1.3.2 Answers

1. Applying the Euler-Lagrange equation $d_t(\partial_{\dot{\phi}_n} L) - \partial_{\phi_n} L = 0$ to the discrete Lagrangian of the lattice model, one finds that the N equations of motion take the form of a three-term difference equation,[14]

$$m\ddot{\phi}_n = k_s\left(\phi_{n+1} - 2\phi_n + \phi_{n-1}\right).$$

As in the continuum theory, the latter can be brought to diagonal form by turning to the Fourier representation. Applying the *Ansatz*

$$\phi_n(t) = \frac{1}{\sqrt{N}}\sum_k e^{-i(\omega_k t - kna)}\phi_k$$

where the discrete quasi-momenta $k = 2\pi m/Na$ take values from the range $m = [-N/2, N/2]$ (i.e. the first **Brillouin zone**), we find $[m\omega_k^2 - 2k_s(1-\cos(ka))]\phi_k = 0$. From this equation one obtains the dispersion relation

$$\omega_k = 2\sqrt{\frac{k_s}{m}}|\sin(ka/2)|.$$

For $k \to 0$, this result collapses to the linear dispersion relation $\omega_k = v|k|$ obtained from the continuum theory. This can be understood simply by comparing the wavelength of the lattice vibration $\lambda = 2\pi/k$ with the lattice spacing a. When $\lambda \gg a$, the *relative* displacement of the atomic sites is small and the continuum approximation is justified. When $\lambda \sim a$, the relative displacement is large and the continuum theory becomes inapplicable.

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2. Applying the Euler-Lagrange equations we obtain the $2 \times N$ coupled equations of motion

$$\begin{aligned} m_A\ddot{\phi}_n^{(A)} &= k_s\left(\phi_n^{(B)} - 2\phi_n^{(A)} + \phi_{n-1}^{(B)}\right), \\ m_B\ddot{\phi}_n^{(B)} &= k_s\left(\phi_{n+1}^{(A)} - 2\phi_n^{(B)} + \phi_n^{(A)}\right). \end{aligned}$$

[14]Note that, looking for stationary solutions $\phi_n(t) = e^{-i\omega t}$, the difference equation can be written as the eigenvalue equation $m\omega^2\phi_n = \sum_m^N M_{nm}\phi_n$, where

$$M = k_s\begin{pmatrix} \cdots & \cdots & \cdots & & & & 0 \\ & -1 & 2 & -1 & & & \\ & & -1 & 2 & -1 & & \\ 0 & & & \cdots & \cdots & \cdots & \end{pmatrix}.$$

The latter has eigenfunctions corresponding to the discrete Fourier transform: i.e. writing the eigenvalue equation as $m\omega^2|n\rangle = \hat{M}|n\rangle$, the normalised eigenfunctions $|k\rangle$, indexed by the wavenumber $k \in [-\pi/a, \pi/a]$, are given by $\phi_n(k) \equiv \langle n|k\rangle = \frac{1}{\sqrt{N}}e^{ikna}$. Later, in the next chapter, we will see that these eigenfunctions (of the discrete lattice Laplacian) will present a convenient basis for expansion of more complicated lattice models.

Applying the *Ansatz* $\phi_n^{(A/B)} = \frac{1}{\sqrt{N}}\sum_k e^{-i(\omega_k t - kna)}\phi_k^{(A/B)}$, one obtains

$$\begin{pmatrix} m_A\omega_k^2 - 2k_s & k_s(1+e^{-ika}) \\ k_s(1+e^{ika}) & m_B\omega_k^2 - 2k_s \end{pmatrix}\begin{pmatrix}\phi_k^{(A)} \\ \phi_k^{(B)}\end{pmatrix} = 0.$$

Diagonalizing the 2×2 matrix one recovers the secular equation shown in the question and from which we obtain the dispersion relation (see Fig. 1.9)

$$\omega_k^{(\pm)} = \omega_0\left[1 \pm \left(1 - \frac{4m_Am_B}{(m_A+m_B)^2}\sin^2(ka/2)\right)^{1/2}\right]^{1/2},$$

where $\omega_0 = \sqrt{k_s/\mu}$ and $\mu = 1/(m_A^{-1}+m_B^{-1})$ denotes the reduced mass.

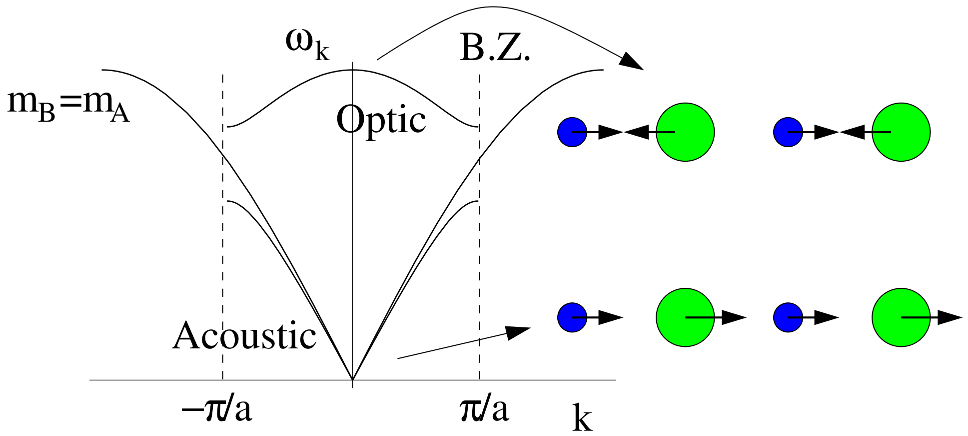

Figure 1.9: Spectrum of the two-atom discrete linear chain. Note that when $m_A = m_B$ we recover the spectrum of the single atom chain with period $a/2$. For $m_A \neq m_B$, a gap opens at the Brillounin zone boundary. The lower energy band is known as the acoustic branch where atoms in each unit cell move in phase. The higher energy optic branch involves atoms in each cell moving in antiphase.

An expansion in the limit $k \to 0$ yields

$$\omega_k^{(\pm)} \to \omega_0\begin{cases}\sqrt{2}\left(1 - \dfrac{m_Am_B}{8(m_A+m_B)^2}(ka)^2\right) + O(k^4) \\ \sqrt{\dfrac{m_Am_B}{2}}\dfrac{1}{(m_A+m_B)}|ka| + O(k^3)\end{cases}$$

from which we deduce that the lower branch describes acoustic phonons with a linear dispersion relation, while the optic phonons are massive with a quadratic spectrum.

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3. To complete this problem, one must generalise the Euler-Lagrange equation derived in lectures. E.g., for case 2., a variation of the action obtains

$$\begin{aligned}\delta S &= \int\left[\mathcal{L}(\dot\phi + \epsilon\dot\eta, \partial_x^2\phi + \epsilon\partial_x^2\eta) - \mathcal{L}(\dot\phi, \partial_x^2\phi)\right] \\ &= \epsilon\int\left[\dot\eta\partial_{\dot\phi}\mathcal{L} + \partial_x^2\eta\partial_{\partial_x^2\phi}\mathcal{L}\right] = \epsilon\int\eta\left[-d_t\partial_{\dot\phi}\mathcal{L} + d_x^2\left(\partial_{\partial_x^2\phi}\mathcal{L}\right)\right]\end{aligned}$$

from which we obtain the Euler-Lagrange equation

$$-d_t\partial_{\dot\phi}\mathcal{L} + d_x^2\left(\partial_{\partial_x^2\phi}\mathcal{L}\right) = 0.$$

Applied to the Lagrangian functionals at hand, one finds the equation of motion

$$\begin{aligned}
&1. \qquad \ddot\phi - \frac{k_s a^2}{m}\partial_x^2\phi + \omega^2\phi = 0,\\
&2. \qquad \ddot\phi + \frac{\kappa}{m}\partial_x^4\phi = 0,\\
&3. \qquad \ddot\phi + \omega^2\phi + \frac{\eta}{m}\phi^3 = 0\\
&4. \qquad \ddot\phi_i - \frac{k_s a^2}{m}\partial_x^2\phi_i = 0.
\end{aligned}$$

Finally, turning to case 5., it is necessary to generalise the Euler-Lagrange equation to account for complex fields. Since the real and imaginary parts fluctuate independently, we can consider a variation of each independently. Separating $\phi = \phi' + i\phi''$ into its real and imaginary parts, and applying a variation to each component, one obtains

$$\ddot\phi' - \frac{k_s a^2}{m}\partial_x^2\phi' = 0, \qquad \ddot\phi'' - \frac{k_s a^2}{m}\partial_x^2\phi'' = 0.$$

In fact, this result shows that the components ϕ and the complex conjugate ϕ^* can be treated as independent. A variation of the action with respect to ϕ^* obtains

$$5. \qquad \ddot\phi - \frac{k_s a^2}{m}\partial_x^2\phi = 0.$$

Physically, one can interpret the last term in 1. as a harmonic lattice binding potential. Its effect is to render the fluctuations massive, viz. $\omega_k = \sqrt{\omega^2 + v^2k^2}$.

For case 2. the momentum conjugate to the field ϕ is given by $\pi = \partial_{\dot\phi}\mathcal{L} = m\dot\phi$. The Hamiltonian corresponding to case 2. is given by

$$\mathcal{H} = \pi\dot\phi - \mathcal{L} = \frac{\pi^2}{2m} + \frac{k_s a^2}{2}(\partial_x^2\phi)^2.$$

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4. (a) Using the definition provided, together with the canonical commutation relations of the field operators, one obtains

$$[\hat\pi_k, \hat\phi_{k'}] = \frac{1}{L}\int_0^L dx \int_0^L dx' e^{ikx - ik'x'} \overbrace{[\hat\pi(x), \hat\phi(x')]}^{-i\hbar\delta(x-x')} = -i\hbar\, \overbrace{\frac{1}{L}\int_0^L dx\ e^{i(k-k')x'}}^{\delta_{kk'}} = -i\hbar\delta_{kk'}.$$

(b) Again, using the definition, the kinetic component of the Hamiltonian takes the form

$$\int_0^L dx\ \frac{\hat\pi^2}{2m} = \sum_{kk'}\frac{1}{L}\int_0^L dx\ e^{-i(k+k')x}\frac{1}{2m}\ \hat\pi_k\hat\pi_{k'} = \sum_k \frac{1}{2m}\hat\pi_k\hat\pi_{-k}.$$

Similarly, applied to the potential component one obtains the Hamiltonian as advertised.

(c) Using the commutation relation derived above, one finds

$$[a_k, a^\dagger_{k'}] = \frac{i}{2\hbar}\left([\hat{\phi}_{-k}, \hat{\pi}_{-k'}] - [\hat{\pi}_k \hat{\phi}_{k'}]\right) = \delta_{kk'}, \qquad [a^\dagger_k, a^\dagger_{k'}] = 0.$$

(d) Inverting the expression for the field operators, one finds

$$\hat{\phi}_k = \left(\frac{\hbar}{2m\omega_k}\right)^{1/2}\left(a_k + a^\dagger_{-k}\right), \qquad \hat{\pi}_k = i\left(\frac{m\hbar\omega_k}{2}\right)^{1/2}\left(a^\dagger_k - a_{-k}\right).$$

Using the identity

$$\begin{aligned}\frac{1}{2m}\left(\hat{\pi}_k\hat{\pi}_{-k} + \hat{\pi}_{-k}\hat{\pi}_k\right) + \frac{k_s a^2}{2}k^2\left(\hat{\phi}_k\hat{\phi}_{-k} + \hat{\phi}_{-k}\hat{\phi}_k\right)\\ = \frac{1}{2}\hbar\omega_k\left(a^\dagger_k a_k + a_k a^\dagger_k + a^\dagger_{-k}a_{-k} + a_{-k}a^\dagger_{-k}\right).\end{aligned}$$

together with the commutation relations, after summation over k, we obtain the harmonic oscillator Hamiltonian.