5.73

Quiz 9 ANSWERS

Grid Points $x_{i}, x_{i+1} = x_{i} + h \text{ (h is step size, not Planck's constant)}$ $\psi = \psi(x_{i})$ U(x) is potential $\left[\frac{d^{2}}{dx^{2}} - \frac{2m}{\hbar^{2}}(U(x) - E)\right] \psi = 0 \text{ is Schrödinger Equation}$ V(x) = C[U(x) - E] $C = \frac{2m}{\hbar^{2}}$ $V_{i} = V(x_{i})$

A. What is the grid definition of $\frac{d\psi}{dx}\Big|_{x=x_i}$?

$$\left. \frac{d\psi}{dx} \right|_{x_i} = \frac{\psi_{i+1} - \psi_i}{h}$$

B. What quantity has the grid definition $h^{-2} [\psi_{i+i} - 2\psi_i + \psi_{i-1}]$?

$$\frac{d^2\Psi}{dx^2}\Big|_{x_i}$$

C. Use $\{\psi_i\}$, h, V_i to write the grid form of the Schrödinger Equation. $h^{-2} \left[\psi_{i+1} - 2\psi_i + \psi_{i-1} \right] - V_i \psi_i = 0$

$$h^{-2} \left[\psi_{i+1} - 2\psi_i + \psi_{i-1} \right] - V_i \psi_i = 0$$

$$h^{-2} \left[\psi_{i+1} - \left(2 + h^2 V_i \right) \psi_i + \psi_{i-1} \right] = 0$$

Suppose you are searching for values of E which satisfy a nonlinear D. equation

$$F(E) = 0$$
.

You know that

$$F(E_I) = a$$

and
 $F(E_1 + \delta) = a + \gamma$.

If you expand F(E) about E_1

$$F(E) = F(E_1) + \frac{dF}{dE} \bigg|_{E_1} (E - E_1)$$

then what value of E is your first iterative solution of $F(E_i) = 0$? To solve for E_i , you need $\frac{dF}{dE}\Big|_{E_1}$, which you obtain from the definition of the

derivative, and $F(E_i) = 0 = F(E_1) + \frac{dF}{dE} \Big|_{E_1} (E_i - E_1)$.

$$0 = F(E_1) + \frac{dF}{dE}\Big|_{E_1} (E_i - E_1)$$

$$0 = a + \frac{\gamma}{\delta} (E_i - E_1)$$

$$-\frac{a\delta}{\gamma} = E_i - E_1$$

$$E_i = E_1 - \frac{a\delta}{\gamma}$$

$$0 = a + \frac{\gamma}{\delta} \left(E_i - E_1 \right)$$

$$-\frac{a\delta}{\gamma} = E_i - E$$

$$E_{i} = E_{1} - \frac{a\delta}{\gamma}$$

MIT OpenCourseWare https://ocw.mit.edu/

5.73 Quantum Mechanics I Fall 2018

For information about citing these materials or our Terms of Use, visit: https://ocw.mit.edu/terms.