Numerical Solution of a Finite Wave Function*

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Abstract—This paper describes how to solve the Schrodinger Equation given a valid wave function.

Index Terms—Wave function, Schrodinger Equation, Root finding, Integration, Interval, Limits

I. Introduction

II. Schrodinger Equation

The time dependent general Schrödinger equation [1] is

$$i\hbar\frac{d}{dt}\left|\Psi(t)\right\rangle = \hat{H}\left|\Psi(t)\right\rangle \tag{1}$$

Where the Hamiltonian $\hat{H}$ is:

$$\hat{H} = \hat{T} + \hat{V} \tag{2}$$

$$\hat{T} = \frac{\hat{\mathbf{p}}\cdot\hat{\mathbf{p}}}{2m} = \frac{\hat{p}^2}{2m} = -\frac{\hbar^2}{2m}\nabla^2; \qquad \hat{\mathbf{p}} = -i\hbar\nabla \tag{3}$$

$$\hat{V} = V = V(\mathbf{r}, t) \tag{4}$$

being $\hat{V}$ the potential energy, $\hat{H}$ the kinetic energy and $\hat{\mathbf{p}}$ the momentum operator. The equation can be written more completely as

$$i\hbar\frac{d}{dt}\left|\Psi(t)\right\rangle = \left[-\frac{\hbar}{2m}\nabla^2 + V(\mathbf{r}, t)\right]\left|\Psi(t)\right\rangle \tag{5}$$

Now, if the basis is relative to some point in the space we use [2]

$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r}, t) = \left[\frac{-\hbar^2}{2m}\nabla^2 + V(\mathbf{r}, t)\right]\Psi(\mathbf{r}, t) \tag{6}$$

instead of a normal derivative we indicate that Ψ depends on $\mathbf{r}$ (a position in the space) so that there is more meaning in the notation.[1]

III. Approaching Numerical Solutions

IV. Probability in a Closed Interval

References

[1] R. Shankar, "Principles of Quantum Mechanics". Springer, 2012.
[2] "Schrodinger equation." http://hyperphysics.phy-astr.gsu.edu/hbase/quantum/Scheq.html (accessed: Sep. 20, 2020).

[1] note that equation (5) is in terms of kets while (6) is in scalar terms.