

### 5. Normal Modes of a Three-Dimensional Crystal

Consider a face-centered cubic monatomic Bravais lattice in which each ion interacts only with its (twelve) nearest neighbors. Assume that the interaction between a pair of neighboring ions is described by a pair potential  $\phi$  that depends only on the distance  $r$  between the pair of ions.

(a) Show that the frequencies of the three normal modes with wave vector  $\mathbf{k}$  are given by

$$\omega = \sqrt{\lambda/M} \quad (22.96)$$

where the  $\lambda$  are the eigenvalues of the  $3 \times 3$  matrix:

$$\mathbf{D} = \sum_{\mathbf{R}} \sin^2(\tfrac{1}{2}\mathbf{k} \cdot \mathbf{R}) [A\mathbf{1} + B\hat{\mathbf{R}}\hat{\mathbf{R}}]. \quad (22.97)$$

Here the sum is over the twelve nearest neighbors of  $\mathbf{R} = 0$ :

$$\frac{a}{2}(\pm\hat{x} \pm \hat{y}), \quad \frac{a}{2}(\pm\hat{y} \pm \hat{z}), \quad \frac{a}{2}(\pm\hat{z} \pm \hat{x}); \quad (22.98)$$

$\mathbf{1}$  is the unit matrix ( $(\mathbf{1})_{\mu\nu} = \delta_{\mu\nu}$ ), and  $\hat{\mathbf{R}}\hat{\mathbf{R}}$  is the diadic formed from the unit vectors  $\hat{\mathbf{R}} = \mathbf{R}/R$  (i.e.,  $(\hat{\mathbf{R}}\hat{\mathbf{R}})_{\mu\nu} = \hat{R}_\mu\hat{R}_\nu$ ). The constants  $A$  and  $B$  are:  $A = 2\phi'(d)/d$ ,  $B = 2[\phi''(d) - \phi'(d)/d]$ , where  $d$  is the equilibrium nearest-neighbor distance. (This follows from Equations (22.59) and (22.11).)

(b) Show that when  $\mathbf{k}$  is in the (100) direction ( $\mathbf{k} = (k, 0, 0)$  in rectangular coordinates), then one normal mode is strictly longitudinal, with frequency

$$\omega_L = \sqrt{\frac{8A + 4B}{M}} \sin \tfrac{1}{4}ka, \quad (22.99)$$

and the other two are strictly transverse and degenerate, with frequency

$$\omega_T = \sqrt{\frac{8A + 2B}{M}} \sin \tfrac{1}{4}ka. \quad (22.100)$$

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## **Table of Contents Ashcroft Mermin Solutions Chapter 22**

1. Understanding the eBook Ashcroft Mermin Solutions Chapter 22
  - The Rise of Digital Reading Ashcroft Mermin Solutions Chapter 22
  - Advantages of eBooks Over Traditional Books
2. Identifying Ashcroft Mermin Solutions Chapter 22
  - Exploring Different Genres
  - Considering Fiction vs. Non-Fiction
  - Determining Your Reading Goals
3. Choosing the Right eBook Platform
  - Popular eBook Platforms
  - Features to Look for in an Ashcroft Mermin Solutions Chapter 22
  - User-Friendly Interface
4. Exploring eBook Recommendations from Ashcroft Mermin Solutions Chapter 22
  - Personalized Recommendations
  - Ashcroft Mermin Solutions Chapter 22 User Reviews and Ratings
  - Ashcroft Mermin Solutions Chapter 22 and Bestseller Lists
5. Accessing Ashcroft Mermin Solutions Chapter 22 Free and Paid eBooks
  - Ashcroft Mermin Solutions Chapter 22 Public Domain eBooks
  - Ashcroft Mermin Solutions Chapter 22 eBook Subscription Services
  - Ashcroft Mermin Solutions Chapter 22 Budget-Friendly Options

6. Navigating Ashcroft Mermin Solutions Chapter 22 eBook Formats
  - ePub, PDF, MOBI, and More
  - Ashcroft Mermin Solutions Chapter 22 Compatibility with Devices
  - Ashcroft Mermin Solutions Chapter 22 Enhanced eBook Features
7. Enhancing Your Reading Experience
  - Adjustable Fonts and Text Sizes of Ashcroft Mermin Solutions Chapter 22
  - Highlighting and Note-Taking Ashcroft Mermin Solutions Chapter 22
  - Interactive Elements Ashcroft Mermin Solutions Chapter 22
8. Staying Engaged with Ashcroft Mermin Solutions Chapter 22
  - Joining Online Reading Communities
  - Participating in Virtual Book Clubs
  - Following Authors and Publishers Ashcroft Mermin Solutions Chapter 22
9. Balancing eBooks and Physical Books Ashcroft Mermin Solutions Chapter 22
  - Benefits of a Digital Library
  - Creating a Diverse Reading Collection Ashcroft Mermin Solutions Chapter 22
10. Overcoming Reading Challenges
  - Dealing with Digital Eye Strain
  - Minimizing Distractions
  - Managing Screen Time
11. Cultivating a Reading Routine Ashcroft Mermin Solutions Chapter 22
  - Setting Reading Goals Ashcroft Mermin Solutions Chapter 22
  - Carving Out Dedicated Reading Time
12. Sourcing Reliable Information of Ashcroft Mermin Solutions Chapter 22
  - Fact-Checking eBook Content of Ashcroft Mermin Solutions Chapter 22
  - Distinguishing Credible Sources
13. Promoting Lifelong Learning
  - Utilizing eBooks for Skill Development
  - Exploring Educational eBooks
14. Embracing eBook Trends
  - Integration of Multimedia Elements

- Interactive and Gamified eBooks

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