## Quiz 9 ANSWERS

1. 

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

A. What is the grid definition of $\left.\frac{d \psi}{d x}\right|_{x=x_{i}}$ ?

$$
\left.\frac{d \psi}{d x}\right|_{x_{i}}=\frac{\psi_{i+1}-\psi_{i}}{h}
$$

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

$$
\left|\frac{d^{2} \psi}{d x^{2}}\right|_{x_{i}}
$$

C. Use $\left\{\psi_{i}\right\}, h, V_{i}$ to write the grid form of the Schrödinger Equation.

$$
\begin{aligned}
& h^{-2}\left[\psi_{i+1}-2 \psi_{i}+\psi_{i-1}\right]-V_{i} \psi_{i}=0 \\
& h^{-2}\left[\Psi_{i+1}-\left(2+h^{2} V_{i}\right) \psi_{i}+\psi_{i-1}\right]=0
\end{aligned}
$$

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

$$
F(E)=0 .
$$

You know that $\quad F\left(E_{I}\right)=a$
and

$$
F\left(E_{1}+\delta\right)=a+\gamma
$$

If you expand $F(E)$ about $\mathrm{E}_{1}$

$$
F(E)=F\left(E_{1}\right)+\left.\frac{d F}{d E}\right|_{E_{1}}\left(E-E_{1}\right)
$$

then what value of $E$ is your first iterative solution of $F\left(E_{i}\right)=0$ ? To solve for $E_{i}$, you need $\left.\frac{d F}{d E}\right|_{E_{1}}$, which you obtain from the definition of the derivative, and $F\left(E_{i}\right)=0=F\left(E_{1}\right)+\left.\frac{d F}{d E}\right|_{E_{1}}\left(E_{i}-E_{1}\right)$.

$$
\begin{aligned}
0 & =F\left(E_{1}\right)+\left.\frac{d F}{d E}\right|_{E_{1}}\left(E_{i}-E_{1}\right) \\
0 & =a+\frac{\gamma}{\delta}\left(E_{i}-E_{1}\right) \\
-\frac{a \delta}{\gamma} & =E_{i}-E_{1} \\
E_{i} & =E_{1}-\frac{a \delta}{\gamma}
\end{aligned}
$$

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