Solid State Physics IV
-Part II : Macroscopic Quantum Phenomena

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We first study why harmonic oscillators are so ubiquitous and see that not only a point mass in a harmonic potential but also an LC circuit as well as the electromagnetic wave in a cavity behave like a harmonic oscillator. Second, we learn an important idea of *normal modes* to deal with coupled harmonic oscillators. Third, taking the *continuum limit* we study that a (1+1)-dimensional boson field is emerged from N coupled (0+1)-dimensional harmonic oscillators.

I. HARMONIC OSCILLATORS, COUPLED HARMONIC OSCILLATORS, AND BOSON FIELDS

A. Harmonic oscillators

1. Point mass in a harmonic potential

Let us begin by considering a point mass with mass m and coordinate x situated in a potential $U(x)$. Suppose that the mass is oscillating with small amplitude around the equilibrium position x_0. Then the potential energy of the mass can be Taylor-expanded around x_0:

$$U(x) = U(x_0) + \frac{\partial U(x_0)}{\partial x}x + \frac{1}{2}\frac{\partial^2 U(x_0)}{\partial x^2}x^2. \tag{1}$$

Since the force, $F = \frac{\partial U(x_0)}{\partial x}$, should be zero in the equilibrium position, neglecting the potential offset $U(x_0)$ we have

$$U(x) = \frac{1}{2}\underbrace{\frac{\partial^2 U(x_0)}{\partial x^2}}_{k}x^2. \tag{2}$$

This suggests that any potential can be considered as a harmonic potential when we are interested in the small motion in the vicinity of the equilibrium position.

With the kinetic part $K = \frac{1}{2}m\dot{x}^2$ we have the standard Lagrangian for the harmonic oscillator:

$$L(x,\dot{x}) = K(\dot{x}) - U(x) = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}kx^2. \tag{3}$$

The motion of the mass from time t_1 to t_2 can be determined so as to minimize the action integral

$$I = \int_{t_1}^{t_2} L(x,\dot{x})dt. \tag{4}$$

The minimum of I can be obtained by a variational principle (Hamilton's principle), which leads to the Euler-Lagrange equation of motion:

$$\frac{d}{dt}\left(\frac{\partial L(x,\dot{x})}{\partial \dot{x}}\right) - \frac{\partial L(x,\dot{x})}{\partial x} = 0, \tag{5}$$

that, in turn, is Newton's second law:

$$m\ddot{x} - kx = 0. \tag{6}$$

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In the formal procedure the conjugate momentum, p, can then be obtained by

$$p = \frac{\partial L(x, \dot{x})}{\partial \dot{x}} = m\dot{x}. \tag{7}$$

We have thus the Hamiltonian $H(x, p)$ from the Legendre transformation:

$$H(x, p) = \dot{x}p - L(x, \dot{x}) = \frac{1}{2m}p^2 + \frac{1}{2}kx^2. \tag{8}$$

The mean value of energy $\bar{H}(x, p)$ in thermal equilibrium can be given by

$$\begin{aligned} \bar{H}(x,p) &= \frac{\int_{-\infty}^{\infty} dxdpH(x,p)e^{-\beta H(x,p)}}{\int_{-\infty}^{\infty} dxdpe^{-\beta H(x,p)}} \\ &= -\frac{\partial}{\partial\beta}\ln\left(\int_{-\infty}^{\infty} dxdpe^{-\beta H(x,p)}\right) \\ &= \frac{1}{\beta} = k_{\mathrm{B}}T. \end{aligned} \tag{9}$$

We can promote x and p to the quantum-mechanical operators by imposing the commutation relation,

$$[\hat{x}, \hat{p}] = i\hbar. \tag{10}$$

Let the annihilation and creation operators be

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + \frac{i}{m\omega}\hat{p}\right) \tag{11}$$

$$\hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} - \frac{i}{m\omega}\hat{p}\right), \tag{12}$$

respectively, where $\omega = \sqrt{\frac{k}{m}}$. The Hamiltonian Eq. (8) can then be written as

$$\begin{aligned} \hat{H}(\hat{x},\hat{p}) &= \frac{1}{2m}\hat{p}^2 + \frac{1}{2}m\omega^2\hat{x}^2 \\ &= \hbar\omega\left(\underbrace{\hat{a}^\dagger\hat{a}}_{\hat{n}} + \frac{1}{2}\right). \end{aligned} \tag{13}$$

The mean value of energy $\langle\hat{H}(\hat{x}, \hat{p})\rangle$ becomes

$$\langle\hat{H}(\hat{x},\hat{p})\rangle = \hbar\omega\left(\langle\hat{n}\rangle + \frac{1}{2}\right), \tag{14}$$

where

$$\langle n\rangle = \frac{1}{e^{\frac{\hbar\omega}{k_{\mathrm{B}}T}} - 1}, \tag{15}$$

which in high temperature limit becomes $\langle n\rangle \to \frac{k_{\mathrm{B}}T}{\hbar\omega}$ as in Eq. (9).

2. LC circuit

Q-representation

An LC circuit can be viewed as a harmonic oscillator, too. Replacing the coordinate x by the charge Q, the mass m

by the inductance L_0, and the spring constant k by the inverse of capacitance C_0, we have the Lagrangian for the LC circuit:

$$L(Q,\dot{Q}) = \frac{1}{2}L_0\dot{Q}^2 - \frac{1}{2C_0}Q^2. \tag{16}$$

The first term is the inductive energy and the second is the charging energy. The conjugate momentum is

$$\frac{\partial L(Q,\dot{Q})}{\partial \dot{Q}} = L_0\dot{Q} = \varphi, \tag{17}$$

which is identified as the flux. The Hamiltonian is thus

$$\begin{aligned} H(Q,\varphi) = \dot{Q}\varphi - L(Q,\dot{Q}) &= \frac{1}{2L_0}\varphi^2 + \frac{1}{2C_0}Q^2 \\ &= \frac{1}{2L_0}\varphi^2 + \frac{1}{2}L_0\omega^2Q^2, \end{aligned} \tag{18}$$

where $\omega = \frac{1}{\sqrt{L_0C_0}}$.

The commutation relation:

$$[Q,\varphi] = i\hbar \tag{19}$$

Let the annihilation and creation operators be

$$\hat{b} = \sqrt{\frac{L_0\omega}{2\hbar}}\left(\hat{Q} + \frac{i}{L_0\omega}\hat{\varphi}\right) \tag{20}$$

$$\hat{b}^\dagger = \sqrt{\frac{L_0\omega}{2\hbar}}\left(\hat{Q} - \frac{i}{L_0\omega}\hat{\varphi}\right). \tag{21}$$

The Hamiltonian Eq. (18) can then be written as

$$\begin{aligned} \hat{H}(\hat{Q},\hat{\varphi}) &= \frac{1}{2L_0}\hat{\varphi}^2 + \frac{1}{2}L_0\omega^2\hat{Q}^2 \\ &= \hbar\omega\left(\hat{b}^\dagger\hat{b} + \frac{1}{2}\right). \end{aligned} \tag{22}$$

φ-representation

We can equally use the flux φ as the coordinate of the LC circuit system, which is more relevant when we deal with a transmission line. Then, the Lagrangian is a function of φ and $\dot{\varphi}$, and is given by

$$L(\varphi,\dot{\varphi}) = \frac{1}{2}C_0\dot{\varphi}^2 - \frac{1}{2L_0}\varphi^2, \tag{23}$$

where the roles of C_0 and L_0^{-1} are the mass and the spring constant, respectively, and are switched from the first case. The first term is then the charging energy and the second is the inductive energy. The conjugate momentum becomes

$$\frac{\partial L(\varphi,\dot{\varphi})}{\partial \dot{\varphi}} = C_0\dot{\varphi}. \tag{24}$$

Since $\dot{\varphi} = L_0\dot{I} = V$ (*Faraday's law of induction*) the conjugate momentum of the flux φ is indeed the charge:

$$C_0\dot{\varphi} = C_0V = Q. \tag{25}$$

Consequently, the Hamiltonian is

$$\begin{aligned} H(\varphi,Q) = \dot{\varphi}Q - L(\varphi,\dot{\varphi}) &= \frac{1}{2C_0}Q^2 + \frac{1}{2L_0}\varphi^2 \\ &= \frac{1}{2C_0}Q^2 + \frac{1}{2}C_0\omega^2\varphi^2. \end{aligned} \tag{26}$$

The commutation relation:

$$[\varphi, Q] = i\hbar \tag{27}$$

Let the annihilation and creation operators be

$$\hat{c} = \sqrt{\frac{C_0\omega}{2\hbar}}\left(\hat{\varphi} + \frac{i}{C_0\omega}\hat{Q}\right) \tag{28}$$

$$\hat{c}^\dagger = \sqrt{\frac{C_0\omega}{2\hbar}}\left(\hat{\varphi} - \frac{i}{C_0\omega}\hat{Q}\right). \tag{29}$$

The Hamiltonian Eq. (26) can then be written as

$$\begin{aligned}\hat{H}(\hat{\varphi}, \hat{Q}) &= \frac{1}{2C_0}\hat{Q}^2 + \frac{1}{2}C_0\omega^2\hat{\varphi}^2 \\ &= \hbar\omega\left(\hat{c}^\dagger\hat{c} + \frac{1}{2}\right).\end{aligned} \tag{30}$$

3. Electromagnetic field in a cavity [1, 2]

The same line of argument can be employed to deal with the electromagnetic field in a cavity. Maxwell's equations (first order differential equations) tell us that there are 4 independent degrees of freedom out of apparent 6 degrees of freedom $\{\boldsymbol{E}, \boldsymbol{B}\}$; namely

$$\{\boldsymbol{E}_\perp, \boldsymbol{B}_\perp\}, \tag{31}$$

i.e., the transverse components of electric and magnetic fields since the longitudinal components $\{\boldsymbol{E}_\parallel, \boldsymbol{B}_\parallel\}$ can be fixed by the static equations

$$\nabla \cdot \boldsymbol{E} = \frac{\rho}{\epsilon_0} \tag{32}$$

$$\nabla \cdot \boldsymbol{B} = 0. \tag{33}$$

To *canonically* quantize the electromagnetic field the potentials $\{\boldsymbol{A}, \phi\}$ instead of the field $\{\boldsymbol{E}_\perp, \boldsymbol{B}_\perp\}$ have to be employed since the Euler-Lagrange equations are the second order differential equations. There are then 8 degrees of freedom, $\{\boldsymbol{A}, \phi, \dot{\boldsymbol{A}}, \dot{\phi}\}$. The velocity of scalar potential $\dot{\phi}$ does not appear in the *standard* Lagrangian [1] and thus 2 degrees of freedom $\{\phi, \dot{\phi}\}$ out of 8 can be eliminated as the non-dynamic variables. We could further eliminate the longitudinal 2 components $\{\boldsymbol{A}_\parallel, \dot{\boldsymbol{A}}_\parallel\}$ from the 6 degrees of freedom $\{\boldsymbol{A}, \dot{\boldsymbol{A}}\}$ by fixing the gauge (*Coulomb gauge*). In the Coulomb gauge we have only the transverse components of the vector potential, that is, $\{\boldsymbol{A}_\perp, \dot{\boldsymbol{A}}_\perp\}$, which fit the above fact that there are only 4 independent degrees of freedom. To simplify the notation " $\perp$ " will be henceforth omitted. The free field Lagrangian can then be given by [1]

$$L = \int dV \mathcal{L}(\boldsymbol{A}, \dot{\boldsymbol{A}}) \tag{34}$$

with the Lagrangian density of

$$\mathcal{L}(\boldsymbol{A}, \dot{\boldsymbol{A}}) = \frac{\epsilon_0}{2}\left(\dot{\boldsymbol{A}}^2 - c^2\left(\nabla \times \boldsymbol{A}\right)^2\right), \tag{35}$$

The momentum conjugate with the variable A_i with $i = x, y, z$ is given by

$$\Pi_i = \left(\frac{\partial \mathcal{L}}{\partial \dot{A}_i}\right)^* = \epsilon_0 \dot{A}_i. \tag{36}$$

The free field Hamiltonian in the *Coulomb gauge* can then be given by [1]

$$H_R = \frac{\epsilon_0}{2}\int_{\text{cavity}} dV \left(\underbrace{\left(\frac{\boldsymbol{\Pi}(\boldsymbol{r})}{\epsilon_0}\right)^2}_{\boldsymbol{E}_\perp(\boldsymbol{r})^2} + c^2 \underbrace{\left(\nabla \times \boldsymbol{A}(\boldsymbol{r})\right)^2}_{\boldsymbol{B}_\perp(\boldsymbol{r})^2}\right). \tag{37}$$

	Point mass	LC (Q-rep.)	LC (φ-rep.)	EM cavity mode
Mass	m	L_0	C_0	ϵ_0
Spring const.	k	$\frac{1}{C_0}$	$\frac{1}{L_0}$	$\frac{1}{\mu_0}$
Ang. freq.	$\omega = \sqrt{\frac{k}{m}}$	$\omega = \frac{1}{\sqrt{C_0 L_0}}$	$\omega = \frac{1}{\sqrt{C_0 L_0}}$	$\omega_k = ck$
Position var.	x	Q	φ	A_k
Momentum var.	p	φ	Q	Π_k

In reciprocal space Maxwell's equations are strictly local, so is the Hamiltonian density, which leads to

$$\begin{aligned} H_R &= \sum_{\boldsymbol{k}>0} \sum_{\lambda=1,2} \frac{\epsilon_0}{2} \left(\left(\frac{\boldsymbol{\Pi}^\dagger_{\lambda,\boldsymbol{k}}}{\epsilon_0} \cdot \frac{\boldsymbol{\Pi}_{\lambda,\boldsymbol{k}}}{\epsilon_0} \right) + c^2 k^2 \left(\boldsymbol{A}^\dagger_{\lambda,\boldsymbol{k}} \cdot \boldsymbol{A}_{\lambda,\boldsymbol{k}} \right) \right) \\ &= \sum_k \mathcal{H}_k \end{aligned} \tag{38}$$

where $\mathcal{H}_k$ is the Hamiltonian for a *single mode* with the index k, which has the wave vector $\boldsymbol{k}$ and polarization λ:

$$\mathcal{H}_k = \underbrace{\frac{1}{2\epsilon_0} \Pi^\dagger_k \cdot \Pi_k}_{\text{kinetic part}} + \underbrace{\frac{1}{2} \epsilon_0 \omega_k^2 A^\dagger_k \cdot A_k}_{\text{potential part}}, \tag{39}$$

where $\omega_k = ck$. The form of Eq. (39) is quite analogous to the Hamiltonian for harmonic oscillators appeared in Eqs. (8), (18) and (26). In this sense we can consider the single-mode free electromagnetic field in the Coulomb gauge (in reciprocal space) as a harmonic oscillator with the position variable $A(\omega)$, the momentum variable $\Pi(\omega)$, and the mass ϵ_0 .

The commutation relation:

$$[A_k, \Pi_{k'}] = i\hbar \delta_{k,k'} \tag{40}$$

With the annihilation and creation operators

$$\hat{d}_k = \sqrt{\frac{\epsilon_0 \omega_k}{2\hbar}} \left(\hat{A}_k + \frac{i}{\epsilon_0 \omega_k} \hat{\Pi}_k \right) \tag{41}$$

$$\hat{d}^\dagger_k = \sqrt{\frac{\epsilon_0 \omega_k}{2\hbar}} \left(\hat{A}^\dagger_k - \frac{i}{\epsilon_0 \omega_k} \hat{\Pi}^\dagger_k \right), \tag{42}$$

the Hamiltonian Eq. (39) can then be rewritten as

$$\mathcal{H}_k = \hbar \omega_k \left(\hat{d}^\dagger_k \hat{d}_k + \frac{1}{2} \right). \tag{43}$$

B. Coupled harmonic oscillators

1. LC-mechanical oscillator coupling

Let us consider first the situation in which a metallic membrane oscillator with the angular frequency of ω_m is capacitively coupled to a LC circuit with the angular frequency of ω_{LC}. The coupled system's potential can then be given by $H(x, q)$, where x is the membrane displacement and q is the charge in the capacitor of the LC circuit. Suppose that with certain external voltage the equilibrium position is $x = X_0$, and the equilibrium charge is $q = Q_0$. Then, around the equilibrium point, the potential can be written as

$$H(x,q) = H(X_0, Q_0) + (\frac{\partial H}{\partial x}\hat{x} + \frac{\partial H}{\partial q}\hat{q}) + (\frac{1}{2}\frac{\partial^2 H}{\partial x^2}\hat{x}^2 + \frac{1}{2}\frac{\partial^2 H}{\partial q^2}\hat{q}^2 + \frac{\partial^2 H}{\partial x \partial q}\hat{x}\hat{q}), \tag{44}$$

with $x = X_0 + \hat{x}, q = Q_0 + \hat{q}$. The linear terms in Eq. (44), however, vanish becasue of the definition of the equilibrium condition $\frac{\partial H}{\partial x}|_{x=X_0} = 0$ and $\frac{\partial H}{\partial q}|_{q=Q_0} = 0$. Neglecting the equilibrium potential energy $H(X_0, Q_0)$, we have

$$\hat{H}(\hat{x}, \hat{q}) = \frac{1}{2} m\omega_m \hat{x}^2 + \frac{1}{2C}\hat{q}^2 + G\hat{x}\hat{q}, \tag{45}$$

where $\frac{\partial^2 H}{\partial x^2}|_{x=X_0} = k = m\omega_m^2$, $\frac{\partial^2 H}{\partial q^2}|_{q=Q_0} = \frac{1}{C}$, and $\frac{\partial^2 H}{\partial x \partial q}|_{x=X_0, q=Q_0} = G$.

By adding the kinetic energy parts, $\frac{1}{2m}p^2 = \frac{1}{2}m(\frac{dx}{dt})^2$ for mechanics and $\frac{1}{2L}\phi^2 = \frac{1}{2}L(\frac{dq}{dt})^2$ for LC-circuit, we have the Hamiltonian,

$$\hat{H} = \underbrace{\frac{1}{2m}\hat{p}^2 + \frac{1}{2}m\omega_m\hat{x}^2}_{\text{mechanics}} + \underbrace{\frac{1}{2L}\hat{\phi}^2 + \frac{1}{2C}\hat{q}^2}_{\text{LC}} + \underbrace{G\hat{x}\hat{q}}_{\text{coupling}} . \tag{46}$$

The Hamiltonian Eq. (46) can be rewritten as

$$\begin{aligned}
\hat{H} &= \frac{1}{2m}\hat{p}^2 + \frac{1}{2}m\omega_m\hat{x}^2 + \frac{1}{2L}\hat{\phi}^2 + \frac{1}{2}L\omega_{LC}\hat{q}^2 + G\hat{x}\hat{q} \\
&= \hbar\omega_m\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right) + \hbar\omega_{LC}\left(\hat{b}^\dagger\hat{b} + \frac{1}{2}\right) + G\left(\sqrt{\frac{\hbar}{2m\omega_m}}\left(\hat{a}^\dagger + \hat{a}\right)\right)\left(\sqrt{\frac{\hbar}{2L\omega_{LC}}}\left(\hat{b}^\dagger + \hat{b}\right)\right) \\
&= \hbar\omega_m\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right) + \hbar\omega_{LC}\left(\hat{b}^\dagger\hat{b} + \frac{1}{2}\right) + \frac{\hbar}{2}\underbrace{\frac{G}{\sqrt{m\omega_m}\sqrt{L\omega_{LC}}}}_{g}\left(\hat{a}^\dagger + \hat{a}\right)\left(\hat{b}^\dagger + \hat{b}\right).
\end{aligned} \tag{47}$$

Using the *rotating-wave approximation* which neglect rapidly oscillating terms $\hat{a}\hat{b}$ and $\hat{a}^\dagger\hat{b}^\dagger$ in the last term in Eq. (47) we have the *canonical* Hamiltonian for the coupled oscillator system:

$$\hat{H} = \hbar\omega_m\hat{a}^\dagger\hat{a} + \hbar\omega_{LC}\hat{b}^\dagger\hat{b} + \frac{\hbar}{2}g\left(\hat{a}^\dagger\hat{b} + \hat{b}^\dagger\hat{a}\right). \tag{48}$$

Here the vacuum energy terms are omitted since the energy can be offset arbitrary.

Let us analyze the energy level structure for the coupled system. First, suppose that the two oscillators are resonant, that is, $\omega_m = \omega_{LC} = \omega$. We then easily guess that the *normal modes*, which diagonalize the Hamiltonian Eq. (48), are

$$\hat{c} = \frac{1}{\sqrt{2}}\left(\hat{a} - \hat{b}\right) \tag{49}$$

$$\hat{d} = \frac{1}{\sqrt{2}}\left(\hat{a} + \hat{b}\right). \tag{50}$$

With these normal mode operators the Hamiltonian can be indeed rewritten in a diagonal form as

$$\hat{H} = \left(\hbar\omega - \frac{\hbar g}{2}\right)\hat{c}^\dagger\hat{c} + \left(\hbar\omega + \frac{\hbar g}{2}\right)\hat{d}^\dagger\hat{d}. \tag{51}$$

The eigen-energies are shifted from the originally degenerate $\hbar\omega$ by $\hbar g$, which called *normal mode splitting*.

Next, let us consider the situation where the mechanical and LC oscillators have different resonance angular frequencies, ω_m and $\omega_{LC} = \omega_m + \Delta$, respectively. The normal modes in this case become

$$\hat{c} = \cos\theta\ \hat{a} - \sin\theta\ \hat{b} \tag{52}$$

$$\hat{d} = \sin\theta\ \hat{a} + \cos\theta\ \hat{b}, \tag{53}$$

where the *mixing angle* θ is defined by

$$\cot 2\theta = \frac{\Delta}{\omega}. \tag{54}$$

The resultant diagonalized Hamiltonian is

$$\hat{H} = \left(\underbrace{\hbar\omega_m + \frac{\hbar\Delta}{2}}_{\frac{1}{2}(\omega_m + \omega_{LC})} - \frac{\hbar g}{2}\frac{1}{\sin 2\theta}\right)\hat{c}^\dagger\hat{c} + \left(\underbrace{\hbar\omega_m + \frac{\hbar\Delta}{2}}_{\frac{1}{2}(\omega_m + \omega_{LC})} + \frac{\hbar g}{2}\frac{1}{\sin 2\theta}\right)\hat{d}^\dagger\hat{d}. \tag{55}$$

2. 1D atomic chain -phonon modes [3]

Let us consider one-dimensional monatomic atomic chain with the periodic (Born-von Karman) boundary condition, $q(N_{\rm a}a) = q(0)$, where a is the inter-atomic distance. The potential energy of an atom in the chain is now dependent on the configurations of the nearest-neighbor atoms and the total potential energy is

$$V = \frac{1}{2}\kappa \sum_{n=1}^{N_{\rm a}} \left(q(na) - q([n+1]a)\right)^2, \tag{56}$$

where we assume that the neighboring atoms interact with the spring constant of κ. The equations of motion for the coordinates $\{q(a), \cdots, q(N_{\rm a}a)\}$ are coupled equations, i.e.,

$$\begin{aligned} m\ddot{q}(na) &= -\frac{\partial V}{\partial q(na)} \\ &= -\kappa \left(2q(na) - q([n-1]a) - q([n+1]a)\right). \end{aligned} \tag{57}$$

It is again possible to diagonalize the potential energy, Eq. (56) into independent quasi-particles' potential energies by linear transformation of the coordinates and thus by defining the normal modes (phonon modes). Taking advantage of the periodicity due to the periodic boundary condition ($q(N_{\rm a}a) = q(0)$) we can employ a type of Fourier transformation as the required transformation, that is,

$$q(na) = \frac{1}{\sqrt{N_{\rm a}}} \sum_{k_l} e^{ik_l na} u_{k_l}, \tag{58}$$

where $k_l = \frac{2\pi}{N_{\rm a}a} l$ with $l = 0, \pm 1, \pm 2, \cdots, \frac{N_{\rm a}}{2}$.

In terms of the normal coordinates u_{k_l}, the kinetic energy becomes

$$\begin{aligned} K &= \frac{1}{2N_{\rm a}} \sum_{na} \sum_{k_l} \sum_{k_{l'}} m\dot{u}_{k_l} \dot{u}_{k_{l'}} e^{i(k_l + k_{l'})na} \\ &= \frac{m}{2} \sum_{k_l} \dot{u}_{k_l} \dot{u}_{-k_l}, \end{aligned} \tag{59}$$

and the potential energy Eq. (56) becomes

$$\begin{aligned} V &= \frac{\kappa}{2N_{\rm a}} \sum_{na} \sum_{k_l} \sum_{k_{l'}} u_{k_l} u_{k_{l'}} e^{ik_l na} \left(e^{ik_l a} - 1\right) e^{ik_{l'} na} \left(e^{ik_{l'} a} - 1\right) \\ &= \frac{\kappa}{2} \sum_{k_l} 2\left(1 - \cos(k_l a)\right) u_{k_l} u_{-k_l}, \end{aligned} \tag{60}$$

where we used

$$\sum_{na} e^{i(k_l - k_{l'})na} = N_{\rm a} \delta_{k_l k_{l'}}. \tag{61}$$

Since the Lagrangian can be given by

$$L = \frac{m}{2} \sum_{k_l} \dot{u}_{k_l} \dot{u}_{-k_l} - \frac{\kappa}{2} \sum_{k_l} 2\left(1 - \cos(k_l a)\right) u_{k_l} u_{-k_l}, \tag{62}$$

the canonical momenta are systematically deduced, i.e.,

$$p_{k_l} = \frac{\partial L}{\partial \dot{u}_{k_l}} = m\dot{u}_{-k_l} \tag{63}$$

$$p_{-k_l} = \frac{\partial L}{\partial \dot{u}_{-k_l}} = m\dot{u}_{k_l}. \tag{64}$$

In terms of these new coordinates the Hamiltonian becomes

$$H = \frac{1}{2m} \sum_{k_l} p_{k_l} p_{-k_l} + \kappa \sum_{k_l} \left(1 - \cos(k_l a)\right) u_{k_l} u_{-k_l}. \tag{65}$$

The Hamiltonian Eq. (65) is still not in the desired form because of the terms contain both k_l and $-k_l$, which stems from the fact that $\{u_{k_l}, p_{k_l}\}$ are not hermitian but $u^\dagger_{k_l} = u_{-k_l}$ and $p^\dagger_{k_l} = p_{-k_l}$. We can rectify this situation by introducing manifestly hermitian coordinates (*standing wave solutions*)

$$u^{(c)}_{k_l} = \frac{1}{\sqrt{2}}\left(u_{k_l} + u_{-k_l}\right) = \frac{1}{\sqrt{2}}\left(u_{k_l} + u^\dagger_{k_l}\right) \tag{66}$$

$$u^{(s)}_{k_l} = \frac{1}{\sqrt{2}i}\left(u_{k_l} - u_{-k_l}\right) = \frac{1}{\sqrt{2}i}\left(u_{k_l} - u^\dagger_{k_l}\right), \tag{67}$$

and their respective canonical momenta

$$p^{(c)}_{k_l} = m\dot{u}^{(c)}_{k_l} = \frac{1}{\sqrt{2}}\left(p_{k_l} + p_{-k_l}\right) = \frac{1}{\sqrt{2}}\left(p_{k_l} + p^\dagger_{k_l}\right) \tag{68}$$

$$p^{(s)}_{k_l} = m\dot{u}^{(s)}_{k_l} = \frac{1}{\sqrt{2}i}\left(p_{k_l} - p_{-k_l}\right) = \frac{1}{\sqrt{2}i}\left(p_{k_l} - p^\dagger_{k_l}\right). \tag{69}$$

Note that for new coordinates and momenta k_l runs over only positive values up to $\frac{N_\mathrm{a}}{2}$. With these coordinates the Hamiltonian Eq. (65) becomes a sum of the Hamiltonians for the N_a independent harmonic oscillators;

$$H = \sum_{k_l}{}' \left(\frac{1}{2m}p^{(c)\ 2}_{k_l} + \frac{1}{2}m\omega^2_{k_l}u^{(c)\ 2}_{k_l}\right) + \sum_{k_l}{}' \left(\frac{1}{2m}p^{(s)\ 2}_{k_l} + \frac{1}{2}m\omega^2_{k_l}u^{(s)\ 2}_{k_l}\right), \tag{70}$$

where $k_l = \frac{2\pi}{N_\mathrm{a}a}l$ with $l = 0, 1, 2, \cdots, \frac{N_\mathrm{a}}{2}$ and ω_{k_l} is the doubly-degenerate eigen angular frequency defined as

$$\omega_{k_l} = \sqrt{\frac{2\kappa\left(1 - \cos(k_l a)\right)}{m}} = 2\sqrt{\frac{\kappa}{m}}\sin(\frac{k_l a}{2}). \tag{71}$$

Note that the relation between the eigen angular frequency ω (energy) and the wave number k (momentum) is generally called the *dispersion relation*. We have now N_a solutions of eigen energies $\{\hbar\omega_{k_l}\}$, and the mean total energy per mole is

$$\bar{E} = 2\sum_{l=1}^{\frac{N_\mathrm{a}}{2}} \hbar\omega_{k_l}\left(\frac{1}{2} + \frac{1}{e^{\beta\hbar\omega_{k_l}} - 1}\right). \tag{72}$$

For an atomic chain made up of two atoms, the two eigen angular frequencies are

$$\omega_{k_0} = 0 \tag{73}$$

$$\omega_{k_1} = 2\sqrt{\frac{\kappa}{m}}, \tag{74}$$

which reproduce the aforementioned normal mode splitting.

C. Boson fields

1. 1D atomic chain -continuum limit [3]

Suppose that $a \ll 1$, then

$$q([n+1]a) - q(na) \equiv q(x_n + a) - q(x_n) = \frac{\partial q(x_n + a)}{\partial x}a \tag{75}$$

and

$$q([n]a) - q([n-1]a) \equiv q(x_n) - q(x_n - a) = \frac{\partial q(x_n)}{\partial x}a, \tag{76}$$

thus

$$\begin{aligned} 2q(na) - q([n-1]a) - q([n+1]a) &\equiv (q(x_n) - q(x_n - a)) - (q(x_n + a) - q(x_n)) \\ &= -\left(\frac{\partial q(x_n + a)}{\partial x} - \frac{\partial q(x_n)}{\partial x}\right) a \\ &= -\left(\frac{\partial^2 q(x_n + a)}{\partial x^2}\right) a^2. \end{aligned} \tag{77}$$

Plugging this in Eq. (57) the equation of motion for $q(x)$ in the *continuum limit* can be written as

$$m\ddot{q}(x) = \kappa \left(\frac{\partial^2 q(x)}{\partial x^2}\right) a^2, \tag{78}$$

or rather

$$\left(\frac{1}{v_s^2}\frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial x^2}\right) q(x,t) = 0, \tag{79}$$

that is, a (1+1)-dimensional boson field equation with the velocity,

$$v_s = \sqrt{\frac{\kappa a^2}{m}} = \sqrt{\frac{\kappa a}{\left(\frac{m}{a}\right)}} = \sqrt{\frac{c_{11}}{\rho}}, \tag{80}$$

where $c_{11} = K + \frac{4}{3}\mu = \kappa a$ and $\rho = \frac{m}{a}$ are the elastic constant (K being the bulk modulus and μ being the shear modulus) and the mass density of the chain. This wave equation is essentially for the longitudinal acoustic phonon mode. For the transverse acoustic phonon mode, the velocity becomes

$$v_{sT} = \sqrt{\frac{\kappa_T a^2}{m}} = \sqrt{\frac{c_{12}}{\rho}} = \sqrt{\frac{\mu}{\rho}}. \tag{81}$$

The dispersion relation in the continuum limit is linear:

$$\omega_k = v_s k. \tag{82}$$

We see that in the continuum limit, $a \to 0, N_a \to \infty$, the displacement *field* $q(x,t)$ is emerged from the discrete atomic chain. Note that x is now the index as opposed to the coordinate. From the view point of the field theory the above point mass equation, Eq. (6) is in fact (0+1)-dimensional boson field equation.

As in Eq. (58) the (0+1)-dimensional coordinate is

$$q_n(t) = \frac{1}{\sqrt{N_a}} \sum_{k_l} e^{ik_l(na)} u_{k_l}(t), \tag{83}$$

and the canonical momentum is

$$p_n(t) = \frac{1}{\sqrt{N_a}} \sum_{k_l} e^{-ik_l(na)} p_{k_l}(t). \tag{84}$$

The commutation relations are

$$[q_n(t), p_{n'}(t)] = i\hbar\delta_{n,n'}. \tag{85}$$

for the real space operators and

$$\left[u_{k_l}(t), p_{k_{l'}}(t)\right] = i\hbar\delta_{k_l,k_{l'}} \tag{86}$$

for the reciprocal space operators.

The (1+1)-dimensional operators are defined, on the other hand, by

$$q(x,t) = \lim_{\substack{a\to 0 \\ N_a\to\infty}} \frac{q_n(t)}{\sqrt{a}} = \lim_{\substack{a\to 0 \\ N_a\to\infty}} \frac{1}{\sqrt{N_a a}} \sum_k u_k(t) e^{ikx} = \frac{1}{\sqrt{L}} \sum_k u_k(t) e^{ikx} \tag{87}$$

and

$$p(x,t) = \lim_{\substack{a\to 0 \\ N_a\to\infty}} \frac{p_n(t)}{\sqrt{a}} = \lim_{\substack{a\to 0 \\ N_a\to\infty}} \frac{1}{\sqrt{N_a a}} \sum_k p_k(t) e^{-ikx} = \frac{1}{\sqrt{L}} \sum_k p_k(t) e^{-ikx}. \tag{88}$$

Note that the factor $\frac{1}{\sqrt{a}}$ in introduced in each definition in order to make sense when the limit operation $a \to 0, N_a \to \infty$ with $N_a a = L$ finite is performed on the original (0+1)-dimensional forms in Eqs. (83) and (84). The Fourier-transforms are then properly defined with the periodic boundary condition over the length L

$$u_k(t) = \frac{1}{\sqrt{L}} \int_{-\frac{L}{2}}^{\frac{L}{2}} dx q(x,t) e^{-ikx} \tag{89}$$

and

$$p_k(t) = \frac{1}{\sqrt{L}} \int_{-\frac{L}{2}}^{\frac{L}{2}} dx p(x,t) e^{ikx}. \tag{90}$$

The commutation relations are

$$[q(x,t), p(x',t)] = i\hbar\delta(x-x') \tag{91}$$

for the real space operators and

$$[u_k, p_{k'}] = i\hbar\delta_{k,k'} \tag{92}$$

for the reciprocal space operators.

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