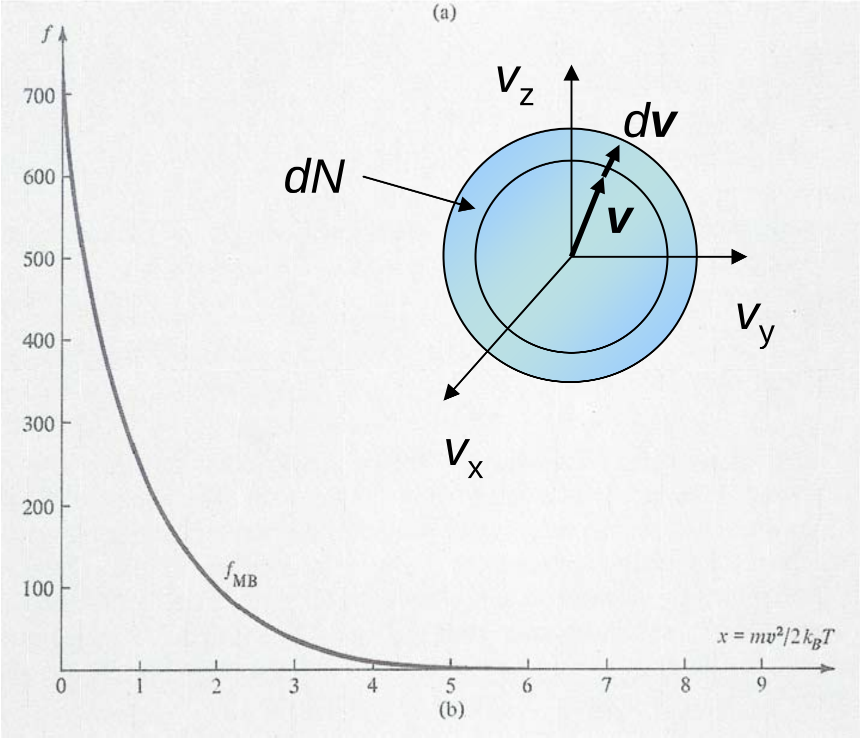
Lecture 7: Free Electron Model

Statistical Distributions

Drude model: electron gas of density $n = N/V$, V-volume
Classical Maxwell-Boltzmann distribution:

$$f_B(\mathbf{v}) = n\left(\frac{m}{2\pi k_B T}\right)^{3/2} e^{-mv^2/2k_B T}.$$

$$dN = f_B(\mathbf{v})\, d\mathbf{v} = f_B(\mathbf{v})\, dv_x dv_y dv_z$$

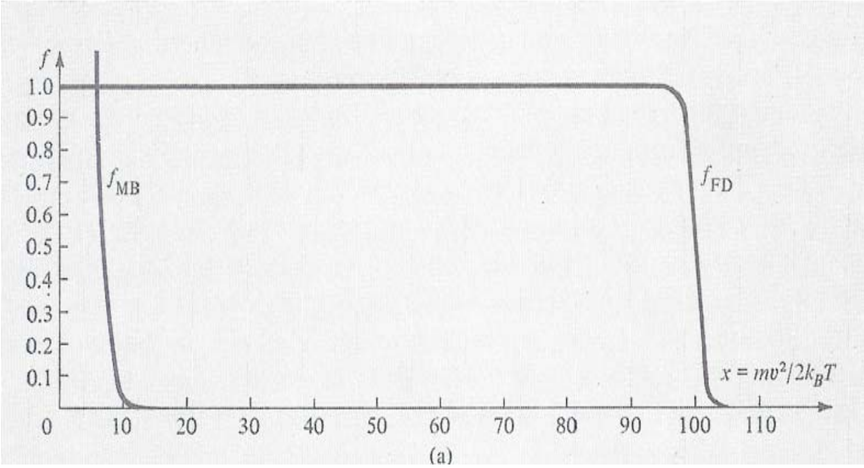


Sommerfeld model: same classical gas, but with quantum Fermi-Dirac distribution:

$$f(\mathbf{v}) = \frac{(m/\hbar)^3}{4\pi^3} \frac{1}{\exp\left[\left(\frac{1}{2}mv^2 - k_B T_0\right)/k_B T\right] + 1}.$$

T_0 – temperature determined by the normalization:

$$n = \int d\mathbf{v}\, f(\mathbf{v})$$



Properties of Fermi-Dirac distribution:

Ground state T→0:
For $mv^2/2 < k_B T_0$ $f(v) = 1$ – **Consequence of Pauli exclusion principle**
For $mv^2/2 > k_B T_0$ $f(v) = 0$

Transition to Maxwell-Boltzman distribution require $T >> T_0$ whereas in practice in metals $T << T_0$ (in Figure $T = 0.01T_0$).

Ground-State Properties of the Electron Gas

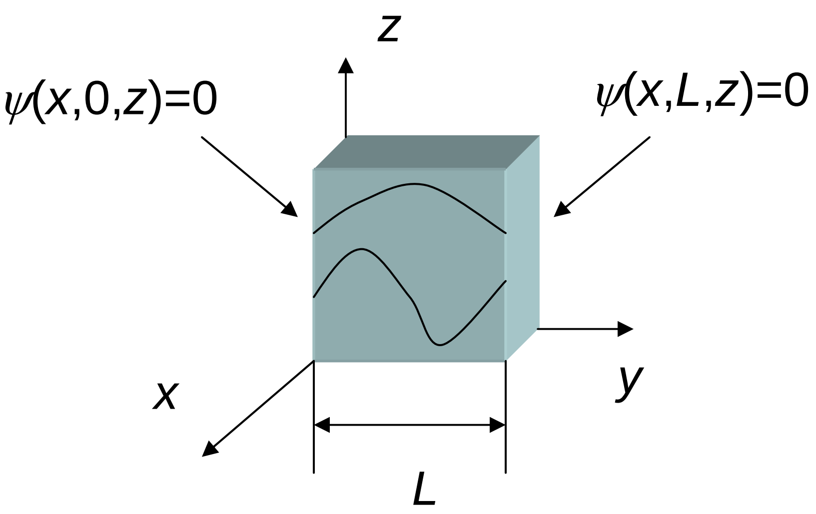
Find at first the energy spectrum and then fill it up by electrons according to Pauli.

One electron wave function ***without interactions*** satisfies the time-independent Schrödinger equation:

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{z^2}\right)\psi(\mathbf{r}) = \mathrm{E}\psi(\mathbf{r})$$

Boundary Conditions

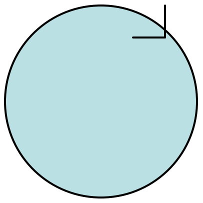
Natural choice, zero conditions, lead to standing-wave solutions whereas the transport should be discussed in terms of running waves.



Born-von Karman (or periodic) boundary conditions:

$$\psi(x,y,z+L) = \psi(x,y,z)$$
$$\psi(x,y+L,z) = \psi(x,y,z)$$
$$\psi(x+L,y,z) = \psi(x,y,z)$$

In 1-D case:
$\psi(x+L) = \psi(x)$



Electron coming to the surface is not reflected back in, but reenters the metal from opposite surface. **Excludes the surfaces from any role in transport phenomena.**

The Solutions are Plane Waves

$$\psi_{\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{V}} e^{i\mathbf{k}\cdot\mathbf{r}} \qquad E(\mathbf{k}) = \frac{\hbar^2 k^2}{2m}$$

Can be easily verified by substituting into the equation in a 1-D form.
The constant was defined due to:

$$1 = \int d\mathbf{r} \left|\psi(\mathbf{r})\right|^2$$

Momentum:

Since $\boxed{\frac{\hbar}{i}\frac{\partial}{\partial \mathbf{r}}} e^{i\mathbf{k}\cdot\mathbf{r}} = \hbar\mathbf{k} e^{i\mathbf{k}\cdot\mathbf{r}}$

With eigenvalue:

$\mathbf{p} = \hbar\mathbf{k}$ and a velocity: $\mathbf{v} = \mathbf{p}/m = \frac{\hbar\mathbf{k}}{m}$

$\mathbf{p} = \frac{\hbar}{i}\frac{\partial}{\partial \mathbf{r}}$ - Introduce the momentum operator

Particles: This allows particle analogy: $E = p^2/(2m) = mv^2/2$ – classical result

Matter waves: the plane wave e^{ikr} = Const in the plane ⊥ **k** (since **kr** = Const) and periodic along **k** with wavelength: $\lambda = 2\pi/k$ – de Broglie wavelength – quantum result

Discrete Nature of k-vector

From the boundary conditions: $e^{ik_xL} = e^{ik_yL} = e^{ik_zL} = 1$

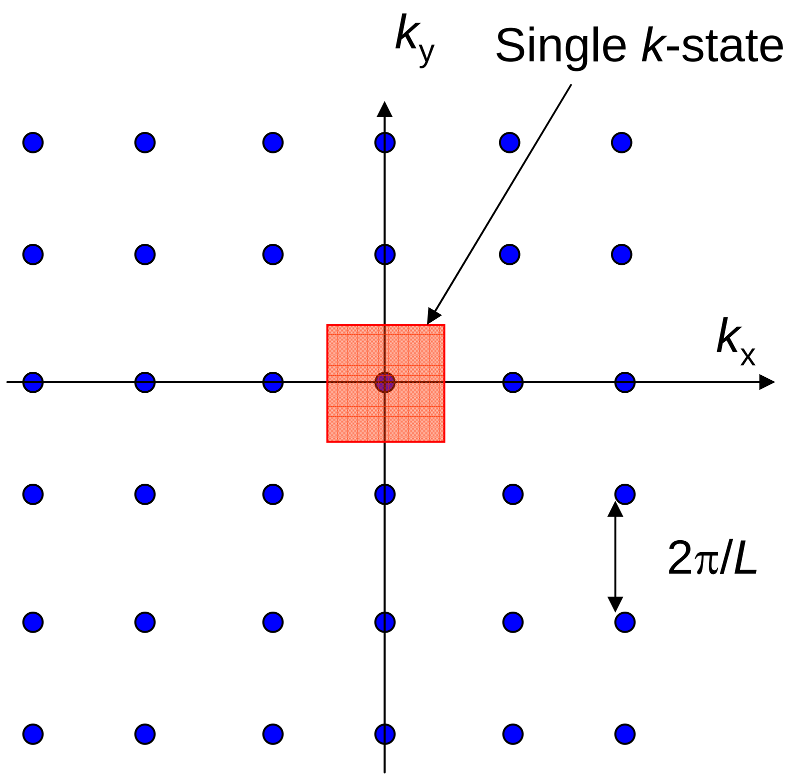
$k_x = 2\pi n_x/L = 2\pi n_y/L = 2\pi n_z/L$, where n_i - integers

2-D lattice in reciprocal space

The number of states in a *k*-space volume (Ω):

$\Omega/(2\pi/L)^3 = \Omega V/8\pi^3$, V – init cell volume

The density of *k*-states is $V/8\pi^3$

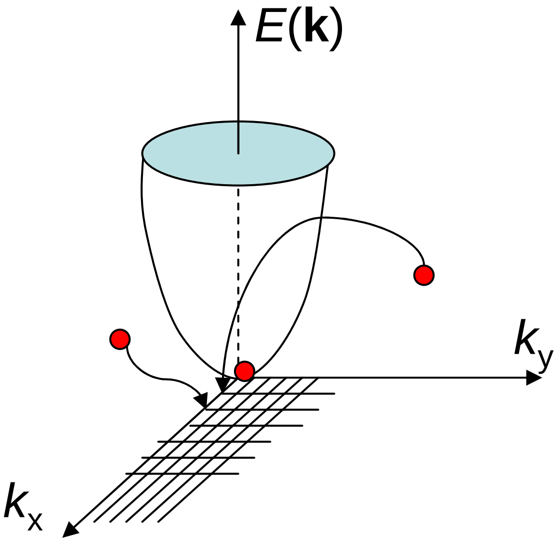


Filling k-space with electrons

Building the N-electron ground state by placing electrons into single electron levels.

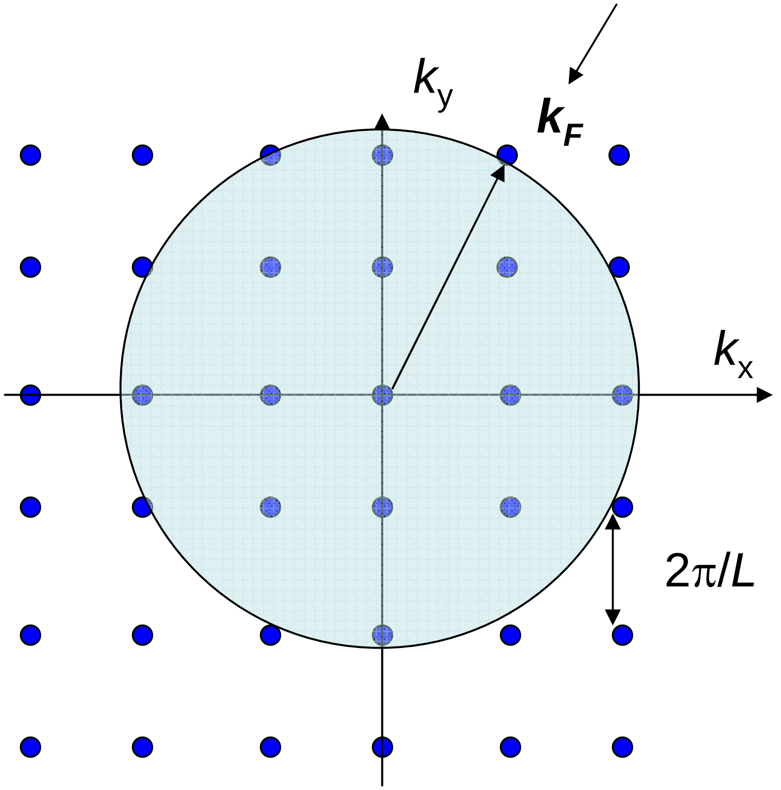
Consider $$E(\mathbf{k}) = \frac{\hbar^2 k^2}{2m}$$ combined with the Pauli exclusion principle.

Since it is a lowest energy state (T = 0) we have a tight packing starting from k=0.
For large N the occupied region is a sphere in 3-D case.



The Fermi wave vector

In 2-D:



Lecture 8: Fermi Surface, Energy, Wavevector, and Velocity

In 3-D: Number of k-states within the sphere is:

V - volume of material

$$\left(\frac{4\pi k_F^3}{3}\right)\left(\frac{V}{8\pi^3}\right) = \frac{k_F^3}{6\pi^2}V \xrightarrow{\times 2} N = \frac{k_F^3}{3\pi^2}V$$

Since each state is occupied with 2 electrons:

As a result: $\boxed{n = N/V = \frac{k_F^3}{3\pi^2}}$

The surface of the Fermi sphere, which separates the occupied from the unoccupied states called the ***Fermi surface***.

$p_F = hk_F/2\pi$ - ***Fermi momentum***, $v_F = p_F/m$ – ***Fermi velocity***

$v_F \sim 1\% c$ – Surprising result since in a classical gas $v \Rightarrow 0$ if $T \Rightarrow 0$

$$E_F = \frac{\hbar^2 k_F^2}{2m}$$

- ***Fermi energy***

Energy per electron *E*/*N* in the ground state and T_F

Energy of N electrons inside Fermi sphere:

$$E = 2\sum_{k<k_F} \frac{\hbar^2}{2m} k^2$$

Define

$$F(\mathbf{k}) = \frac{\hbar^2}{2m} k^2$$

Replace summation with integration:

$$E = 2\int \frac{V d\mathbf{k}}{8\pi^3} F(\mathbf{k})$$

Where $V/(8\pi^3)$ – density of states in k-space

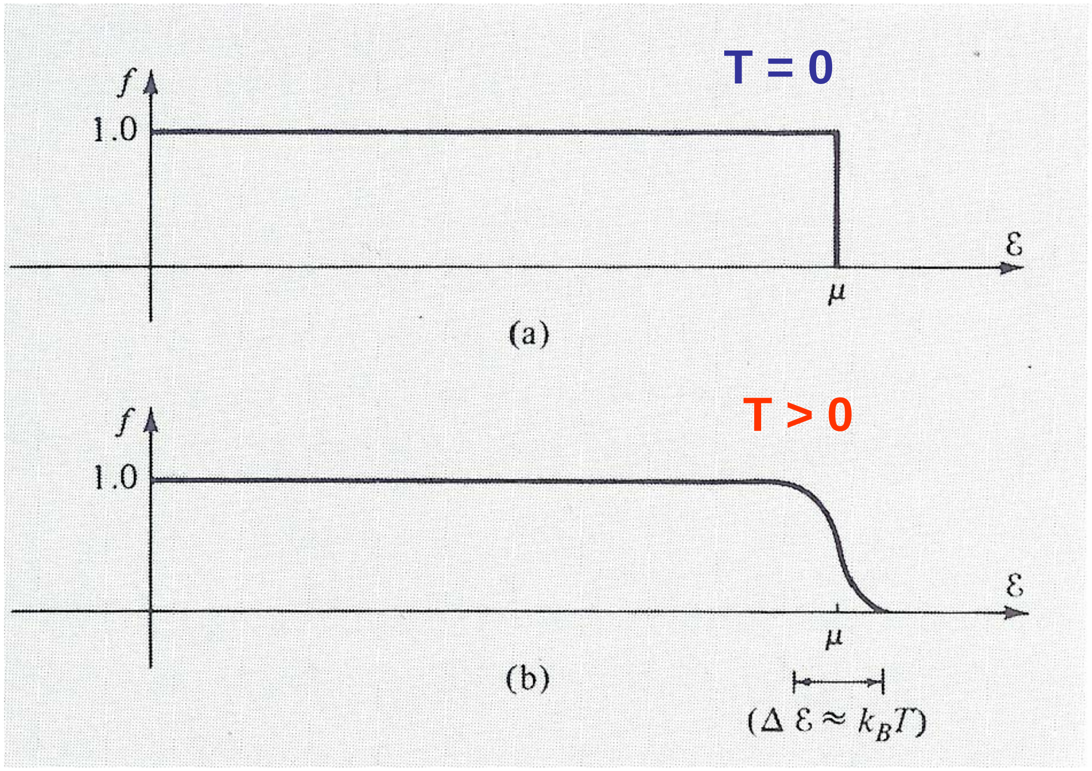
$$\frac{E}{V} = \frac{1}{4\pi^3}\int_{k<k_F} d\mathbf{k}\, \frac{\hbar^2 k^2}{2m} = \frac{1}{4\pi^3}\int_{k<k_F} 4\pi k^2 dk\, \frac{\hbar^2 k^2}{2m} = \frac{1}{\pi^2}\frac{\hbar^2 k_F^5}{10m}$$

Taking into account that $N/V = k_F^3/3\pi^2$ $\Rightarrow$ $E/N = (3/5)k_B T_F$, where $T_F = E_F/k_B$ - ***Fermi temperature***

What if the temperature is non zero?

Fermi-Dirac distribution:

$$f(E) = \frac{1}{e^{(E-\mu)/k_B T} + 1}$$



μ - chemical potential

lim $f(E)$ ($T \Rightarrow 0$) = 1 for $E(\mathbf{k}) < \mu$

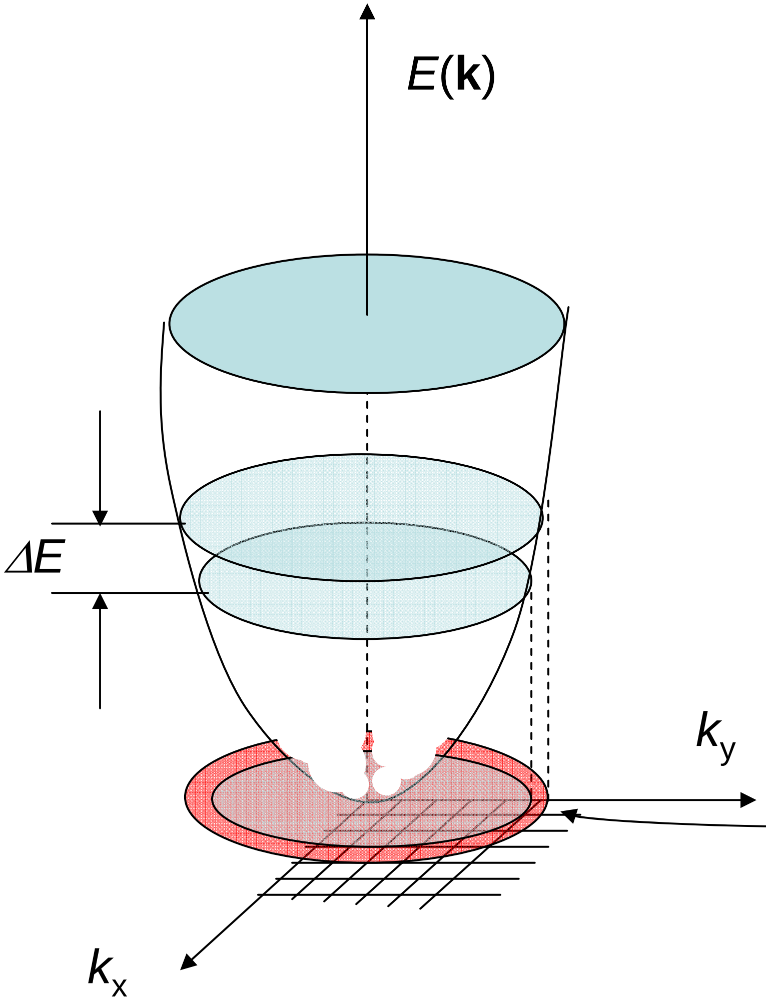
= 0 for $E(\mathbf{k}) > \mu$

Lim μ ($T \Rightarrow 0$) = E_F

In fact μ can be changed for increased *T*, in many cases it can be neglected

Density of States Distribution Function *g*(*E*) in 2D Case

$$g(E) = \frac{dn}{dE} = \frac{1}{V}\frac{dN}{dE}$$



$$E = \frac{\hbar^2 k^2}{2m} \Rightarrow \boxed{dE = \frac{\hbar^2 k}{m} dk}, k = \sqrt{\frac{2mE}{\hbar^2}}$$

This is always true (any D) since *k* here is a magnitude of the *k*-vector:
$k = (k_x^2 + k_y^2 + k_z^2)^{1/2}$

However expression for *dN* depends on D. In 2D:

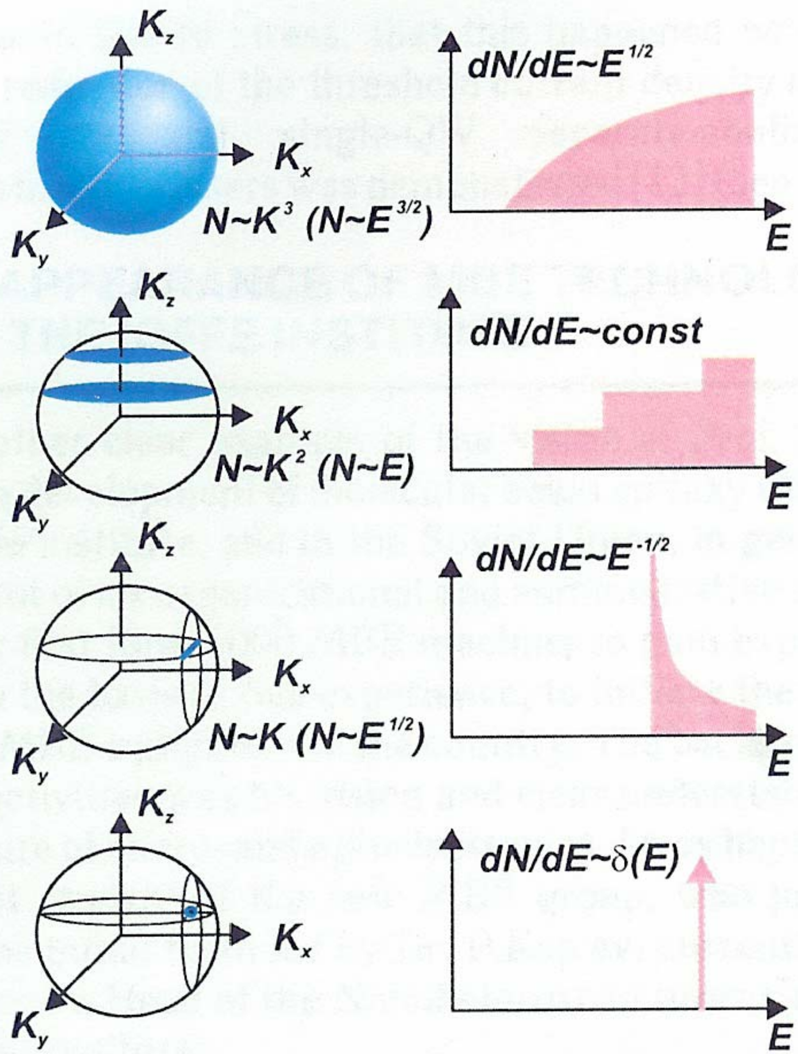
$dN = 2\pi k \, dk \, (V/8\pi^3)$

Leading to:

$$\frac{dn}{dE} = \frac{1}{V}\frac{dN}{dE} = \frac{m}{4\pi^2\hbar^2}$$

Taking into account spin **×2**

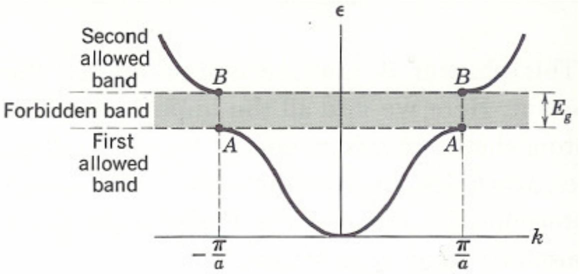
Density of states for carriers in structures with different dimensionalities



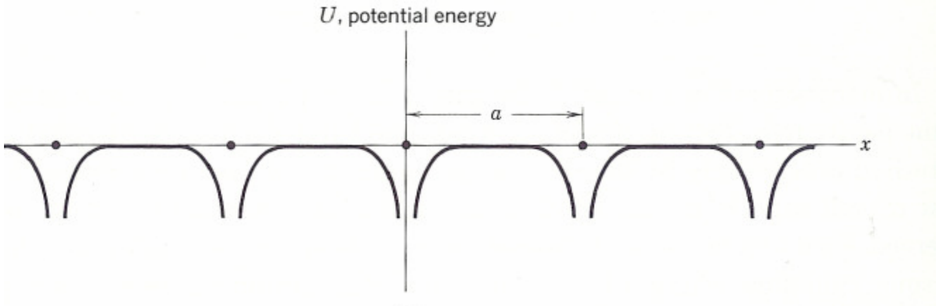
Lecture 9: Two Models, Nearly Free Electron Model

Two Models

Nearly Free Electrons (Kittel)

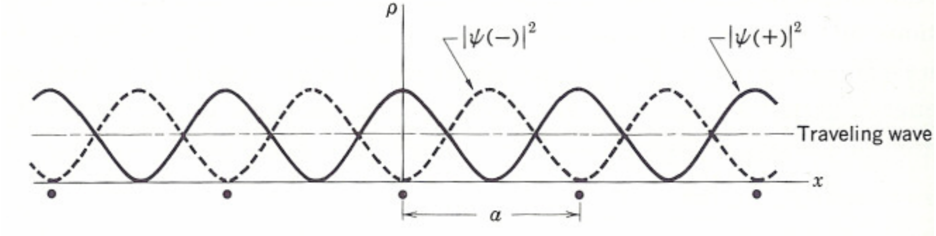


Bragg: $k = \pm G/2 = \pm n\pi/a$

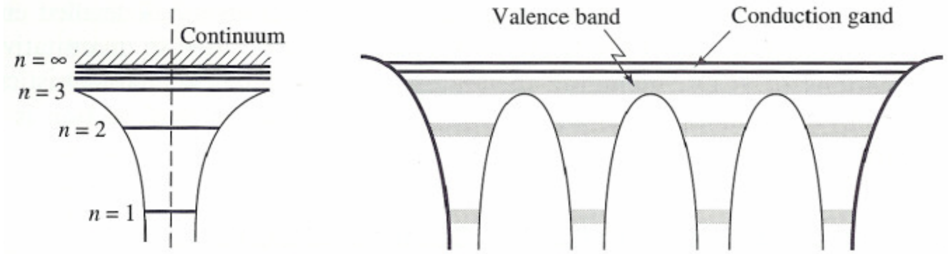


(a)

$\psi(-) \sim \sin(\pi x/a)$ $\psi(+) \sim \cos(\pi x/a)$

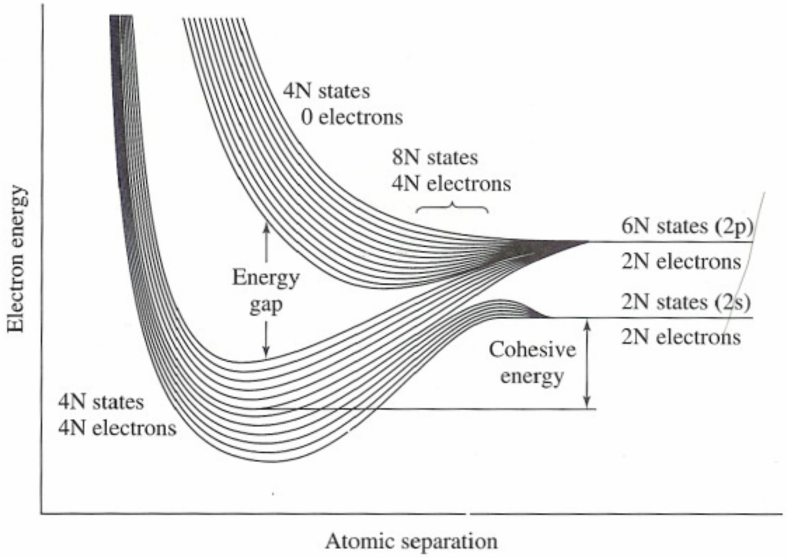


Tight Binding Model



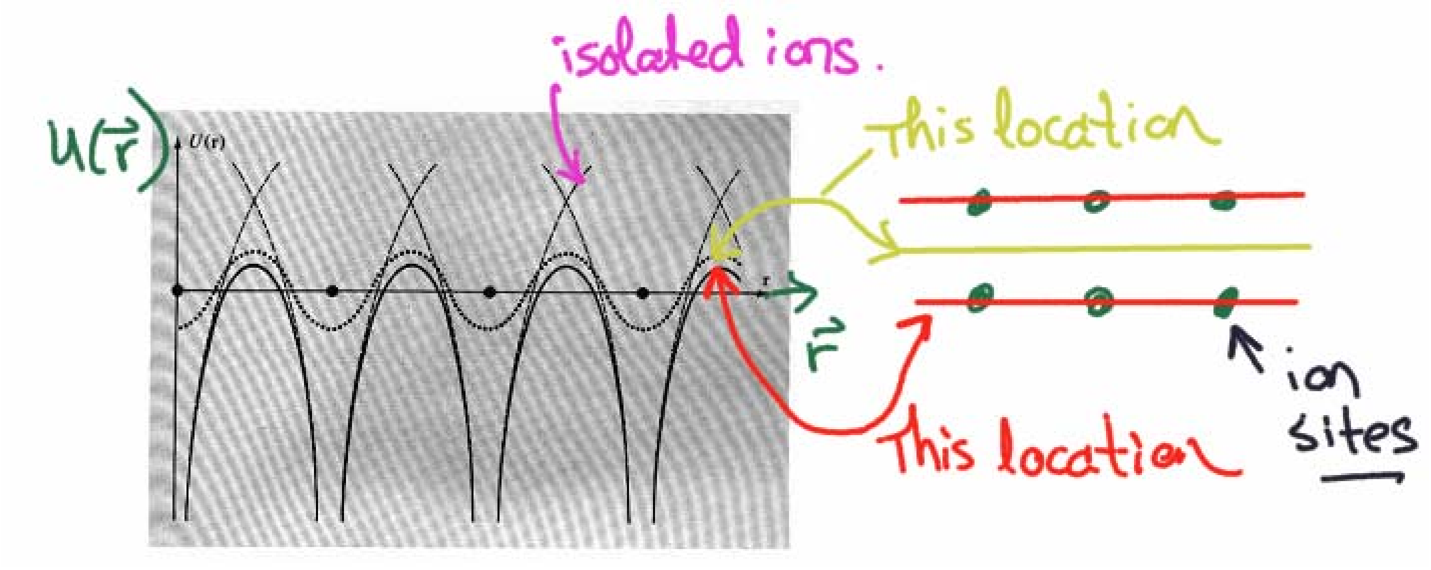
(a) Energy levels of isolated atom

(b) Energy bands of crystals



Nearly Free Electron Model

One-electron effective potential:



Single electron Schrödinger equation:

$$H\psi = \left(-\frac{\hbar^2}{2m}\nabla^2 + U(\mathbf{r})\right)\psi = E\psi$$

$U(\mathbf{r})$ – periodic potential

Bloch's Theorem

The eigenfunction ψ is a product of a plane wave and a periodic function:

$\boxed{\psi_{n\mathrm{k}}(\mathbf{r}) = e^{i\mathbf{kr}} u_{n\mathrm{k}}(\mathbf{r}),}$ where u_{nk} has periodicity of Bravais lattice:

$u_{n\mathbf{k}}(\mathbf{r}+\mathbf{R}) = u_{n\mathbf{k}}(\mathbf{r})$ for all $\mathbf{R}$ in the Bravais lattice

$\boxed{\psi_{n\mathrm{k}}(\mathbf{r}+\mathbf{R}) = e^{i\mathbf{kR}} \psi(\mathbf{r})}$ – equivalent formulation of the Bloch's theorem

The Born-von Karman Boundary Conditions

$\psi(\mathbf{r}+N_i\mathbf{a}_i) = \psi(\mathbf{r})$, i = 1, 2, 3,… , where N_i – number of primitive cells in "*I*" direction.

$N = N_1N_2N_3$ – total number of primitive cells in the crystal

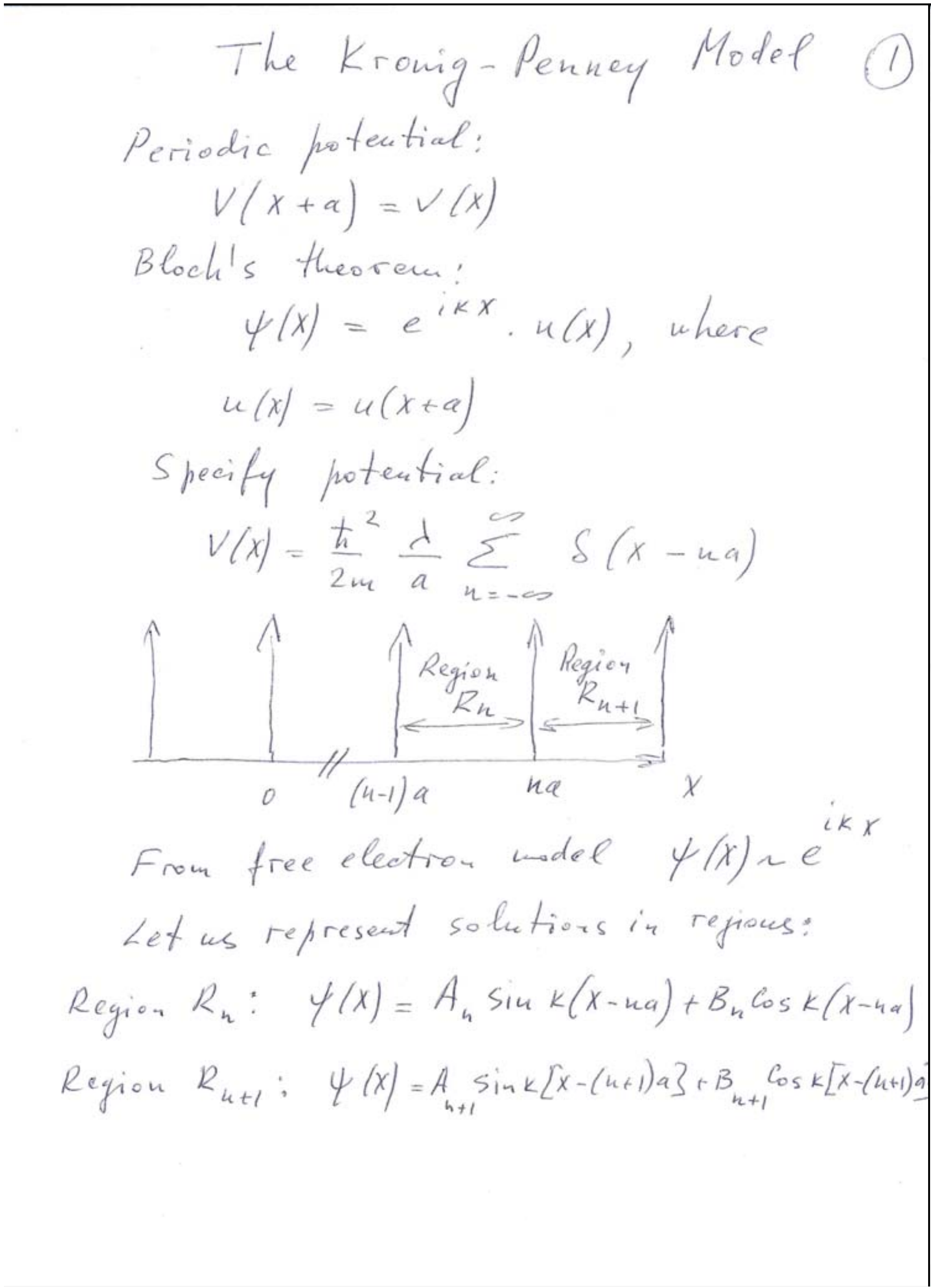
Applying Bloch's theorem to the boundary condition:

$\psi_{n\mathbf{k}}(\mathbf{r} + N_i\mathbf{a}_i) = e^{iN_i\mathbf{ka}_i}\,\psi_{n\mathbf{k}}(\mathbf{r})$, i = 1, 2, 3,… $\Rightarrow e^{iN_i\mathbf{ka}_i} = 1$

by representing $\mathbf{k} = x_1\mathbf{b}_1 + x_2\mathbf{b}_2 + x_3\mathbf{b}_3$ we have $e^{2\pi i N_i x_i} = 1 \Rightarrow x_i = m_i/N_i$, $m_i = 0, 1, 2,\ldots$

The size of the cell in k-space ~ $\Delta k_i = 2\pi/L_i \Rightarrow$ Volume of the cell $\Delta\mathbf{k} = (2\pi)^3/V$

Solution in 1D case: Kronig-Penney Model



The Kronig-Penney Model ①

Periodic potential:

$$V(x+a)=V(x)$$

Bloch's theorem:

$$\psi(x)=e^{ikx}\cdot u(x),$$ where

$$u(x)=u(x+a)$$

Specify potential:

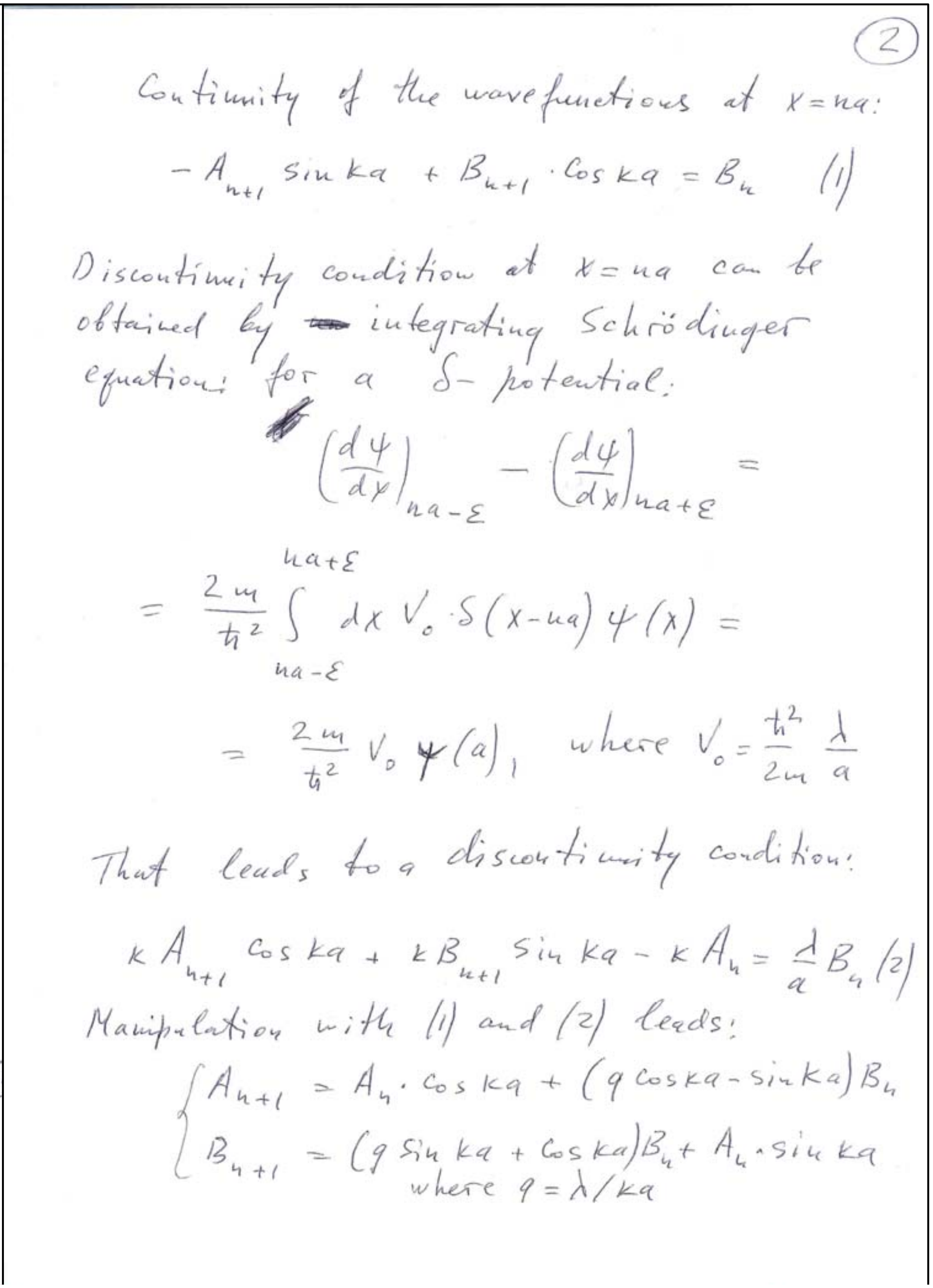
$$V(x)=\frac{\hbar^2}{2m}\frac{\lambda}{a}\sum_{n=-\infty}^{\infty}\delta(x-na)$$

From free electron model $\psi(x)\sim e^{ikx}$

Let us represent solutions in regions:

Region R_n: $\psi(x)=A_n\sin k(x-na)+B_n\cos k(x-na)$

Region R_{n+1}: $\psi(x)=A_{n+1}\sin k[x-(n+1)a]+B_{n+1}\cos k[x-(n+1)a$



②

Continuity of the wavefunctions at $x=na$:

$$-A_{n+1}\sin ka+B_{n+1}\cdot\cos ka=B_n \qquad (1)$$

Discontinuity condition at $x=na$ can be obtained by integrating Schrödinger equation for a δ-potential:

$$\left(\frac{d\psi}{dx}\right)_{na-\varepsilon}-\left(\frac{d\psi}{dx}\right)_{na+\varepsilon}=$$

$$=\frac{2m}{\hbar^2}\int_{na-\varepsilon}^{na+\varepsilon}dx\,V_0\cdot\delta(x-na)\,\psi(x)=$$

$$=\frac{2m}{\hbar^2}V_0\,\psi(a),$$ where $V_0=\frac{\hbar^2}{2m}\frac{\lambda}{a}$

That leads to a discontinuity condition:

$$kA_{n+1}\cos ka+kB_{n+1}\sin ka-kA_n=\frac{\lambda}{a}B_n \qquad (2)$$

Manipulation with (1) and (2) leads:

$$\begin{cases}A_{n+1}=A_n\cdot\cos ka+(q\cos ka-\sin ka)B_n\\ B_{n+1}=(q\sin ka+\cos ka)B_n+A_n\cdot\sin ka\end{cases}$$

where $q=\lambda/ka$

Bloch's theorem:

$$\psi(x+a) = e^{i(x+a)k} \cdot u(x+a) = e^{i\varphi} \cdot e^{ikx} \cdot u(x) =$$

$$= e^{i\varphi} \cdot \psi(x) \quad (3)$$

Implies; $\psi(R_{n+1}) = e^{i\varphi} \cdot \psi(R_n)$

That is satisfied if:

$$A_{n+1} = e^{i\varphi} \cdot A_n$$

$$B_{n+1} = e^{i\varphi} \cdot B_n$$

Once it is inserted in (3), we have a consistency condition:

$$(e^{i\varphi} - \cos ka)(e^{i\varphi} - q \sin ka - \cos ka) =$$

$$= \sin ka(q \cdot \cos ka - \sin ka)$$

that is

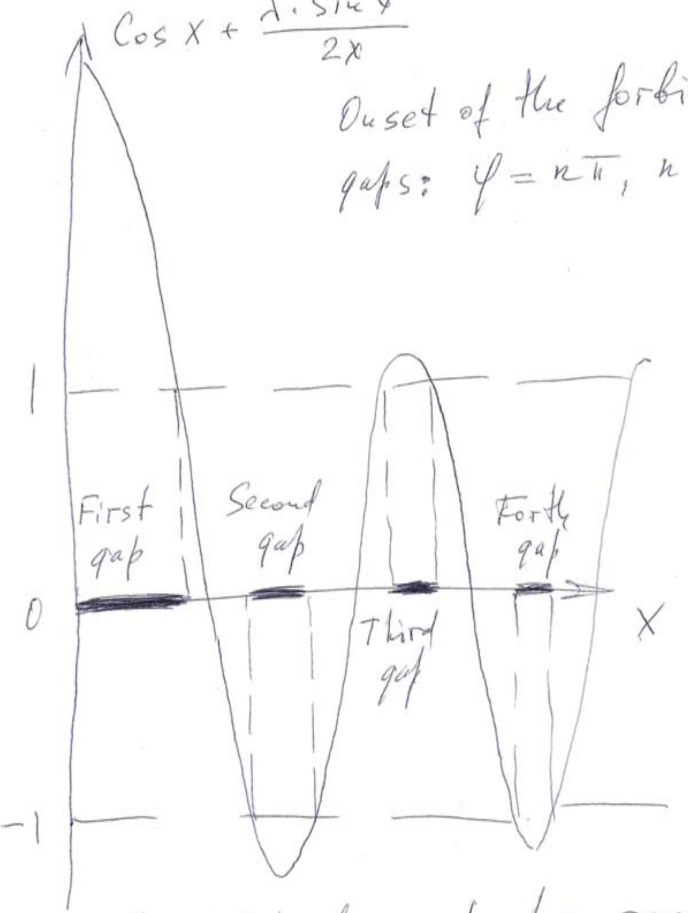
$$e^{2i\varphi} - e^{i\varphi}(2\cos ka + q \sin ka) + 1 = 0$$

by multiplying by $e^{-i\varphi}$:

$$\cos\varphi = \cos ka + \frac{1}{2} q \sin ka$$

In the equation $\cos\varphi = \cos ka + \frac{1}{2}\lambda \frac{\sin ka}{ka}$

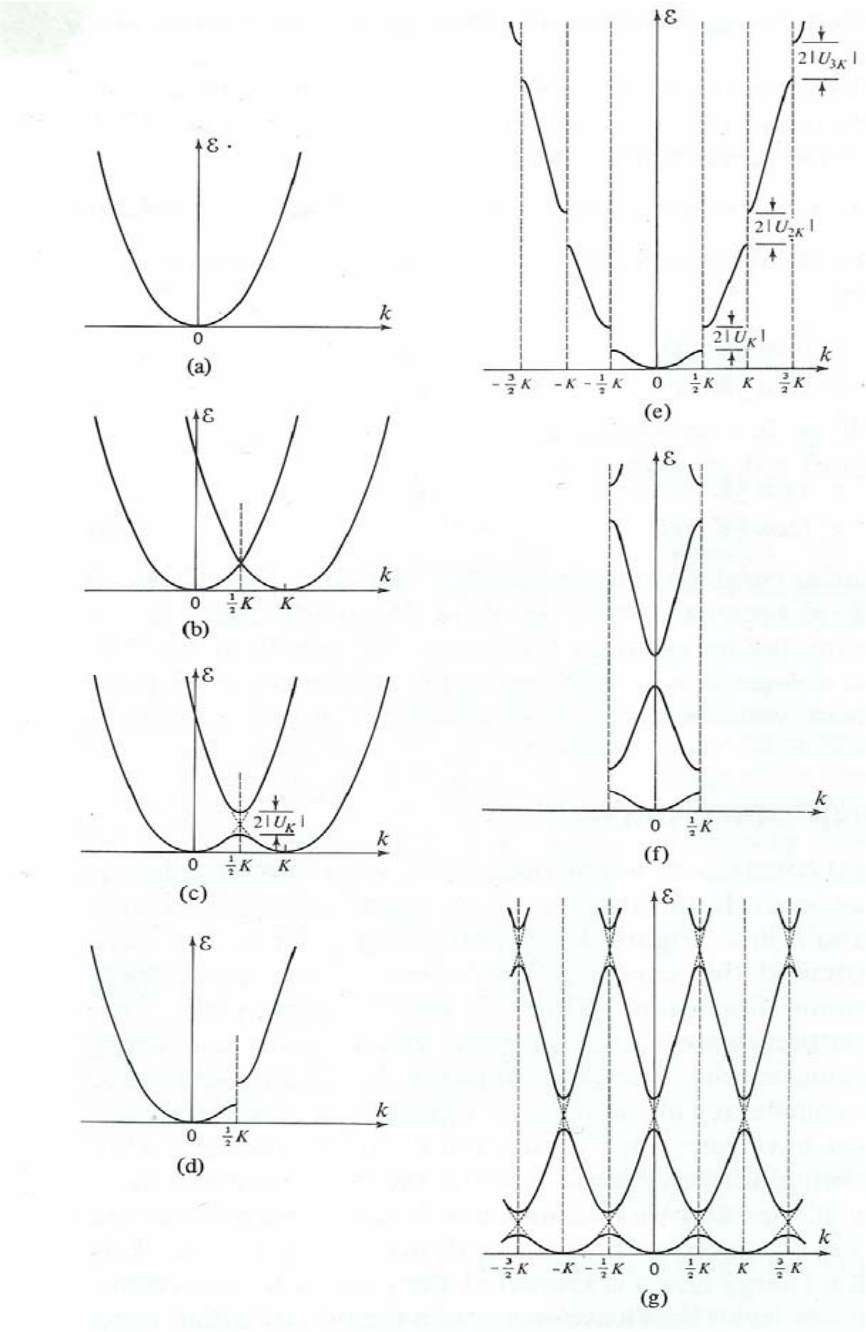
Bounded by 1



Onset of the forbidden gaps: $\varphi = n\pi$, $n = \pm 1, \pm 2$.

The plot demonstrates restrictions on $X = ka$, but due to $E = \frac{\hbar^2 k^2}{2m}$ these restrictions translate into E: $\boxed{\text{Forbidden Bands}}$

Photonic Band Structure in 1D Case



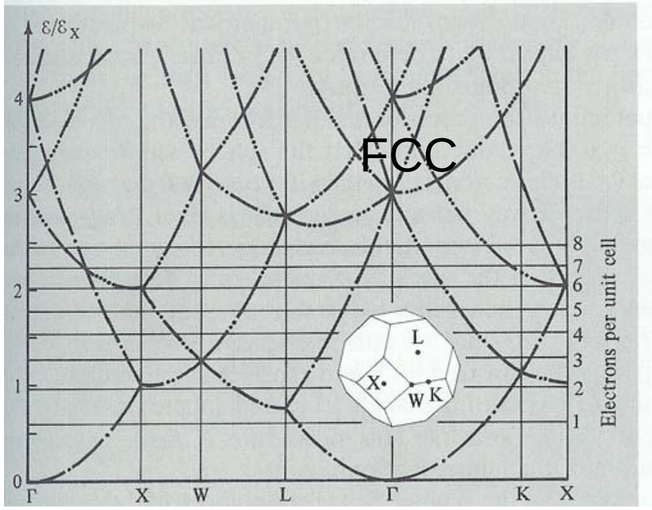
Degeneracy of the parabolic behavior is lifted at $k = K/2 = \pi/a$

Expanded-zone scheme

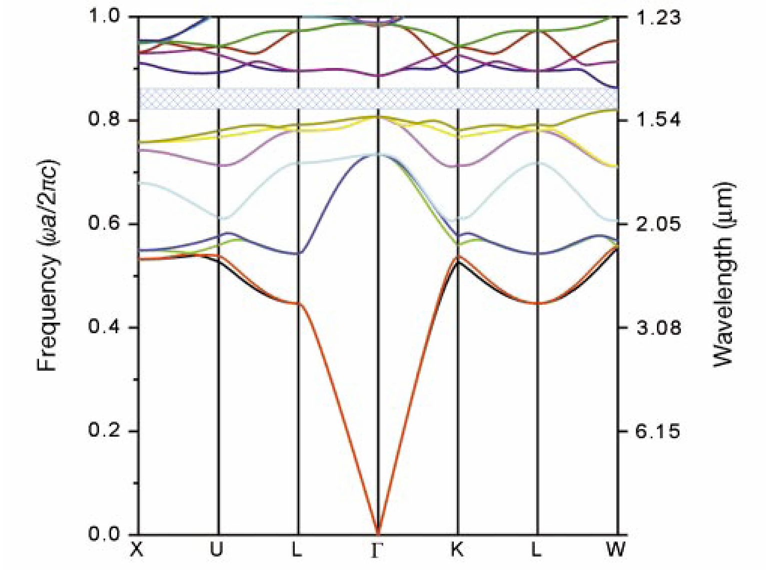
Reduced-zone scheme

Repeated-zone scheme

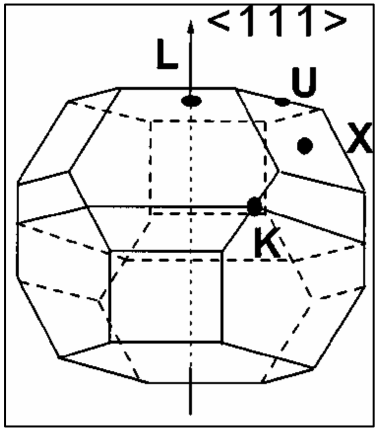
Photonic Band Structure in 3D Case

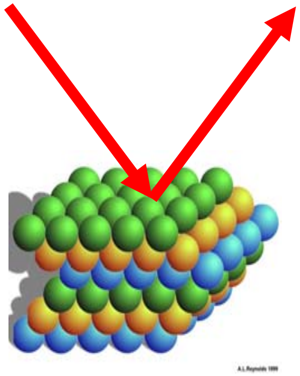


Electronic Band Structure



Photonic Band Structure



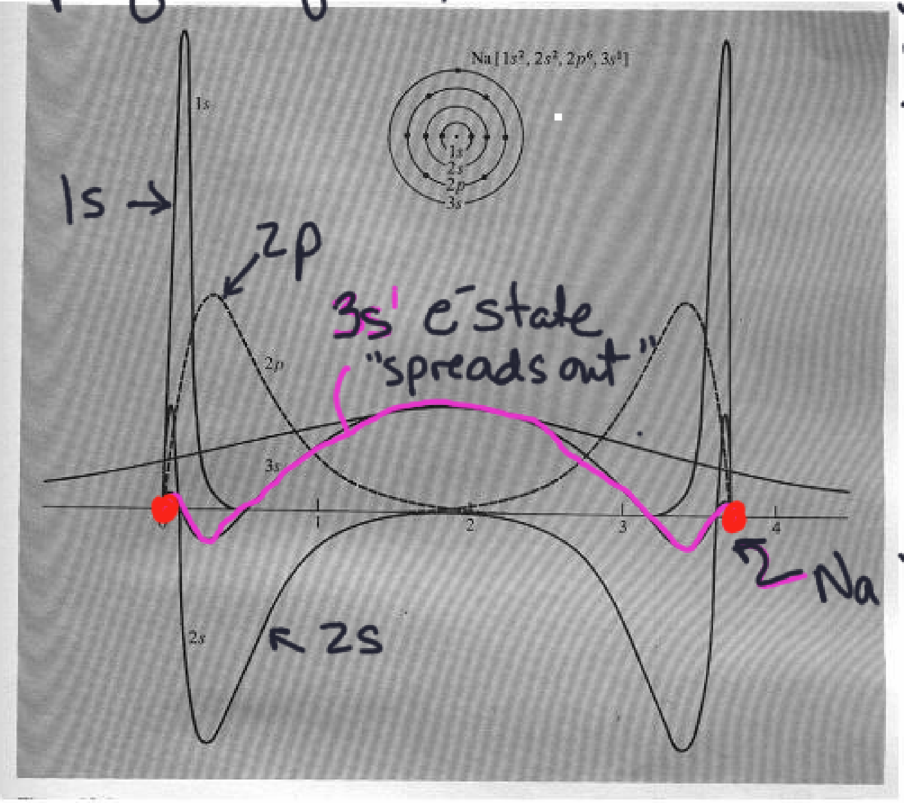


A.Blanko et al., Nature 405, 437 (2000)

Lecture 10: The Tight-Binding Method

The Tight-Binding approximation:
- Overlap of atomic wave functions is enough to perturb the picture of isolated atoms
- But not so strong to make the atomic description completely irrelevant
- Reconciliation between contradictory features of atomic and free electron gas models

Example of wavefctns, $\Psi(\vec{r})$ when you bring 2 Na atoms together...



General Formulation

$H_{at}\psi_n = E_n\psi_n$ - for bound levels of the atomic Hamiltonian

To calculate corrections the crystal Hamiltonian is represented as:

$H = H_{at} + \Delta U(\mathbf{r})$

To preserve Bloch description: $\psi(\mathbf{r}+\mathbf{R}) = e^{i\mathbf{kR}}\psi(\mathbf{r})$ (1)

We can try linear combinations of atomic wave functions:

$$\psi_{n\mathbf{k}}(\mathbf{r}) = \sum_{\mathbf{R}} e^{i\mathbf{kR}}\psi_n(\mathbf{r}-\mathbf{R}) \qquad (2)$$

The Bloch condition (1) is verified for wavefunctions (2)

Since the atomic functions can be slightly different in the presence of $\Delta U(\mathbf{r})$ the general form of (2) is:

$$\psi_{n\mathbf{k}}(\mathbf{r}) = \sum_{\mathbf{R}} e^{i\mathbf{kR}}\phi(\mathbf{r}-\mathbf{R})$$

In its turn: $\phi(r) = \sum_n b_n\psi_n(\mathbf{r})$ - Linear combination of atomic orbitals LCAO

Wannier Functions

Function ϕ that play the role of the atomic wave functions are ***Wannier functions***.

If the band formed by these functions is narrow tight-binding band then ϕ are very close to atomic functions ψ_n. If it is broad, then these functions will differ.

Any Bloch function can be represented in the basis of Wannier functions. To prove note that Bloch function $\psi_{n\mathbf{k}}(\mathbf{r})$ can be considered as a function of **k** for a given **r**. However, since it is periodic in k-space, it can be represented as a Fourier series expansion in the reciprocal of the receiprocal, i.e., in the ***real*** lattice:

$$\psi_{n\mathbf{k}}(\mathbf{r}) = \sum_{\mathbf{R}} f_n(\mathbf{R},\mathbf{r}) e^{i\mathbf{R}\mathbf{k}}$$

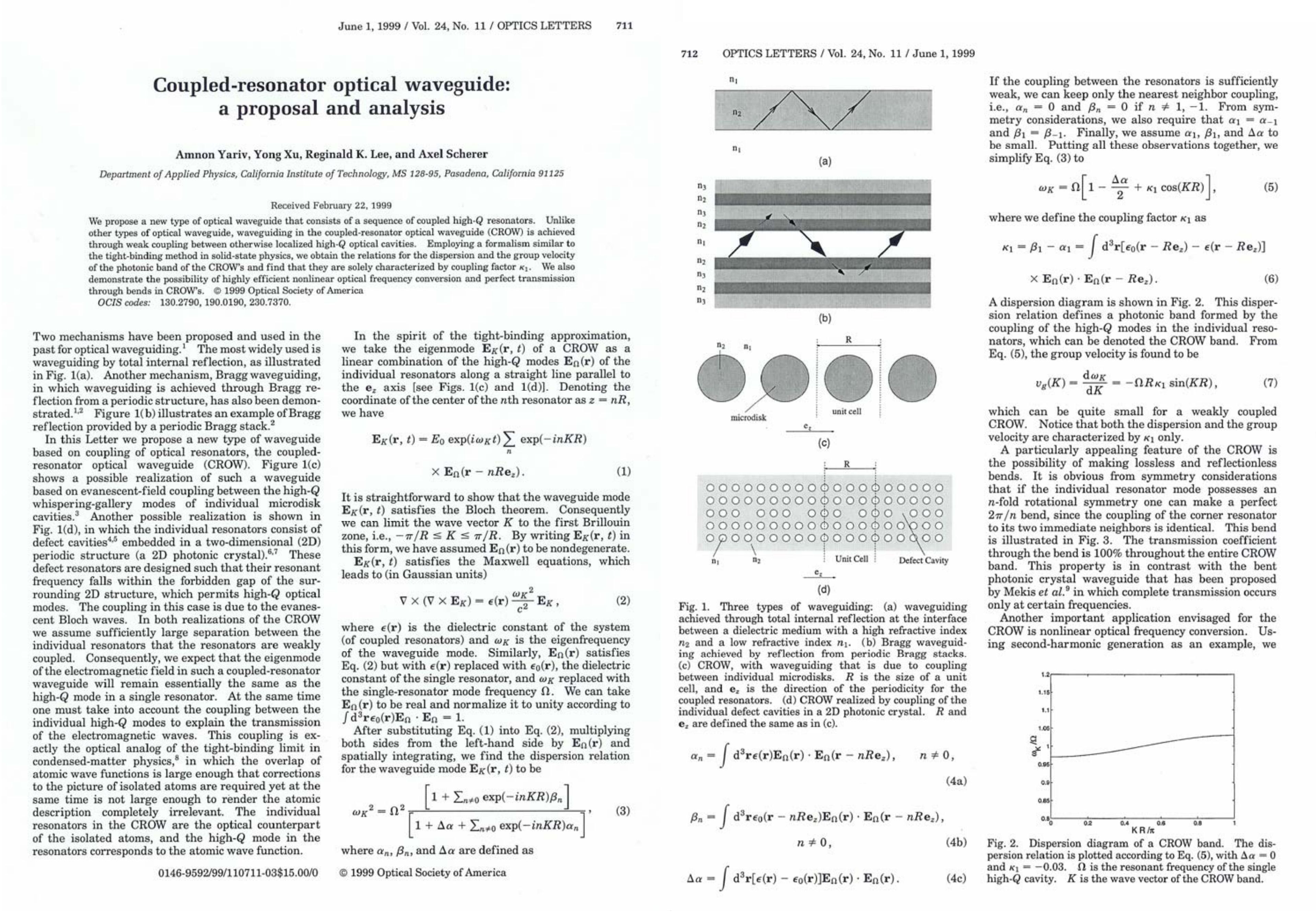
This equation is of the form of Wannier series expansion:

$$\psi_{n\mathbf{k}}(\mathbf{r}) = \sum_{\mathbf{R}} e^{i\mathbf{k}\mathbf{R}} \psi_n(\mathbf{r}-\mathbf{R})$$

Where $f_n(\mathbf{R},\mathbf{r}) = \phi_n(\mathbf{r}-\mathbf{R})$

The Wannier functions are orthogonal at different sites. They form a complete orthogonal set alternative to Bloch functions.

Wannier Functions with Maxwell Equations



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Coupled-resonator optical waveguide: a proposal and analysis

Amnon Yariv, Yong Xu, Reginald K. Lee, and Axel Scherer

Department of Applied Physics, California Institute of Technology, MS 128-95, Pasadena, California 91125

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We propose a new type of optical waveguide that consists of a sequence of coupled high-Q resonators. Unlike other types of optical waveguide, waveguiding in the coupled-resonator optical waveguide (CROW) is achieved through weak coupling between otherwise localized high-Q optical cavities. Employing a formalism similar to the tight-binding method in solid-state physics, we obtain the relations for the dispersion and the group velocity of the photonic band of the CROW's and find that they are solely characterized by coupling factor κ_1. We also demonstrate the possibility of highly efficient nonlinear optical frequency conversion and perfect transmission through bends in CROW's. © 1999 Optical Society of America

OCIS codes: 130.2790, 190.0190, 230.7370.

Two mechanisms have been proposed and used in the past for optical waveguiding.[1] The most widely used is waveguiding by total internal reflection, as illustrated in Fig. 1(a). Another mechanism, Bragg waveguiding, in which waveguiding is achieved through Bragg reflection from a periodic structure, has also been demonstrated.[1,2] Figure 1(b) illustrates an example of Bragg reflection provided by a periodic Bragg stack.[2]

In this Letter we propose a new type of waveguide based on coupling of optical resonators, the coupled-resonator optical waveguide (CROW). Figure 1(c) shows a possible realization of such a waveguide based on evanescent-field coupling between the high-Q whispering-gallery modes of individual microdisk cavities.[3] Another possible realization is shown in Fig. 1(d), in which the individual resonators consist of defect cavities[4,5] embedded in a two-dimensional (2D) periodic structure (a 2D photonic crystal).[6,7] These defect resonators are designed such that their resonant frequency falls within the forbidden gap of the surrounding 2D structure, which permits high-Q optical modes. The coupling in this case is due to the evanescent Bloch waves. In both realizations of the CROW we assume sufficiently large separation between the individual resonators that the resonators are weakly coupled. Consequently, we expect that the eigenmode of the electromagnetic field in such a coupled-resonator waveguide will remain essentially the same as the high-Q mode in a single resonator. At the same time one must take into account the coupling between the individual high-Q modes to explain the transmission of the electromagnetic waves. This coupling is exactly the optical analog of the tight-binding limit in condensed-matter physics,[8] in which the overlap of atomic wave functions is large enough that corrections to the picture of isolated atoms are required yet at the same time is not large enough to render the atomic description completely irrelevant. The individual resonators in the CROW are the optical counterpart of the isolated atoms, and the high-Q mode in the resonators corresponds to the atomic wave function.

In the spirit of the tight-binding approximation, we take the eigenmode $\mathbf{E}_K(\mathbf{r}, t)$ of a CROW as a linear combination of the high-Q modes $\mathbf{E}_\Omega(\mathbf{r})$ of the individual resonators along a straight line parallel to the $\mathbf{e}_z$ axis [see Figs. 1(c) and 1(d)]. Denoting the coordinate of the center of the nth resonator as $z = nR$, we have

$$\mathbf{E}_K(\mathbf{r}, t) = E_0 \exp(i\omega_K t) \sum_n \exp(-inKR) \times \mathbf{E}_\Omega(\mathbf{r} - nR\mathbf{e}_z)\,. \tag{1}$$

It is straightforward to show that the waveguide mode $\mathbf{E}_K(\mathbf{r}, t)$ satisfies the Bloch theorem. Consequently we can limit the wave vector K to the first Brillouin zone, i.e., $-\pi/R \le K \le \pi/R$. By writing $\mathbf{E}_K(\mathbf{r}, t)$ in this form, we have assumed $\mathbf{E}_\Omega(\mathbf{r})$ to be nondegenerate.

$\mathbf{E}_K(\mathbf{r}, t)$ satisfies the Maxwell equations, which leads to (in Gaussian units)

$$\nabla \times (\nabla \times \mathbf{E}_K) = \epsilon(\mathbf{r}) \frac{{\omega_K}^2}{c^2} \mathbf{E}_K\,, \tag{2}$$

where $\epsilon(\mathbf{r})$ is the dielectric constant of the system (of coupled resonators) and ω_K is the eigenfrequency of the waveguide mode. Similarly, $\mathbf{E}_\Omega(\mathbf{r})$ satisfies Eq. (2) but with $\epsilon(\mathbf{r})$ replaced with $\epsilon_0(\mathbf{r})$, the dielectric constant of the single resonator, and ω_K replaced with the single-resonator mode frequency Ω. We can take $\mathbf{E}_\Omega(\mathbf{r})$ to be real and normalize it to unity according to $\int \mathrm{d}^3\mathbf{r}\epsilon_0(\mathbf{r})\mathbf{E}_\Omega \cdot \mathbf{E}_\Omega = 1$.

After substituting Eq. (1) into Eq. (2), multiplying both sides from the left-hand side by $\mathbf{E}_\Omega(\mathbf{r})$ and spatially integrating, we find the dispersion relation for the waveguide mode $\mathbf{E}_K(\mathbf{r}, t)$ to be

$${\omega_K}^2 = \Omega^2 \frac{\left[1 + \sum_{n\neq 0} \exp(-inKR)\beta_n\right]}{\left[1 + \Delta\alpha + \sum_{n\neq 0} \exp(-inKR)\alpha_n\right]}, \tag{3}$$

where α_n, β_n, and $\Delta\alpha$ are defined as

Fig. 1. Three types of waveguiding: (a) waveguiding achieved through total internal reflection at the interface between a dielectric medium with a high refractive index n_2 and a low refractive index n_1. (b) Bragg waveguiding achieved by reflection from periodic Bragg stacks. (c) CROW, with waveguiding that is due to coupling between individual microdisks. R is the size of a unit cell, and $\mathbf{e}_z$ is the direction of the periodicity for the coupled resonators. (d) CROW realized by coupling of the individual defect cavities in a 2D photonic crystal. R and $\mathbf{e}_z$ are defined the same as in (c).

$$\alpha_n = \int \mathrm{d}^3\mathbf{r}\epsilon(\mathbf{r})\mathbf{E}_\Omega(\mathbf{r}) \cdot \mathbf{E}_\Omega(\mathbf{r} - nR\mathbf{e}_z)\,, \qquad n \neq 0\,, \tag{4a}$$

$$\beta_n = \int \mathrm{d}^3\mathbf{r}\epsilon_0(\mathbf{r} - nR\mathbf{e}_z)\mathbf{E}_\Omega(\mathbf{r}) \cdot \mathbf{E}_\Omega(\mathbf{r} - nR\mathbf{e}_z)\,, \quad n \neq 0\,, \tag{4b}$$

$$\Delta\alpha = \int \mathrm{d}^3\mathbf{r}[\epsilon(\mathbf{r}) - \epsilon_0(\mathbf{r})]\mathbf{E}_\Omega(\mathbf{r}) \cdot \mathbf{E}_\Omega(\mathbf{r})\,. \tag{4c}$$

If the coupling between the resonators is sufficiently weak, we can keep only the nearest neighbor coupling, i.e., $\alpha_n = 0$ and $\beta_n = 0$ if $n \neq 1, -1$. From symmetry considerations, we also require that $\alpha_1 = \alpha_{-1}$ and $\beta_1 = \beta_{-1}$. Finally, we assume α_1, β_1, and $\Delta\alpha$ to be small. Putting all these observations together, we simplify Eq. (3) to

$$\omega_K = \Omega\left[1 - \frac{\Delta\alpha}{2} + \kappa_1 \cos(KR)\right], \tag{5}$$

where we define the coupling factor κ_1 as

$$\kappa_1 = \beta_1 - \alpha_1 = \int \mathrm{d}^3\mathbf{r}[\epsilon_0(\mathbf{r} - R\mathbf{e}_z) - \epsilon(\mathbf{r} - R\mathbf{e}_z)] \times \mathbf{E}_\Omega(\mathbf{r}) \cdot \mathbf{E}_\Omega(\mathbf{r} - R\mathbf{e}_z)\,. \tag{6}$$

A dispersion diagram is shown in Fig. 2. This dispersion relation defines a photonic band formed by the coupling of the high-Q modes in the individual resonators, which can be denoted the CROW band. From Eq. (5), the group velocity is found to be

$$v_g(K) = \frac{\mathrm{d}\omega_K}{\mathrm{d}K} = -\Omega R \kappa_1 \sin(KR)\,, \tag{7}$$

which can be quite small for a weakly coupled CROW. Notice that both the dispersion and the group velocity are characterized by κ_1 only.

A particularly appealing feature of the CROW is the possibility of making lossless and reflectionless bends. It is obvious from symmetry considerations that if the individual resonator mode possesses an n-fold rotational symmetry one can make a perfect $2\pi/n$ bend, since the coupling of the corner resonator to its two immediate neighbors is identical. This bend is illustrated in Fig. 3. The transmission coefficient through the bend is 100% throughout the entire CROW band. This property is in contrast with the bent photonic crystal waveguide that has been proposed by Mekis *et al.*[9] in which complete transmission occurs only at certain frequencies.

Another important application envisaged for the CROW is nonlinear optical frequency conversion. Using second-harmonic generation as an example, we

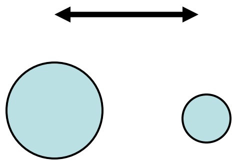
Fig. 2. Dispersion diagram of a CROW band. The dispersion relation is plotted according to Eq. (5), with $\Delta\alpha = 0$ and $\kappa_1 = -0.03$. Ω is the resonant frequency of the single high-Q cavity. K is the wave vector of the CROW band.

Lectures 11-12: Lattice Vibrations: Phonons

Assumptions

- Mean equilibrium position corresponds to a Bravais lattice site.
- Ions displacements are small compared with the interionic spacing.

Classical oscillations in a molecule



$x = x_0 \sin\omega t$, $v = dx/dt = x_0\omega \cos\omega t$, $a = -x_0\omega^2 \sin\omega t$

Hooke's Law: $F = -Kx$

Since $F = ma$

$-Kx_0 \sin\omega t = -mx_0\omega^2 \sin\omega t$

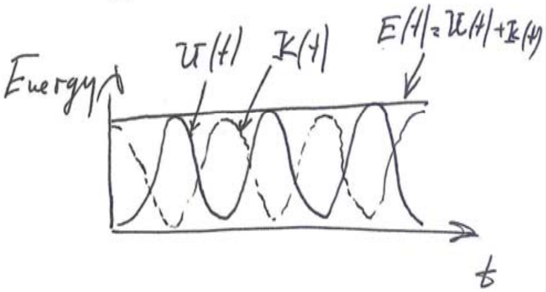
$K = m\omega^2 \Rightarrow \omega = \sqrt{(K/m)}$

Energy:

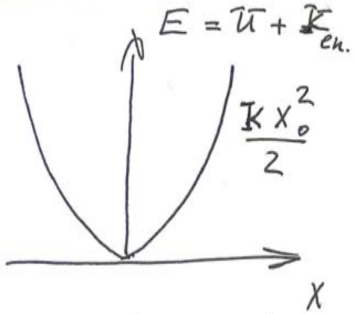
$$\Delta U = -A = -\int_i^f (-Kx)\cdot dx = K\int_i^f x\cdot dx = \frac{Kx_f^2}{2} - \frac{Kx_i^2}{2}.$$

$$u_f - u_i = \frac{Kx_f^2}{2} - \frac{Kx_i^2}{2} \Rightarrow$$

$$u = \frac{Kx^2}{2}$$

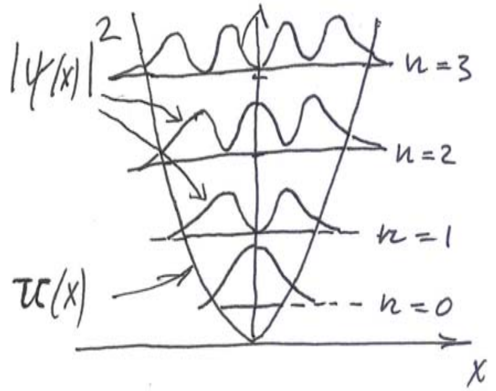


Classical Picture



- Oscillations at a single frequency $\omega = \sqrt{\frac{K}{m}}$
- Any energy is allowed: $E = \frac{Kx_0^2}{2}$

QM Harmonic Oscillator



Hamiltonian:

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + U(x)\right]u(x) = Eu(x)$$

$$\psi(x,t) = T(t)\cdot u(x)$$

Continuation

Classical Oscillator

It is seen that

$$\frac{\partial U}{\partial x} = \frac{2Kx}{2} = Kx = -F$$

In further, considering chains and lattices, we will use $\boxed{\frac{\partial U}{\partial x} = -F}$

QM Harmonic Oscillator

Discrete, equally spaced eigenvalues:

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

For $n = 0$

$$E = \hbar\omega/2$$

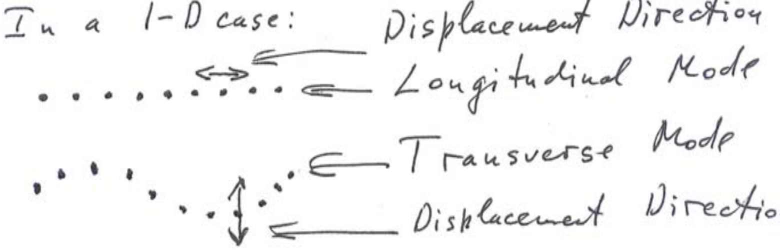
- zero point energy

Consider now a 1-D chain

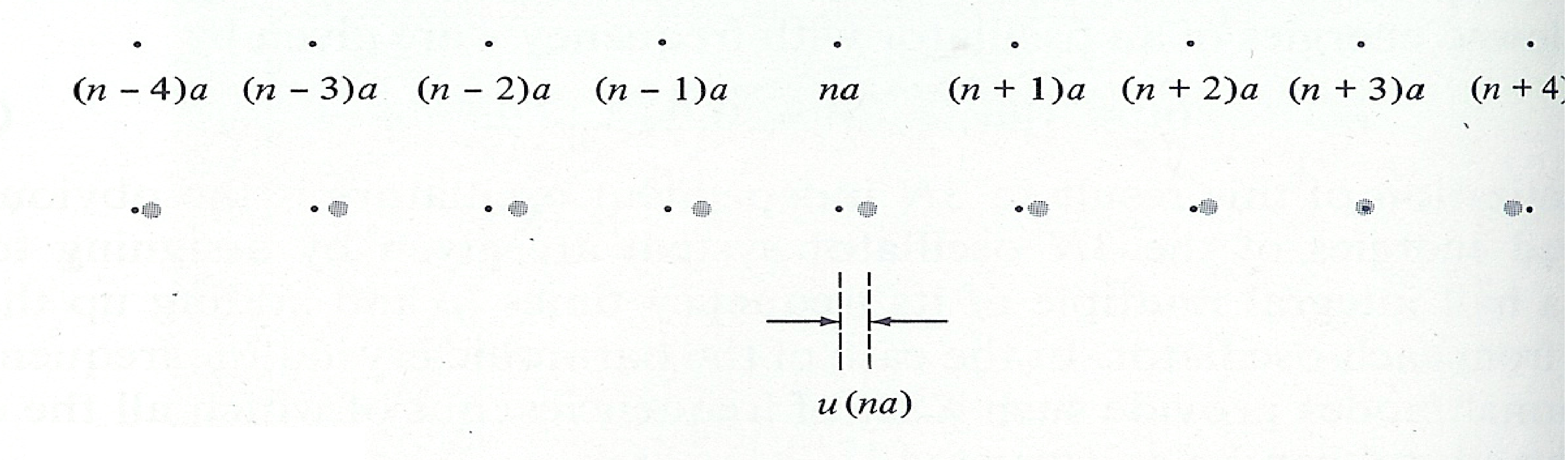
Periodic Boundary Conditions

We have now waves, $\psi \sim e^{ikx}$, instead of localized oscillations in molecules

In a 1-D case:

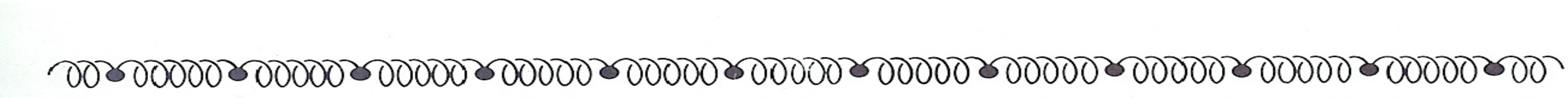


Normal Modes of a 1- D Monatomic Lattice



$u(na,t) \sim e^{i(kx-\omega t)}$ - displacements from equilibrium for each ion,
where $k = 2\pi/\lambda$ - wavevector. It should not be confused with K – Hooke’s constant.

Assuming that only neighbors interact we can express U as for a system of springs:

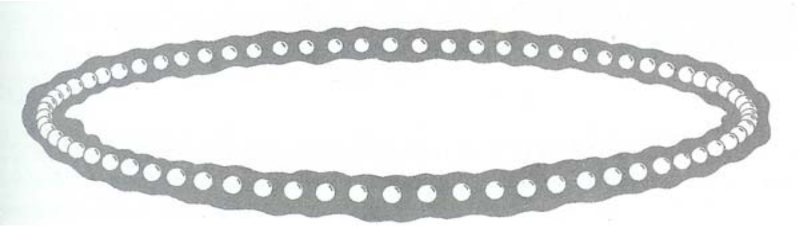


$$U^{harm} = \frac{1}{2} K \sum_{n} [u(na) - u([n+1]a)]^2$$

$$\frac{\partial U^{harm}}{\partial u(na)} = -F(na) = K[\underbrace{(u([n-1]a) - u(na))(-1)}_{\text{For } (n\text{-1)-th term}} + \underbrace{u(na) - u([n-1]a)}_{\text{For } n\text{-th term}}] \qquad (1)$$

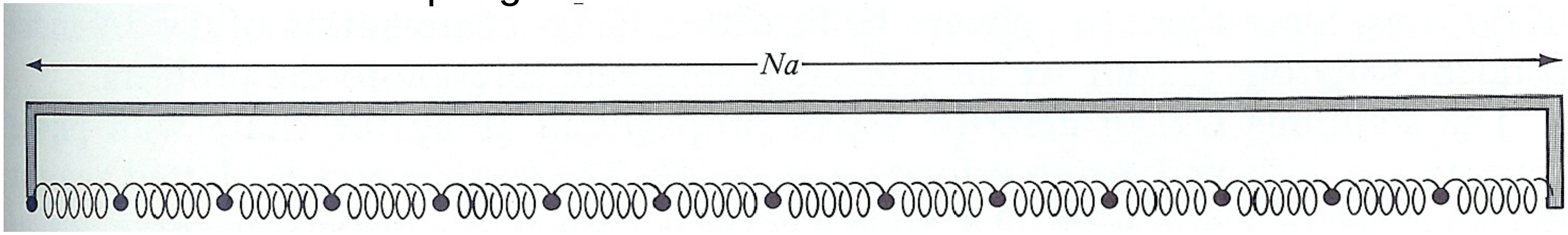
The Born-von Karman periodic boundary conditions

$u([N+1]a) = u(a); u(0) = u(Na)$



Joining the remote ends of the chain back together by the same spring

Alternative interpretaion: explicit mechanical constraint forcing ion N to interact with ion 1 via the same spring K:



$u(na,t) \sim e^{i(kx-\omega t)}$, $e^{i(kx-\omega t)} = e^{i(kx-\omega t)}\, e^{ikL},$

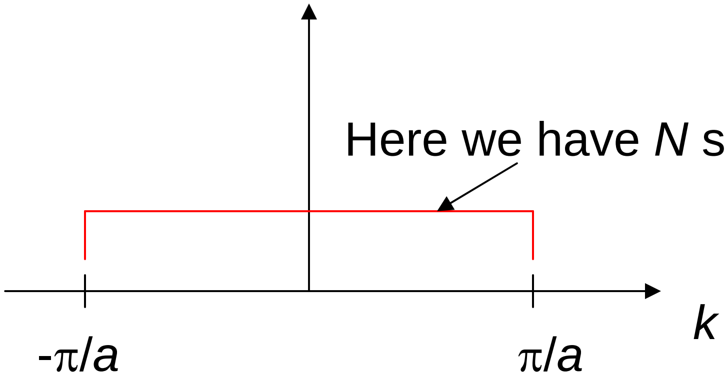
$e^{ikNa} = 1 \Rightarrow k = (2\pi/a)(m/N)$, where m – an integer

If $m = N$ when $k = 2\pi/a \Rightarrow \lambda = a$ – all atoms are moving in phase…

For this reason instead of $0 < k < (2\pi/a)$ we select first Brillouin zone according to:

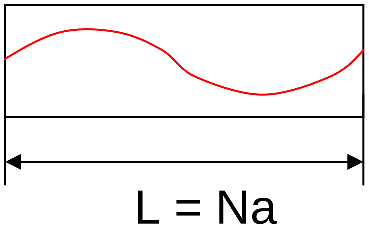
$-\pi/a < k < \pi/a$ – same reasoning as for electronic band structure

First Brillouin zone for phonons



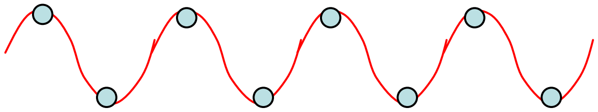
What are the extreme wavelengths (k-vectors)?

Longest $\lambda = Na$ ($m = 1$),



$k = 2\pi/Na$

Shortest $\lambda = 2a$ ($m = N/2$)



$k = +\pi/a$

→

$k = -\pi/a$

←

Continuing solving equation of motion

Substituting $u(na,t) \sim e^{i(kx-\omega t)}$ in the Eq. (1) and taking into account that

$F(na) = \mathrm{M}\, du(na,t)/dt \sim -M\omega^2 e^{i(kx-\omega t)}$ we have:

$M\omega^2 \exp i(kx-\omega t) = K[2 \exp i(kx - \omega t) - \exp(ika) \exp i(kx - \omega t) - \exp(-ika) \exp i(kx - \omega t)]$

$M\omega^2 = 2\mathrm{K}[1 - (\exp(ika) + \exp(-ika))/2] = 2\mathrm{K}\,[1 - \cos \mathrm{ka}]$

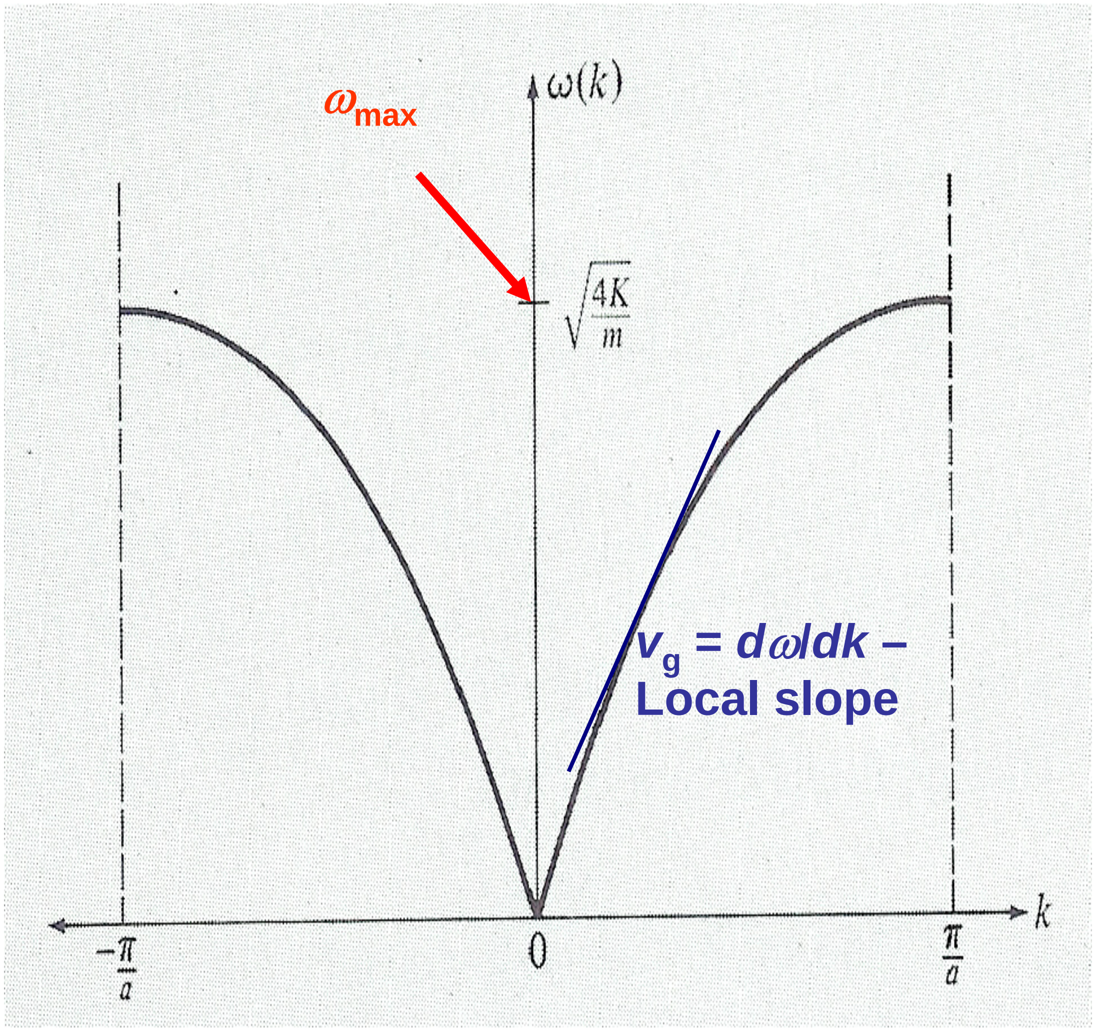
$$\omega(k) = \sqrt{\frac{2K(1-\cos ka)}{M}} = 2\sqrt{\frac{K}{M}}\left|\sin\frac{1}{2}ka\right|$$

The solutions are plane waves:

$u(na,\mathrm{t}) \sim \cos(kna-\omega t)$ or $\sin(kna-\omega t)$

Since $\omega(k) = \omega(-k)$

Phonon Dispersion Relations for a 1- D Monatomic Lattice



$\mathcal{E}(k)$ – dispersion relationship:

- ω_{max} ~ (10^{12} – 10^{14}) Hz or

  λ ~ (5 – 500) μm

  hν ~ (2 – 200) meV

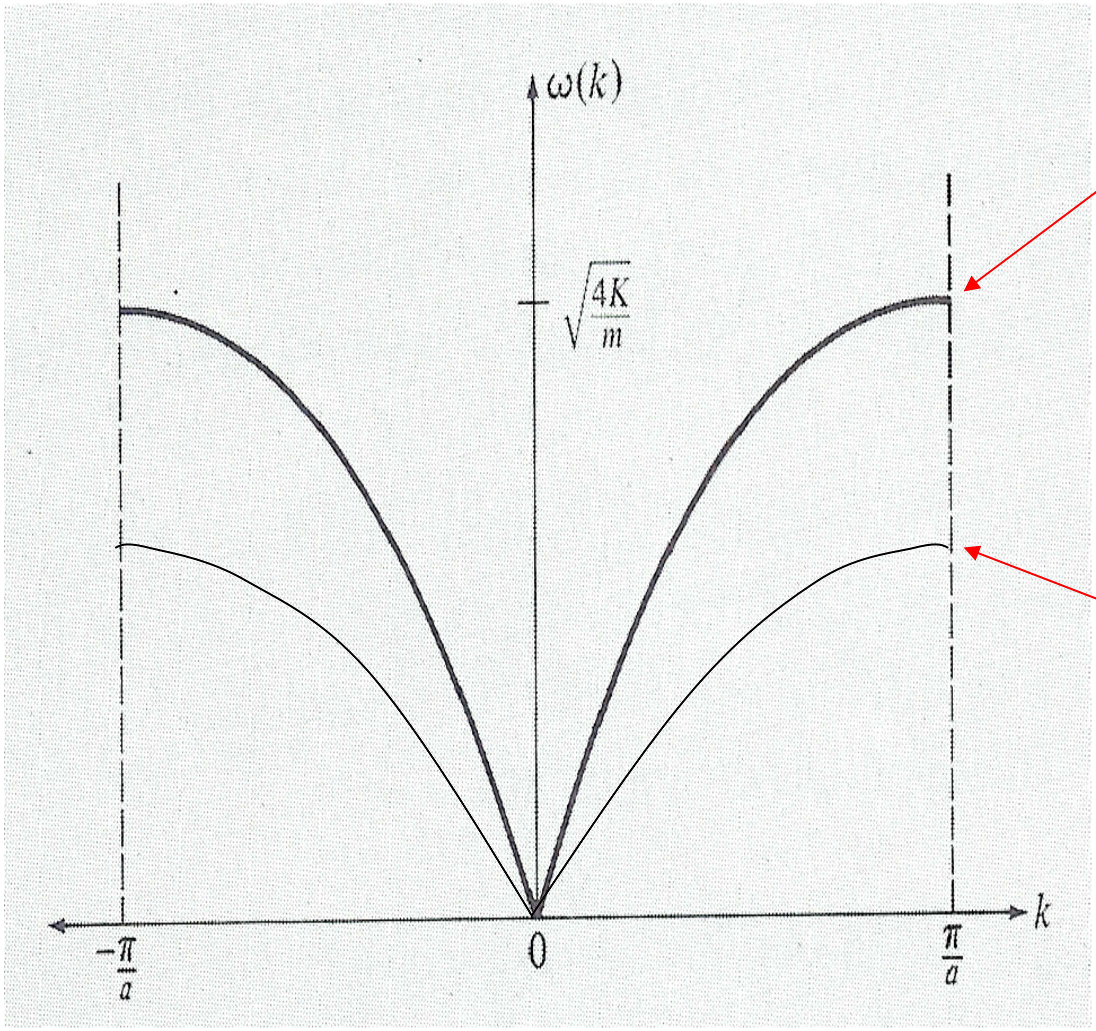
- Phase velocity $v_{ph} = \omega/k$ – weakly dependent on k

- Group velocity $v_g = d\omega/dk$,

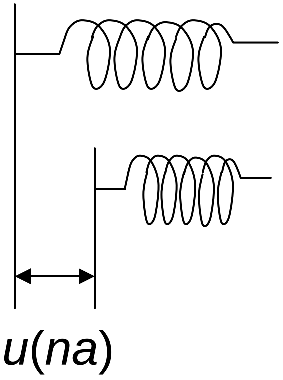
At long-wavelength limit (k~0): $v_g \approx v_{ph}$

At $k = \pm \pi/a$ $v_g \sim 0$

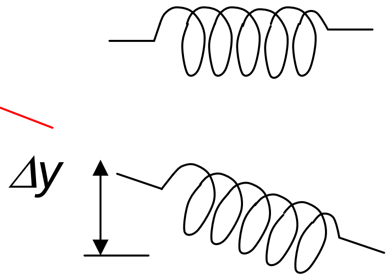
Phonon Dispersion Relations for a 3- D Monatomic Lattice



1 Longitudinal Mode



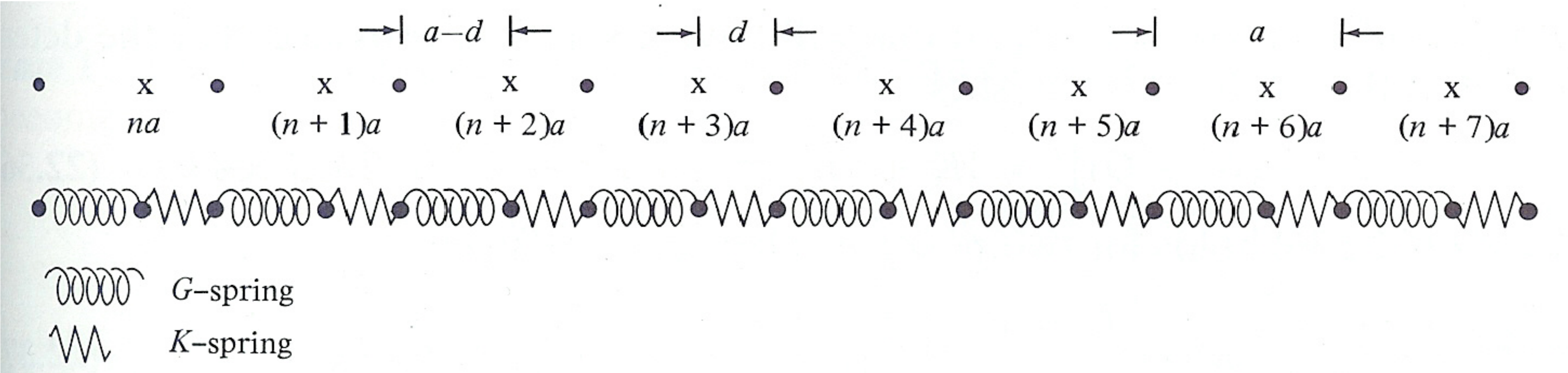
2 Transverse Modes



Which oscillations disturb the spring more?

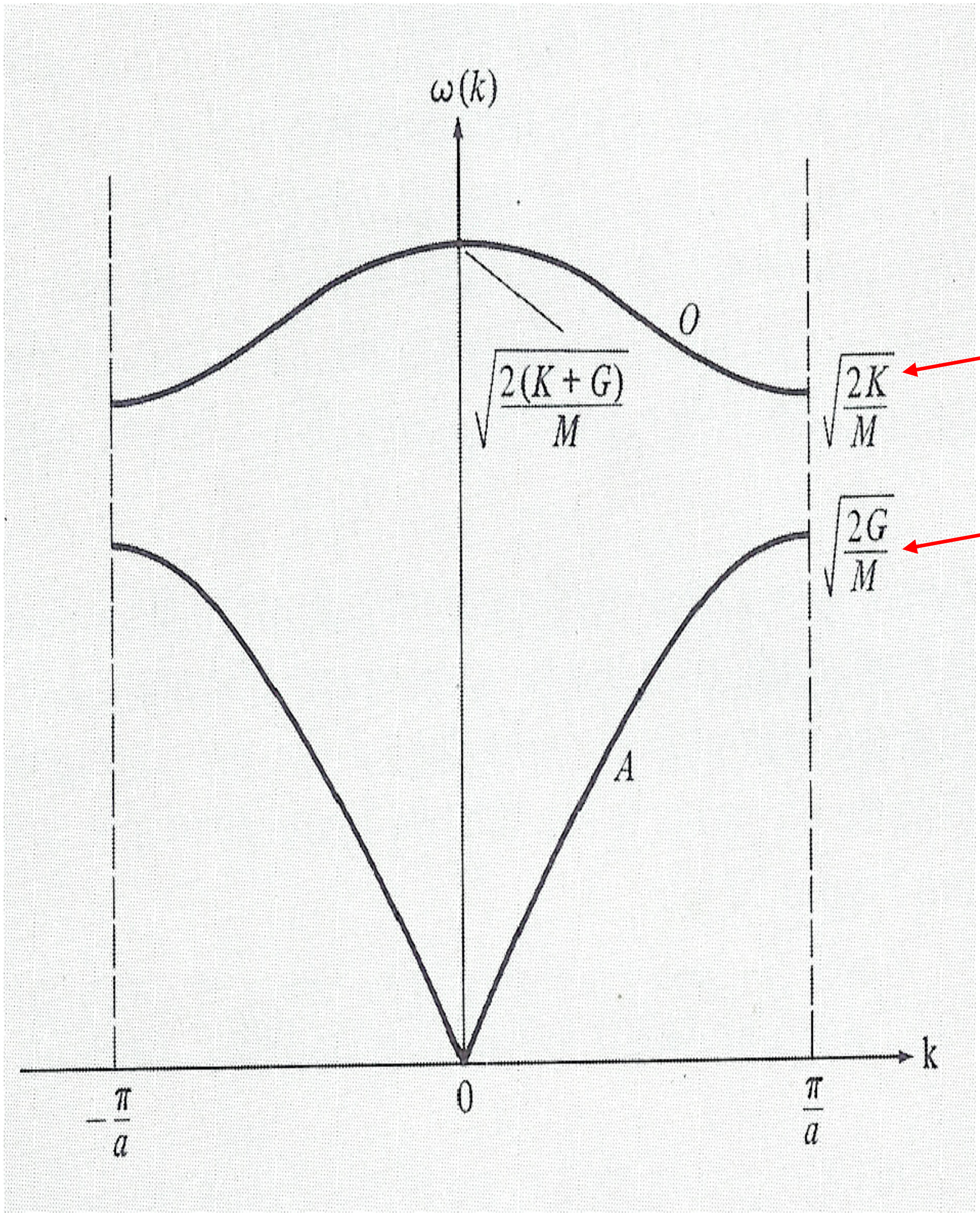
Why longitudinal modes have higher energy?

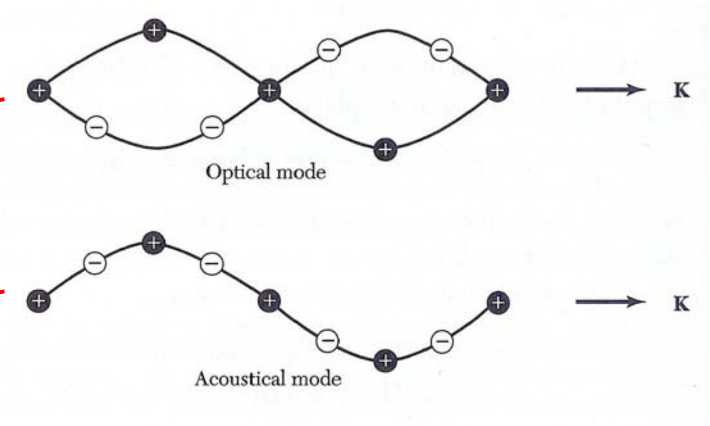
Normal Modes of a 1-D Lattice with a Two Ions Basis



Equilibrium positions are (na) and ($na + d$).
Two ions are identical, but $d < a/2$ $\Rightarrow$ we have G-spring and K-spring.

Optical and Acoustical Branchas

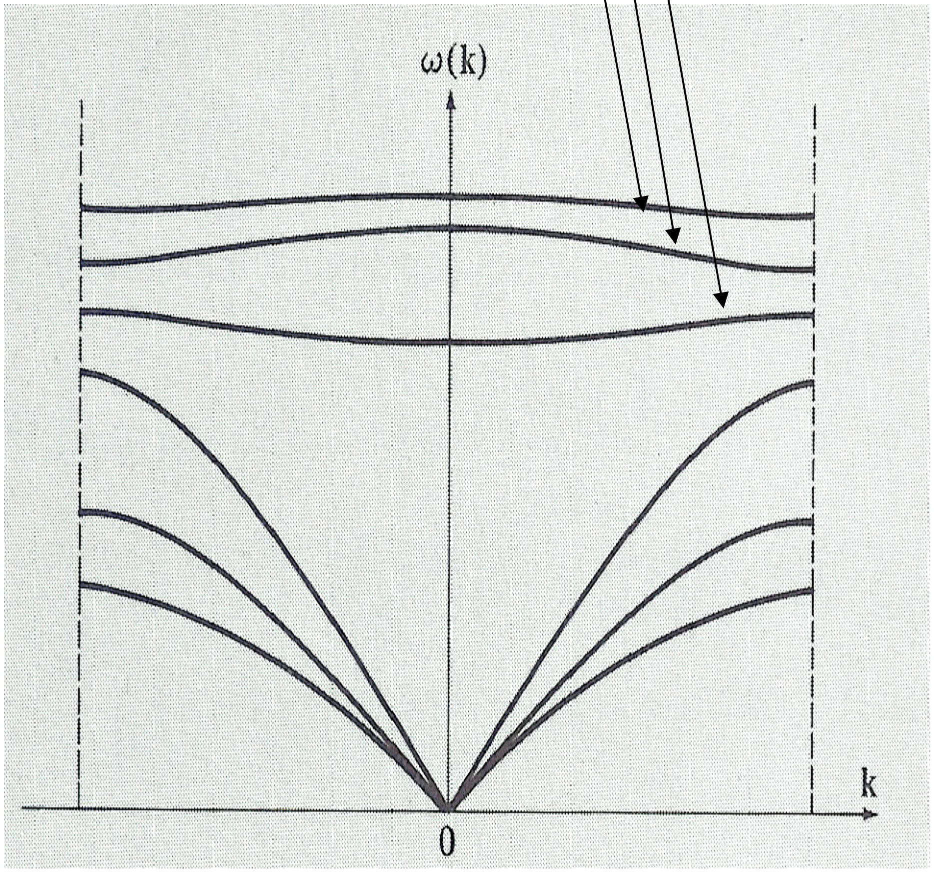




If these two atoms carry opposite charges we may excite this motion with a light wave, see top branch called optical branch.

Phonon Dispersion Relations for a 3- D Lattice with a Basis

3 optical branches interact with light



6N degrees of freedom, N per branch

Lectures 13-15: Lorentz Model of Dipole Oscillators

It does not specify the nature of oscillating dipole and makes very basic assumptions about the forces involved. For these reasons it applies to a variety of situations:

- **Electronic polarization of atoms** (visible and near infrared frequencies 10^{14} – 10^{15} Hz):

$$\omega_0 = \sqrt{\frac{K_s}{\mu}}$$

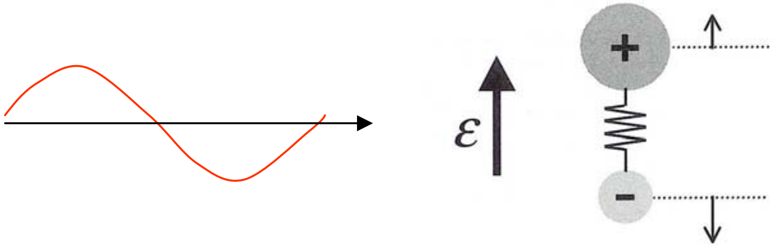
, where $\mu \sim m_e$ – mass of the electron – **small**

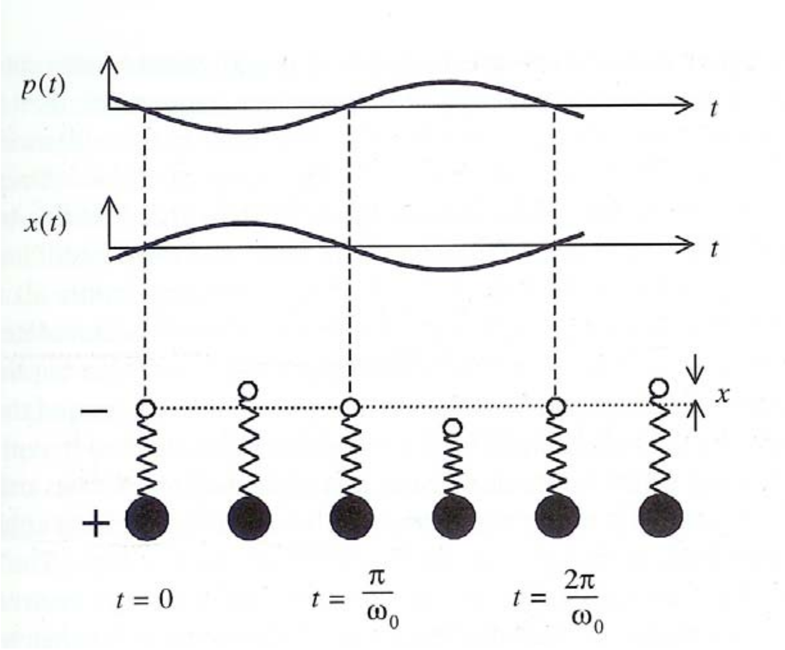
- **Molecular and lattice vibrations** (mid and far infrared frequencies 10^{12} – 10^{13} Hz):
  $\mu \sim M$ – mass of the nucleolus – **large**

- **Free electrons**: special case since we have no restoring force for a dipole

About the model:

Microscopical level: the force $E(\mathrm{t}) = E_0\ \mathrm{e}^{-i\omega t}$ and the solutions $x(\mathrm{t}) = \boldsymbol{X}_0\ \mathrm{e}^{-i\omega t}$
Basic assumptions: driving, returning and friction forces
Goal: express microscopical dipole moment $p(t) = -ex(t)$





Macroscopical level: polarization $P = Np$ and then $D = \varepsilon_0 E + P$ that allows finding ε_r due to the fact that $P \sim E$ and $D = \varepsilon_0\ \varepsilon_r\ E$

Dipersive and absorptive properties: language of $\varepsilon_1(\omega)$ and $\varepsilon_2(\omega)$ or $\mathrm{n}(\omega)$ and $\mathrm{k}(\omega)$

Note Title 2/24/2005

$$\tilde{\varepsilon}(\omega) = \varepsilon_1(\omega) + i\,\varepsilon_2(\omega)$$

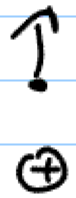
$$\tilde{n}(\omega) = n(\omega) + i\,K(\text{Extinction})(\omega)$$

$1\ \bar{e}$

•

⊕ Bound to $+\,e$ charge (1 proton)

$\bar{E}\downarrow$ $\quad \bar{F} = -q\bar{E}$



$$p = -eX$$

$$ma = \Sigma F$$

$$m_e\ddot{X} = -e\underset{\substack{\uparrow\\ \text{due to}\\ \text{EM field}}}{E} - \underset{\uparrow}{k_s X} - m_e\gamma\underset{\uparrow}{\dot{X}}$$

Hooke's Law (Returning force $k_s = \omega_0^2 \cdot m_e$)

γ – damping constant

$$m_e \ddot{x} + m_e \gamma \dot{x} + \omega_0^2 m_e x = -e\underline{E}$$

$$E = E_0 e^{i(kx - \omega t)}$$ – incoming light wave

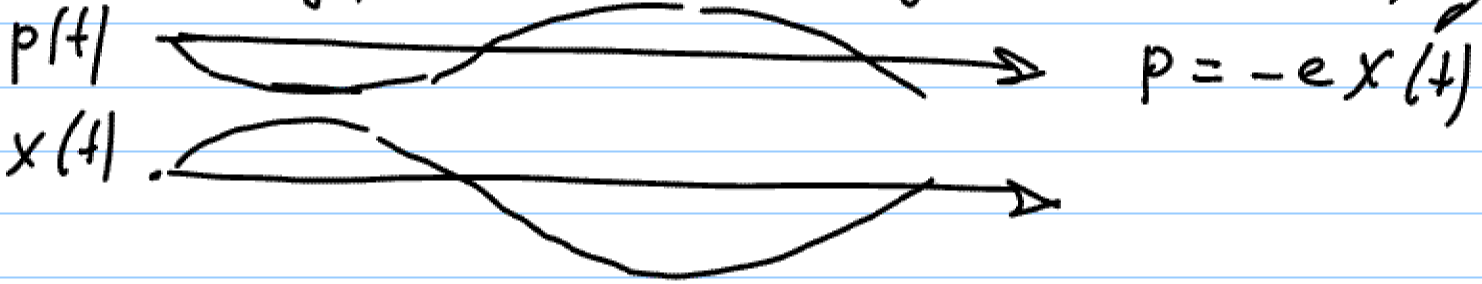
$$x(t) = x_0 e^{-i(\omega t + \Phi)}$$ – expected general solution

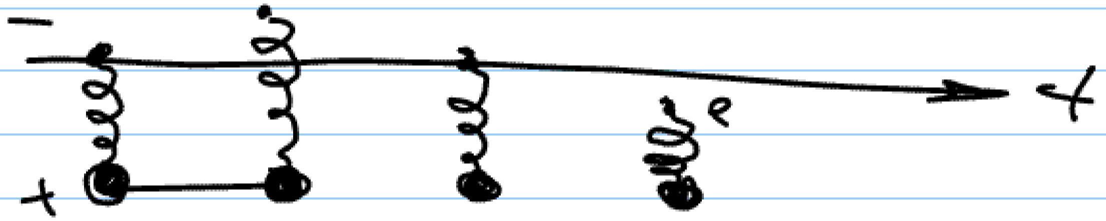
$$x(t) = \tilde{x}_0 \cdot e^{-i\omega t}$$

Plug soln. into D.E.

$$x(t) = \underset{\overset{\|}{\tilde{x}_0}}{\boxed{\frac{-\frac{e}{m_e}E_0\cdot 1\, e^{-i\omega t}}{\omega_0^2-\omega^2-i\omega\gamma}}} = \tilde{x}_0\cdot e^{-i\omega t}$$

Phase difference comes from the damping.





Macroscopical Polarization (P):

$$P = N \cdot p(t)$$

$$D = \varepsilon_0 E + P = \varepsilon_0 E + N p(t) =$$

$$= \varepsilon_0 E + N\left(-e\, x(t)\right) =$$

$$= \varepsilon_0 E + N\left(\frac{e^2/m_e}{\omega_0^2 - \omega^2 - i\gamma\omega}\right) E \Rightarrow$$

$$D = \varepsilon_0 \left[1 + \underbrace{\left[\frac{\frac{N e^2}{\varepsilon_0 m_e}}{\omega_0^2 - \omega^2 - i\gamma\omega} \right]}_{\chi_e(\omega)} \right] E$$

Now $D = \varepsilon_0 (1 + \tilde{\chi}_e) E$

$D = \varepsilon_0 \varepsilon_r \cdot E$ – used in Maxwell's Eq.

$$\tilde{\varepsilon}_r(\omega) = 1 + \frac{N \frac{e^2}{\varepsilon_0 m_e}}{\underbrace{(\omega_0^2 - \omega^2)}_{a} - i \underbrace{\gamma \omega}_{b}} = \varepsilon_1(\omega) + i \varepsilon_2(\omega)$$

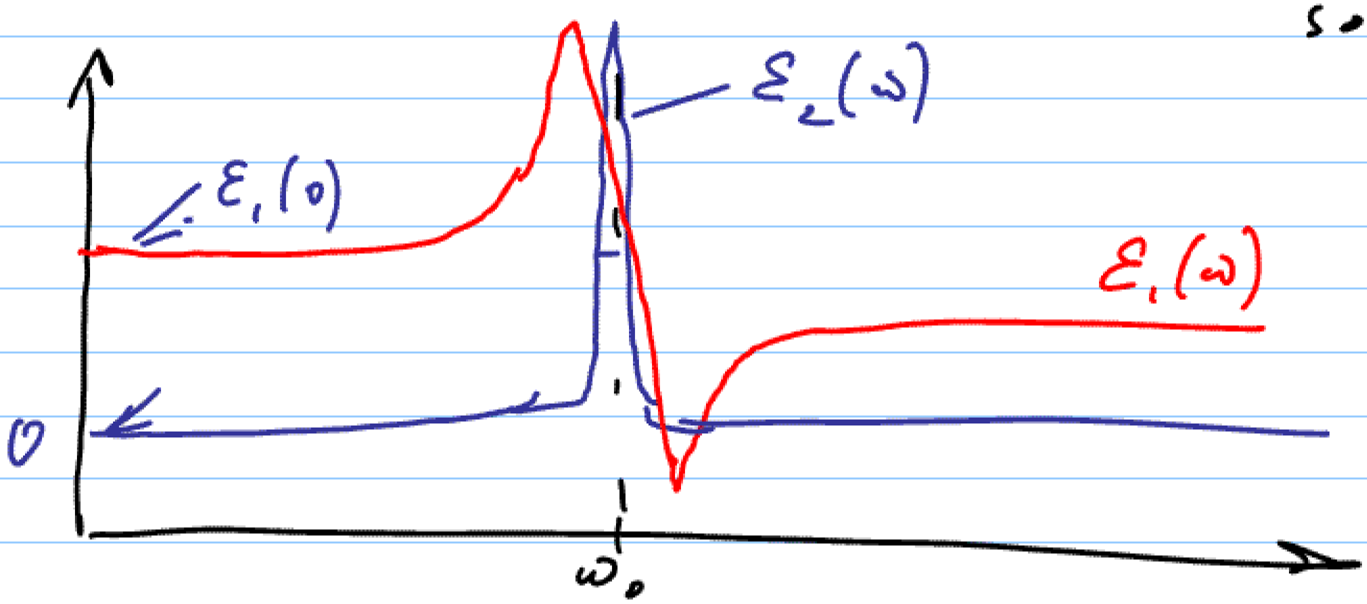
$$\varepsilon_1(\omega) = \mathrm{Re}\{\tilde{\varepsilon}_r(\omega)\} = 1 + \frac{Ne^2}{\varepsilon_0 m_e} \left[\frac{\omega_0^2 - \omega^2}{(\omega_0^2 - \omega^2)^2 + (\omega^2 \gamma} \right.$$

$$\boxed{\begin{aligned} \frac{c(a+ib)}{(a-ib)(a+ib)} &= \frac{ca + icb}{a^2 - (i)^2 \cdot b^2} = \\ &= \frac{ca + icb}{a^2 + b^2} = \frac{ca}{a^2 + b^2} + i \frac{cb}{a^2 + b^2} \end{aligned}}$$

$$= 1 + \frac{Ne^2}{\varepsilon_0 m_e}\left[\frac{\omega_0^2-\omega^2}{(\omega_0^2-\omega^2)^2+(\omega\gamma)^2}\right\}.$$

$$\varepsilon_2(\omega) = \mathrm{Im}\{\tilde{\varepsilon}_r\} = \frac{Ne^2}{\varepsilon_0 m_e}\,\frac{\omega\gamma}{(\omega_0^2-\omega^2)^2+(\omega\gamma)^2}$$

Expression for $\varepsilon_1(\omega)$ and $\varepsilon_2(\omega)$ – general solution.



ω

3. Particular cases:

1. $\omega \ll \omega_0$.
2. $\omega \sim \omega_0$
3. $\omega \gg \omega_0$

1. $\omega \ll \omega_0$.

$$\varepsilon_1(0) = 1 + \frac{Ne^2}{\varepsilon_0 m_e \omega_0^2} = \text{Const}$$

$$\varepsilon_2(0) \simeq 0$$

$$\varepsilon_r(0) = 1 + \underbrace{\frac{Ne^2}{\varepsilon_0 m_e \omega_0^2}}_{\chi(0)}$$

↗

DC susceptibility $\Rightarrow n = \sqrt{\varepsilon_r}$.

$v = \frac{c}{n}$.

③ $\omega \gg \omega_0$

$\varepsilon_1(\infty) \simeq 1 \Rightarrow n = \sqrt{\varepsilon_r} \simeq 1 \Rightarrow v \simeq c$

$\varepsilon_2(\infty) = 0$

② Near Resonance, $\omega \sim \omega_0$

$$\omega_0^2 - \omega^2 = (\omega_0 + \omega)(\omega_0 - \omega) \simeq$$

$$2\omega_0 \Delta\omega$$

$\uparrow$

$\Delta\omega = \omega_0 - \omega$ - Detuning

$$\varepsilon_1(\omega) \simeq 1 + \underbrace{\boxed{\frac{Ne^2}{\varepsilon_0 m_e \omega_0^2}}}_{\nearrow\ \chi(0)} \frac{\omega_0^2 \cdot 2\omega_0 \Delta\omega}{4\omega_0^2 \Delta\omega^2 + (\omega_0 \gamma)^2}$$

$$\varepsilon_1(\omega) \simeq 1 + \chi(0) \frac{2\omega_0 \Delta\omega}{4\Delta\omega^2 + \gamma^2}$$

$$\varepsilon_2(\omega) \simeq \chi(0) \frac{\omega_0 \gamma}{4\Delta\omega^2 + \gamma^2}$$

Single Electron Oscillator Summary

$$\varepsilon_r(\omega) = \varepsilon_1(\omega) + i\,\varepsilon_2(\omega)$$

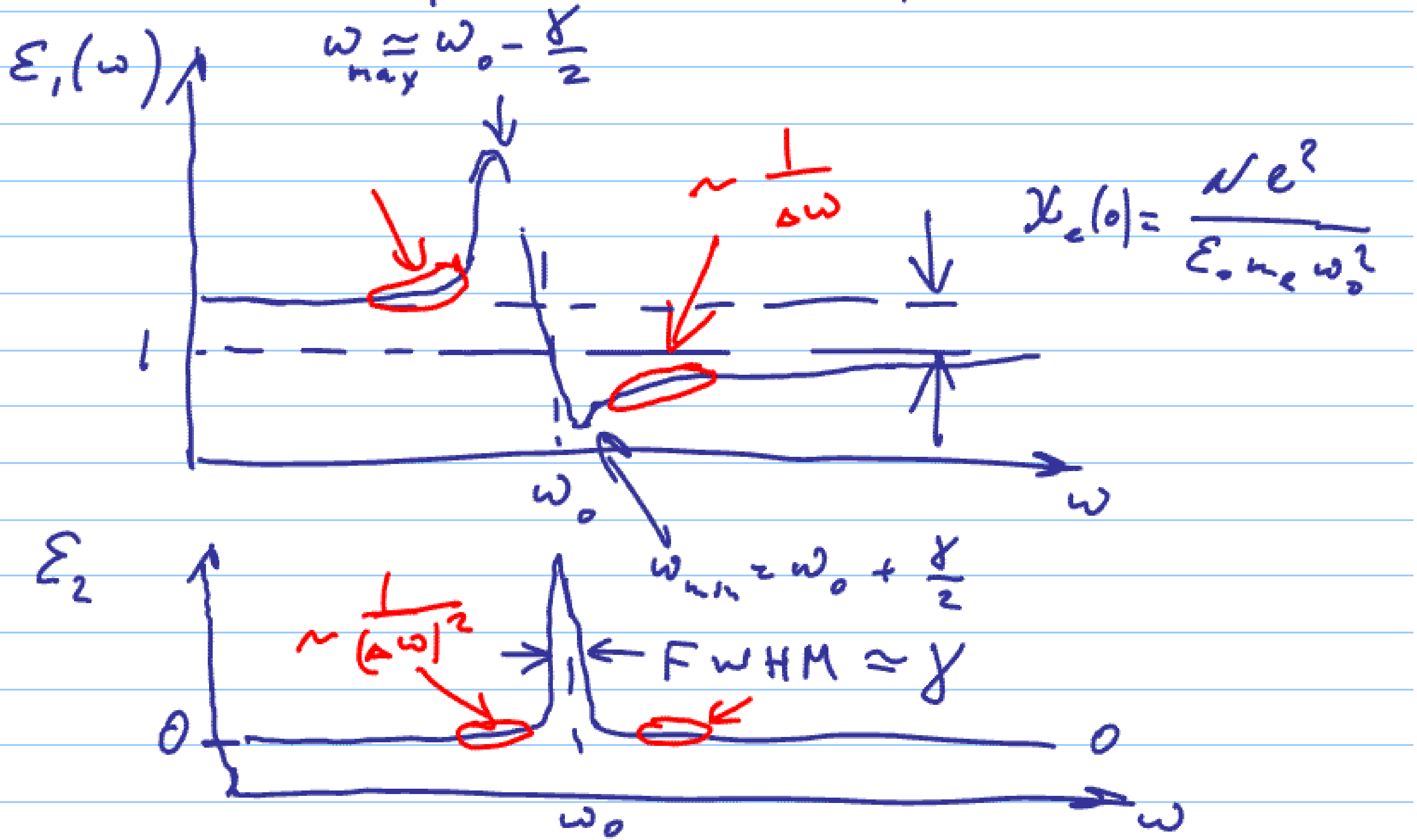
$$\varepsilon_1(\omega) = 1 + \frac{Ne^2}{\varepsilon_0 m_e}\left[\frac{\omega_0^2 - \omega^2}{(\omega_0^2-\omega^2)^2 + (\omega\gamma)^2}\right\}$$

$$\varepsilon_2(\omega) = \frac{Ne^2}{\varepsilon_0 m_e}\,\frac{\omega\gamma}{(\omega_0^2-\omega^2)^2 + (\omega\gamma)^2}$$

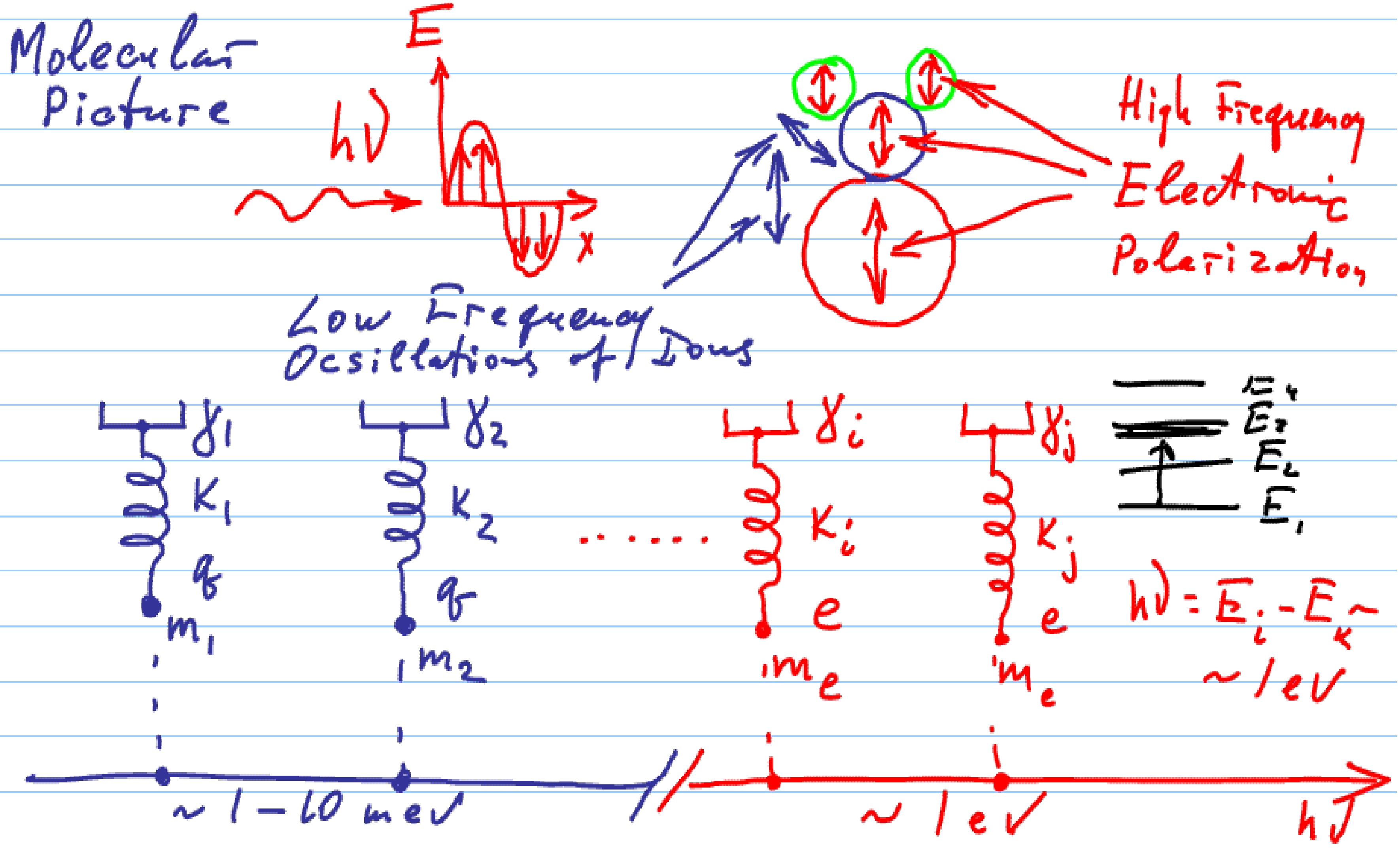
Behaviour in limits

	$\varepsilon_1(\omega)$	$\varepsilon_2(\omega)$	$\varepsilon_r(\omega)$
$\omega \sim 0$ Below resonance	$1 + \chi_e(0)$	0	$1 + \chi_e(0)$
$\omega \sim \omega_0$ Near resonance	$1 + \chi_e(0)\frac{2\omega_0\Delta\omega}{4(\Delta\omega)^2+\gamma^2}$	$\chi_e(0)\frac{\gamma\omega_0}{4(\Delta\omega)^2+\gamma^2}$	$\varepsilon_1(\omega) + i\,\varepsilon_2(\omega)$
$\omega \sim \infty$ Above resonance	1	0	$1 \quad v = c$

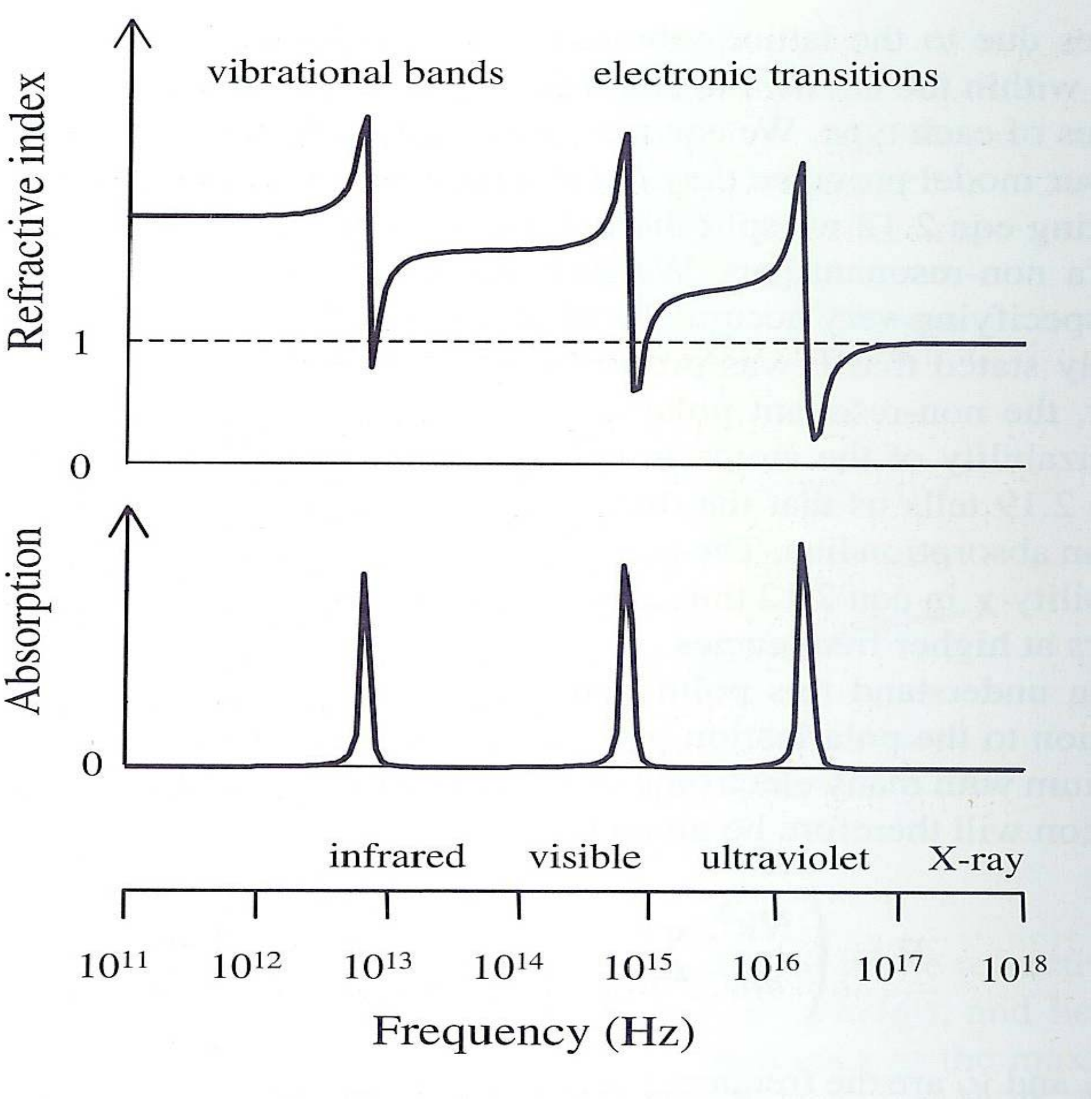
$$\chi_e(0) = \frac{Ne^2}{\varepsilon_0 m_e \omega_0^2}$$ This is DC susceptibility contribution for this resonan



Multiple Oscillators



Multiple Resonances Manifested in Index and Absorption



$p_{tot} = p_1 + p_2 + \dots$ (Σ over all resonances)

$p_j = q\, x_j$ for each $\tilde{x}_j(\omega, t)$

$ma = \Sigma F$

Macroscopic Polarization $P = N \cdot p_{tot}$

$$\underline{P} = \sum_j \frac{N \cdot q_j^2}{m_j} \left[\frac{1}{\omega_j^2 - \omega^2 - i \gamma_j \omega} \right] \cdot E(t)$$

$$E(t) = E_0 \cdot e^{i\omega t}$$

$$\boxed{x(t) = \frac{-\frac{q}{m_e} E_0 e^{-i\omega t}}{\omega_0^2 - \omega^2 - i\omega\gamma}}$$

$$D = \varepsilon_0 E + P \longrightarrow$$

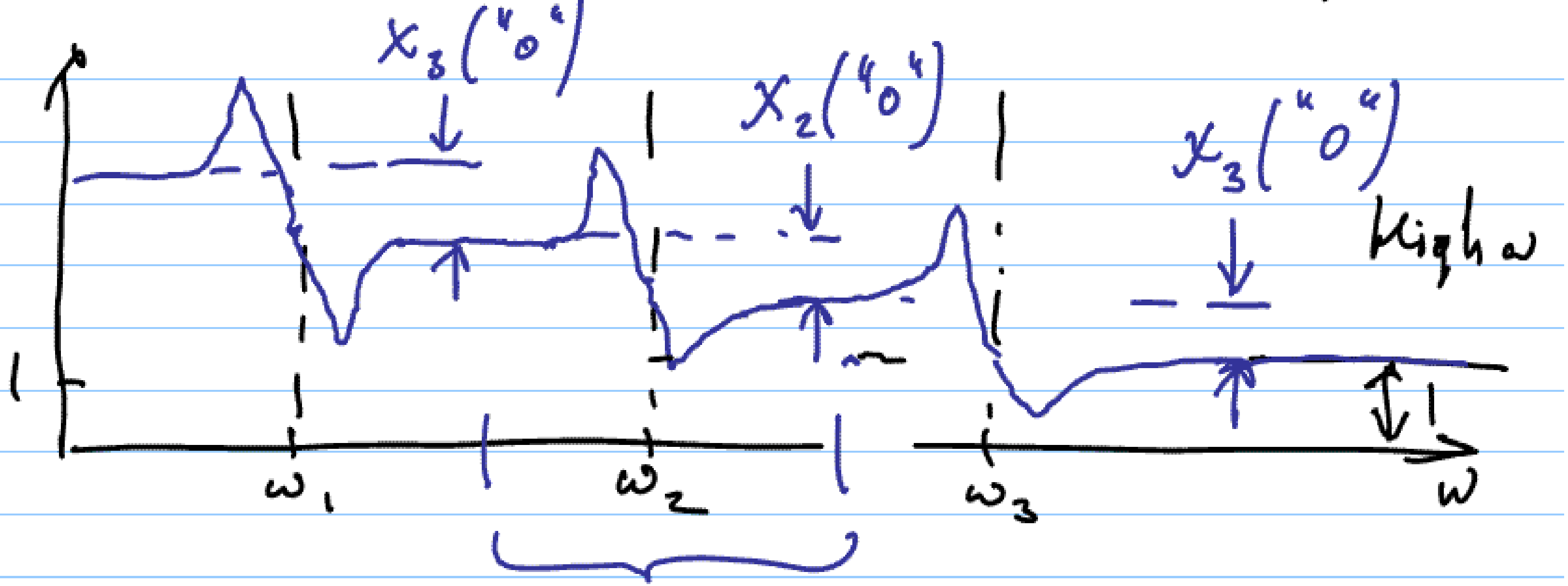
$$\tilde{\varepsilon}_r(\omega) = 1 + \sum_j \frac{N q_j^2}{\varepsilon_0 m_j} \frac{1}{\omega_j^2 - \omega^2 - i\gamma_j \omega}.$$

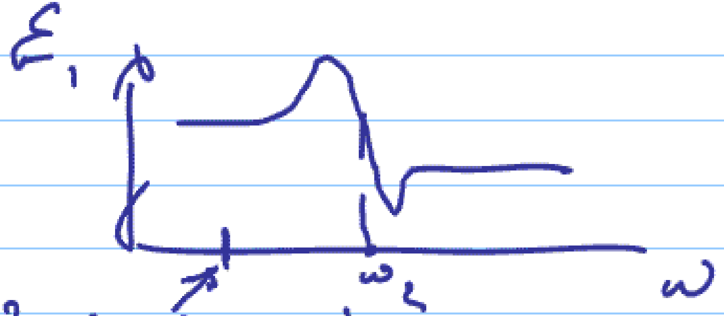
$$\tilde{\varepsilon}_r(\omega) = \varepsilon_1(\omega) + i\,\varepsilon_2(\omega)$$

General Solution

$$\begin{cases} \varepsilon_1(\omega) = 1 + \sum_j \frac{N q_j^2}{\varepsilon_0 m_j} \frac{\omega_j^2 - \omega^2}{(\omega_j^2 - \omega^2)^2 + (\omega \gamma_j)^2} \\ \varepsilon_2(\omega) = \sum_j \frac{N q_j^2}{\varepsilon_0 m_j} \left[\frac{\omega \gamma_j}{(\omega_j^2 - \omega^2)^2 + (\omega \gamma_j)^2} \right] \end{cases}$$

General Solution to $\varepsilon_1(\omega)$

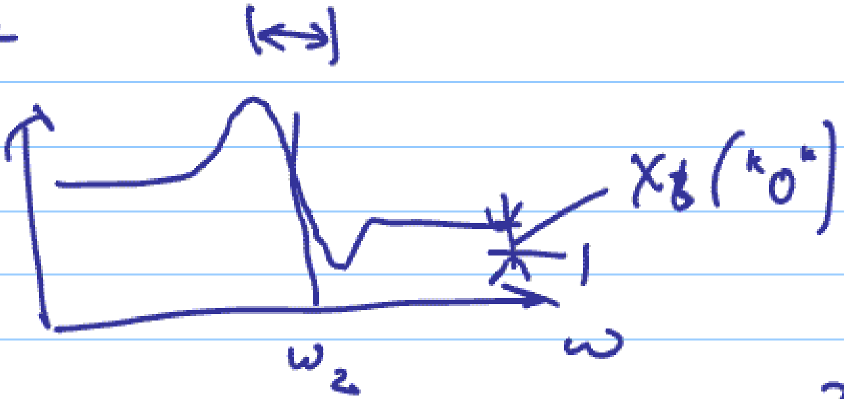




$\omega_1 \ll \omega \ll \omega_2$

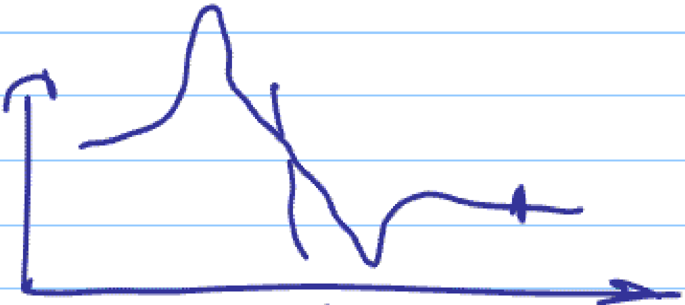
$$\varepsilon_1(\omega) = \text{const} = 1 + \chi_2(\text{"}0\text{"}) + \chi_3(\text{"}0\text{"})$$

$\omega \sim \omega_2$



$$\varepsilon_1(\omega) = 1 + \underbrace{\chi_\gamma(``0")} + \chi_2(``0")\frac{2\omega_2\Delta\omega}{4(\Delta\omega)^2+\gamma^2}$$

$\omega_2 << \omega << \omega_3$



$$\varepsilon_1(\omega) = 1 + \chi_\gamma(\overset{\omega}{``0"})^2$$

Multiple Resonance Summary

General Solution

$$\varepsilon_1(\omega) = 1 + \sum_j \frac{N q_j^2}{\varepsilon_0 m_j} \frac{(\omega_j^2 - \omega^2) \cdot f_j}{(\omega_j^2 - \omega^2)^2 + (\omega \gamma_j)^2}$$

$f_j \leftarrow$ Oscillator strength

$$\varepsilon_2(\omega) = \sum_j \frac{N q_j^2}{\varepsilon_0 m_j} \frac{\omega \gamma_j \cdot f_j}{(\omega_j - \omega^2)^2 + (\omega \gamma_j)^2}$$

	$\varepsilon_1(\omega)$	$\varepsilon_2(\omega)$
below $\omega < \omega_\ell$	$1 + \sum_{j \geq \ell} X_j(\text{"0"})$	0
$\omega \sim \omega_\ell$	$1 + \sum_{j > \ell} X_j(\text{"0"}) + X_\ell(\text{"0"}) \frac{2\omega_\ell \Delta\omega}{4\Delta\omega^2 + \gamma_\ell^2}$	$X_\ell(\text{"0"}) \frac{\gamma_\ell \omega_\ell}{4\Delta\omega^2 + \gamma_\ell^2}$
$\omega > \omega_\ell$ above	$1 + \sum_{j > \ell} X_j(\text{"0"})$	0

Susceptibility contribution to Resonance j:

$$\chi_j(\text{"0"}) = \frac{N q_j}{\varepsilon_0 m_j \omega_j^2}$$

Departures from this model

- Resonance are close $\omega_{j+1} - \omega_j \gg \gamma_1$
- Each resonance can be characterized by "oscillator strength"
- Electronic Bands of Solids

Comparison with Experimental Data