Physics of Semiconductors and Nanostructures

ECE 4070/MSE 5470

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About the class

ECE 4070/MSE 5470: Physics of Semiconductors and Nanostructures
Instructor: Prof. Debdeep Jena (ECE & MSE)
Instructor's research area: Semiconductor Nano Electronic and Photonic Devices

Why is this course important?

- What lies 'under the hood' of cell phones, laptops, robotic controls, space exploration, modern cryptography, and the energy economy?

- What latest discoveries in these areas will transform the way things will be when you are in your mid-life?

- Google (2000), Facebook (2004), iPhone (2007) … all made possible by semiconductor nanostructures – by understanding and controlling the behavior of electrons, photons, phonons, and fundamental physical phenomena in them.

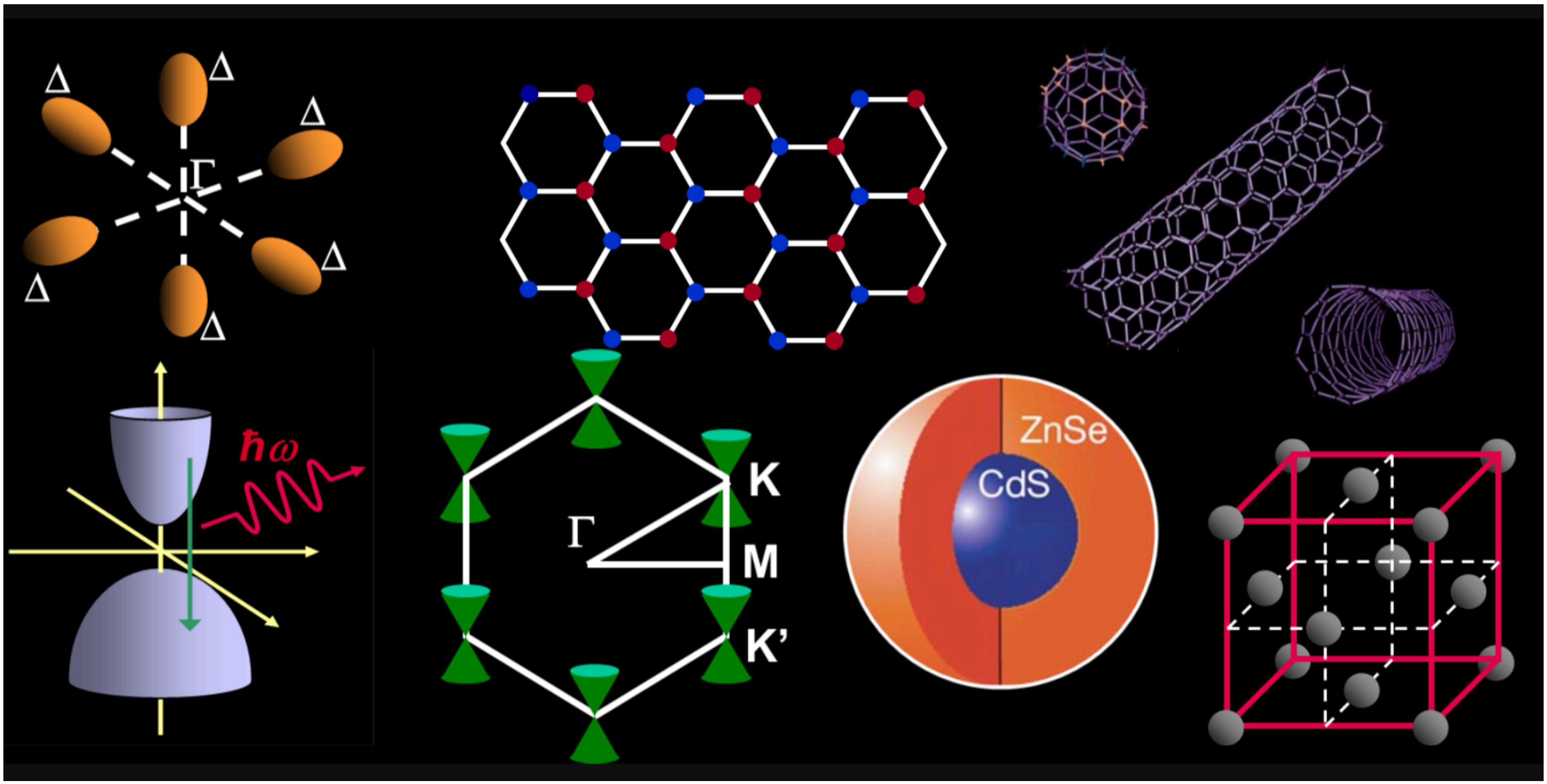
- This is a rare area where you can earn Mega $s doing fundamental science – e.g. the 2014 physics Nobel laureate Prof. Nakamura is a multir  ire and has a startup company on quantum-well LEDs.

+ $$!

- In this class I will teach you how this is done – and enable you to lead your generation!

About the class

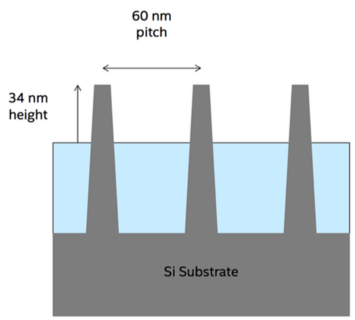
ECE 4070/MSE 5470: Physics of Semiconductors and Nanostructures
Instructor: Prof. Debdeep Jena (ECE & MSE)
Instructor's research area: Semiconductor Nano Electronic and Photonic Devices
We will use Prof. Farhan Rana's notes



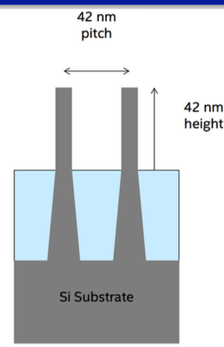
About the class

Electronic switches today

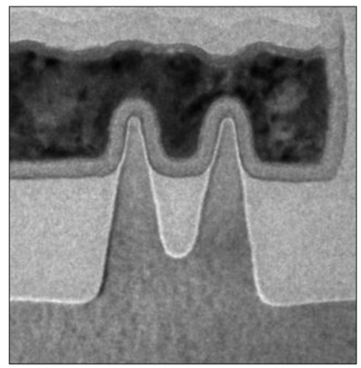
- *Earlier this week (August 11th) Intel announced…*



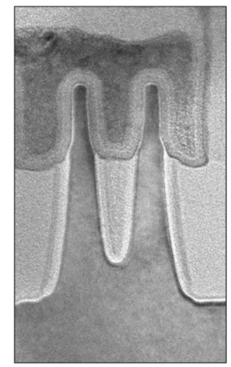
22 nm Process



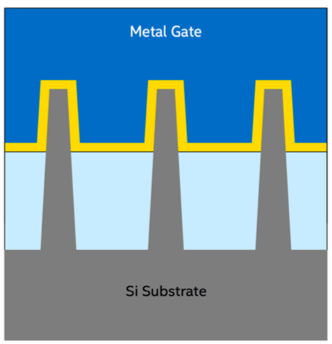
14 nm Process



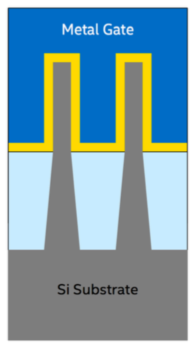
22 nm 1st Generation Tri-gate Transistor



14 nm 2nd Generation Tri-gate Transistor

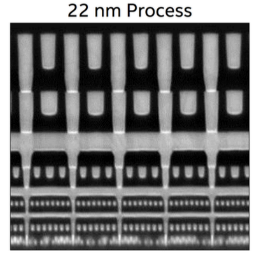


22 nm 1st Generation Tri-gate Transistor



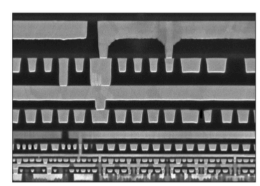
14 nm 2nd Generation Tri-gate Transistor

22 nm Process



80 nm minimum pitch

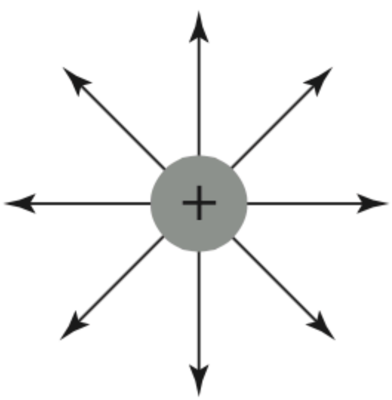
14 nm Process



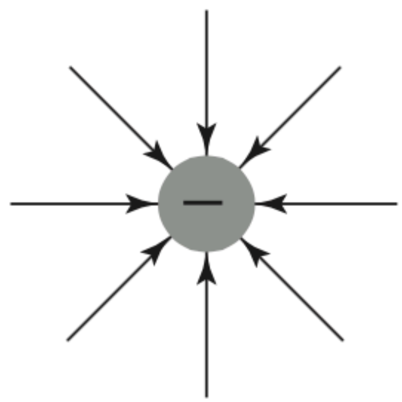
52 nm (0.65x) minimum pitch

Maxwell's equations: Classical EMag

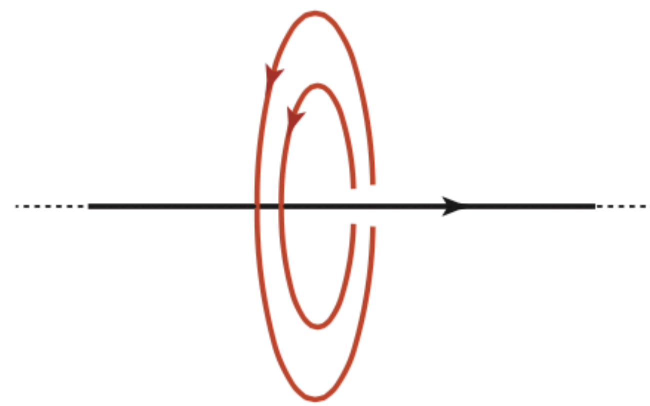
$$
\begin{aligned}
\nabla \cdot \mathbf{D} &= \rho, && \text{Gauss's law} \\
\nabla \cdot \mathbf{B} &= 0, && \text{Gauss's law} \\
\nabla \times \mathbf{E} &= -\frac{\partial \mathbf{B}}{\partial t}, && \text{Faraday's law} \\
\nabla \times \mathbf{H} &= \mathbf{J} + \frac{\partial \mathbf{D}}{\partial t}, && \text{Ampere's law.}
\end{aligned}
$$



$\nabla \cdot \mathbf{E} > 0$



$\nabla \cdot \mathbf{E} < 0$



$\nabla \times \mathbf{H} = \mathbf{J}$

Maxwell's equations: Classical EMag

$$
\begin{aligned}
\left(\nabla^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right)\mathbf{E} &= 0, \quad \text{Wave Equations}\\
\left(\nabla^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right)\mathbf{B} &= 0.
\end{aligned}
$$

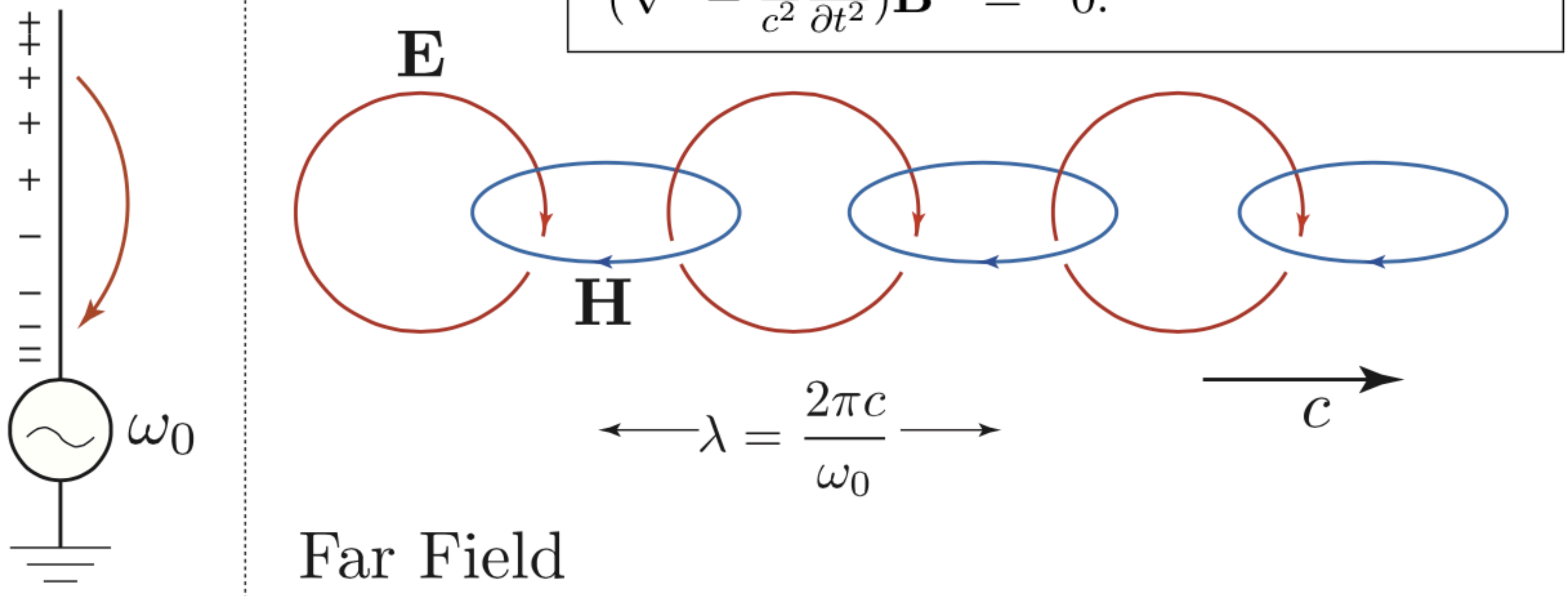


FIGURE 20.2: Antenna producing an electromagnetic wave.

Maxwell's equations: Birth of Light

$$\left(\nabla^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right)\mathbf{E} = 0, \quad \text{Wave Equations}$$
$$\left(\nabla^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right)\mathbf{B} = 0.$$

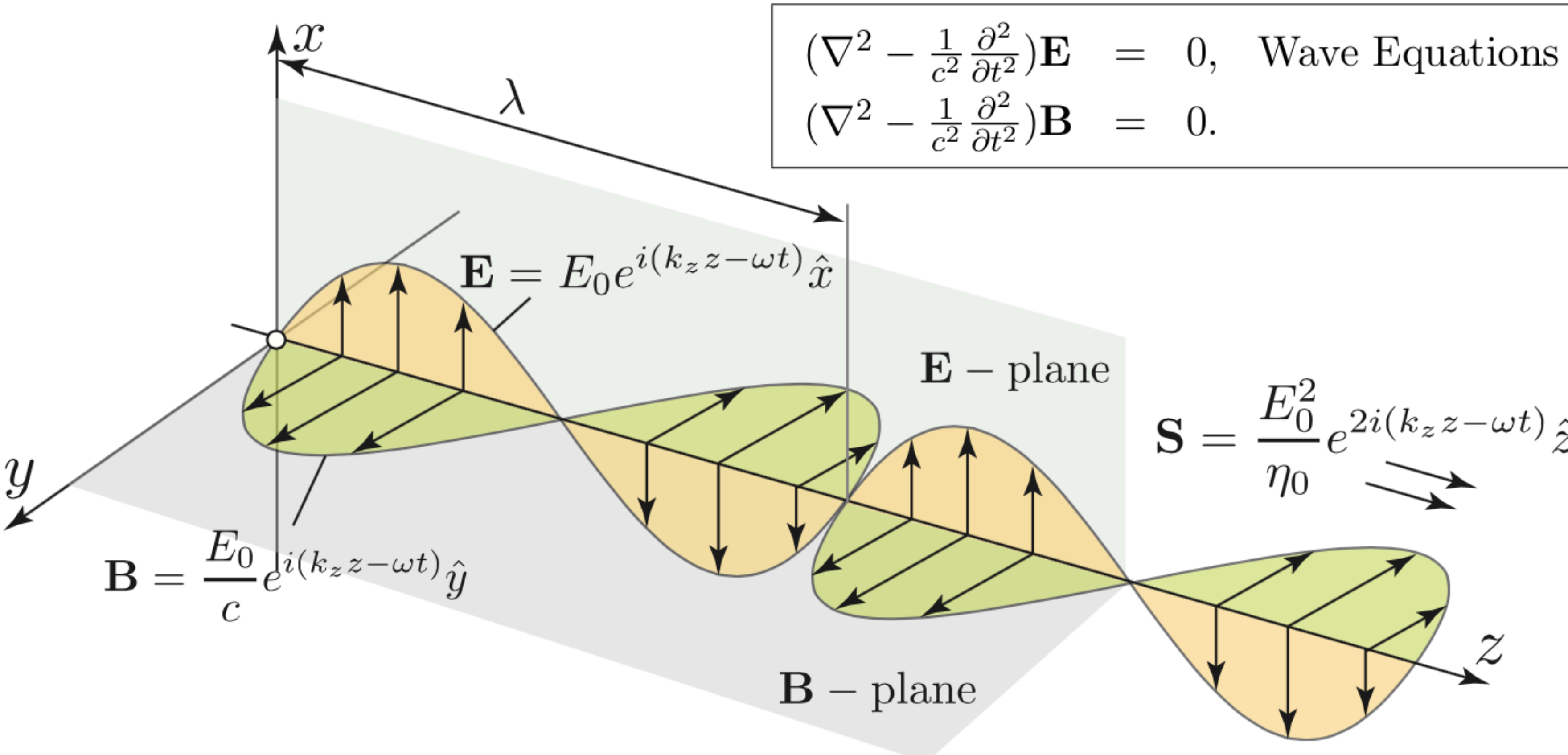
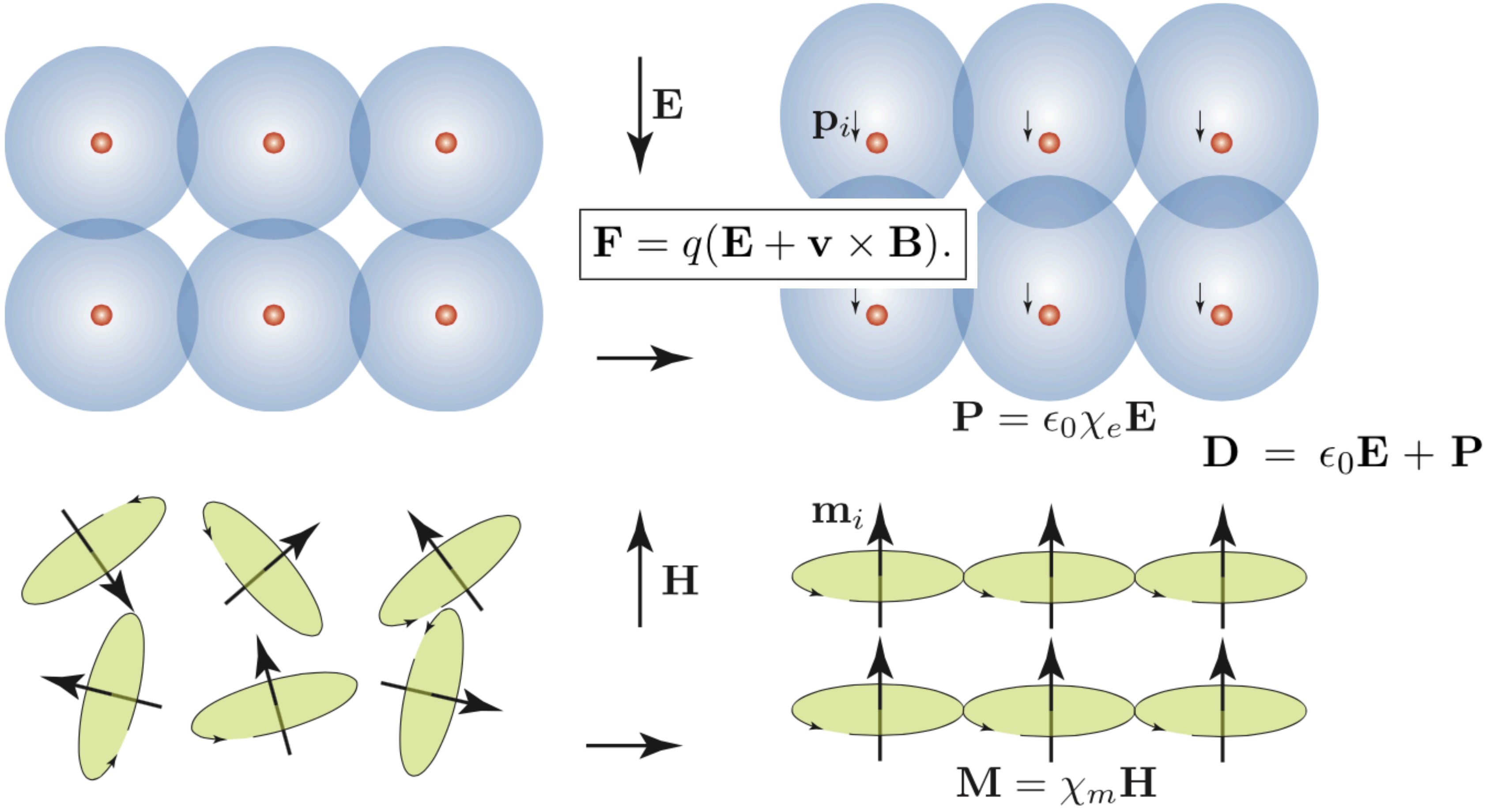


FIGURE 20.3: Electromagnetic wave.

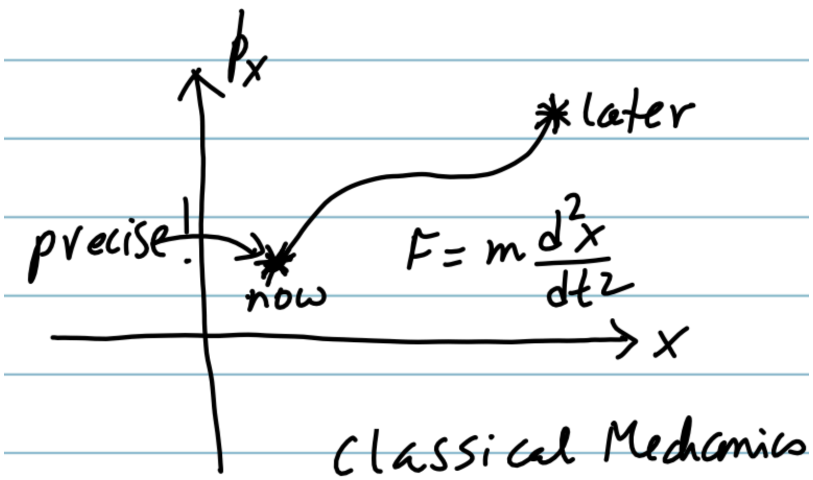
Maxwell's equations: Response of solids



$$\mathbf{B} = \mu_0(\mathbf{H} + \chi_m \mathbf{H}) = \mu_0\underbrace{(1 + \chi_m)}_{\mu_r}\mathbf{H} = \mu \mathbf{H}$$

FIGURE 20.4: Dielectric and Magnetic materials. Orientation of electric and magnetic dipoles by external fields, leading to electric and magnetic susceptibilities.

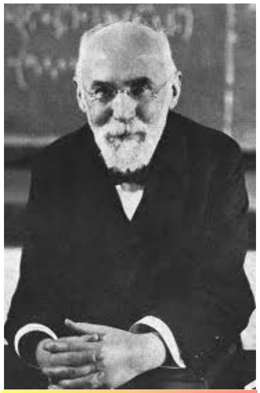
Time-evolution of a classical ‘charged’ object



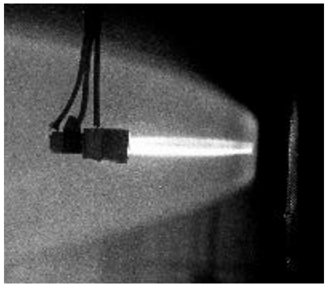
Newton

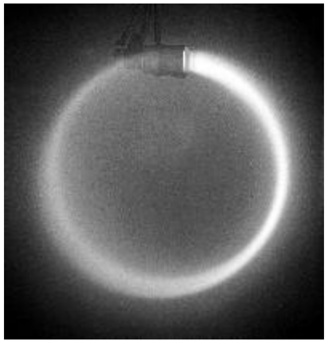
$$\mathbf{F} = -\nabla V(r) = \frac{d\mathbf{p}}{dt}$$

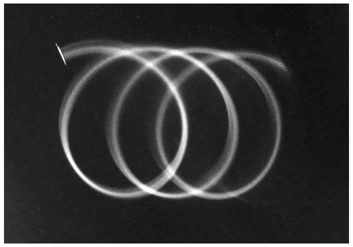
Path is deterministic



Lorentz



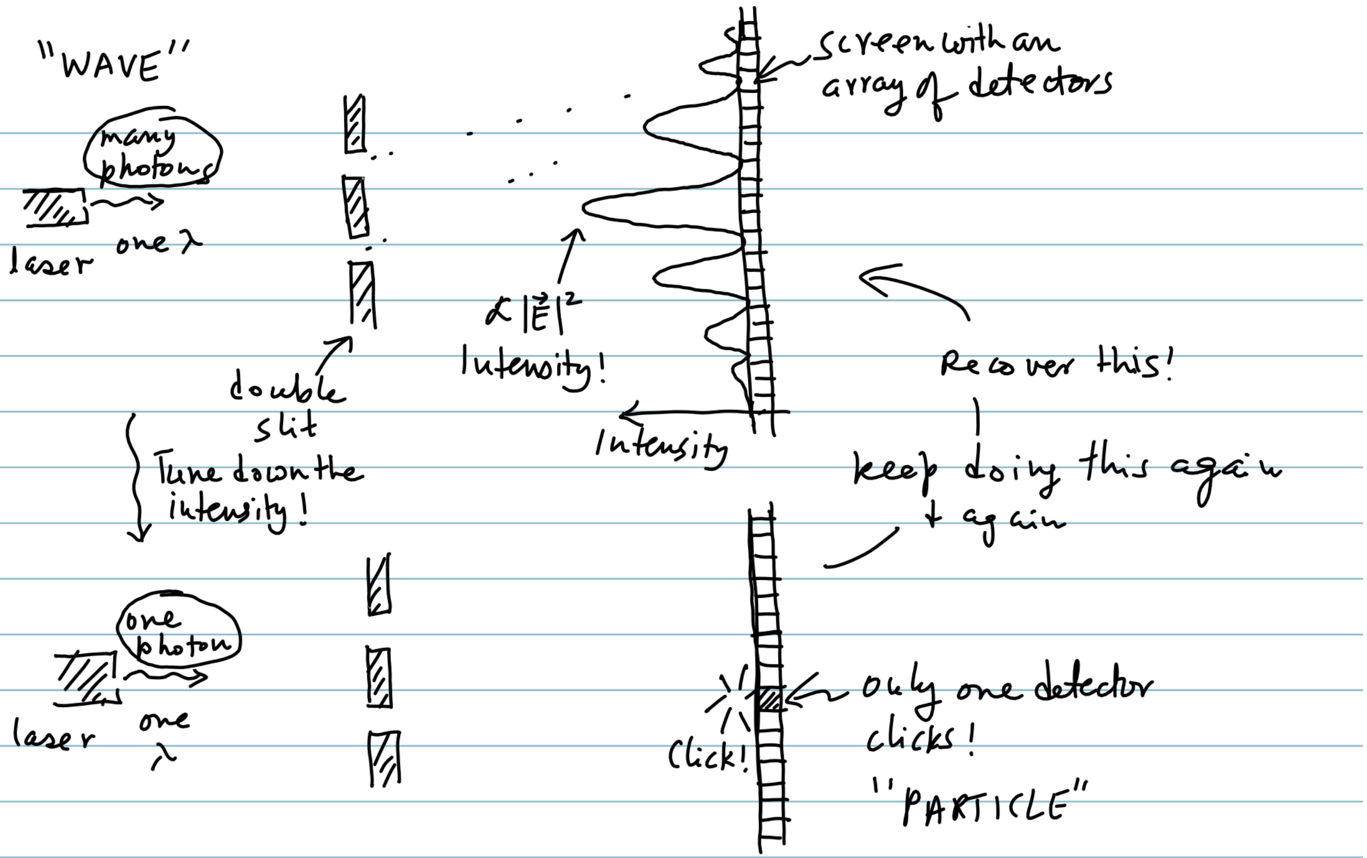




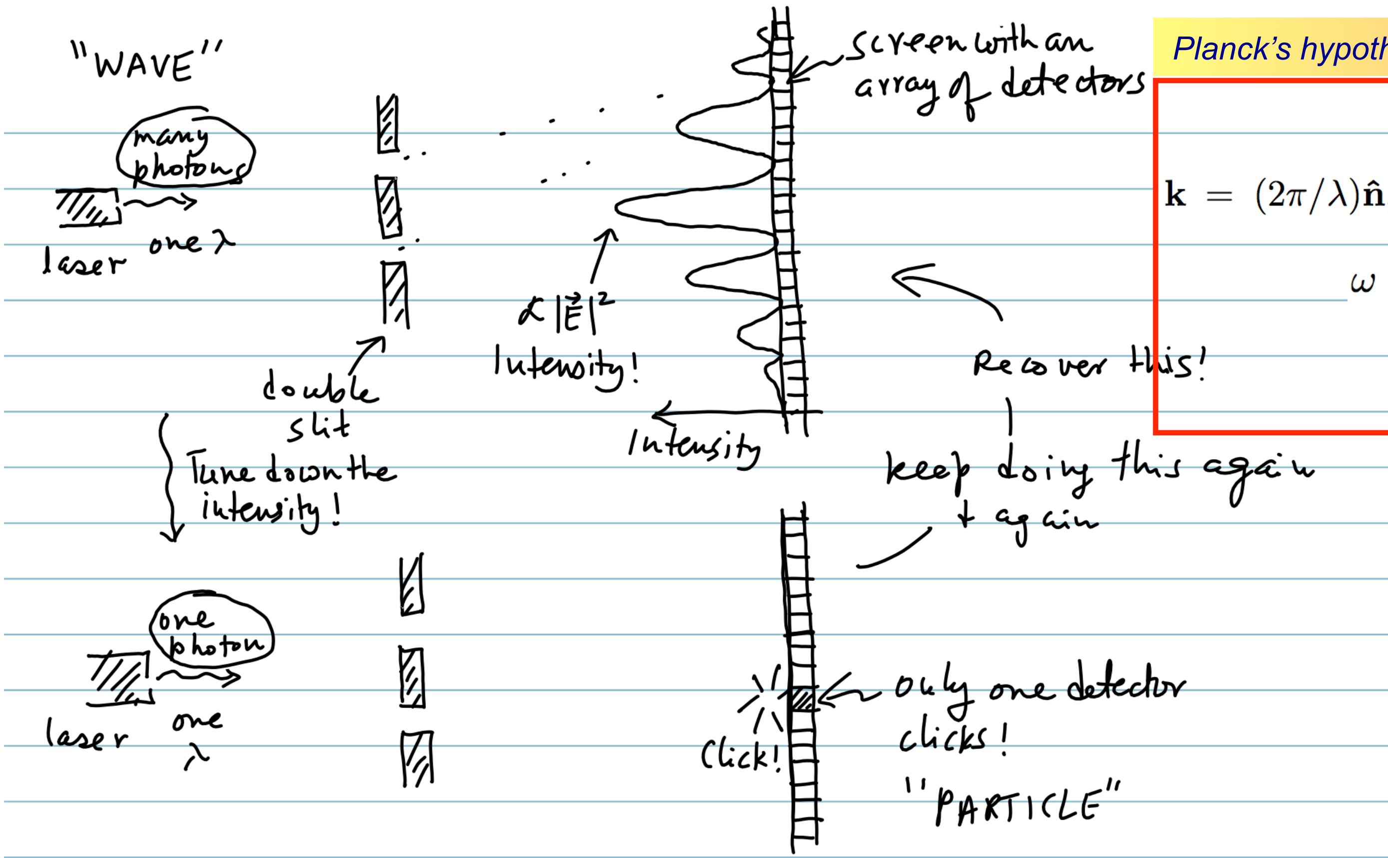
$$\mathbf{F} = q(\mathbf{E} + \mathbf{v} \times \mathbf{B})$$

Path is deterministic

Experiment: Light is a wave… or a particle?



Experiment: Light is a wave… or a particle?



Planck's hypothesis for photons to explain expts:

$$\mathbf{p} = \hbar\mathbf{k}$$

$\mathbf{k} = (2\pi/\lambda)\hat{\mathbf{n}}$, $\hat{\mathbf{n}}$ the direction of propagation

$\omega = c|\mathbf{k}|$ with c the speed of light

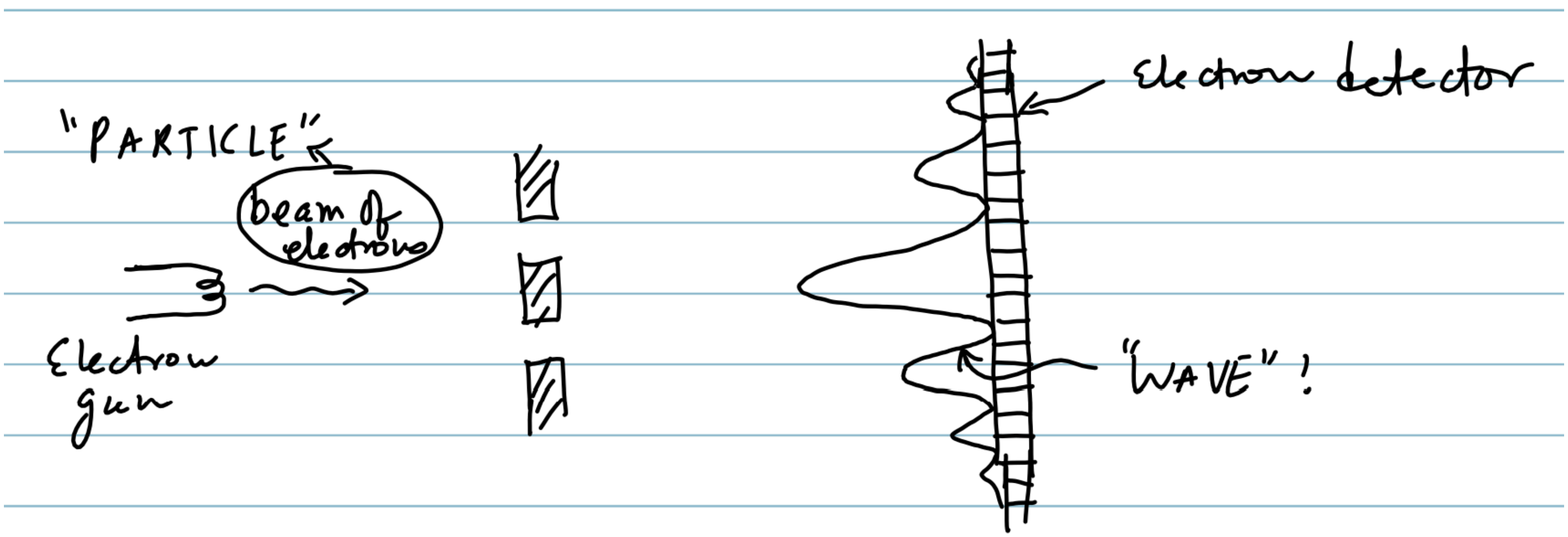
$$E = \hbar\omega$$

Einstein: look downstairs!

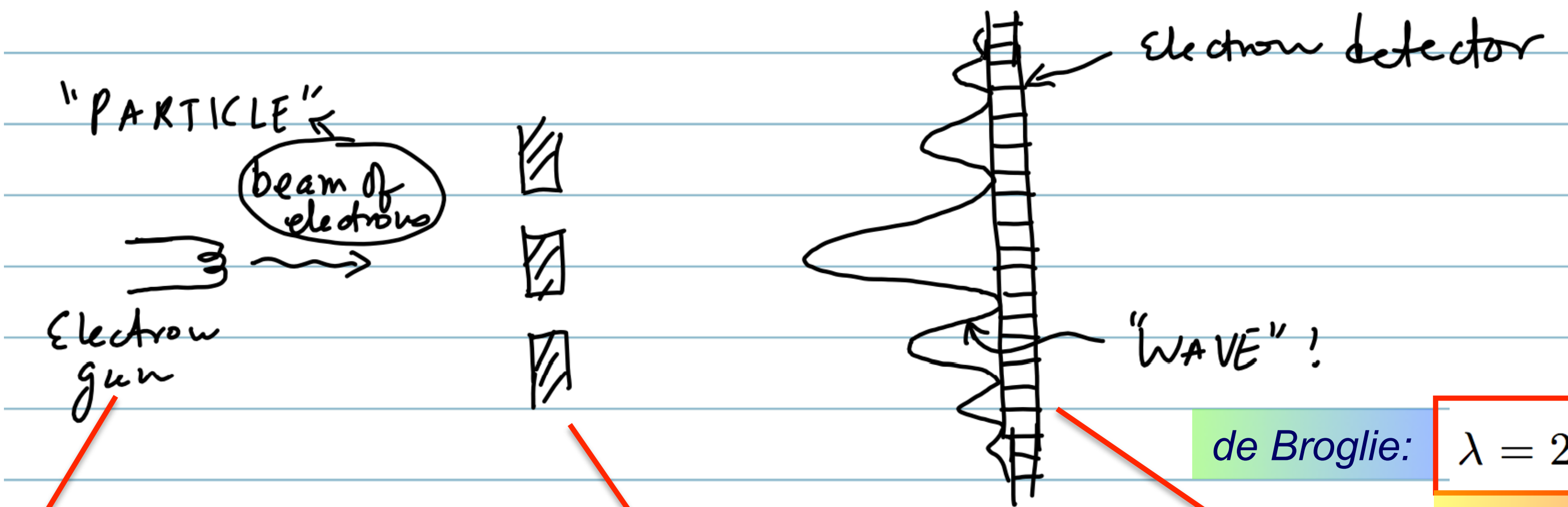
$$p = mv/\sqrt{1-(v/c)^2}$$

- *The only way an object of mass m=0 can have momentum is if its speed v=c, or the speed of light.*
- *A photon is exactly such an object. No mass, all energy, and a finite momentum!*

An electron is a particle… or a wave?



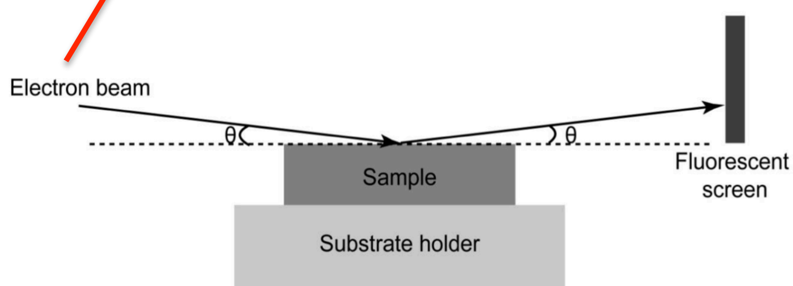
An electron is a particle… or a wave?



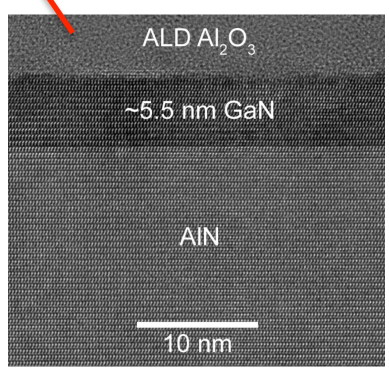
de Broglie: $\lambda = 2\pi\hbar/|\mathbf{p}|$

For both waves, and particles!

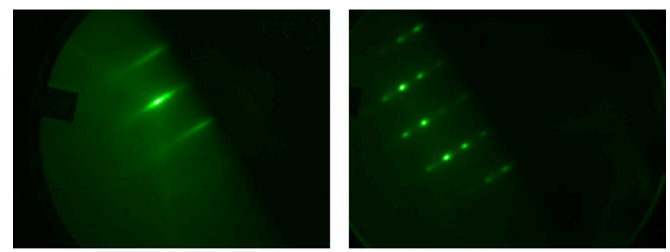
Guowang Li (Results from our lab!)



Electron beam incident on a crystal (RHEED)



Atomic structure of a crystal (grating!)



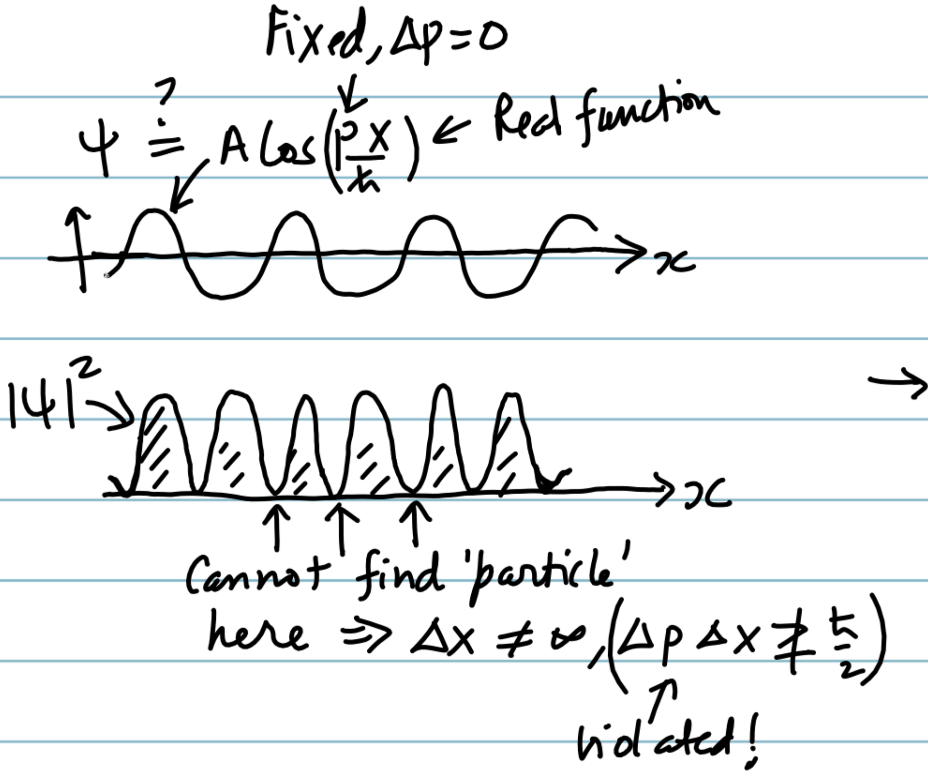
(a) (b)

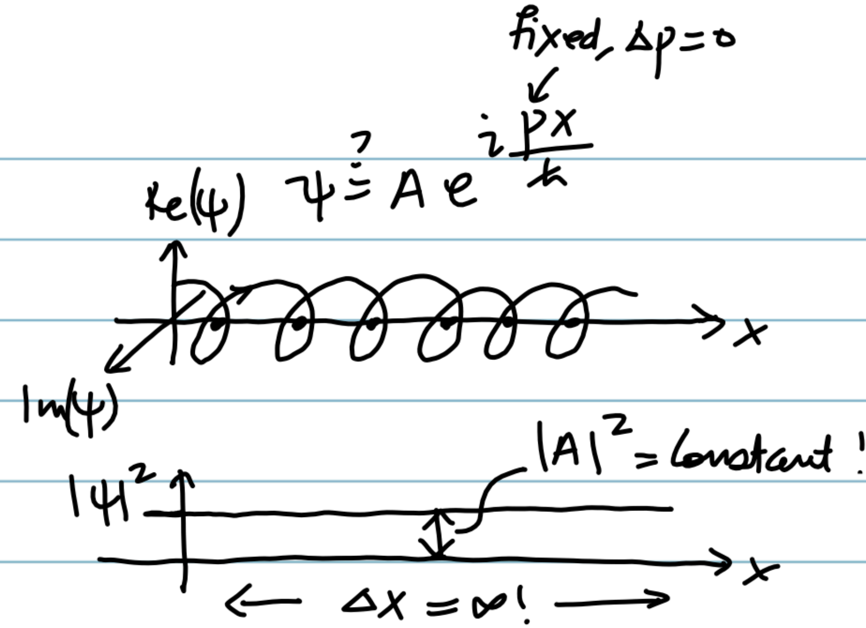
Figure 2.7: RHEED patterns of (a) smooth surface and (b) crystalline but rough of GaN surface.

Electron diffraction pattern on a screen

Wave and particle → need for a wavefunction

Quantum states (electrons, photons) behave as waves AND particles. How do we describe them quantitatively?



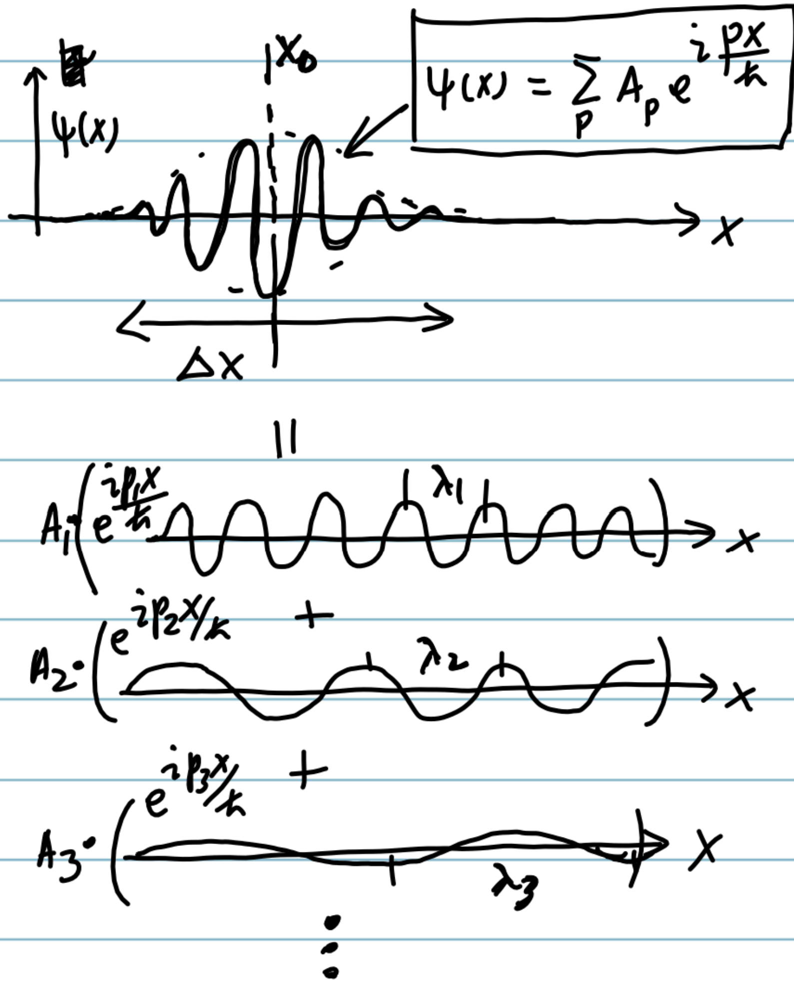


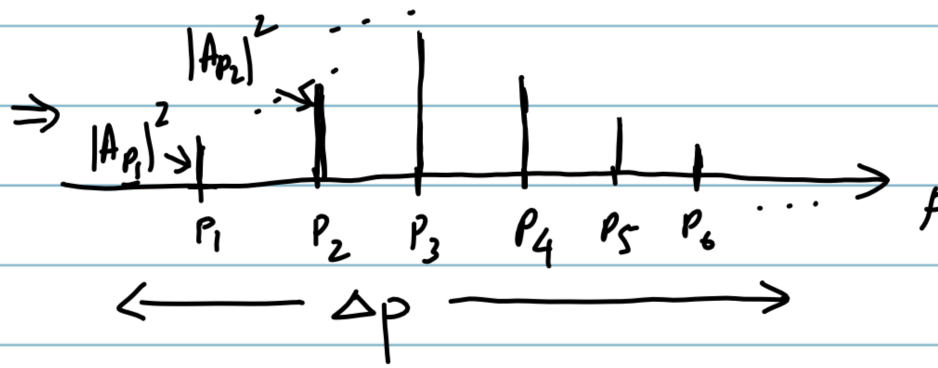
The complex exponential $e^{i\frac{px}{\hbar}} = \psi$ oscillates with x, yet $|\psi|^2$ = Constant ! ⇒ good candidate for a wavefunction that respects $\Delta x \Delta p \geq \frac{\hbar}{2}$.

- *The state of the free quantum particle cannot be represented by independent 'numbers' (x, p_x).*
- *We need a function whose amplitude oscillates in space, yet its magnitude never goes to zero.*
- *The complex exponential e^{ikx} satisfies these requirements, and respects the uncertainty relation.*

Constructing wavefunctions: superposition

By linear superposition of complex exponentials, we can create 'particle' like or 'wave' like states as desired for the problem.



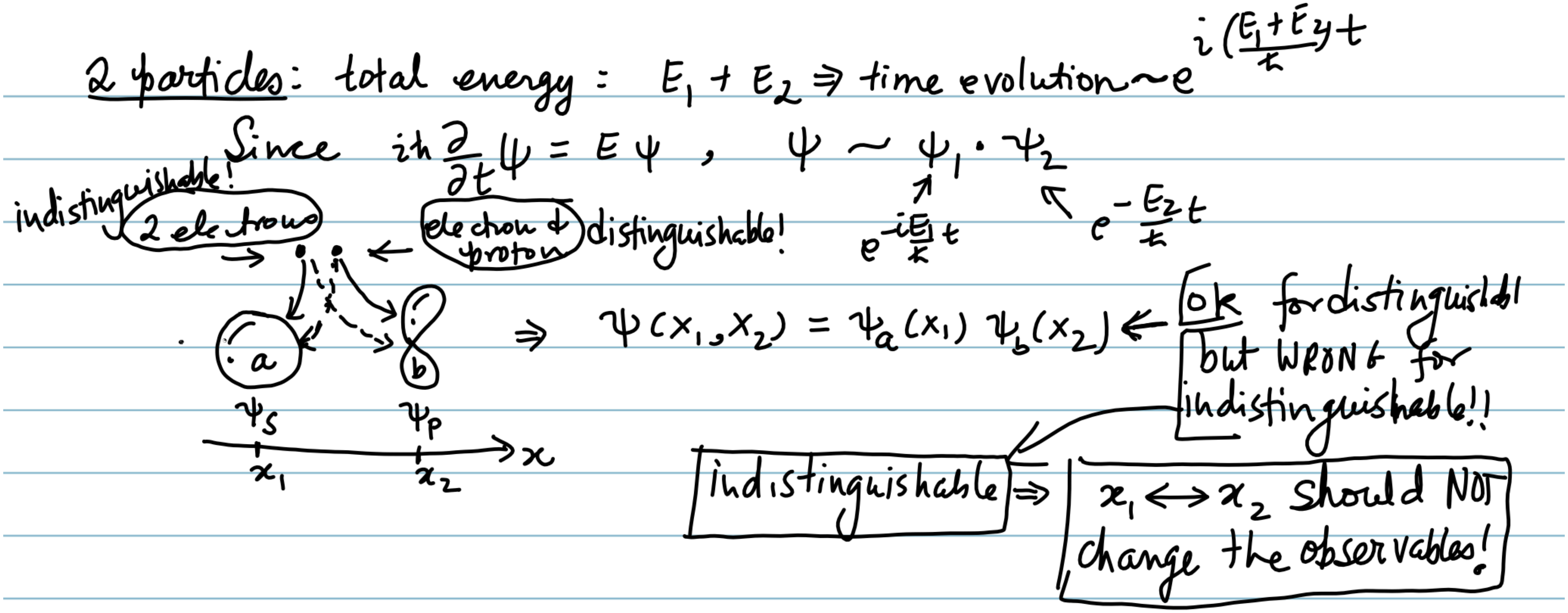


The best we can do to locate a "particle" ⇒ a '<u>wave packet</u>'.

$$\Rightarrow \boxed{\psi(x) = \sum_p A_p e^{i\frac{px}{\hbar}}}$$ is an allowed "wavefunction".

- *Drawing on Fourier series, we realize that we can create any wavefunction shape to capture the correct physics of the problem. Note the corresponding reciprocal space weight distribution.*

Identity crisis: Indistinguishable particles



$$\psi(x_1, x_2) = \psi_a(x_1)\psi_b(x_2)$$

This is OK for distinguishable particles such as a proton and an electron.
*But NOT OK for **indistinguishable particles** such as two electrons!*
For example, |psi|^2 should not change on swapping $x_1 \leftrightarrow x_2$.
How must we then write the wavefunction for two identical particles?

Resolution of identity crisis: Bosons & Fermions

This is necessary for indistinguishable particles.

$$P(x_2, x_1) = P(x_1, x_2) \rightarrow |\psi(x_2, x_1)|^2 = |\psi(x_1, x_2)|^2.$$

$$\psi(x_1, x_2) = \psi_a(x_1)\psi_b(x_2)$$

$$\psi(x_1, x_2) = \psi_a(x_1)\psi_b(x_2) + \psi_a(x_2)\psi_b(x_1)$$

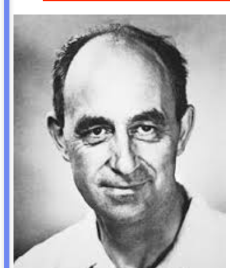
$$\psi(x_2, x_1) = +\psi(x_1, x_2)$$

$$\psi(x_1, x_1) = +\psi(x_1, x_1)$$

$$f_{BE}(E) = \frac{1}{e^{\frac{E-\mu}{kT}} - 1}$$

The Bose-Einstein distribution!
Particles are called ***Bosons.***
Examples: Photons, Phonons

Bose



Fermi

$$\psi(x_1, x_2) = \psi_a(x_1)\psi_b(x_2) - \psi_a(x_2)\psi_b(x_1)$$

$$\psi(x_2, x_1) = -\psi(x_1, x_2),$$

$$\psi(x_1, x_1) = -\psi(x_1, x_1) \rightarrow \psi(x_1, x_1) = 0.$$

The Pauli exclusion principle!

$$f_{FD}(E) = \frac{1}{1 + e^{\frac{E-E_F}{kT}}}$$

The Fermi-Dirac distribution!
Particles are called ***Fermions.***
Examples: Electrons, Protons

- *Note: Why not* $\psi(x_2, x_1) = e^{i\phi}\psi(x_1, x_2)$ *? Majorana particles → later…*

Math preliminaries before the physics…

$$\psi_p(x) = Ae^{ipx/\hbar}$$

Wavefunction ties x and p together.
Must respect the uncertainty principle.

$$\hat{p} = -i\hbar\partial/\partial x$$

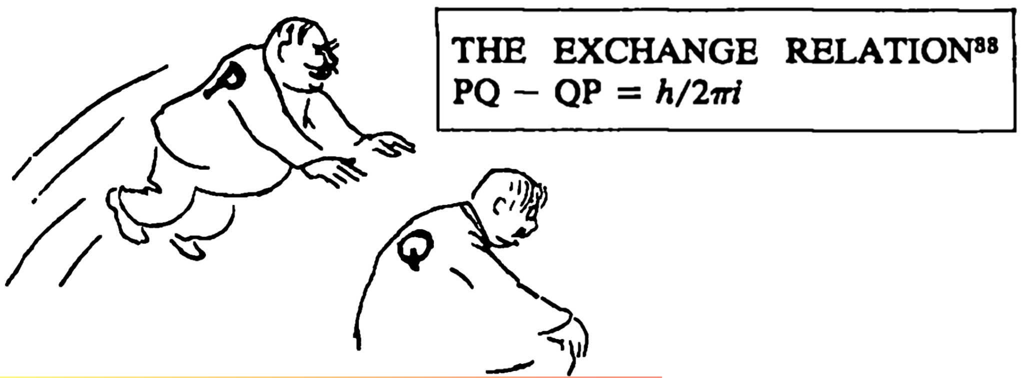
Obervables are mathematical operators.
They act on the wavefunction to extract info.

$$\hat{p}\psi_p(x) = (\hbar k)\psi_p(x)$$

The states of definite value of an operator are called the eigenstates of that operator.

$$x\hat{p} - \hat{p}x = [x, \hat{p}] = i\hbar.$$

Unlike classical mechanics, some operators fail to commute!



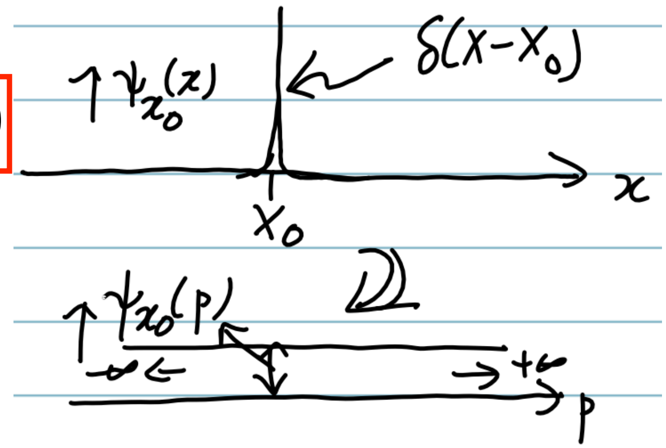
Non-commuting actions…
Ref: Gamow, Thirty years that shook physics.

Definite momentum, and definite location states

A state of definite location x_0:
Must be an eigenstate of operator x, with eigenvalue x_0:

$$x\psi_{x_0}(x) = x_0\psi_{x_0}(x) \implies \boxed{\psi_{x_0}(x) = \delta(x - x_0)}$$

Definite in real space → spread out in momentum

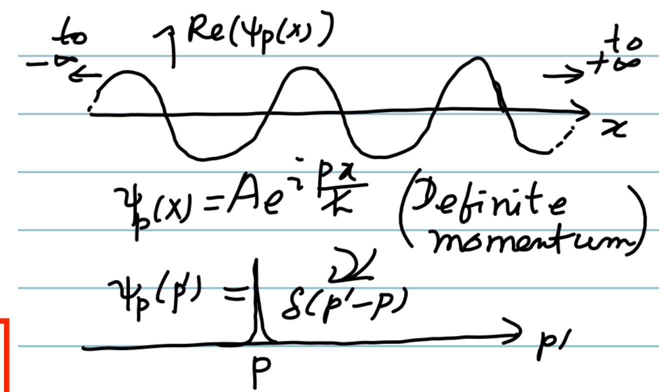


A state of definite momentum p:
Must be an eigenstate of operator –ih(d/dx), with eigenvalue p:

$$\hat{p}_x\psi_p(x) = p_x\psi_p(x) \implies -i\hbar\frac{d}{dx}\psi_p(x) = p_x\psi_p(x)$$

$$\boxed{\psi_p(x) = Ae^{i\frac{p_x x}{\hbar}} = Ae^{ik_x x}}$$

Definite in momentum → spread out in real space



States of definite location and definite momentum are unique in quantum mechanics.

States of definite energy: Schrodinger equation

States of definite energy are not unique, because they depend on the 'potential' V(x)

In classical mechanics, the energy of a particle is:

$$E_{cl} = \frac{p^2}{2m} + V(r)$$

In quantum mechanics, r & p cannot be simultaneously determined because [x,p]=ih. Thus, we must solve an equation to obtain the energy.

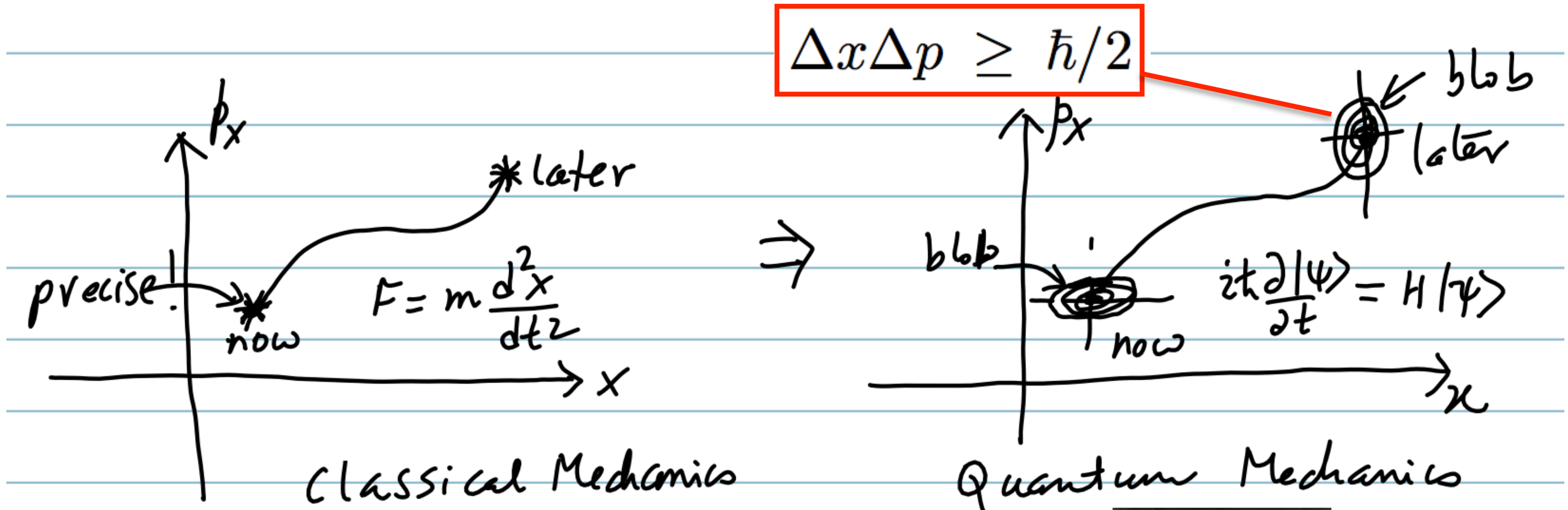
Schrodinger

$$[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)]\psi_E(x) = E\psi_E(x).$$

The Schrodinger equation gives us the prescription to find the states of definite energy.

$$\underbrace{[\frac{\hat{p}^2}{2m} + V(r)]}_{\hat{H}}|\psi\rangle = E|\psi\rangle$$

Time-evolution of states: Time-dep. Schr. Eqn.



Newton

Schrodinger

$$\mathbf{F} = -\nabla V(r) = \frac{d\mathbf{p}}{dt}$$

Path is deterministic

$$i\hbar\frac{\partial|\psi\rangle}{\partial t} = [\frac{\hat{\mathbf{p}}^2}{2m} + V(\mathbf{r},t)]|\psi\rangle$$

Path respects uncertainty relation

States of definite energy are stationary states

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t}=\underbrace{[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x)]}_{\hat{H}}\Psi(x,t).$$

$$\frac{d\langle\hat{A}\rangle}{dt}=-\frac{i}{\hbar}\langle[\hat{A},\hat{H}]\rangle$$

Ehrenfrest's theorem for the time evolution of an operator.

$$\Psi(x,t)=\chi(t)\psi(x)$$

Try set of solutions that allow the separation of x and t.

$$i\hbar\frac{\dot{\chi}(t)}{\chi(t)}=\frac{\hat{H}\psi(x)}{\psi(x)}=E.$$

$$\Psi_E(x,t)=\psi_E(x)e^{-i\frac{E}{\hbar}t}$$

*This means that the **amplitude** of states of definite energy oscillate with time with frequency E/h*

$$|\Psi_E(x,t)|^2=|\psi_E(x)|^2$$

*But observables relate to the probability, which is time independent → this is why they care called **stationary states**.*

- *States of definite energy (energy eigenvalues of the time-independent Schrodinger equation) are states of definite energy.*
- *Their probability density does not change with time → they are called stationary states.*
- *This is analogous to the 1st law of classical mechanics: quantum states of definite energy will continue to remain in those states unless perturbed by a potential.*

The Postulates of Quantum Mechanics

The five basic postulates of quantum mechanics are:

(1) The state of any physical system at a given time t is completely represented by a state vector $|\Psi\rangle = |\Psi(\mathbf{r}, t)\rangle$.

(2) For an observervable quantity A there is an operator $\hat{\mathbf{A}}$. The eigenvalues of $\hat{\mathbf{A}}$ are the possible results of the measurements of A, that is, denoting the eigenvalues of $\hat{\mathbf{A}}$ by a,

$$\hat{\mathbf{A}}|a\rangle = a|a\rangle, \tag{2.23}$$

and the probability of a measurement of A yielding the value a at time t is $|\langle a|\Psi(t)\rangle|^2$. The a's, which are the results of possible measurements, must be real. This implies that $\hat{\mathbf{A}}$ must be a linear hermitian operator.

(3) A measurement of $|\Psi\rangle$ that leads to an eigenvalue a_i leads the quantum mechanical system to *collapse* into the eigenstate $|\Psi_i\rangle$, which is the eigenstate corresponding to the eigenvalue a_i. So a measurement affects the state of the quantum system.

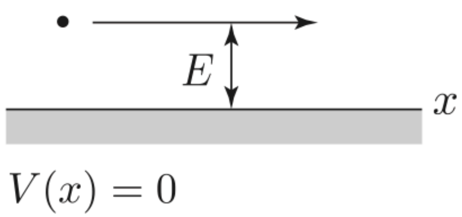
(4) There exists a hermitian operator $\hat{\mathbf{H}}$ such that

$$i\hbar \frac{\partial |\Psi(\mathbf{r}, t)\rangle}{\partial t} = \hat{\mathbf{H}}|\Psi(\mathbf{r}, t)\rangle. \tag{2.24}$$

(5) Two classical dynamical variables a, b, which are conjugate in the Hamiltonian sense, are represented by Schrodinger operators $\hat{\mathbf{A}}$,$\hat{\mathbf{B}}$, which obey

$$\hat{\mathbf{A}}_i \hat{\mathbf{B}}_j - \hat{\mathbf{B}}_j \hat{\mathbf{A}}_i = i\hbar \delta_{ij}. \tag{2.25}$$

The free electron



Free Electron

$$-\frac{\hbar^2}{2m_e}\frac{d^2}{dx^2}\psi(x) = E\psi(x)$$

V(x) = 0

$$\psi(x) = Ae^{ikx} + Be^{-ikx}$$

$$k = \sqrt{\frac{2m_e E}{\hbar^2}} = \frac{2\pi}{\lambda}$$

Allowed momenta are continuous

$$E = \frac{\hbar^2 k^2}{2m_e}$$

Energy spectrum is continuous

$$\hat{p}_x\psi(x) = -i\hbar\frac{d}{dx}\psi(x) = -i\hbar(ikAe^{ikx} - ikBe^{-ikx}) = \hbar k(Ae^{ikx} - Be^{-ikx}) \neq p\psi(x)$$

Not a momentum eigenstate

but... for $\psi_{\rightarrow}(x) = Ae^{ikx}$,

$$\hat{p}_x\psi_{\rightarrow}(x) = -i\hbar\frac{d}{dx}\psi_{\rightarrow}(x) = -i\hbar(ikAe^{ikx}) = \hbar k\psi_{\rightarrow}(x) = p\psi_{\rightarrow}(x)$$

momentum eigenstate

Restrict particle in space → Quantization

If we restrict the 'particle' in one space, it quantizes the allowed 'vectors' in the reciprocal space.

$\psi_p(x+L) = \psi_p(x)$ → $e^{ikL} = 1 = e^{i2\pi \times n}$, and $k_n = n \times (2\pi/L)$. Here $n = 0, \pm1, \pm2, \ldots$

Particle on a 'RING'

$\psi_n(x) = \frac{1}{\sqrt{L}} e^{ik_n x}$ $k_n = \frac{2\pi}{L} \cdot n$ $n = 0, \pm1, \pm2, \ldots$

Call this 'state vector' $|n\rangle$.

The state functions form a 'set'

$\{ \ldots \psi_{-3}(x), \psi_{-2}(x), \psi_{-1}(x), \psi_0(x), \psi_{+1}(x), \psi_{+2}(x), \ldots \}$

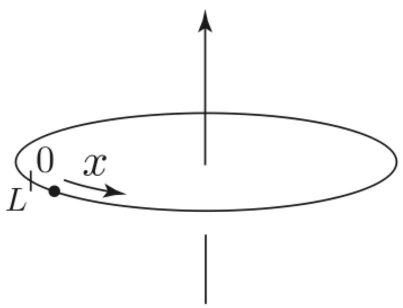
Note: $\int_0^L \psi_n^*(x) \psi_m(x) dx = \delta_{nm}$! ⇒ functions are ORTHOGONAL!

$\langle n | m \rangle = \delta_{nm}$ ⇐ Vectors are "perpendicular"!

The set of wave functions $[\ldots\psi_{-2}(x), \psi_{-1}(x), \psi_0(x), \psi_1(x), \psi_2(x), \ldots] = [\psi_n(x)]$ are special. We note that $\int_0^L dx \psi_m^\star(x)\psi_n(x) = \delta_{nm}$, i.e., the functions are orthogonal. *Any* general wavefunction representing the particle $\psi(x)$ can be expressed as a linear combination of this set. This is the principle of superposition, and a basic mathematical result from Fourier theory. Thus the quantum mechanical state of a particle may be represented as $\psi(x) = \sum_n A_n \psi_n(x)$. Clearly, $A_n = \int dx \psi_n^\star(x)\psi(x)$. Every wavefunction constructed in this fashion represents a permitted state of the particle, as long as $\sum_n |A_n|^2 = 1$.

- *The set of states {...|-1>,|0>,|+1>,…} is an orthogonal basis for constructing the wavefunction.*
- *One can draw an analogy to vector spaces, and use the tools of linear algebra on states.*

The particle on a ring



Particle on a ring

3.4 Not so free: particle in a ring

$$\psi(x+L) = \psi(x) \rightarrow e^{ik(x+L)} = e^{ikx} \rightarrow e^{ikL} = 1 \rightarrow kL = 2n\pi$$

Momentum is quantized

$$\boxed{k_n = \frac{2\pi}{L}n}, n = 0, \pm 1, \pm 2, \ldots$$

$$\psi(n,x) = Ae^{ik_n x}.$$

$$\int_0^L dx|\psi(n,x)|^2 = 1 \rightarrow |A|^2 \times L = 1 \rightarrow A = \frac{1}{\sqrt{L}} \rightarrow \boxed{\psi(n,x) = \frac{1}{\sqrt{L}}e^{ik_n x}}$$

Note that $n = 0$ is *allowed* as a result of the periodic boundary condition.

Energy spectrum is discrete,
Zero energy is allowed

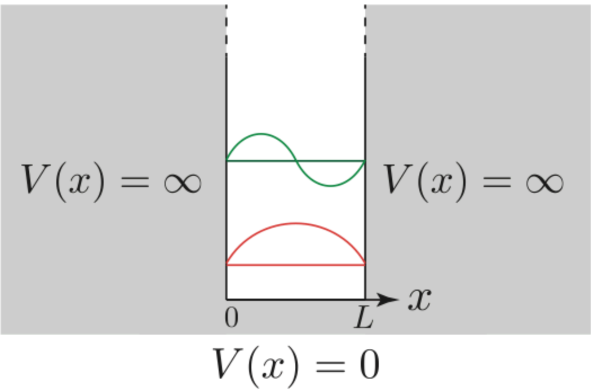
$$E_n = \frac{\hbar^2 k_n^2}{2m_e} = n^2 \frac{(2\pi\hbar)^2}{2m_e L^2} = n^2 \frac{h^2}{2m_e L^2}$$

Angular momentum is quantized

$$L = p \times r = \hbar k_n \times \frac{L}{2\pi} = \frac{2\pi\hbar}{L}n \times \frac{L}{2\pi} = n\hbar$$

The particle in a box

$$V(x) = 0, \quad 0 \leq x \leq L$$
$$V(x) = \infty, \quad x < 0, x > L$$



Particle in a box

The major change is that $\psi(x) = 0$ in regions where $V(x) = \infty$.

$$\psi(x) = Ae^{ikx} + Be^{-ikx} \rightarrow \psi(0) = 0 = A + B, \psi(L) = Ae^{ikL} + Be^{-ikL} = 0$$

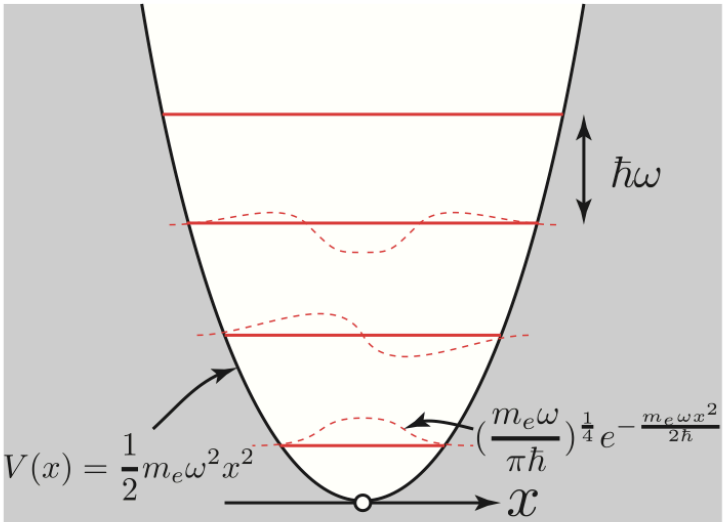
$$\frac{A}{B} = -e^{-i2kL} = -1 \rightarrow 2kL = 2n\pi \rightarrow \boxed{k_n = n\frac{\pi}{L}}, n = \pm1, \pm2, \pm3, ...$$

Note that $n = 0$ is *not allowed*, because then $\psi(x) = 0$ and there is no particle wavefunction after normalization over the length L is

$$\psi(n, x) = \sqrt{\frac{2}{L}}\sin(n\frac{\pi}{L}x) = \sqrt{\frac{2}{L}}\sin(k_n x)$$

Energy spectrum is discrete, zero energy NOT allowed!

$$E_n = n^2\frac{(\pi\hbar)^2}{2m_e L^2} = n^2\frac{h^2}{8m_e L^2}$$



Harmonic Oscillator

$$V(x) = \frac{1}{2}m_e\omega^2 x^2$$

$$a = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + \frac{i}{m\omega}\hat{p}\right)$$

$$a^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} - \frac{i}{m\omega}\hat{p}\right)$$

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(a^\dagger + a)$$

$$\hat{p} = i\sqrt{\frac{m\omega\hbar}{2}}(a^\dagger - a)$$

Can solve the problem using raising and lowering operators

$$\psi_n(x) = \frac{1}{\sqrt{2^n\, n!}} \cdot \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \cdot e^{-\frac{m\omega x^2}{2\hbar}} \cdot H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right), \qquad n = 0, 1, 2, \ldots.$$

The functions H_n are the Hermite polynomials,

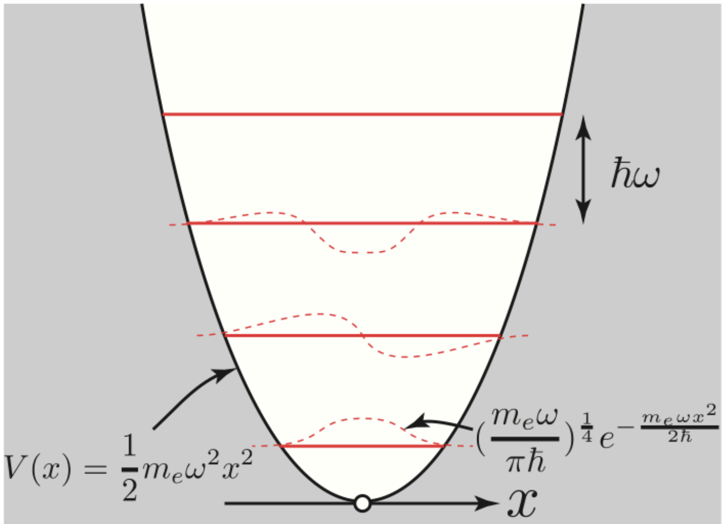
$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n}\left(e^{-x^2}\right).$$

The corresponding energy levels are

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right).$$

Energy levels equally spaced
Zero energy NOT allowed!

The harmonic oscillator



$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(a^\dagger + a)$$

$$V(x) = \frac{1}{2}m_e\omega^2x^2$$

$$\hat{p} = i\sqrt{\frac{m\omega\hbar}{2}}(a^\dagger - a)$$

$$E_n = (n + \frac{1}{2})\hbar\omega$$

$$[a, a^\dagger] = 1$$

Annihilation operator

$$a = \sqrt{\frac{m\omega}{2\hbar}}(\hat{x} + \frac{i}{m\omega}\hat{p})$$

$$a|n\rangle = \sqrt{n}|n-1\rangle$$

Creation operator

$$a^\dagger = \sqrt{\frac{m\omega}{2\hbar}}(\hat{x} - \frac{i}{m\omega}\hat{p})$$

$$a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$$

$$\hat{n} = a^\dagger a$$

$$\hat{H} = \hbar\omega(a^\dagger a + \frac{1}{2})$$

The creation/annihilation operator formalism will be key in the 'second quantization' methods to be developed later in the course!

The hydrogen atom

Energy levels [edit source | edit beta]

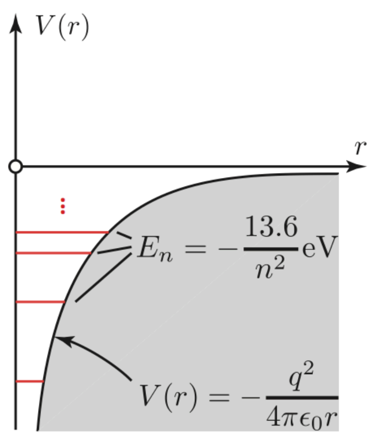
The energy levels of hydrogen, including fine structure, are given by the Sommerfeld expression:

$$E_{j\,n} = -m_e c^2 \left[\left(1+\left[\frac{\alpha}{n-j-\frac{1}{2}+\sqrt{\left(j+\frac{1}{2}\right)^2-\alpha^2}}\right]^2\right)^{-1/2} - 1\right]$$
$$\approx -\frac{m_e c^2 \alpha^2}{2n^2}\left[1+\frac{\alpha^2}{n^2}\left(\frac{n}{j+\frac{1}{2}}-\frac{3}{4}\right)\right],$$

where α is the fine-structure constant and j is the "total angular momentum" quantum number, which is equal to $|\ell \pm 1/2|$ depending on the direction of the electron spin. The factor in square brackets in the last expression is nearly one; the extra term arises from relativistic effects (for details, see #Features going beyond the Schrödinger solution).

The value

$$\frac{m_e c^2 \alpha^2}{2} = \frac{0.51\,\text{MeV}}{2\cdot 137^2} = 13.6\,\text{eV}$$



Hydrogen Atom

Wavefunction [edit source | edit beta]

The normalized position wavefunctions, given in spherical coordinates are:

$$\psi_{n\ell m}(r,\vartheta,\varphi) = \sqrt{\left(\frac{2}{na_0}\right)^3 \frac{(n-\ell-1)!}{2n(n+\ell)!}} e^{-\rho/2}\rho^\ell L^{2\ell+1}_{n-\ell-1}(\rho) Y^m_\ell(\vartheta,\varphi)$$

where:

$\rho = \frac{2r}{na_0}$,

a_0 is the Bohr radius,

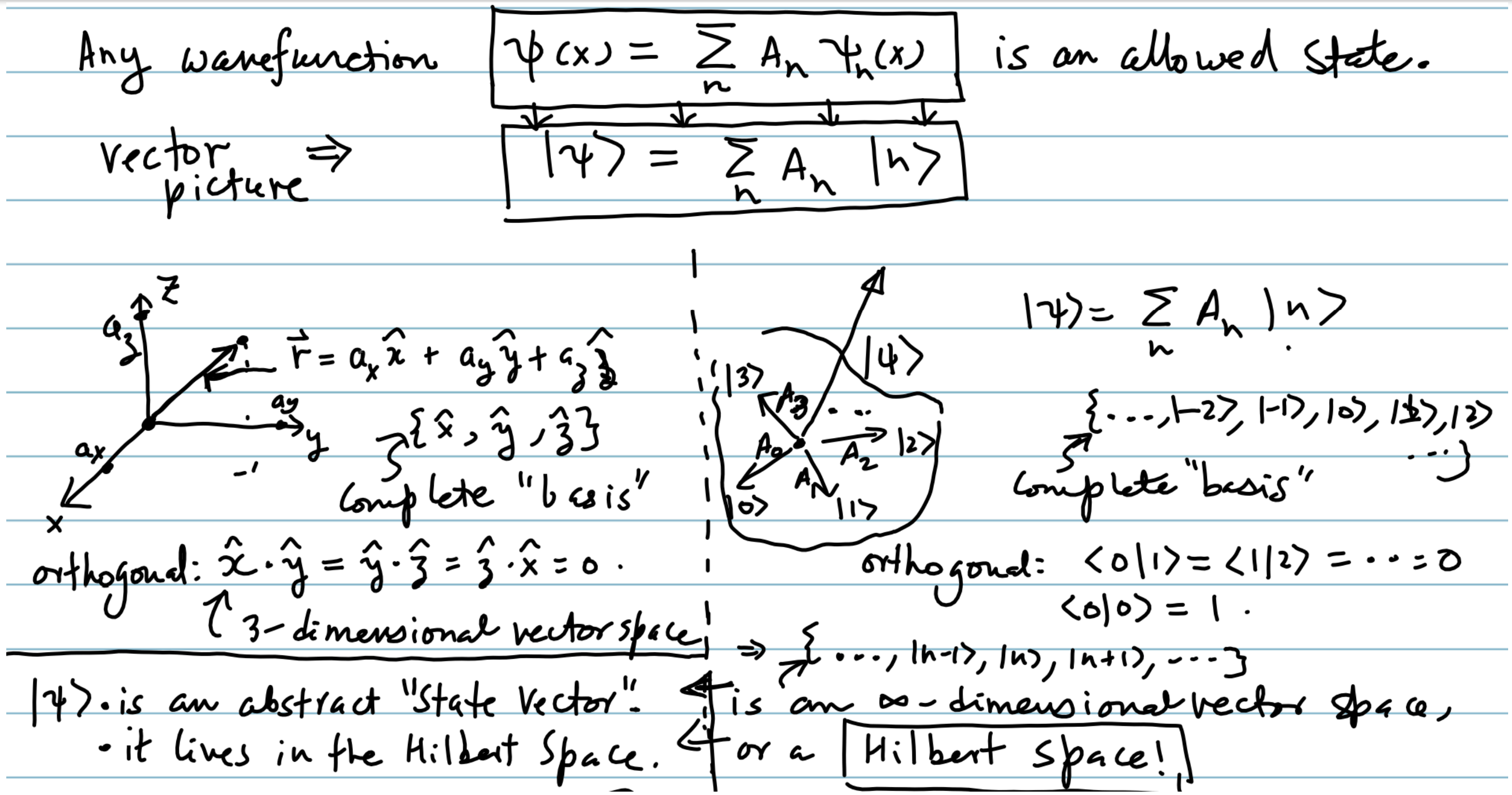
$L^{2\ell+1}_{n-\ell-1}(\rho)$ is a generalized Laguerre polynomial of degree $n - \ell - 1$, and

$Y^m_\ell(\vartheta,\varphi)$ is a spherical harmonic function of degree ℓ and order m. Note that the generalized Laguerre polynomials are defined differently by different authors. The usage here is consistent with the definitions used by Messiah,[8] and Mathematica.[9] In other places, the Laguerre polynomial includes a factor of $(n+\ell)!$,[10] or the generalized Laguerre polynomial appearing in the hydrogen wave function is $L^{2\ell+1}_{n+\ell}(\rho)$ instead. [11]

The quantum numbers can take the following values:

$$n = 1, 2, 3, \ldots$$
$$\ell = 0, 1, 2, \ldots, n-1$$
$$m = -\ell, \ldots, \ell.$$

Quantum states are vectors in the Hilbert space



It is useful here to draw an analogy to the decomposition of a vector into specific coordinates. The 'hybrid' state function $\psi(x)$ is pictured as a vector $|\psi\rangle$ in an abstract space. The definite momentum wavefunctions $\psi_n(x)$ are pictured as the 'coordinate' vectors $|n\rangle$ in that space of vectors. This set of vectors is called the basis. Since there are an infinite set of integers $n = 0, \pm1, \pm2, ...$, the vector space is infinite dimensional. It is called the Hilbert space. One may then consider the coefficients A_n as the length of the projections of the state on the basis states. The abstract picture allows great economy of expression by writing $|\psi\rangle = \sum_n A_n |n\rangle$. The orthogonality of the basis states

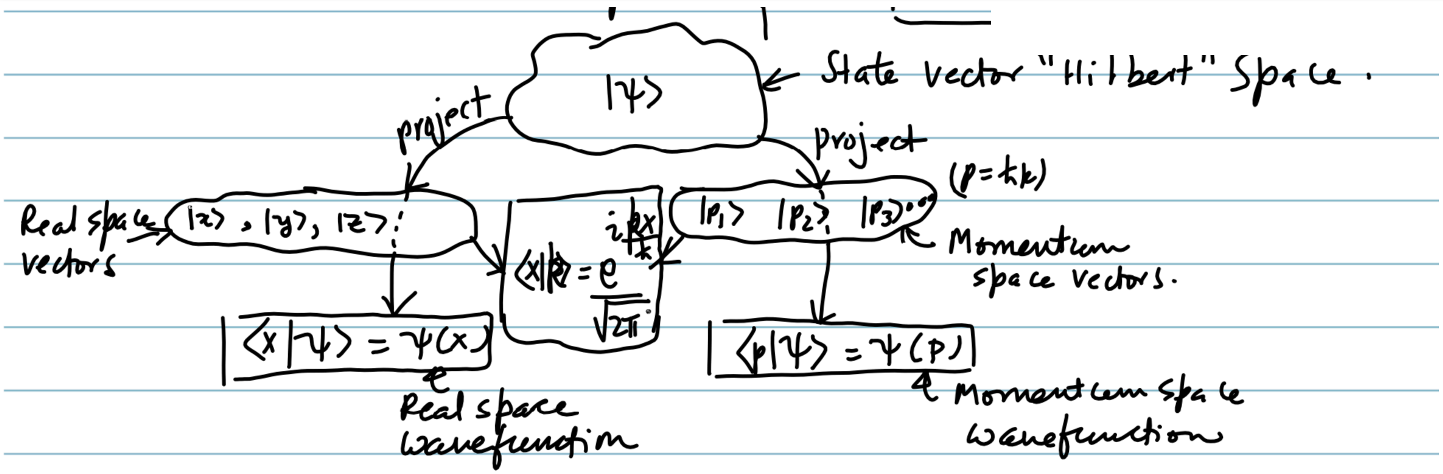
$$|\psi\rangle = \sum_n A_n |n\rangle \qquad \langle m|n\rangle = \delta_{mn}$$

$$A_n = \langle n|\psi\rangle$$

$$|\psi\rangle = \sum_n \langle n|\psi\rangle |n\rangle = \sum_n |n\rangle\langle n|\psi\rangle$$

$$\sum_n |n\rangle\langle n| = 1$$

By projecting states, get various representations



$|\psi\rangle = \sum_n A_n |n\rangle \Rightarrow A_n = \langle n|\psi\rangle$ ← a number

$\Rightarrow |\psi\rangle = \sum_n \langle n|\psi\rangle |n\rangle = \left(\sum_n |n\rangle\langle n|\right)|\psi\rangle$ Same as LHS!

$\Rightarrow \boxed{\sum_n |n\rangle\langle n| = 1}$ Similarly, $\boxed{\int d^3x\, |x\rangle\langle x| = 1}$

"outer product"

$$\langle x|\psi\rangle = \psi(x)$$
$$\langle k|\psi\rangle = \psi(k)$$
$$\langle x|k_x\rangle = \frac{e^{ik_x x}}{\sqrt{2\pi}}$$

$$\langle\psi_2|\psi_1\rangle = \int_{-\infty}^{\infty} dx \langle\psi_2|x\rangle\langle x|\psi_1\rangle = \int_{-\infty}^{\infty} dx \psi_2^\star(x)\psi_1(x)$$

- *We can think of the states as vectors.*
- *The 'inner product' is a complex number generated by projection to the appropriate space.*
- *This number is the wavefunction – it can be found in real space, momentum space, etc…*

Electron in a periodic potential (no analytic soln!)

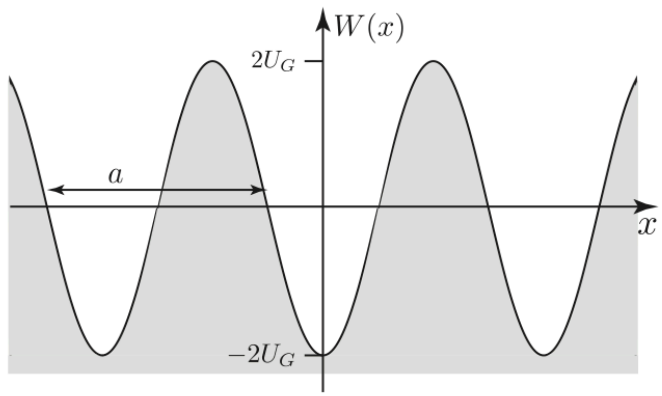


FIGURE 13.1: A periodic potential $W(x) = -2U_G \cos(Gx)$ acts as a perturbation to the free electron.

We will first attack this problem using perturbation theory!

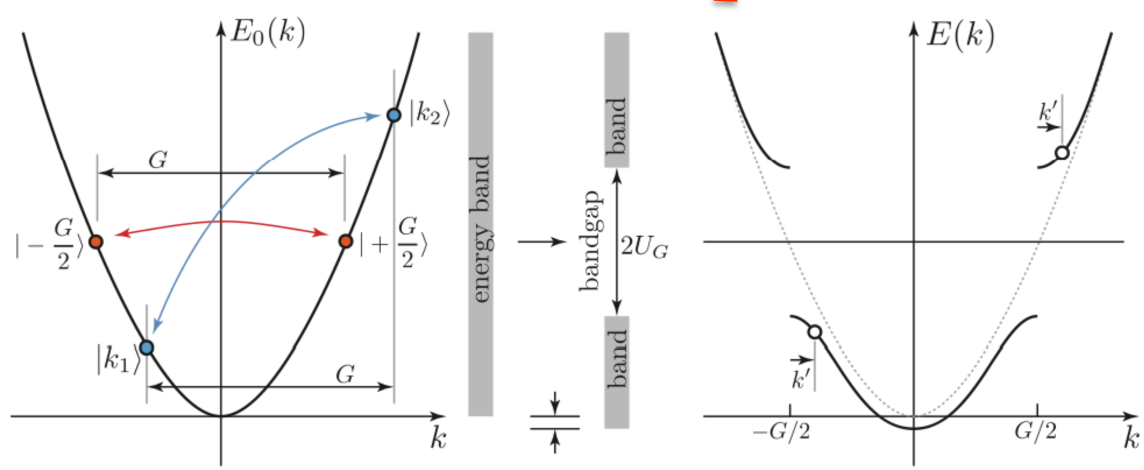


FIGURE 13.2: Bandgap opening in the energy spectrum of a free electron upon perturbation by a periodic potential.