Mineral Physics I
Chapter 3. Lattice vibration
Section 3. 1D Quantum-mechanical harmonic oscillator

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This section

q Lattice vibrations: collection of oscillating atoms

q à The physical law that oscillating microscopic particles follow should be understood

q The motions in microscopic scales: governed by quantum physics

Ø à some introduction of quantum physics

Schrödinger Equation

- We will argue a given state of a collection of oscillating atoms

- The time-independent Schrödinger equation for one particle with mass m and energy E in one-dimensional space:

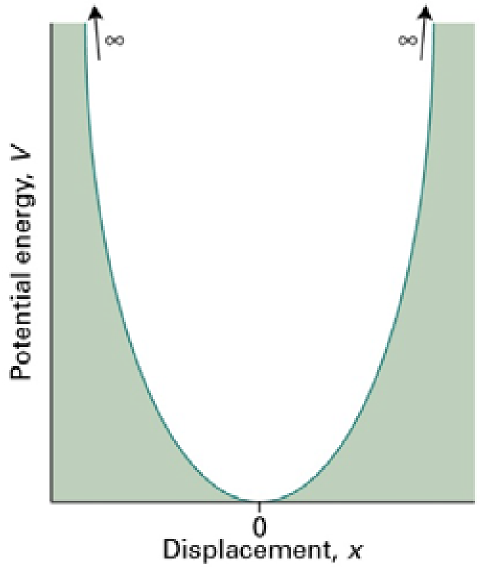
  - $$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + V(x)\psi = E\psi \qquad (3.4.1)$$

    - h: the Planck constant, $6.626\ldots \times 10^{-34}$ Js
    - $\hbar = h/2\pi$: the reduced Planck constant, $1.05457\ldots \times 10^{-34}$ Js
    - $\psi(x)$: the wavefunction giving probability finding the particle at the position x
    - $V(x)$: the potential energy that is operated to the particle at the position x

  - The wavefunction contains all information about the motion of the particle

1D harmonic oscillation

- Harmonic oscillation
  - a particle with a restoring force proportional to its displacement:
    - $F = -kx$ (3.4.2)
      - k : the force constant:
  - The force can be related to the potential energy
    - $F = -\mathrm{d}V/\mathrm{d}x$ (3.4.3)
  - The potential energy for the harmonic oscillation
    - $V = (1/2)kx^2$ (3.4.4)
      - parabolic potential energy



- The Schrodinger equation for the particle in the parabolic potential:

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + \frac{1}{2}kx^2\psi = E\psi \qquad (3.4.5)$$

Solution of 1D harmonic oscillator -1

- In classical mechanics,
  - Equation of spring: $F = -kx$
  - Equation of motion: $F = m\frac{\mathrm{d}^2x}{\mathrm{d}t^2}$

$$m\frac{\mathrm{d}^2x}{\mathrm{d}t^2} = -kx \tag{3.4.6}$$

  - Solution: $x = A\cos(\omega t + \theta)$

$$x = A\cos(\omega t + \theta) \text{ with } \omega = \sqrt{k/m} \tag{3.4.7}$$

  - The parameter k is replaced by

$$k = m\omega^2 \tag{3.4.8}$$

  - The potential energy is written as $V(x) = m\omega^2x^2/2$ (3.4.9)

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + \frac{m\omega^2}{2}x^2\psi = E\psi \tag{3.4.5'}$$

Solution of 1D harmonic oscillator -2

q The equation (3.4.9) $-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + \frac{m\omega^2}{2}x^2\psi = E\psi$ is difficult to solve

q Modified as $-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi(x)}{\mathrm{d}x^2} = \left(E - \frac{1}{2}m\omega^2x^2\right)\psi(x)$ (3.4.10)

q The valuables x and E are replaced by

Ø $x = \sqrt{\hbar/m\omega}\,\xi$ (3.4.11)

Ø $E = (\hbar\omega/2)\varepsilon$ (3.4.12)

q Then the equation become in a simple form

Ø $\frac{\mathrm{d}^2\phi(\xi)}{\mathrm{d}\xi^2} + (\varepsilon - \xi^2)\phi(\xi) = 0$ (3.4.13)

ü $\psi(x)$ à $\phi(\xi)$

ü However, this equation is still difficult to solve…

Solution of 1D harmonic oscillator -3

- Assuming the solution of (3.4.13) $\frac{\mathrm{d}^2\phi(\xi)}{\mathrm{d}\xi^2} + (\varepsilon - \xi^2)\phi(\xi) = 0$ as:
  - $\phi = H(\xi)\exp\left(-\frac{\xi^2}{2}\right)$ (3.4.14)
- We substitute Eq. (3.4.17) into (3.4.13), then we find
  - $\frac{\mathrm{d}^2\phi(\xi)}{\mathrm{d}\xi^2} = \frac{\mathrm{d}^2}{\mathrm{d}\xi^2}\left[H(\xi)\exp\left(-\frac{\xi^2}{2}\right)\right] = \frac{\mathrm{d}}{\mathrm{d}\xi}\left[\frac{\mathrm{d}H(\xi)}{\mathrm{d}\xi}\exp\left(-\frac{\xi^2}{2}\right) - H(\xi)\frac{\mathrm{d}}{\mathrm{d}\xi}\left\{\exp\left(-\frac{\xi^2}{2}\right)\right\}\right]$

    $= \frac{\mathrm{d}}{\mathrm{d}\xi}\left[\frac{\mathrm{d}H}{\mathrm{d}\xi}\exp\left(-\frac{\xi^2}{2}\right) - H\xi\exp\left(-\frac{\xi^2}{2}\right)\right] = \left[\frac{\mathrm{d}^2H}{\mathrm{d}\xi^2} - 2\xi\frac{\mathrm{d}H}{\mathrm{d}\xi} + (\xi^2 - 1)H\right]\exp\left(-\frac{\xi^2}{2}\right)$
  - $\left[\frac{\mathrm{d}^2H}{\mathrm{d}\xi^2} - 2\xi\frac{\mathrm{d}H}{\mathrm{d}\xi} + (\xi^2 - 1)H\right]\exp\left(-\frac{\xi^2}{2}\right) + (\varepsilon - \xi^2)H\exp\left(-\frac{\xi^2}{2}\right) = 0$ (3.4.15)
  - $\left[\frac{\mathrm{d}^2H}{\mathrm{d}\xi^2} - 2\xi\frac{\mathrm{d}H}{\mathrm{d}\xi} + (\varepsilon - 1)H\right]\exp\left(-\frac{\xi^2}{2}\right) = 0$ (3.4.16)

Solution of 1D harmonic oscillator -4

- By removing $\exp\left(-\frac{\xi^2}{2}\right)$ from (3.4.16)
  - $\left[\frac{\mathrm{d}^2}{\mathrm{d}\xi^2} - 2\xi\frac{\mathrm{d}}{\mathrm{d}\xi} + (\varepsilon - 1)\right]H(\xi) = 0$ (3.4.17)
- We assume the H can be expanded by an algebra series
  - $H(\xi) = \sum_{k=0}^{\infty} a_k \xi^k$ (3.4.18)
- We substitute (3.3.17) into (3.3.16), and we have:
  - $\sum_{k=2}^{\infty} k(k-1)a_k\xi^{k-2} - 2\xi\sum_{k=1}^{\infty} ka_k\xi^{k-1} + (\varepsilon - 1)\sum_{k=0}^{\infty} a_k\xi^k = 0$
  - $\sum_{k=2}^{\infty} k(k-1)a_k\xi^{k-2} - 2\left(0 \cdot a_0 \cdot \xi^0 + \sum_{k=1}^{\infty} ka_k\xi^k\right) + (\varepsilon - 1)\sum_{k=0}^{\infty} a_k\xi^k = 0$
  - $\sum_{k=0}^{\infty}(k+2)(k+1)a_{k+2}\xi^k - 2\sum_{k=0}^{\infty} ka_k\xi^k + (\varepsilon - 1)\sum_{k=0}^{\infty} a_k\xi^k = 0$
  - $\sum_{k=0}^{\infty}[(k+1)(k+2)a_{k+2} - (2k - \varepsilon + 1)a_k]\xi^k = 0$ (3.4.19)

fórmula de recursividad; fórmula de recurrencia

Solution of 1D harmonic oscillator -5

q To make (3.4.19) $\sum_{k=0}^{\infty}[(k+1)(k+2)a_{k+2}-(2k-\varepsilon+1)a_k]\xi^k$ always 0, the inside of the square bracket must be zero by:

Ø $a_{k+2}=\frac{2k-\varepsilon+1}{(k+1)(k+2)}a_k$ (3.4.20)

q Using (3.4.20), $H(\xi)=\sum_{k=0}^{\infty}a_k\xi^k$ becomes,

Ø $$H(\xi)=a_0\left(1-\frac{\varepsilon-1}{1\cdot2}\xi^2+\frac{\varepsilon-1}{1\cdot2}\frac{\varepsilon-4-1}{3\cdot4}\xi^4-\cdots\right)$$
$$+a_1\left(\xi-\frac{\varepsilon-1}{2\cdot3}\xi^3+\frac{\varepsilon-2-1}{2\cdot3}\frac{\varepsilon-6-1}{4\cdot5}\xi^5-\cdots\right) \quad (3.4.21)$$

q The formula (3.4.21): an infinite series.

Ø Without special conditions, the series diverges at large ξ

Ø The conditions for the convergence of (3.4.21) at any ξ

Solution of 1D harmonic oscillator -6

- When k is large, the recurrence formula (3.4.20) becomes
  - $a_{k+2} = \frac{2}{k} a_k$ (3.4.22)
- If a function $\exp \xi^2$ is expanded,
  - $\exp \xi^2 = 1 + \xi^2 + \frac{1}{2}\xi^4 + \frac{1}{3!}\xi^6 + \cdots + \frac{1}{(k/2)!}\xi^k + \cdots$ (3.4.23)
- The recurrence (3.4.21) expresses the term of (3.4.22). Thus $H(\xi)$ diverges when $\xi \to \infty$
  - $H(\xi) \approx A \exp(\xi^2) \xrightarrow[\xi \to \infty]{} \infty$ (3.4.24)
    - The series $\sum_{k=0}^{\infty} a_k \xi^k$ must be finite.
- The n^{th} term is zero so that the higher terms are zero and the series is finite.

Solution of 1D harmonic oscillator -7

q If

Ø $\varepsilon = 2n - 1$ (3.4.25)

q then even a_n is non-zero, the higher terms are zero: the series becomes finite.

Ø $a_{n+2} = -\frac{\varepsilon - 2n + 1}{(n+1)(n+2)} a_n = 0$

(3.4.26)

q $H(\xi)$ changes by the value of $\varepsilon = 2n - 1$

q Each $H(\xi)$ is expressed using $H_n(\xi)$

Ø Hermite polynomials

Ø $H_0(\xi) = a_0$

Ø $H_1(\xi) = a_1 \xi$

Ø $H_2(\xi) = a_0 \left(1 - \frac{4}{1 \cdot 2} \xi^2\right)$

Ø $H_3(\xi) = a_1 \left(1 - \frac{4}{2 \cdot 3} \xi^3\right)$

Ø $H_4(\xi) = a_0 \left(1 - \frac{8}{1 \cdot 2} \xi^2 + \frac{8}{1 \cdot 2} \frac{4}{3 \cdot 4} \xi^4\right)$

Ø $H_5(\xi) = a_1 \left(1 - \frac{8}{2 \cdot 3} \xi^3 + \frac{8}{2 \cdot 3} \frac{4}{4 \cdot 5} \xi^5\right)$

Ø $\vdots$

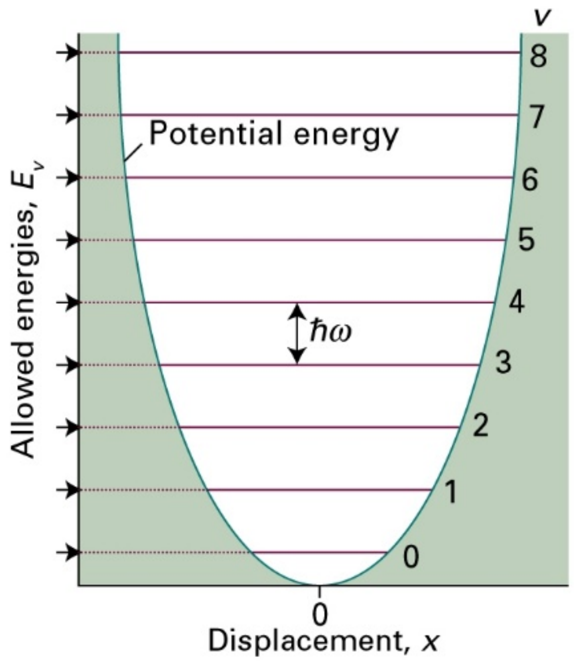
(3.4.27)

Solution of 1D harmonic oscillator -8

- From (3.4.15) and (3.4.27), the wavefunction under the potential of the harmonic oscillator:
  - $\phi(\xi) = cH(\xi)\exp\left(-\frac{\xi^2}{2}\right)$ (3.4.28)
  - $\psi(x) = cH\left(\sqrt{\frac{m\omega}{\hbar}}x\right)\exp\left(-\frac{m\omega}{2\hbar}x^2\right)$ (3.4.29)
  - Allowed energies: $E = \frac{\hbar\omega}{2}(2n+1) = \hbar\omega\left(n+\frac{1}{2}\right)$ (3.4.30)
    - Eq. (3.4.12): $E = \frac{\hbar\omega}{2}\varepsilon$
    - Eq. (3.4.25): $\varepsilon = 2n+1$

Energy levels

- The permitted energy levels:
  - $E_v = \frac{\hbar\omega}{2}\varepsilon_v = \frac{\hbar\omega}{2}\left(v + \frac{1}{2}\right)$ (3.4.30)
    - $v = 0, 1, 2, \ldots,$ quantum number
    - $\omega = (k/m)^{1/2}$, (3.4.31)
      - ω increases with increasing k and decreasing m.
    - $E_0 = 1/2\hbar\omega$ at $v = 0$ (3.4.32)
      - non-zero zero-point energy



- The separation between adjacent levels:
  - $E_{v+1} - E_v = \hbar\omega$ (3.4.33)
    - Identical for all v.
    - The energy levels $\hbar\omega$ form a uniform ladder of spacing.

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Section 3. One-dimensional quantum-mechanical harmonic oscillator

End