillation in the absence of any driving or damping forces. For the RLC circuit, the natural frequency of oscillation is given by $\omega_0 = \frac{1}{\sqrt{LC}}$, and making use of ω_0, we can define a dimensionless time τ t and a dimensionless charge Q by

$$\tau = \omega_0 t,\ \ Q = \frac{\omega_0^2 L}{\varepsilon_0} q \tag{3}$$

The resulting dimensionless equation for the RLC circuit can then be found to be

$$\frac{d^2Q}{d\tau^2} + \alpha \frac{dQ}{d\tau} + Q = \cos \beta t, \tag{4}$$

with $\alpha = \frac{R}{L\omega_0},\ \beta = \frac{\omega}{\omega_0}$.

We have an RLC circuit, a simple electrical engineering circuit with an AC current, easy to recognize the form of the equation (4) is an inhomogeneous term to the second-order with constant coefficients. We learned how to solve these problems, so we totally can apply them to solve the equation (4).

By redefining dimensionless variables, we end up with an equation without dimensions with fewer parameters, alpha and beta are constant and unit-less. We can solve the equation (4) more quickly and the computation takes less time.

3. Hydrogen atom models

Then the Schrödinger equation for hydrogen atom is found to be

$$\hat{H}(\vec{r})\psi(\vec{r}) = E\psi(\vec{r}), \tag{5}$$

where the Hamiltonian is given by

$$\hat{H}(\vec{r}) = -\frac{\hbar^2}{2m_e}\nabla^2 - \frac{e^2}{4\pi\varepsilon_0 |\vec{r}|}, \tag{6}$$

With the Schrödinger equation (5), our variables are x, y, z, E and constants are $e, m_e, \varepsilon_0, \hbar, \pi$. We realize that the relevant numbers that govern the character of physical phenomena are not dimensional variables $(e, m_e, \varepsilon_0, \hbar, \pi)$, but rather, dimensionless numbers (x, y, z, E). In the computational, the dimensional variables $(e, m_e, \varepsilon_0, \hbar, \pi)$ make the computational time become longer and exhibit round-off errors. It will affect the accuracy of the calculation. So, we should remove them leaving a much simpler equation.

To obtain a dimensionless Schrödinger equation, we first define dimensionless coordinate and dimensionless energy by:

$$\vec{\rho} = \frac{\vec{r}}{a},\ \ E_\rho = \frac{E}{b}, \tag{7}$$

where a and b are corresponding a unit of length and energy that we choose conveniently for problem.

To rewrite the equation (5) with variables x, y, z, E to variables $\rho_x, \rho_y, \rho_z, E_\rho$, we transform:

$$\begin{cases} \frac{\partial}{\partial x} = \frac{\partial}{\partial \rho_x}\frac{\partial \rho_x}{\partial x} = \frac{1}{a}\frac{\partial}{\partial \rho_x} \\ \frac{\partial}{\partial y} = \frac{\partial}{\partial \rho_y}\frac{\partial \rho_y}{\partial y} = \frac{1}{a}\frac{\partial}{\partial \rho_y} \\ \frac{\partial}{\partial z} = \frac{\partial}{\partial \rho_z}\frac{\partial \rho_z}{\partial z} = \frac{1}{a}\frac{\partial}{\partial \rho_z} \end{cases} \to \begin{cases} \frac{\partial^2}{\partial x^2} = \frac{1}{a^2}\frac{\partial^2}{\partial \rho_x^2} \\ \frac{\partial^2}{\partial y^2} = \frac{1}{a^2}\frac{\partial^2}{\partial \rho_y^2} \\ \frac{\partial^2}{\partial z^2} = \frac{1}{a^2}\frac{\partial^2}{\partial \rho_z^2} \end{cases} \to \nabla^2 = \frac{1}{a^2}\nabla_\rho^2 \tag{8}$$

$$|r| = \sqrt{x^2 + y^2 + z^2} = a\sqrt{\rho_x^2 + \rho_y^2 + \rho_z^2} = a|r_\rho|. \tag{9}$$

Replace (8), (9) into (5) we have

$$\left[-\frac{1}{2}\nabla_\rho^2 - \frac{m_e a e^2}{4\pi\hbar^2\varepsilon_0}\frac{1}{|\vec{\rho}|}\right]\psi(\vec{\rho}) = \frac{m_e a^2 b}{\hbar^2}E_\rho\psi(\vec{\rho}), \tag{10}$$

Continue, we choose

$$\begin{cases} \dfrac{m_e a e^2}{4\pi\hbar^2\varepsilon_0} = 1 \\ \dfrac{m_e a^2 b}{\hbar^2} = 1 \end{cases} \rightarrow \begin{cases} a = \dfrac{4\pi\hbar^2\varepsilon_0}{m_e e^2} \\ b = \dfrac{m_e e^2}{16\pi^2\hbar^2\varepsilon_0^2} \end{cases} \tag{11}$$

We have the dimensionless Schrödinger as:

$$\left[-\frac{1}{2}\nabla_\rho^2 - \frac{1}{|\vec{\rho}|}\right]\psi(\vec{\rho}) = E_\rho\psi(\vec{\rho}) \tag{12}$$

With:

- $a = \dfrac{4\pi\varepsilon_0\hbar^2}{e^2 m_e} = a_0$ is the unit of length (a_0: the Bohr radius).
- $b = \dfrac{me^4}{16\pi^2\varepsilon_0^2\hbar^2} = \dfrac{me^4}{4\varepsilon_0^2 h^2} = 2R_y$ is the unit of energy (R_y: the Rydberg constant).

We realize that the dimensionless Schrödinger (12) is a simplified version of the equation (5) and that the algebraic manipulation of the dimensionless equation and its numerical treatment are significantly less time-consuming.

4. Two-dimensional negatively charged exciton models

In this section, we focus on the two-dimensional negatively charged exciton. The bound complexes of electrons and holes were predicted by Lampert (Lampert, 1958). Charged excitons (or trions) are three-particle excitonic complexes resulting from the binding of an exciton (an electron-hole pair) with an extra electron or hole in semiconductors, in which the negatively charged exciton consists of two electrons bound to a hole.

The Schrödinger equation of a negatively charged exciton is given by (Hoang, 2016; Nguyen, 2019; Ly, 2023)

$$\hat{H}(\vec{r})\psi(\vec{r}_1,\vec{r}_2) = E\psi(\vec{r}_1,\vec{r}_2), \tag{13}$$

$$\hat{H} = -\frac{\hbar^2}{2\mu^*}\nabla_1^2 - \frac{\hbar^2}{2\mu^*}\nabla_2^2 - \frac{\hbar^2}{m_h^*}\left(\frac{\partial^2}{\partial x_1\partial x_2} + \frac{\partial^2}{\partial y_1\partial y_2}\right) - \frac{Z^*e^2}{4\pi\varepsilon_0 r_1} - \frac{Z^*e^2}{4\pi\varepsilon_0 r_2} + \frac{e^2}{4\pi\varepsilon_0|r_1 - r_2|}. \tag{14}$$

Where m_e^*, m_h^* are the electron's effective mass and the hole's effective mass; Z^* is the effective charge of the hole, ε_0 is the static dielectric constant; r_1, r_2 are the coordinates vectors of electrons and holes in two-dimensional respectively; the effective reduced mass μ^* is defined by the formula

$$\mu^* = \frac{m_e^* m_h^*}{m_h^* + m_e^*}. \tag{15}$$

To convert a dimensionless Schrödinger equation, we denoted:

$$\rho_{x_1} = \frac{x_1}{a}, \rho_{y_1} = \frac{y_1}{a}, \rho_{x_2} = \frac{x_2}{a}, \rho_{y_2} = \frac{y_2}{a}, E_\rho = \frac{E}{b}, \tag{16}$$

here a and b are corresponding a unit of length and energy that we choose conveniently for the problem.

We have:

$$\frac{\partial}{\partial x_1} = \frac{\partial \rho_{x_1}}{\partial x_1}\frac{\partial}{\partial \rho_{x_1}} = \frac{1}{a}\frac{\partial}{\partial \rho_{x_1}} \quad \Rightarrow \frac{\partial^2}{\partial x_1^2} = \frac{1}{a^2}\frac{\partial^2}{\partial \rho_{x_1}^2}$$

$$\frac{\partial}{\partial y_1} = \frac{\partial \rho_{y_1}}{\partial y_1}\frac{\partial}{\partial \rho_{y_1}} = \frac{1}{a}\frac{\partial}{\partial \rho_{y_1}} \quad \Rightarrow \frac{\partial^2}{\partial y_1^2} = \frac{1}{a^2}\frac{\partial^2}{\partial \rho_{y_1}^2}$$

$$\Rightarrow \begin{cases} \nabla_1^2 = \frac{1}{a^2}\nabla_{\rho_1}^2, \nabla_2^2 = \frac{1}{a^2}\nabla_{\rho_2}^2 \\ r_1 = a\left|r_{\rho_1}\right|; \quad r_2 = ar_{\rho_1}; \quad \left|r_1 - r_2\right| = a\left|r_{\rho_1} - r_{\rho_2}\right| \\ \frac{\partial^2}{\partial x_1 \partial x_2} = \frac{1}{a^2}\frac{\partial^2}{\partial \rho_{x_1}\partial \rho_{x_2}}; \quad \frac{\partial^2}{\partial y_1 \partial y_2} = \frac{1}{a^2}\frac{\partial^2}{\partial \rho_{y_1}\partial \rho_{y_2}} \end{cases} \tag{17}$$

Replace (17) into (13) we have

$$\left[-\frac{1}{2}\nabla_{\rho_1}^2 - \frac{1}{2}\nabla_{\rho_2}^2 - \frac{\mu^*}{m_h^*}\left(\frac{\partial^2}{\partial \rho_{x_1}\partial \rho_{x_2}} + \frac{\partial^2}{\partial \rho_{y_1}\partial \rho_{y_2}}\right) - \frac{e^2\mu^* a}{4\pi\hbar^2\varepsilon_0}\frac{Z^*}{\left|r_{\rho_1}\right|} - \frac{e^2\mu^* a}{4\pi\hbar^2\varepsilon_0}\frac{Z^*}{\left|r_{\rho_2}\right|} + \frac{e^2\mu^* a}{4\pi\hbar^2\varepsilon_0}\frac{1}{\left|r_{\rho_1} - r_{\rho_2}\right|}\right]\psi\left(\vec{\rho}_1, \vec{\rho}_2\right) = \frac{\mu^* a^2 b}{\hbar^2}E_\rho \psi\left(\vec{\rho}_1, \vec{\rho}_2\right). \tag{18}$$

We choose

$$\begin{cases} \frac{e^2\mu^* a}{4\pi\hbar^2\varepsilon_0} = 1 \\ \frac{\mu^* a^2 b}{\hbar^2} = 1 \end{cases} \rightarrow \begin{cases} a = \frac{4\pi\hbar^2\varepsilon_0}{\mu^* e^2} \\ b = \frac{\mu^* e^2}{16\pi^2\hbar^2\varepsilon_0^2} \end{cases} \tag{19}$$

We have the dimensionless Schrödinger as:

$$\left[-\frac{1}{2}\nabla_{\rho_1}^2 - \frac{1}{2}\nabla_{\rho_2}^2 - \frac{\mu^*}{m_h^*}\left(\frac{\partial^2}{\partial \rho_{x_1}\partial \rho_{x_2}} + \frac{\partial^2}{\partial \rho_{y_1}\partial \rho_{y_2}}\right) - \frac{Z^*}{\left|r_{\rho_1}\right|} - \frac{Z^*}{\left|r_{\rho_2}\right|} + \frac{1}{\left|r_{\rho_1} - r_{\rho_2}\right|}\right]\psi\left(\vec{\rho}_1, \vec{\rho}_2\right) = E_\rho \psi\left(\vec{\rho}_1, \vec{\rho}_2\right). \tag{20}$$

With:

- $a = \frac{4\pi\varepsilon_0\hbar^2}{e^2\mu^*} = a_0$ is the unit of length (a_0: the Bohr radius).

• $b = \dfrac{\mu^* e^4}{16\pi^2 \varepsilon_0^2 \hbar^2} = \dfrac{\mu^* e^4}{4\varepsilon_0^2 h^2} = 2R_y$ is the unit of energy (R_y : the Rydberg constant).

We demonstrate the conversion of the dimensionless Schrödinger simplier in the two-dimensional negatively charged exciton models, not only by choosing units such that $\hbar = m = e = c = 1$ or expressions of a similar nature (Fernández, 2020) but also by providing a method for doing so that can be used to solve a wide range of issues. Applying this method to a two-dimensional exciton in a constant magnetic field (Hoang, 2016; Nguyen, 2019; Ly, 2023) allowed us to optimize the computation process and minimize errors due to its dimensionless Schrödinger.

5. Conclusion

The work discusses the benefits of using dimensionless equations in physics, especially when solving problems with numerical methods. Dimensionless equations are simpler and less prone to rounding errors. The study also introduces a method for transforming dimensional equations into dimensionless ones. This method is applied to various examples, including the RLC circuit, hydrogen atom models, and two-dimensional negatively charged exciton models. This technique shows that these fundamental constants and other model parameters not only by choosing units such that or expressions of a similar nature but also by providing a method for doing so that can be used to solve a wide range of issues. We applied this technique for more complex problems such as a two-dimensional exciton in a constant magnetic field, a two-dimensional exciton screened by reduced dimensionality with the presence of a constant magnetic field, and other problems. It is worth adding that dimensionless equations are a valuable tool for solving complex problems in physics, not just quantum mechanics.

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