# **Study Circle Session**

#### 04/09/2015

# **Topic: Quantum Mechanics**

- Time dependent free particle Schrodinger equation in 3 dimensions
- Particle in an external potential
- Time-independent Schrodinger equation
- Operators, eigen functions, eigenvalues; meaning of degeneracy
- Laplacian operator in spherical polar co-ordinates
- Hydrogen atom ground state and first excited state

# Topic: Elastic collisions

The meaning of elastic collisions was discussed both in the context of billiard ball collisions and atomic collisions. The usefulness of the expression  $E = p^2/2m$  was highlighted to discuss recoil energy of heavy targets. How Bohr relation  $E_2 - E_1 = hx$  frequency is modified to include recoil energy of the atom radiating a photon. An order of magnitude estimate showed that the correction due to recoil is negligible.

Inelastic collisions of electrons with atoms; how Franck-Hertz experiments show that atomic energy levels are quantized.

# Topic: Partial derivatives in thermodynamics

Meaning of total or exact differential, its relation to path-independence.

Maxwell relations; relating derivatives of entropy w.r.t P, V to other more measurable derivatives.

# General learning points

- Practicing to 'read' functions and the significance of constants they carry for the given context.
- Looking at dimensionless ratios to assert something is small or negligible, or large.
- The idea of field and waves; how classical wave equation differs from Schrödinger wave equation.
- Basic laws of mechanics, electrodynamics and quantum mechanics are differential equations; they need to be supplemented by initial conditions/boundary conditions.
- To focus on ideas, not so much what they are named and their symbols, though the latter are also important for learning and communication.

# **Study Circle Session**

#### 11/09/2015

# **Topic: The Gaussian function**

The function  $\exp(-ax^2)$  was discussed in detail. The qualitative properties of its bell-shaped graph (maximum at the origin, two inflexion points on either side of it, etc.) were related to the vanishing of its first order derivative (with negative second order derivative), the vanishing of its second order derivative, etc. The square root of 1/a which has the dim of length (if x is length) was related to the 'width' of the curve. We digressed to revise introductory calculus, in particular, the indefinite and definite integral, and the fundamental theorem of calculus. The value of the definite integral of the Gaussian function was quoted (proof in next week's session); this is needed at many places. The topic of complex numbers was also revised.

# **Topic: Quantum Mechanics**

A problem was taken up in which a wavefunction was given explicitly as a function of x and t, and the potential energy V(x) was to be found. Direct substitution in the time-dependent Schrodinger equation easily gave the result: V(x) proportional to  $x^2$ . Further the given wavefunction had a separable dependence in x and t (product of function of x and function of t); its t dependence was just a phase factor exp (--i a t). Clearly it was a stationary wave function (modulus squared of the function time-independent). The x-dependent part was a gaussian in x, which is known to be the ground state energy eigenfunction of linear harmonic oscillator. As expected, *a* turned out to be *w*/2, where *w* is the angular frequency of the oscillator which appeared in V(x)=1/2 m  $w^2 x^2$ .

By the usual methods of QM, we will determine  $\langle x \rangle$ ,  $\langle p \rangle$ ,  $\langle x^2 \rangle$ ,  $\langle p^2 \rangle$ , etc. for this function in the next session.

# **Topic:** Thermodynamics

The definitions of isothermal compressibility k and volume expansivity were motivated. They are intensive characteristics of a substance. They involve partial derivatives of V w,r,t P and T respectively. They are not constants necessarily; in general they are functions of P and T.

A problem was taken up in which these functions of P and T were given, and the equation of state was to be found out. This involved integration of one equation; the result has an unknown 'constant', which, however, could depend on the variable kept fixed (T in case of k). This when fed into the other equation fixes the equation of state to within a constant.

# General Learning Points

- 1. For a discrete variable *m*, we talk of probability of *m*; for a continuous variable *x*, it is probability density at *x* or probability between *x* and x + dx
- 2. To be alert where and what physical inputs have gone into a mathematical derivation in physics and chemistry.

18/09/2015

There were only internal HBCSE members at the session. We worked on some problems involving the First Law of Thermodynamics. The problems essentially focused on the fundamental distinction between state variables ( like U, P) and the process variables (like Q and W).