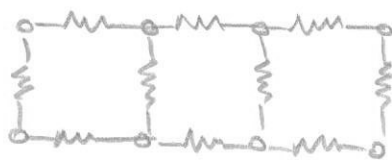


Lattice vibrations

①



Model of lattice

Phonon

Def: The phonon is the energy quantum of the elastic wave

Compare photon - energy quantum of electromagn. wave

A phonon is described completely by

$$\omega$$

$$E = \hbar \omega$$

$$\vec{K}$$

Wave vector, $\lambda = \frac{2\pi}{|\vec{K}|}$ (Propagation along $\vec{K}$)

polarization direction

$$\begin{cases} 3D: & 1L, 2T \\ 2D: & 1L, 1T \\ 1D: & 1L \end{cases}$$

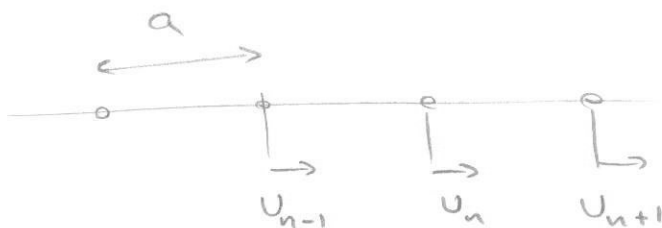
Useful statements

- ① There is a highest frequency $\omega_{\max}$
- ② The number of $\vec{K}$ -values is discrete due to boundary cond.
In practise, it is quasicontinuous, $\sum_{\vec{K}} \rightarrow \int d^3K$ or $\int d\omega$
- ③ All possible vibration modes can be described with a $\vec{K}$ -vector in the 1st Brillouin zone
- ④ In a crystal with N atoms there are N vibration modes per polarization direction.

① Highest frequency $\omega_{\max}$

" $F = C \cdot x$ " spring

Models: 1-dim chain, harmonic forces between nearest neighbors



$$L = N \cdot a$$

mass M per atom

Eg:
$$M \cdot \ddot{U}_n = C \cdot (U_{n+1} - U_n) - C (U_n - U_{n-1}) =$$

$$= C (U_{n+1} - 2U_n + U_{n-1})$$

Ansatz:
$$U_n = A \cdot e^{i(K \cdot n \cdot a - \omega t)} \quad (x = n \cdot a)$$

$$\Rightarrow \begin{cases} \ddot{U}_n = -(i\omega)^2 U_n = -\omega^2 U_n \\ U_{n+1} = A e^{i(K(n+1)a - \omega t)} = e^{iKa} U_n \\ U_{n-1} = e^{-iKa} U_n \end{cases}$$

$$-M\omega^2 U_n = C (e^{iKa} - 2 + e^{-iKa}) U_n$$

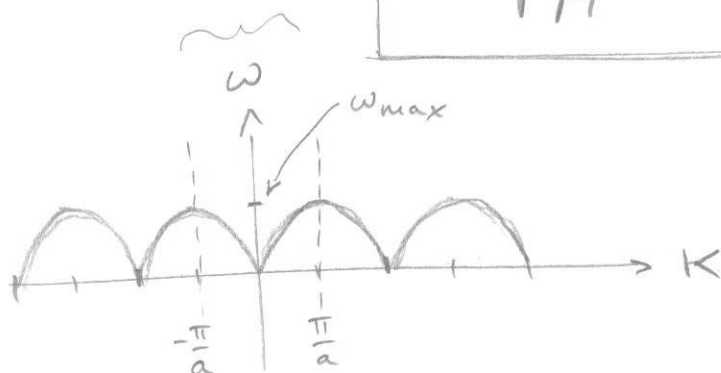
$$M\omega^2 = 2C (1 - \cos Ka)$$

$$2 \sin^2 \frac{Ka}{2}$$

1st B.Z.

$$\boxed{\omega = \sqrt{\frac{4C}{M}} \left| \sin \frac{Ka}{2} \right|}$$

$$\omega_{\max} = \sqrt{\frac{4C}{M}}$$



A lattice cannot vibrate with arbitrarily high frequencies

Dispersion relation

② Number of $\bar{K}$ -values

Assume periodic boundary conditions

$$U_n(na) = U_n(na+L)$$

$$e^{iKna} = e^{iK(na+L)} \Rightarrow e^{iKL} = 1$$

$$K \cdot L = p \cdot 2\pi$$

$$K_x = 0, \pm \frac{2\pi}{L}, \pm \frac{4\pi}{L} \dots$$

$$K_y = \dots$$

$$K_z = \dots$$

③ All vibration modes in 1st B.Z.

$$U_n = A \cdot e^{i(Kna - \omega t)}$$

Let $K' = K + p \cdot G = K + p \cdot \frac{2\pi}{a}$, p integer

$$\Rightarrow U'_n = \underbrace{e^{iG \cdot na}}_{e^{ip \cdot \frac{2\pi}{a} \cdot na}} U_n = U_n$$

Same state/wave

$$e^{ip \cdot \frac{2\pi}{a} \cdot na} = e^{i2\pi \cdot p \cdot n} = 1$$

Example

$$K' = \frac{15}{7} \cdot \frac{\pi}{a} > \frac{2\pi}{a}$$

$$\lambda' = \frac{2\pi}{K'} = \frac{14}{15} a$$

$$K = K' - G = \frac{1}{7} \cdot \frac{\pi}{a}$$

$$\Rightarrow \lambda = \frac{2\pi}{K} = 14a$$

Wavelengths shorter than lattice parameter can be better described with a longer wavelength

④ N vibration modes per polarization direction

Proof: If N is even ($L = N \cdot a$):

$$K = 0, \pm \frac{2\pi}{L}, \pm \frac{4\pi}{L}, \dots \pm \frac{N\pi}{a} = \pm \frac{\pi}{a}$$

but $\frac{\pi}{a} - \frac{2\pi}{a} = -\frac{\pi}{a}$ same state $\Rightarrow$ keep only $+\frac{n\pi}{L}$

$$\begin{array}{c} 0 \\ \uparrow \\ 1 \end{array} + \begin{array}{c} \pm \\ \uparrow \\ 2 \end{array} \cdot \frac{(N-2)}{2} + \begin{array}{c} +\frac{N\pi}{a} \\ \uparrow \\ 1 \end{array} \text{ states} = N - 2 + 2 = \underline{N \text{ states}}$$

If N is odd: (1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74, 75, 76, 77, 78, 79, 80, 81, 82, 83, 84, 85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 96, 97, 98, 99, 100, 101, 102, 103, 104, 105, 106, 107, 108, 109, 110, 111, 112, 113, 114, 115, 116, 117, 118, 119, 120, 121, 122, 123, 124, 125, 126, 127, 128, 129, 130, 131, 132, 133, 134, 135, 136, 137, 138, 139, 140, 141, 142, 143, 144, 145, 146, 147, 148, 149, 150, 151, 152, 153, 154, 155, 156, 157, 158, 159, 160, 161, 162, 163, 164, 165, 166, 167, 168, 169, 170, 171, 172, 173, 174, 175, 176, 177, 178, 179, 180, 181, 182, 183, 184, 185, 186, 187, 188, 189, 190, 191, 192, 193, 194, 195, 196, 197, 198, 199, 200, 201, 202, 203, 204, 205, 206, 207, 208, 209, 210, 211, 212, 213, 214, 215, 216, 217, 218, 219, 220, 221, 222, 223, 224, 225, 226, 227, 228, 229, 230, 231, 232, 233, 234, 235, 236, 237, 238, 239, 240, 241, 242, 243, 244, 245, 246, 247, 248, 249, 250, 251, 252, 253, 254, 255, 256, 257, 258, 259, 260, 261, 262, 263, 264, 265, 266, 267, 268, 269, 270, 271, 272, 273, 274, 275, 276, 277, 278, 279, 280, 281, 282, 283, 284, 285, 286, 287, 288, 289, 290, 291, 292, 293, 294, 295, 296, 297, 298, 299, 300, 301, 302, 303, 304, 305, 306, 307, 308, 309, 310, 311, 312, 313, 314, 315, 316, 317, 318, 319, 320, 321, 322, 323, 324, 325, 326, 327, 328, 329, 330, 331, 332, 333, 334, 335, 336, 337, 338, 339, 340, 341, 342, 343, 344, 345, 346, 347, 348, 349, 350, 351, 352, 353, 354, 355, 356, 357, 358, 359, 360, 361, 362, 363, 364, 365, 366, 367, 368, 369, 370, 371, 372, 373, 374, 375, 376, 377, 378, 379, 380, 381, 382, 383, 384, 385, 386, 387, 388, 389, 390, 391, 392, 393, 394, 395, 396, 397, 398, 399, 400, 401, 402, 403, 404, 405, 406, 407, 408, 409, 410, 411, 412, 413, 414, 415, 416, 417, 418, 419, 420, 421, 422, 423, 424, 425, 426, 427, 428, 429, 430, 431, 432, 433, 434, 435, 436, 437, 438, 439, 440, 441, 442, 443, 444, 445, 446, 447, 448, 449, 450, 451, 452, 453, 454, 455, 456, 457, 458, 459, 460, 461, 462, 463, 464, 465, 466, 467, 468, 469, 470, 471, 472, 473, 474, 475, 476, 477, 478, 479, 480, 481, 482, 483, 484, 485, 486, 487, 488, 489, 490, 491, 492, 493, 494, 495, 496, 497, 498, 499, 500, 501, 502, 503, 504, 505, 506, 507, 508, 509, 510, 511, 512, 513, 514, 515, 516, 517, 518, 519, 520, 521, 522, 523, 524, 525, 526, 527, 528, 529, 530, 531, 532, 533, 534, 535, 536, 537, 538, 539, 540, 541, 542, 543, 544, 545, 546, 547, 548, 549, 550, 551, 552, 553, 554, 555, 556, 557, 558, 559, 560, 561, 562, 563, 564, 565, 566, 567, 568, 569, 570, 571, 572, 573, 574, 575, 576, 577, 578, 579, 580, 581, 582, 583, 584, 585, 586, 587, 588, 589, 590, 591, 592, 593, 594, 595, 596, 597, 598, 599, 600, 601, 602, 603, 604, 605, 606, 607, 608, 609, 610, 611, 612, 613, 614, 615, 616, 617, 618, 619, 620, 621, 622, 623, 624, 625, 626, 627, 628, 629, 630, 631, 632, 633, 634, 635, 636, 637, 638, 639, 640, 641, 642, 643, 644, 645, 646, 647, 648, 649, 650, 651, 652, 653, 654, 655, 656, 657, 658, 659, 660, 661, 662, 663, 664, 665, 666, 667, 668, 669, 670, 671, 672, 673, 674, 675, 676, 677, 678, 679, 680, 681, 682, 683, 684, 685, 686, 687, 688, 689, 690, 691, 692, 693, 694, 695, 696, 697, 698, 699, 700, 701, 702, 703, 704, 705, 706, 707, 708, 709, 710, 711, 712, 713, 714, 715, 716, 717, 718, 719, 720, 721, 722, 723, 724, 725, 726, 727, 728, 729, 730, 731, 732, 733, 734, 735, 736, 737, 738, 739, 740, 741, 742, 743, 744, 745, 746, 747, 748, 749, 750, 751, 752, 753, 754, 755, 756, 757, 758, 759, 760, 761, 762, 763, 764, 765, 766, 767, 768, 769, 770, 771, 772, 773, 774, 775, 776, 777, 778, 779, 780, 781, 782, 783, 784, 785, 786, 787, 788, 789, 790, 791, 792, 793, 794, 795, 796, 797, 798, 799, 800, 801, 802, 803, 804, 805, 806, 807, 808, 809, 810, 811, 812, 813, 814, 815, 816, 817, 818, 819, 820, 821, 822, 823, 824, 825, 826, 827, 828, 829, 830, 831, 832, 833, 834, 835, 836, 837, 838, 839, 840, 841, 842, 843, 844, 845, 846, 847, 848, 849, 850, 851, 852, 853, 854, 855, 856, 857, 858, 859, 860, 861, 862, 863, 864, 865, 866, 867, 868, 869, 870, 871, 872, 873, 874, 875, 876, 877, 878, 879, 880, 881, 882, 883, 884, 885, 886, 887, 888, 889, 890, 891, 892, 893, 894, 895, 896, 897, 898, 899, 900, 901, 902, 903, 904, 905, 906, 907, 908, 909, 910, 911, 912, 913, 914, 915, 916, 917, 918, 919, 920, 921, 922, 923, 924, 925, 926, 927, 928, 929, 930, 931, 932, 933, 934, 935, 936, 937, 938, 939, 940, 941, 942, 943, 944, 945, 946, 947, 948, 949, 950, 951, 952, 953, 954, 955, 956, 957, 958, 959, 960, 961, 962, 963, 964, 965, 966, 967, 968, 969, 970, 971, 972, 973, 974, 975, 976, 977, 978, 979, 980, 981, 982, 983, 984, 985, 986, 987, 988, 989, 990, 991, 992, 993, 994, 995, 996, 997, 998, 999, 1000)

$$K = 0, \pm \frac{2\pi}{L}, \pm \frac{4\pi}{L}, \dots \pm \frac{(N-1)\pi}{L}, \pm \frac{(N+1)\pi}{L}$$

$$1 + 2 \cdot \frac{(N-1)}{2} = \underline{N \text{ states}}$$

Detecting phonons

Elastic scattering $\bar{k}' - \bar{k} = \bar{G}$

modify : $\boxed{\bar{k}' - \bar{k} = \pm \bar{K}_{ph} (+\bar{G})}$ (1)

Energy $\boxed{h\nu' - h\nu = \pm \hbar\omega_{ph}}$ (2)

X-ray : $\lambda \sim 1 \text{ \AA}$ $h\nu = \frac{hc}{\lambda} \sim 10 \text{ keV}$ } x-ray cannot be used
 Phonon : $\hbar\omega \sim 40 \text{ meV}$

Visible light : $\lambda \sim 500 \text{ nm}$, $h\nu \sim 2 \text{ eV}$ maybe possible to resolve 40 meV

BUT : $k = \frac{2\pi}{\lambda} \sim 10^7 \text{ m}^{-1}$

$|\bar{K}| \lesssim \frac{\pi}{a} \sim 10^{10} \text{ m}^{-1}$

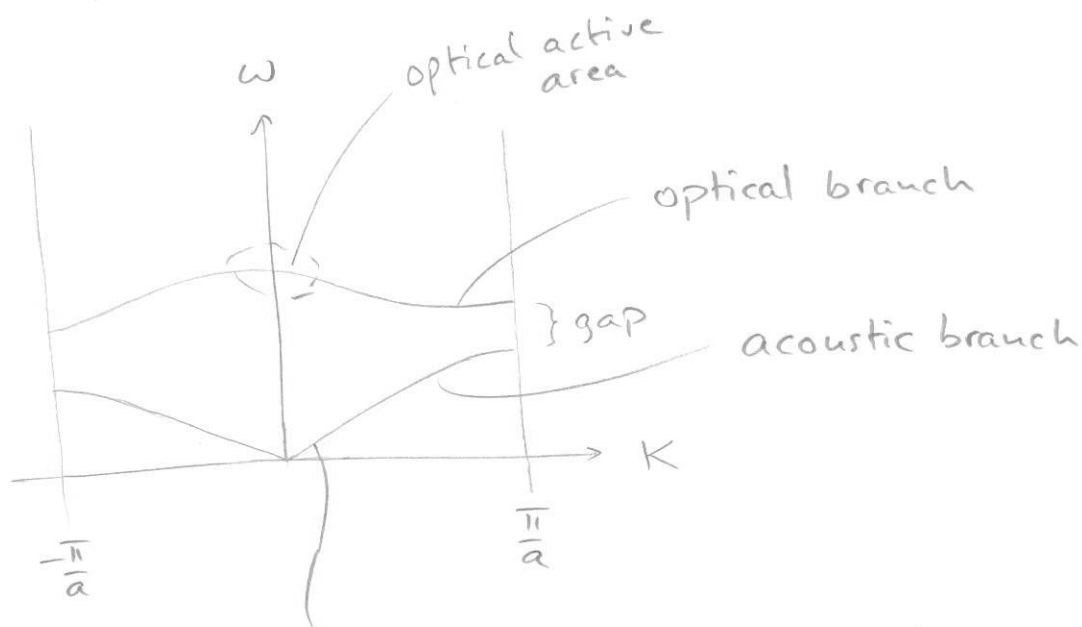
maximum change in k : $\Longleftrightarrow 2 \cdot k = 2 \cdot 10^7 \text{ m}^{-1}$
 much smaller than 10^{10} m^{-1}

$\Rightarrow |\bar{K}|$ cannot be "absorbed"

Neutrons With neutrons both (1) and (2) can be fulfilled over the entire B.Z.

Dispersion relation

ω vs k



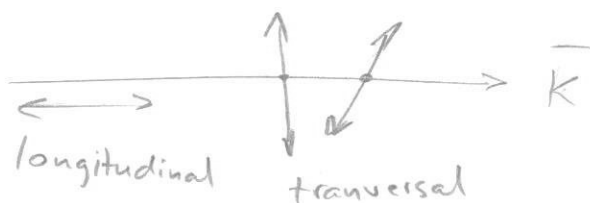
Sound velocity $v_s = \lim_{k \rightarrow 0} \frac{\partial \omega}{\partial k}$

p atoms/ions per cell



$\left\{ \begin{array}{l} 3p \text{ acoustic branches} \longrightarrow \omega \rightarrow 0 \text{ when } k \rightarrow 0 \\ 3(p-1) \text{ optical branches} \end{array} \right.$

$3 \longrightarrow 1 \text{ longitudinal, } 2 \text{ transverse } \underline{\text{polarizations}}$
 (3D crystals)



Wave equation for continuous media

$$\frac{\partial^2 u}{\partial x^2} - \sqrt{\frac{\rho}{E}} \frac{\partial^2 u}{\partial t^2} = 0$$

E = elasticity modulus

ρ = density

$$v_s = \sqrt{\frac{E}{\rho}}$$

Lattice model : $\omega = \sqrt{\frac{4C}{M}} \left| \sin \frac{ka}{2} \right|$

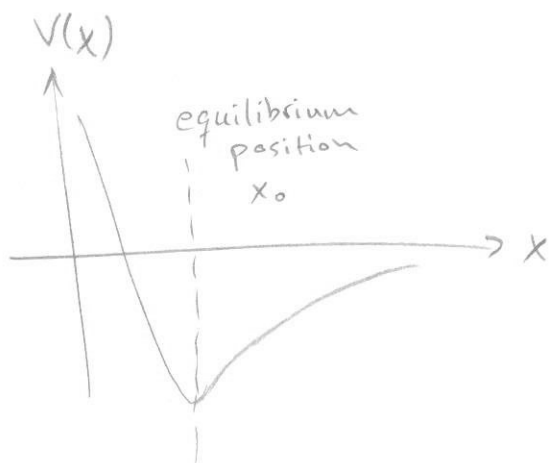
$$v_s = \lim_{k \rightarrow 0} \frac{\partial \omega}{\partial k} = \sqrt{\frac{4C}{M}} \cdot \frac{a}{2} = a \cdot \sqrt{\frac{C}{M}}$$

$$M = \rho \cdot a^3$$

Compare $\sqrt{\frac{E}{\rho}} = a \cdot \sqrt{\frac{C}{\rho a^3}} = \sqrt{\frac{C}{\rho a}}$

$$\Rightarrow \boxed{C = a \cdot E}$$

Harmonicity



Small displacements

$$V(x) \approx V(x_0) + A \cdot (x - x_0)^2$$

$$F = - \frac{dV}{dx} = - \underbrace{2A}_{\substack{C \\ \text{spring constant}}} (x - x_0)$$

Hooke's law:

$$F = -C \cdot (x - x_0)$$

Harmonic force

$\Rightarrow$ harmonic oscillations etc.

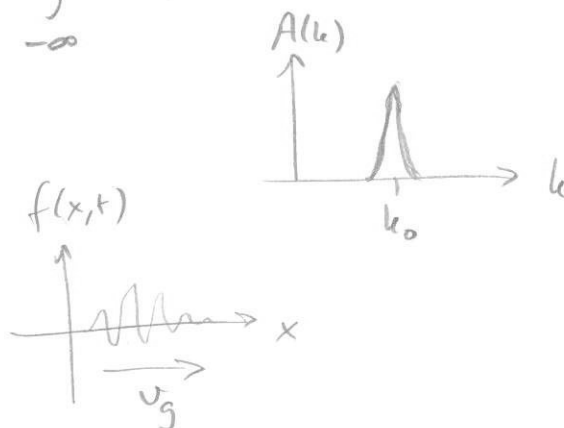
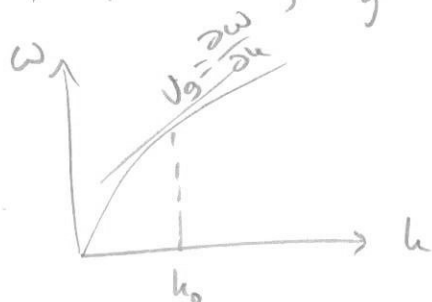
Larger amplitudes / displacements

$\Rightarrow$ anharmonic effects

Wave packages

$$f(x, t) = \int_{-\infty}^{\infty} A(k) e^{i(kx - \omega t)} dk$$

Group velocity $v_g = \frac{\partial \omega}{\partial k}$



$$3D: \vec{v}_g = \nabla_{\vec{k}} \omega(k) = \left(\frac{\partial \omega}{\partial k_x}, \frac{\partial \omega}{\partial k_y}, \frac{\partial \omega}{\partial k_z} \right)$$

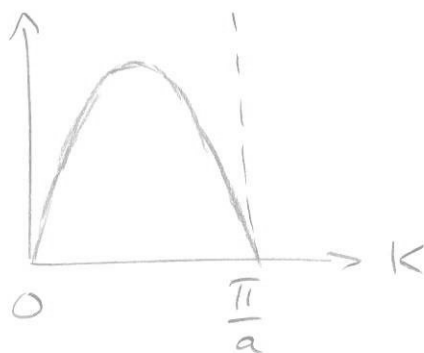
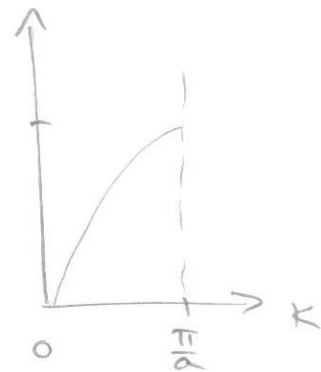
Plane waves : Practical set of basis

Interaction beyond nearest neighbors

$$\omega^2 = \frac{2}{M} \sum_{j>0} C_j (1 - \cos(Kja))$$

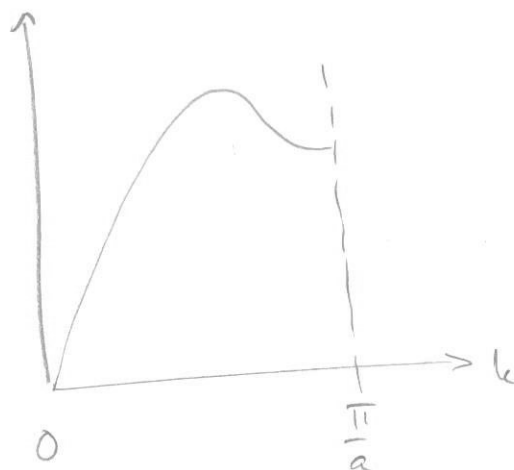
$$j=1 \quad \omega^2 = \frac{2}{M} \cdot C_j \cdot \underbrace{2 \cdot \sin\left(\frac{Ka}{2}\right)}_{1 - \cos(Ka)}$$

$$j=2 \quad 1 - \cos(2Ka)$$



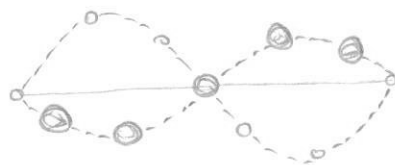
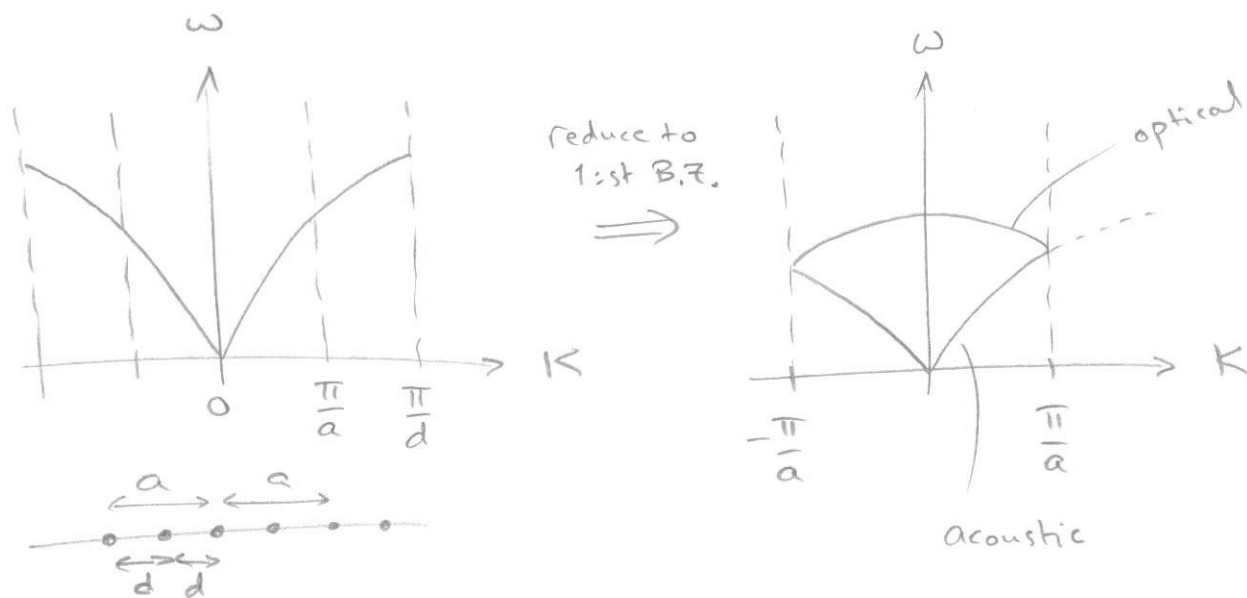
$$j=1 + j=2$$

$$\omega(k) = \sqrt{\omega^2}$$

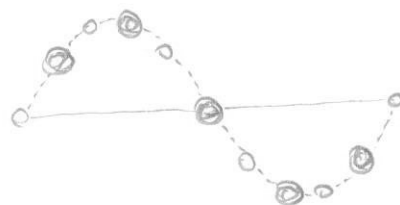


$$\omega^2 = \frac{2C}{M} \left[(1 - \cos Ka) + (1 - \cos 2Ka) \right]$$

One-dimensional, basis with 2 ions

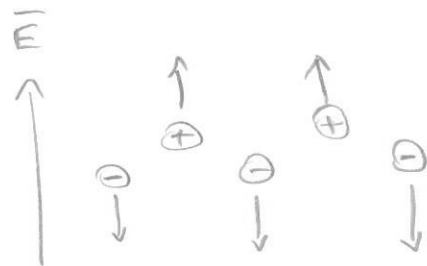


optical mode

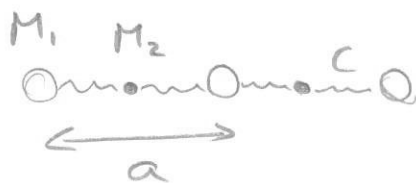


acoustic mode

Optical excitation $\sim$ IR



ex. NaCl



$$M_1: u_s$$

$$M_2: v_s$$

Assume same C

$$\begin{cases} M_1 \cdot \frac{d^2 u_s}{dt^2} = C(v_s + v_{s-1} - 2u_s) \\ M_2 \cdot \frac{d^2 v_s}{dt^2} = C(u_{s+1} + u_s - 2v_s) \end{cases}$$

Ansatz:
$$\begin{cases} u_s = u \cdot e^{i(Ksa - \omega t)} \\ v_s = v \cdot e^{i(Ksa - \omega t)} \end{cases}$$

$$\Rightarrow \begin{cases} -\omega^2 M_1 u = C \cdot v (1 + e^{-iKa}) - 2Cu \\ -\omega^2 M_2 v = C \cdot u (1 + e^{iKa}) - 2Cv \end{cases}$$

or
$$\begin{cases} (2C - M_1 \omega^2) u = C \cdot (1 + e^{-iKa}) v \\ (2C - M_2 \omega^2) v = C \cdot (1 + e^{iKa}) u \end{cases}$$

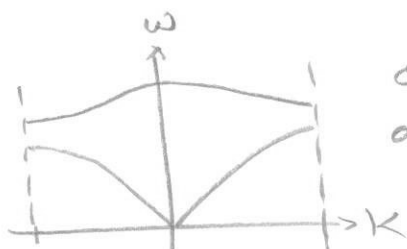
if $u \cdot v \neq 0$

$$\Rightarrow (2C - M_1 \omega^2)(2C - M_2 \omega^2) = C^2 (1 + e^{-iKa})(1 + e^{iKa})$$

2nd degree equation for ω^2

$\Rightarrow$ 2 solutions for each ω^2 for each K

with $\omega = +\sqrt{\omega^2}$ ($\omega > 0$) $\Rightarrow$ 2 solutions $\omega(K)$



optical
acoustic

— can also have longitudinal/
transversal branches

in 3D $\Rightarrow$ 6 branches (2 ions/cell)