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Quiz 9 ANSWERS

1.

Grid Points	x_i, $x_{i+1} = x_i + h$ (h is step size, not Planck's constant)
	$\psi_i \equiv \psi(x_i)$
	$U(x)$ is potential
	$\left[\frac{d^2}{dx^2} - \frac{2m}{\hbar^2}(U(x) - E)\right]\psi = 0$ 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 $\left.\frac{d\psi}{dx}\right|_{x=x_i}$?

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

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

$$\left.\frac{d^2\psi}{dx^2}\right|_{x_i}$$

C. Use $\{\psi_i\}$, h, V_i to write the grid form of the Schrödinger Equation.

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

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

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

$$F(E) = 0.$$

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

If you expand $F(E)$ about E_1

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

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

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

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

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

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