
MM2090

An Introduction to Scientific Computing



Team 2

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1 ME20B004 - Abhaumika Bijudith

1.1 The Equation - Hall Effect

$$V = \frac{Bi}{ned} \quad (1)$$

1.2 Analysis

Following contains a brief explanation of the variables and the importance of the equation:

- The given equation 1 has terms V , B , i , n , e and d .

Here,

V represents the voltage across the two plates

B represents the magnetic field between the two plates

i represents the current flowing between the two plates

n represents the density of charge carrier

e represents the electronic charge

d represents the distance between the two plates

If an electric current flows through a conductor in a magnetic field, the magnetic field exerts a transverse force on the moving charge carriers which tends to push them to one side of the conductor. This is most evident in a thin flat conductor as illustrated. A buildup of charge at the sides of the conductors will balance this magnetic influence, producing a measurable voltage between the two sides of the conductor. The presence of this measurable transverse voltage is called the Hall effect after E. H. Hall who discovered it in 1879. [6]

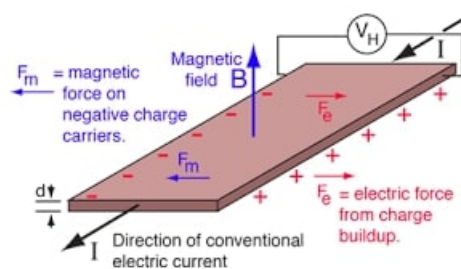


Figure 1: Hall Effect [7]

1.3 Applications

Hall probes are often used as magnetometers, i.e. to measure magnetic fields, or inspect materials (such as tubing or pipelines) using the principles of magnetic flux leakage. Hall effect devices produce a very low signal level and thus require amplification. While suitable for laboratory instruments, the vacuum tube amplifiers available in the first half of the 20th century were too expensive, power consuming, and unreliable for everyday applications. It was only with the development of the low cost integrated circuit that the Hall effect sensor became suitable for mass application. Many devices now sold as

Hall effect sensors in fact contain both the sensor as described above plus a high gain integrated circuit (IC) amplifier in a single package. Recent advances have further added into one package an analog-to-digital converter and I²C (Inter-integrated circuit communication protocol) IC for direct connection to a microcontroller's I/O port. Hall effect sensors are readily available from a number of different manufacturers, and may be used in various sensors such as rotating speed sensors (bicycle wheels, gear-teeth, automotive speedometers, electronic ignition systems), fluid flow sensors, current sensors, and pressure sensors. Common applications are often found where a robust and contactless switch or potentiometer is required. These include: electric airsoft guns, triggers of electropneumatic paintball guns, go-cart speed controls, smart phones, and some global positioning systems. [9]

2 ME20B022 - Amar Muhammed

2.1 The Equation

Van der Waals Equation:

$$\left(P + \frac{an^2}{V^2}\right)(V - nb) = nRT \quad (2)$$

2.2 Analysis

Following contains a brief explanation of the variables in the equation :

The equation 7 has terms **P** , **V** , **n**, **R** , **T** , **a** and **b**

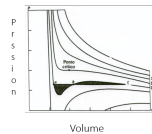
Here,

- **P** represents the pressure of the system
- **V** represents the volume of the system
- **n** represents the number of moles of gas present in the system
- **R** represents the universal gas constant
- **T** represents the temperature of the system
- **a** represents the Van der Waals constant that provides the correction for inter-molecular forces.
- **b** represents the Van der Waals constant that adjusts for the volume occupied by gas molecules in the system

The Van der Waals equation is an equation of state that generalizes the ideal gas law based on plausible reasons that real gases do not act ideally. The ideal gas law treats gas molecules as point particles that interact with their containers but not each other, meaning they neither take up space nor change kinetic energy during collisions. It is available via its traditional derivation (a mechanical equation of state), or via a derivation based in statistical thermodynamics, the latter of which provides the partition function of the system and allows thermodynamic functions to be specified. It successfully approximates the behavior of real fluids above their critical temperatures and is qualitatively reasonable for their liquid and low-pressure gaseous states at low temperatures. However, near the phase transitions between gas and liquid, in the range of p , V , and T where the liquid phase and the gas phase are in equilibrium, the Van der Waals equation fails to accurately model observed experimental behaviour, in particular that p is a constant function of V at given temperatures. As such, the Van der Waals model is not useful only for calculations intended to predict real behavior in regions near the critical point. Corrections to address these predictive deficiencies have since been made, such as the equal area rule or the principle of corresponding states.

van der Waals Equation

$$p = \frac{RT}{v - b} - \frac{a}{v^2}$$



$p \leftrightarrow$ Pressure

$T \leftrightarrow$ Temperature

$v \leftrightarrow$ Molar volume

$R \leftrightarrow$ Universal constant of gases

$a \text{ and } b \leftrightarrow$ Empirical constants.

Figure 2: The Van der Waals equation [5]

2.3 Validity

The Van der Waals equation is mathematically simple, but it nevertheless predicts the experimentally observed transition between vapor and liquid, and predicts critical behaviour.[12]:289 It also adequately predicts and explains the Joule–Thomson effect (temperature change during adiabatic expansion), which is not possible in ideal gas.

Above the critical temperature, T_C , the Van der Waals equation is an improvement over the ideal gas law, and for lower temperatures, i.e., $T < T_C$, the equation is also qualitatively reasonable for the liquid and low-pressure gaseous states; however, with respect to the first-order phase transition, i.e., the range of (p, V, T) where a liquid phase and a gas phase would be in equilibrium, the equation appears to fail to predict observed experimental behaviour, in the sense that p is typically observed to be constant as a function of V for a given temperature in the two-phase region. This apparent discrepancy is resolved in the context of vapour–liquid equilibrium: at a particular temperature, there exist two points on the Van der Waals isotherm that have the same chemical potential, and thus a system in thermodynamic equilibrium will appear to traverse a straight line on the p – V diagram as the ratio of vapour to liquid changes. However, in such a system, there are really only two points present (the liquid and the vapour) rather than a series of states connected by a line, so connecting the locus of points is incorrect: it is not an equation of multiple states, but an equation of (a single) state. It is indeed possible to

compress a gas beyond the point at which it would typically condense, given the right conditions, and it is also possible to expand a liquid beyond the point at which it would usually boil. Such states are called "metastable" states. Such behaviour is qualitatively (though perhaps not quantitatively) predicted by the Van der Waals equation of state. [10]

3 ME20B050 - Cecil Jacob Thomas

3.1 Equation - Halley's Method

$$x_{n+1} = x_n - \frac{2f(x_n)f'(x_n)}{2[f'(x_n)]^2 - f(x_n)f''(x_n)} \quad (3)$$

3.2 Terms Involved

- $\mathbf{x_n}$: is the test value we input to the function to get the next closest approximation
- $\mathbf{x_{n+1}}$: is the next best approximation to the root achieved by taking x_{n+1} as the starting point
- $\mathbf{f(x)}$: is the function whose roots we are trying to find by finding successively better approximations to the root

3.3 Description

Halley's method also called *method of tangent hyperbolas* is a numerical method for calculating the roots of a function by producing successively better approximations to the roots of a real-valued function. It is generally more convergent than say the Newton-Rhapson method. Unlike the Newton-Rhapson method, Halley's method uses Tangent hyperbola's to approximate the next point. This method was invented by Edmond Halley

3.4 Derivation

Equation 3 can be derived by the use of a 2^{nd} order Taylor polynomial

$$y(x) = f(x_n) + f'(x_n)(x - x_n) + \frac{f''(x_n)(x - x_n)^2}{2} \quad (4)$$

Then by setting $y(x_{n+1}) = 0$ and rearranging we get:

$$x_{n+1} = x_n - \frac{2f(x_n)}{2f'(x_n) + f''(x_n)(x - x_n)} \quad (5)$$

Finally we can put in the Newton-Rhapson approximation

$x_{n+1} - x_n = -\frac{f(x_n)}{f'(x_n)}$ in the LHS to get:

$$x_{n+1} = x_n - \frac{2f(x_n)f'(x_n)}{2f'(x_n)^2 - f''(x_n)f(x_n)} \quad (6)$$

Which is essentially **Halley's root-finding algorithm**

3.5 Applications

Numerical algorithms such as these are very important as sometimes there might not exist a method to calculate an exact root by symbolic manipulation alone.

For example Kepler's equation needs to be solved many times for a variety of problems in Celestial Mechanics[4]. Therefore, computing the solution to Kepler's equation in an efficient manner is of great importance as we could use it to solve Kepler's Equation numerically[4]. The below graph contrasts the performance of Halley's method to different root finding algorithms when applied to solve the Kepler's equation numerically for different eccentricities [4]

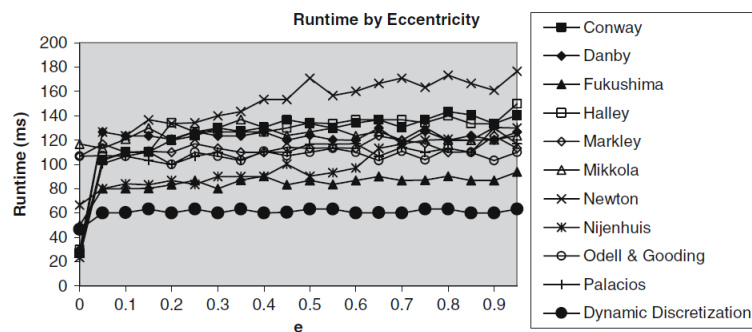


Figure 3: Runtime varying with eccentricity

Figure 3 shows us that Halley's method does certainly do better than the Newton-Rhapson method but recent techniques such as Dynamic Discretization are far more efficient

4 MM20B017 - Divya Jyothi D

4.1 The Equation

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}}e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2}$$

Variables:

$f(x)$ = probability density function

σ = standard deviation

μ = mean

$\pi \approx 3.14159...$

$e \approx 2.71828...$

4.2 Description

The above is the equation for normal distribution or probability density function. It is also called as the equation of **Bell Curve** or the **Gaussian Equation** named after the scientist *Carl Friedrich Gauss*. This equation can be used to express any bell curve as a function of x. This equation is used to represent the probability density distribution of a normally distributed random variable.

Let us consider a case where tiny steel balls in a container are made to pass through a narrow neck separating the container into two halves. The situation is illustrated in fig.1 below.

The tiny steel balls from the top half fall through the narrow neck into the bottom chamber. Observe that the number of balls collecting at the centre is maximum and it gradually diminishes towards the sides giving rise to a bell-shaped profile.

This shows that the probability of a random variable occurring at its mean value is maximum and diminishes for values away from the mean. [11] [8]

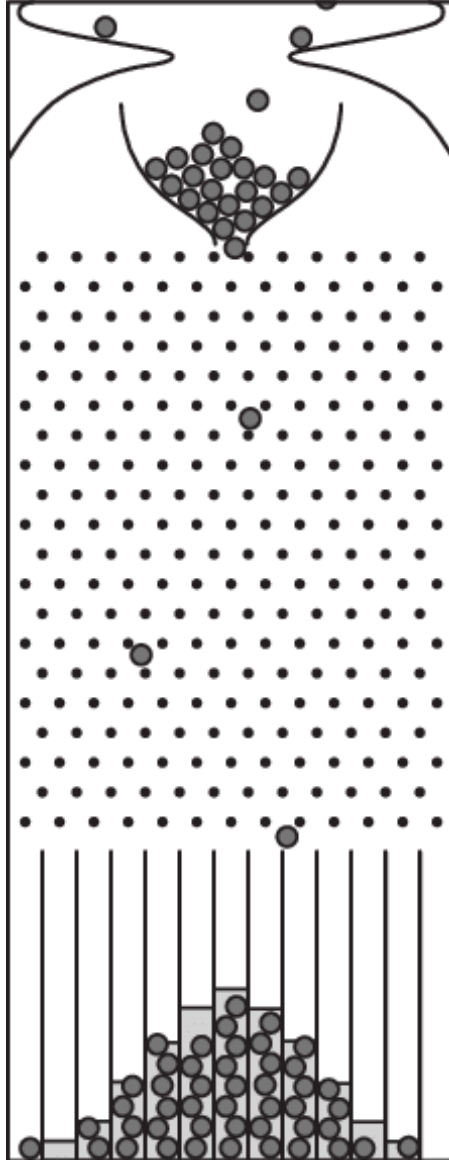


Figure 4: Illustration of the above case

5 MM20B057 - Shreya Rajesh

5.1 The Langevin Equation

$$m \frac{dv}{dt} = -\lambda v + \eta(t) \quad (7)$$

5.2 Terms of the Equation

In the above equation,

m denotes the mass of the particle

λ represents the viscous force

v represents the velocity of the particle

$\eta(t)$ is the *noise term* which describes the force

5.3 Description

The Langevin Equation is used to describe *Brownian Motion*.

Brownian motion is the observed random movement that is portrayed by a particle when in a fluid due to its collisions with the other molecules.

The Langevin equation is a phenomenological stochastic differential equation of motion (see Equation 7). It describes the time evolution of a subset of the various degrees of freedom where it slowly relaxes the macroscopic variables and rapidly relaxes the microscopic variables. Thus, the equation is stochastic in nature. [3] [7]

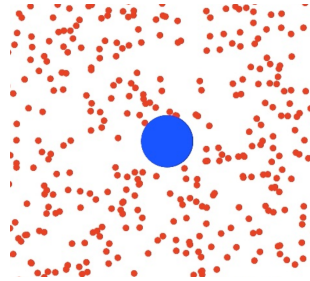


Figure 5: Brownian Motion

Brownian motion (see Figure 5) is by far the simplest way to approximate the dynamics of the particles of a non equilibrium system. In the given equation, the net force has been split into a systematic part (*friction*) and a fluctuating part (*noise*). Both these forces arise due to the interaction of the Brownian particle with the environment. [2]

5.4 Importance

The original Langevin equation helps you describe the Brownian motion of the given Brownian particle, but the application of this equation sees no boundaries. Various forms of this equation has been used in electrical resistors, critical dynamics, harmonic oscillators in a fluid, to find trajectories of Brownian particles and in Boltzmann statistics. [1]

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