elegant. *Disadvantages:* It is less explicit than the microscopic approach. Most importantly, it does not fix the coefficients of the different contributions to the action.

Thus far, we have introduced some basic concepts of field theoretical modeling in condensed matter physics. Starting from a microscopic model Hamiltonian, we have illustrated how principles of universality and symmetry can be applied to distill effective continuum field theories capturing the low-energy content of the system. We have formulated such theories in the language of Lagrangian and Hamiltonian continuum mechanics, respectively, and shown how variational principles can be applied to extract concrete physical information. Finally, we have seen that field theory provides a unifying framework whereby analogies between seemingly different physical systems can be uncovered. In the next section we discuss how the formalism of classical field theory can be elevated to the quantum level.

## 1.4 Quantum chain

Earlier we saw that, at low temperatures, the excitation profile of the classical atomic chain differs drastically from that observed in experiment. Generally, in condensed matter physics, low-energy phenomena with pronounced temperature sensitivity are indicative of a quantum mechanism at work. To introduce and exemplify a general procedure whereby quantum mechanics can be incorporated into continuum models, we next consider the low-energy physics of the quantum mechanical atomic chain.

The first question to ask is conceptual: how can a model like Eq. (1.4) be quantized in general? Indeed, there exists a standard procedure for quantizing continuum theories, which closely resembles the quantization of Hamiltonian point mechanics. Consider the defining Eq. (1.9) and (1.10) for the canonical momentum and the Hamiltonian, respectively. Classically, the momentum $\pi(x)$ and the coordinate $\phi(x)$ are canonically conjugate variables: $\{\pi(x), \phi(x')\} = -\delta(x-x')$ where $\{,\}$ is the Poisson bracket and the $\delta$-function arises through continuum generalization of the discrete identity $\{P_I, R_{I'}\} = -\delta_{II'}$, $I, I' = 1, \ldots, N$. The theory is quantized by generalization of the canonical quantization procedure for the discrete pair of conjugate coordinates $(R_I, P_I)$ to the continuum: (i) promote $\phi(x)$ and $\pi(x)$ to operators, $\phi \mapsto \hat{\phi}$, $\pi \mapsto \hat{\pi}$, and (ii) generalize the canonical commutation relation $[P_I, R_{I'}] = -i\hbar\delta_{II'}$ to[12]

$$\boxed{[\hat{\pi}(x), \hat{\phi}(x')] = -i\hbar\delta(x - x').} \tag{1.25}$$

Operator-valued functions like $\hat{\phi}$ and $\hat{\pi}$ are generally referred to as **quantum fields**. For clarity, the relevant relations between canonically conjugate classical and quantum fields are summarized in Table 1.2.

INFO By introducing quantum fields, we have departed from the conceptual framework laid out on page 6: being operator-valued, the quantized field no longer represents a mapping into an

[12] Note that the dimensionality of both the quantum and the classical continuum field is compatible with the dimensionality of the Dirac $\delta$-function, $[\delta(x - x')] = [\text{length}]^{-1}$, i.e. $[\phi(x)] = [\phi_I] \cdot [\text{length}]^{-1/2}$ and similarly for $\pi$.

Table 1.2 *Relations between discrete and continuum canonically conjugate variables/operators.*

| | Classical | Quantum |
|---|---|---|
| Discrete | $\{P_I, R_{I'}\} = -\delta_{II'}$ | $[\hat{P}_I, \hat{R}_{I'}] = -i\hbar\delta_{II'}$ |
| Continuum | $\{\pi(x), \phi(x')\} = -\delta(x - x')$ | $[\hat{\pi}(x), \hat{\phi}(x')] = -i\hbar\delta(x - x')$ |

ordinary differentiable manifold.[13] It is thus legitimate to ask why we bothered to give a lengthy exposition of fields as "ordinary" functions. The reason is that, in the not too distant future, after the framework of functional field integration has been introduced, we will return to the comfortable ground of the definition of page 6.

Employing these definitions, the classical Hamiltonian density (1.10) becomes the quantum operator

$$\hat{\mathcal{H}}(\hat{\phi}, \hat{\pi}) = \frac{1}{2m}\hat{\pi}^2 + \frac{k_s a^2}{2}(\partial_x \hat{\phi})^2. \tag{1.26}$$

The Hamiltonian above represents a quantum field theoretical *formulation* of the problem but not yet a solution. In fact, the development of a spectrum of methods for the analysis of quantum field theoretical models will represent a major part of this text. At this point the objective is merely to exemplify the way physical information can be extracted from models like Eq. (1.26). As a word of caution, let us mention that the following manipulations, while mathematically straightforward, are conceptually deep. To disentangle different aspects of the problem, we will first concentrate on plain operational aspects. Later, in Section 1.4, we will reflect on "what has really happened."

As with any function, operator-valued functions can be represented in a variety of different ways. In particular, they can be subjected to Fourier transformation,

$$\left\{\begin{matrix}\hat{\phi}_k \\ \hat{\pi}_k\end{matrix}\right. \equiv \frac{1}{L^{1/2}}\int_0^L dx\, e^{\{\ \ ikx}\left\{\begin{matrix}\hat{\phi}(x) \\ \hat{\pi}(x)\end{matrix}\right., \qquad \left\{\begin{matrix}\hat{\phi}(x) \\ \hat{\pi}(x)\end{matrix}\right. = \frac{1}{L^{1/2}}\sum_k e^{\{\pm ikx}\left\{\begin{matrix}\hat{\phi}_k \\ \hat{\pi}_k\end{matrix}\right., \tag{1.27}$$

where $\sum_k$ represents the sum over all Fourier coefficients indexed by quantized momenta $k = 2\pi m/L$, $m \in \mathbb{Z}$ (not to be confused with the "operator momentum" $\hat{\pi}$!). Note that the *real* classical field $\phi(x)$ quantizes to a *Hermitian* quantum field $\hat{\phi}(x)$, implying that $\hat{\phi}_k = \hat{\phi}^\dagger_{-k}$ (and similarly for $\hat{\pi}_k$). The corresponding Fourier representation of the canonical commutation relations reads (exercise)

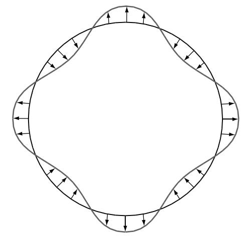
$$[\hat{\pi}_k, \hat{\phi}_{k'}] = -i\hbar\delta_{kk'}. \tag{1.28}$$

[13] At least if we ignore the mathematical subtlety that a linear operator can also be interpreted as an element of a certain manifold.

When expressed in the Fourier representation, making use of the identity

$$\int dx\,(\partial_x\hat{\phi})^2 = \sum_{k,k'}(-ik\hat{\phi}_k)(-ik'\hat{\phi}_{k'})\overbrace{\frac{1}{L}\int dx\, e^{-i(k+k')x}}^{\delta_{k+k',0}} = \sum_k k^2\hat{\phi}_k\hat{\phi}_{-k} = \sum_k k^2|\hat{\phi}_k|^2$$

together with a similar relation for $\int \mathrm{d}x\ \hat{\pi}^2$, the Hamiltonian $\hat{H} = \int \mathrm{d}x\ \mathcal{H}(\hat{\phi},\hat{\pi})$ assumes the near diagonal form



$$\hat{H} = \sum_k \left[\frac{1}{2m}\hat{\pi}_k\hat{\pi}_{-k} + \frac{m\omega_k^2}{2}\hat{\phi}_k\hat{\phi}_{-k}\right], \tag{1.29}$$

where $\omega_k = v|k|$ and $v = a\sqrt{k_s/m}$ denotes the classical sound wave velocity. In this form, the Hamiltonian can be identified as nothing but a superposition of independent **harmonic oscillators**.[14] This result is actually not difficult to understand (see figure): Classically, the system supports a discrete set of wave excitations, each indexed by a wave number $k = 2\pi m/L$. (In fact, we could have performed a Fourier transformation of the classical fields $\phi(x)$ and $\pi(x)$ to represent the Hamiltonian function as a superposition of classical harmonic oscillators.) Within the quantum picture, each of these excitations is described by an oscillator Hamiltonian operator with a $k$-dependent frequency. However, it is important not to confuse the atomic constituents, also oscillators (albeit coupled), with the independent *collective* oscillator modes described by $\hat{H}$.

The description above, albeit perfectly valid, still suffers from a deficiency: our analysis amounts to explicitly describing the effective low-energy excitations of the system (the waves) in terms of their microscopic constituents (the atoms). Indeed the different contributions to $\hat{H}$ keep track of details of the microscopic oscillator dynamics of individual $k$-modes. However, it would be much more desirable to develop a picture where the relevant excitations of the system, the waves, appear as fundamental units, without explicit account of underlying microscopic details. (As with hydrodynamics, information is encoded in terms of collective density variables rather than through individual molecules.) As preparation for the construction of this improved formulation of the system, let us temporarily focus on a single oscillator mode.

### *Revision of the quantum harmonic oscillator*

Consider a standard harmonic oscillator (HO) Hamiltonian

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}\hat{x}^2.$$

[14] The only difference between Eq. (1.29) and the canonical form of an oscillator Hamiltonian $\hat{H} = \hat{p}^2/(2m) + m\omega^2\hat{x}^2/2$ is the presence of the sub-indices $k$ and $-k$ (a consequence of $\hat{\phi}_k^\dagger = \hat{\phi}_{-k}$). As we will show shortly, this difference is inessential.

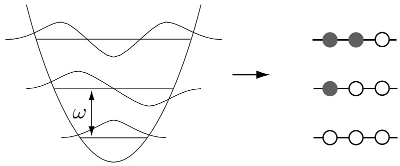



Figure 1.6 Low-lying energy levels/states of the harmonic oscillator.

The first few energy levels $\epsilon_n = \omega\left(n + \frac{1}{2}\right)$ and the associated Hermite polynomial eigenfunctions are displayed schematically in Fig. 1.6. (To simplify the notation we henceforth set $\hbar = 1$.)

The HO has, of course, the status of a single-particle problem. However, the equidistance of its energy levels suggests an alternative interpretation. One can think of a given energy state $\epsilon_n$ as an accumulation of $n$ elementary entities, or **quasi-particles**, each having energy $\omega$. What can be said about the features of these new objects? First, they are structureless, i.e. the only "quantum number" identifying the quasi-particles is their energy $\omega$ (otherwise $n$-particle states formed of the quasi-particles would not be equidistant). This implies that the quasi-particles must be *bosons*. (The same state $\omega$ can be occupied by more than one particle, see Fig. 1.6.)

This idea can be formulated in quantitative terms by employing the formalism of ladder operators in which the operators $\hat{p}$ and $\hat{x}$ are traded for the pair of Hermitian adjoint operators $\hat{a} \equiv \sqrt{\frac{m\omega}{2}}(\hat{x} + \frac{i}{m\omega}\hat{p})$, $\hat{a}^\dagger \equiv \sqrt{\frac{m\omega}{2}}(\hat{x} - \frac{i}{m\omega}\hat{p})$. Up to a factor of $i$, the transformation $(\hat{x}, \hat{p}) \to (\hat{a}, \hat{a}^\dagger)$ is canonical, i.e. the new operators obey the canonical commutation relation

$$[\hat{a}, \hat{a}^\dagger] = 1. \tag{1.30}$$

More importantly, the $a$-representation of the Hamiltonian is very simple, namely

$$\hat{H} = \omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right), \tag{1.31}$$

as can be checked by direct substitution. Suppose, now, we had been given a zero eigenvalue state $|0\rangle$ of the operator $\hat{a}$: $\hat{a}|0\rangle = 0$. As a direct consequence, $\hat{H}|0\rangle = (\omega/2)|0\rangle$, i.e. $|0\rangle$ is identified as the ground state of the oscillator.[15] The complete hierarchy of higher energy states can now be generated by setting $|n\rangle \equiv (n!)^{-1/2}\,(\hat{a}^\dagger)^n|0\rangle$.

EXERCISE Using the canonical commutation relation, verify that $\hat{H}|n\rangle = \omega(n + 1/2)|n\rangle$ and $\langle n|n\rangle = 1$.

Formally, the construction above represents yet another way of constructing eigenstates of the quantum HO. However, its "real" advantage is that it naturally affords a many-particle interpretation. To this end, let us *declare* $|0\rangle$ to represent a "vacuum" state, i.e. a state with zero particles present. Next, imagine that $\hat{a}^\dagger|0\rangle$ is a state with a single featureless particle

[15] This can be verified by explicit construction. Switching to a real-space representation, the solution of the equation $[x + \partial_x/(m\omega)]\langle x|0\rangle = 0$ obtains the familiar ground state wavefunction $\langle x|0\rangle = \sqrt{m\omega/2\pi}e^{-m\omega x^2/2}$.

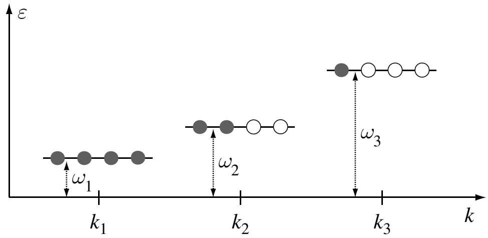



Figure 1.7 Diagram visualizing an excited state of the chain. Here, the number of quasi-particles decreases with increasing energy $\omega_k$.

(the operator $\hat{a}^\dagger$ does not carry any quantum number labels) of energy $\omega$. Similarly, $(\hat{a}^\dagger)^n|0\rangle$ is considered as a many-body state with $n$ particles, i.e. within the new picture, $\hat{a}^\dagger$ is an operator that creates particles. The total energy of these states is given by $\omega \times$ (occupation number). Indeed, it is straightforward to verify (see exercise above) that $\hat{a}^\dagger\hat{a}|n\rangle = n|n\rangle$, i.e. the Hamiltonian basically counts the number of particles. While, at first sight, this may look unfamiliar, the new interpretation is internally consistent. Moreover, it achieves what we had asked for above, i.e. it allows an interpretation of the HO states as a superposition of independent structureless entities.

INFO The representation above illustrates the capacity to think about individual quantum problems in **complementary pictures**. This principle finds innumerable applications in modern condensed matter physics. The existence of different interpretations of a given system is by no means heretical but, rather, reflects a principle of quantum mechanics: there is no "absolute" system that underpins the phenomenology. The only thing that matters is observable phenomena. For example, we will see later that the "fictitious" quasi-particle states of oscillator systems *behave* as "real" particles, i.e. they have dynamics, can interact, be detected experimentally, etc. From a quantum point of view these object are, then, real particles.

### *Quasi-particle interpretation of the quantum chain*

Returning to the oscillator chain, one can transform the Hamiltonian (1.29) to a form analogous to (1.31) by defining the ladder operators[16]

$$\hat{a}_k \equiv \sqrt{\frac{m\omega_k}{2}}\left(\hat{\phi}_k + \frac{i}{m\omega_k}\hat{\pi}_{-k}\right), \quad \hat{a}_k^\dagger \equiv \sqrt{\frac{m\omega_k}{2}}\left(\hat{\phi}_{-k} - \frac{i}{m\omega_k}\hat{\pi}_k\right). \tag{1.32}$$

With this definition, applying the commutation relations Eq, (1.28), one finds that the ladder operators obey commutation relations generalizing Eq. (1.30):

$$\left[\hat{a}_k, \hat{a}_{k'}^\dagger\right] = \delta_{kk'}, \quad [\hat{a}_k, \hat{a}_{k'}] = \left[\hat{a}_k^\dagger, \hat{a}_{k'}^\dagger\right] = 0. \tag{1.33}$$

[16] As to the consistency of these definitions, recall that $\hat{\phi}_k^\dagger = \hat{\phi}_{-k}$ and $\hat{\pi}_k^\dagger = \hat{\pi}_{-k}$. Under these conditions the second of the definitions following in the text follows from the first upon taking the Hermitian adjoint.

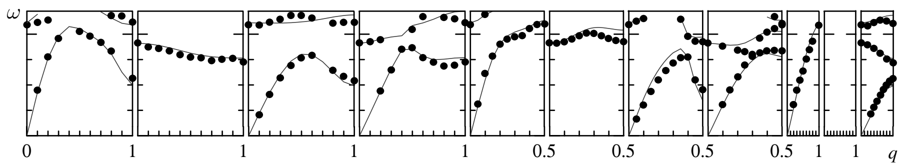



Figure 1.8 Phonon spectra of the transition metal oxide $Sr_2RuO_4$ measured along different axes in momentum space. Notice the approximate linearity of the low-energy branches (acoustic phonons) at small momenta. Superimposed at high frequencies are various branches of optical phonons. (Source: Courtesy of M. Braden, II. Physikalisches Institut, Universität zu Köln.)

Expressing the operators $(\hat{\phi}_k, \hat{\pi}_k)$ in terms of $(\hat{a}_k, \hat{a}_k^\dagger)$, it is now straightforward to bring the Hamiltonian into the quasi-particle oscillator form (exercise)

$$\hat{H} = \sum_k \omega_k \left( \hat{a}_k^\dagger \hat{a}_k + \frac{1}{2} \right). \tag{1.34}$$

Equations (1.34) and (1.33) represent the final result of our analysis. The Hamiltonian $\hat{H}$ takes the form of a sum of harmonic oscillators with characteristic frequencies $\omega_k$. In the limit $k \to 0$ (i.e. long wavelength), one finds $\omega_k \to 0$; excitations with this property are said to be **massless**.

An excited state of the system is indexed by a set $\{n_k\} = (n_1, n_2, \dots)$ of quasi-particles with energy $\{\omega_k\}$ (see Fig. 1.7). Physically, the quasi-particles of the harmonic chain are identified with the **phonon modes** of the solid. A comparison with measured phonon spectra (Fig. 1.8) reveals that, at low momenta, $\omega_k \sim |k|$ in agreement with our simplistic model (even in spite of the fact that the spectrum was recorded for a three-dimensional solid with non-trivial unit cell – universality!). While the linear dispersion was already a feature of the classical sound wave spectrum, the low-temperature specific heat reflected non-classical behavior. It is left as an exercise (problem 1.8) to verify that the quantum nature of the phonons resolves the problem with the low-temperature specific heat discussed in Section 1.1. (For further discussion of phonon modes in atomic lattices we refer to Chapter 2 of the text by Kittel.[17])

## 1.5 Quantum electrodynamics

The generality of the procedure outlined above suggests that the quantization of the EM field Eq. (1.24) proceeds in a manner analogous to the phonon system. However, there are a number of practical differences that make quantization of the EM field a harder (but also more interesting!) enterprise. Firstly, the vectorial character of the vector potential, in combination with the condition of relativistic covariance, gives the problem a non-trivial internal geometry. Closely related, the gauge freedom of the vector potential introduces redundant degrees of freedom whose removal on the quantum level is not easily achieved. For

[17] C. Kittel, *Quantum Theory of Solids*, 2nd edition (Wiley, 1987).