

Uncertainty principle and particle current

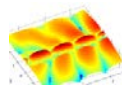
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YONSEI UNIVERSITY



**Advanced Computational
ElectroMagnetics Lab.**

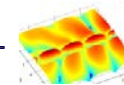
Outline



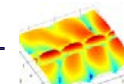
1 Uncertainty principle

2 Particle current

3 Summary



Uncertainty principle



Uncertainty principle



❖ Uncertainty

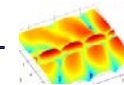
- By using measurable property → position, momentum

❖ Momentum operator

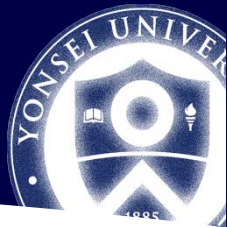
$$\hat{p} = -i\hbar\nabla$$

$$\text{with } \nabla \equiv \mathbf{x}_0 \frac{\partial}{\partial x} + \mathbf{y}_0 \frac{\partial}{\partial y} + \mathbf{z}_0 \frac{\partial}{\partial z}$$

x_0, y_0, z_0 unit vector of each direction



Uncertainty principle



❖ Momentum operator

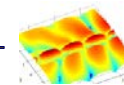
$$\frac{\hat{p}^2}{2m} \equiv -\frac{\hbar^2}{2m} \nabla^2$$

- Classical notation of energy

$$E = \frac{p^2}{2m} + V$$

- Hamiltonian operator of Schrödinger equation

$$\hat{H} = -\frac{\hbar^2}{2m} \nabla^2 + V = \frac{\hat{p}^2}{2m} + V$$



Uncertainty principle



❖ Example of position-momentum uncertainty

- Gaussian wavepacket

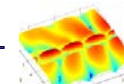
$$\Psi_G(z, t) \propto \int_k \exp\left[-\left(\frac{k - \bar{k}}{2\Delta k}\right)^2\right] \exp\{-i[\omega(k)t - kz]\} dk$$

at time $t = 0$ as

where
$$\Psi(z, 0) = \int_k \Psi_k(k) \exp(ikz) dk$$

$$\Psi_k(k) \propto \exp\left[-\left(\frac{k - \bar{k}}{2\Delta k}\right)^2\right]$$

$\Psi_k(k)$ is the representation of the wavefunction in k space



Uncertainty principle



❖ Example of position-momentum uncertainty

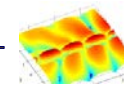
- With wavefunction in K space

$$\Psi_k(k) \propto \exp\left[-\left(\frac{k - \bar{k}}{2\Delta k}\right)^2\right]$$

- Probability of finding value $\hbar k$ for the momentum

$$P_k = |\Psi_k(k)|^2 \propto \exp\left[-\frac{(k - \bar{k})^2}{2(\Delta k)^2}\right]$$

corresponds to statistical Gaussian probability distribution with standard deviation Δk



Uncertainty principle



❖ Example of position-momentum uncertainty

- Gaussian wavepacket at time $t=0$

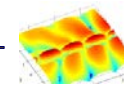
$$\Psi(z, 0) = \int_k \Psi_k(k) \exp(ikz) dk$$

→ Fourier transform of $\Psi_k(k)$

$$\Psi(z, 0) \propto \exp\left[-(\Delta k)^2 z^2\right]$$

Modulus square

$$|\Psi(z, 0)|^2 \propto \exp\left[-2(\Delta k)^2 z^2\right]$$



Uncertainty principle



❖ Example of position-momentum uncertainty

- Standard deviation in momentum space

$$|\Psi(z, 0)|^2 \propto \exp\left[-2(\Delta k)^2 z^2\right]$$

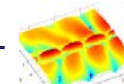
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- Standard deviation in space

$$|\Psi(z, 0)|^2 \propto \exp\left[-\frac{z^2}{2(\Delta z)^2}\right]$$



$$\Delta k \Delta z = 1 / 2$$



Uncertainty principle



❖ Example of position-momentum uncertainty

- Multiplying \hbar to each term

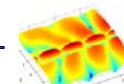
$$\Delta p \Delta z = \frac{\hbar}{2}$$

→ Gaussian pulse will broaden in space as it propagates, even though the range of k values remains the same

- Gaussian shape is the minimum possible product of these standard deviations

$$\Delta p \Delta z \geq \frac{\hbar}{2}$$

→ Uncertainty principle



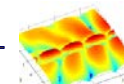
Uncertainty principle



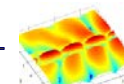
❖ Uncertainty principle to fourier analysis

$$\Delta\omega\Delta t \geq \frac{1}{2}$$

→ One cannot simultaneously have both a well defined frequency and a well defined time for a signal



Particle current



Particle current



❖ Divergence of vector \mathbf{F}

$$\operatorname{div} \mathbf{F} = \nabla \cdot \mathbf{F} = \frac{\partial F_x}{\partial x} + \frac{\partial F_y}{\partial y} + \frac{\partial F_z}{\partial z}$$

❖ Visualize \mathbf{F}

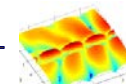
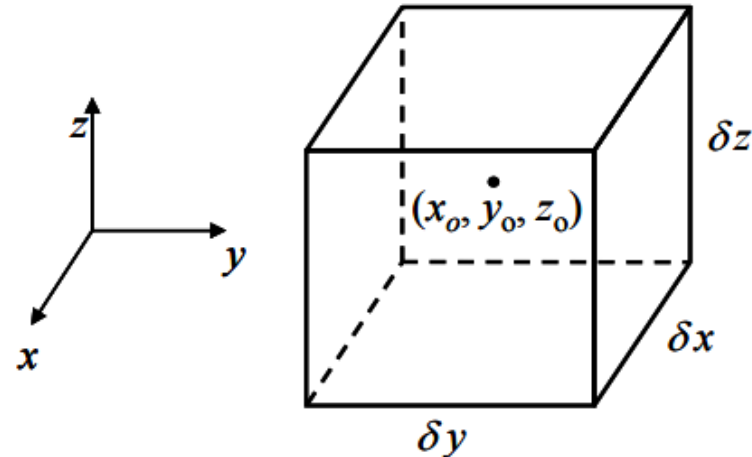
- Flow of some quantity, like mass or charge, through a small cuboidal little box
- Flow leaves the box at front

$$F_x(x_o + \delta x / 2, y_o, z_o) \delta y \delta z$$

$$F_x\left(x_o + \frac{\delta x}{2}, y_o, z_o\right) \delta y \delta z \equiv \mathbf{F}\left(x_o + \frac{\delta x}{2}, y_o, z_o\right) \cdot \delta \mathbf{A}_{yz}$$

- Flow arrives the box at back

$$F_x(x_o - \delta x / 2, y_o, z_o) \delta y \delta z$$



Particle current

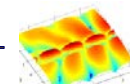


- ❖ Net amount leaving the box through the front or back

$$\begin{aligned} & F_x \left(x_o + \frac{\delta x}{2}, y_o, z_o \right) \delta y \delta z - F_x \left(x_o - \frac{\delta x}{2}, y_o, z_o \right) \delta y \delta z \\ &= \frac{F_x \left(x_o + \frac{\delta x}{2}, y_o, z_o \right) - F_x \left(x_o - \frac{\delta x}{2}, y_o, z_o \right)}{\delta x} \delta x \delta y \delta z \\ &\simeq \frac{\partial F_x}{\partial x} \delta x \delta y \delta z \end{aligned}$$

- ❖ Total amount of flow leaving small box dividing by δV

$$\text{div } \mathbf{F} = \nabla \cdot \mathbf{F} = \frac{\partial F_x}{\partial x} + \frac{\partial F_y}{\partial y} + \frac{\partial F_z}{\partial z}$$



Particle current



❖ Classically, conservation of flow of particles

$$\frac{\partial s}{\partial t} = -\nabla \cdot \mathbf{j}_p$$

s particle density

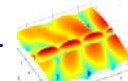
\mathbf{j}_p particle current density

❖ $s = |\Psi(\mathbf{r}, t)|^2$

$$\frac{\partial \Psi(\mathbf{r}, t)}{\partial t} = \frac{1}{i\hbar} \hat{H} \Psi(\mathbf{r}, t) \quad \frac{\partial \Psi^*(\mathbf{r}, t)}{\partial t} = -\frac{1}{i\hbar} \hat{H}^* \Psi^*(\mathbf{r}, t)$$

$$\frac{\partial}{\partial t} [\Psi^* \Psi] = \Psi^* \frac{\partial \Psi}{\partial t} + \Psi \frac{\partial \Psi^*}{\partial t}$$

$$\frac{\partial}{\partial t} [\Psi^* \Psi] + \frac{i}{\hbar} (\Psi^* \hat{H} \Psi - \Psi \hat{H}^* \Psi^*) = 0$$



Particle current



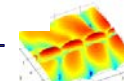
- ❖ Potential V is real and does not depend in time, Hamiltonian to be the form

$$\hat{H} \equiv -\frac{\hbar^2}{2m} \nabla^2 + V(r)$$

$$\begin{aligned} \underline{\Psi^* \hat{H} \Psi - \Psi \hat{H}^* \Psi^*} &= -\frac{\hbar^2}{2m} [\Psi^* \nabla^2 \Psi - \Psi \nabla^2 \Psi^*] + \Psi^* V \Psi - \Psi V \Psi^* \\ &= -\frac{\hbar^2}{2m} [\Psi^* \nabla^2 \Psi - \Psi \nabla^2 \Psi^*] \end{aligned}$$

$$\frac{\partial}{\partial t} [\Psi^* \Psi] + \frac{i}{\hbar} (\underline{\Psi^* \hat{H} \Psi - \Psi \hat{H}^* \Psi^*}) = 0$$

$$\frac{\partial}{\partial t} [\Psi^* \Psi] - \frac{i\hbar}{2m} (\Psi^* \nabla^2 \Psi - \Psi \nabla^2 \Psi^*) = 0$$



Particle current



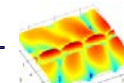
❖ Using algebraic trick

$$\begin{aligned}\Psi \nabla^2 \Psi^* - \Psi^* \nabla^2 \Psi &= \Psi \nabla^2 \Psi^* + \nabla \Psi \nabla \Psi^* - \nabla \Psi \nabla \Psi^* - \Psi^* \nabla^2 \Psi \\ &= \nabla \cdot (\Psi \nabla \Psi^* - \Psi^* \nabla \Psi)\end{aligned}$$

$$\frac{\partial}{\partial t} [\Psi^* \Psi] - \frac{i\hbar}{2m} (\Psi^* \nabla^2 \Psi - \Psi \nabla^2 \Psi^*) = 0$$

$$\frac{\partial (\Psi^* \Psi)}{\partial t} = -\frac{i\hbar}{2m} \nabla \cdot (\Psi \nabla \Psi^* - \Psi^* \nabla \Psi)$$

modulus square of wave function



Particle current



❖ Particle current

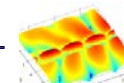
$$j_p = \frac{i\hbar}{2m} (\Psi \nabla \Psi^* - \Psi^* \nabla \Psi)$$

❖ For nth energy eigenstate

$$\Psi_n(\mathbf{r}, t) = \exp\left(-i \frac{E_n}{\hbar} t\right) \psi_n(\mathbf{r})$$

▪ Particle current

$$\mathbf{j}_{pn}(\mathbf{r}, t) = \frac{i\hbar}{2m} (\Psi_n(\mathbf{r}, t) \nabla \Psi_n^*(\mathbf{r}, t) - \Psi_n^*(\mathbf{r}, t) \nabla \Psi_n(\mathbf{r}, t))$$



Particle current



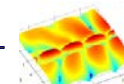
- Gradient has no effect on time factor → particle current

$$\begin{aligned}\mathbf{j}_{pn}(\mathbf{r}, t) &= \frac{i\hbar}{2m} \exp\left(-i\frac{E_n}{\hbar}t\right) \exp\left(i\frac{E_n}{\hbar}t\right) (\psi_n(\mathbf{r}) \nabla \psi_n^*(\mathbf{r}) - \psi_n^*(\mathbf{r}) \nabla \psi_n(\mathbf{r})) \\ &= \frac{i\hbar}{2m} (\psi_n(\mathbf{r}) \nabla \psi_n^*(\mathbf{r}) - \psi_n^*(\mathbf{r}) \nabla \psi_n(\mathbf{r}))\end{aligned}$$

❖ Does not depend on time

$$\mathbf{j}_{pn}(\mathbf{r}, t) = \mathbf{j}_{pn}(\mathbf{r})$$

- Particle current is constant in any energy eigenstate
- For real spatial eigenfunctions particle current is actually zero



❖ Uncertainty principle

$$\Delta p \Delta z \geq \frac{\hbar}{2}$$

- One cannot simultaneously have both a well defined real space and a well defined momentum space for a signal

❖ Particle current

- Particle current is constant in any energy eigenstate
- **Electron in eigenstate does not radiate electromagnetic radiation**

**Thank you
for your attention !!**

