Chapter 2
Heisenberg's Matrix Mechanics

Abstract The quantum selection rule and its generalizations are capable of predicting energies of the stationary orbits; however they should be obtained in a more general framework of a universal theory, which could provide the intensities of spectral lines, scattering cross sections, etc.

Such a dynamical theory has been discovered first by Heisenberg in 1925 by developing Bohr's correspondence principle. The Heisenberg 'matrix mechanics' serves as a tool for extending the quantum selection rule (1.55) to arbitrary quantum systems, independently of the periodicity of trajectories of the corresponding classical models. The stationary energies appear to be the eigenvalues of the matrix Hamiltonian.

All equations and predictions of the Heisenberg theory turn into the classical one as $\hbar \to 0$; this agrees with the Bohr Correspondence Principle.

Heisenberg's theory, as was developed immediately by Born, Jordan, Pauli and others, is capable of producing the Hydrogen spectra, the selection rules and intensities of spectral lines, the quantization of the Maxwell field, etc. Up to now, Heisenberg's theory serves as the ground for the quantum electrodynamics and for modern quantum field theory.

2.1 Heisenberg's Matrix Formalism

Heisenberg suggested a novel revolutionary treatment of classical kinematics by combining Bohr's postulates (1.52) with the quantum selection rule (1.55) and the Bohr's Correspondence Principle.

2.1.1 Classical Oscillator

In 1925, Heisenberg [82] applied the correspondence principle to the one-dimensional oscillator

$$\dot{x}(t) = p(t), \qquad \dot{p}(t) = f\big(x(t)\big), \qquad f(x) = -V'(x) \qquad (2.1)$$

introducing a non commutative algebra of 'quantum' observables and the corresponding dynamical equations. This is the Hamilton equation with the Hamiltonian function

$$H(x, p) = \frac{p^2}{2} + V(x);$$

(2.2)

the energy is conserved,

$$\frac{p^2(t)}{2} + V(x(t)) = E, \quad t \in \mathbb{R}.$$

(2.3)

Let us assume that the potential is confining; i.e.,

$$V(x) \to \infty, \quad |x| \to \infty.$$

Then each solution is periodic in time, the period being given by

$$T = \oint dt = \int_\gamma \frac{dx}{\sqrt{2(E - V(x))}},$$

(2.4)

where γ is the trajectory $H(x, p) = E$, and $dt = dx/dp$. This period can be infinite when E is a critical value of $V(x)$. It can be written as

$$T = \frac{dS}{dE},$$

(2.5)

where $S = \oint p \, dx$ is the action integral over the period; i.e.,

$$S = \int_\gamma \sqrt{2(E - V(x))} \, dx.$$

(2.6)

Equivalently, (2.5) can be written as

$$\omega = \frac{dE}{dJ}, \quad J := S/2\pi,$$

(2.7)

where $\omega = 2\pi/T$ is the angular frequency. The corresponding Fourier series for the trajectories read

$$x(t) = \sum_{\nu \in \mathbb{Z}} x_\nu e^{i\nu\omega t}, \qquad p(t) = \sum_{\nu \in \mathbb{Z}} p_\nu e^{i\nu\omega t},$$

(2.8)

where the frequencies can be expressed as follows:

$$\nu\omega = \lim_{\varepsilon \to 0} \frac{E(J + \nu\varepsilon) - E(J)}{\varepsilon}, \quad \nu \in \mathbb{Z}.$$

(2.9)

Thus the classical framework is capable of yielding only the frequencies $\nu\omega$.

2.1.2 Quantum Oscillator

Main features of the program of Heisenberg are as follows:

I. The position and momentum of an electron in the atom are not observable, since the Bohr postulates treat 'stationary orbits' rather than the electron motion. Respectively, these classical dynamical variables should be *reinterpreted* by taking into account the Bohr's correspondence principle.

II. The *form* of all classical relations between the dynamical variables (the form of dynamical equations, the expressions for the Hamiltonian, for the angular momentum, for the dipole moment, etc.) *should be kept.*

Correspondence Principles and Quantum Observables

The quantum selection rule (1.55) gives $J = n\hbar$ for $n = 1, 2, 3, \ldots$. On the other hand, by the Bohr postulate (1.52),

$$\omega_{mn} = \frac{E(m\hbar) - E(n\hbar)}{\hbar}. \tag{2.10}$$

The key Heisenberg's observation was the parallelism between (2.10) and the relation (2.9), which can be written approximately as follows:

$$(m - n)\omega \approx \frac{E(m\hbar) - E(n\hbar)}{\hbar}, \quad |m - n| \ll m. \tag{2.11}$$

Comparing (2.11) and (2.10), Heisenberg suggested, by the Bohr's correspondence principle, that ω_{mn} should be quantum analogues of the classical 'obertones' $(m - n)\omega$. This suggestion is confirmed by the Rydberg–Ritz Combination Principle (1.1), as written in the form

$$\omega_{mn} = \omega_{mk} + \omega_{kn} \tag{2.12}$$

which agrees with the classical 'combination principle'

$$\omega(m - n) = \omega(m - k) + \omega(k - n). \tag{2.13}$$

Respectively, the classical Fourier coefficients x_{m-n} and p_{m-n} should be substituted by new *quantum amplitudes* $\hat{x}_{mn}$ and $\hat{p}_{mn}$, and the Correspondence Principle should be treated as the asymptotics

$$\begin{aligned}
\hat{x}_{mn} e^{i\omega_{mn}t} &\approx x_{m-n} e^{i\omega(m-n)t}, \\
\hat{p}_{mn} e^{i\omega_{mn}t} &\approx p_{m-n} e^{i\omega(m-n)t}, \quad |m - n| \ll m.
\end{aligned} \tag{2.14}$$

Hence, the quantum analogues $\hat{x}(t)$ and $\hat{p}(t)$ of the classical abservable $x(t)$ and $p(t)$ should be constructed in terms of collections of all quantum amplitudes

$$\begin{aligned}
\hat{x}(t) &= \{\hat{x}_{mn} e^{i\omega_{mn}t} : m, n = 1, 2, \ldots\}, \\
\hat{p}(t) &= \{\hat{p}_{mn} e^{i\omega_{mn}t} : m, n = 1, 2, \ldots\},
\end{aligned} \tag{2.15}$$

representing the system at time t. The form of the observables was intended to give an appropriate description of Bohr's transitions (1.51), introducing the unknown frequencies ω_{mn} and the corresponding amplitudes $\hat{x}_{mn}$ and $\hat{p}_{mn}$, which are provisionally responsible for the transitions.

Matrix Algebra

Heisenberg's main intention was to keep all the classical relations for new 'quantum observables' (2.15), taking the correspondence (2.14) as the 'Ariadne's thread'. First, Heisenberg kept the form of dynamical equations (2.1), postulating

$$\partial_t \hat{x}(t) = \hat{p}(t), \qquad \partial_t \hat{p}(t) = f\big(\hat{x}(t)\big) \tag{2.16}$$

where the derivatives and the first linear equation are well defined for the quantum observables (2.15). On the other hand, the meaning of the nonlinear function $f(\hat{x})$ should be reinterpreted for general nonlinear functions f, at least for the polynomial functions.

For example, let us discuss the case of $f(x) = -\lambda x^2$ considered by Heisenberg. The multiplication of the Fourier series (2.8) gives

$$x^2(t) = \sum_{\mu,\nu \in \mathbb{Z}} x_\mu x_\nu e^{i(\mu+\nu)\omega t}. \tag{2.17}$$

Equivalently, the Fourier component of $x^2(t)$ with frequency $\omega(m-n)$ is given by

$$\big(x^2\big)_{m-n} e^{i\omega(m-n)t} = \sum_{k \in \mathbb{Z}} x_{m-k} e^{i\omega(m-k)t} x_{k-n} e^{i\omega(k-n)t}. \tag{2.18}$$

Now the correspondence principle (2.14) suggests the definition

$$\big(\hat{x}^2\big)_{mn} e^{i\omega_{mn}t} := \sum_{k \in \mathbb{Z}} \hat{x}_{mk}(t) e^{i\omega_{mk}t} \hat{x}_{kn}(t) e^{i\omega_{kn}t}, \tag{2.19}$$

which agrees with the Rydberg–Ritz Combination Principle (2.12). In other words,

$$\big(\hat{x}^2(t)\big)_{mn} := \sum_{k \in \mathbb{Z}} \hat{x}_{mk}(t) \hat{x}_{kn}(t), \tag{2.20}$$

where $\hat{x}_{mk}(t) := \hat{x}_{mk} e^{i\omega_{mk}t}$ and $\hat{x}_{kn}(t) := \hat{x}_{kn} e^{i\omega_{kn}t}$. The rule (2.20) was recognized as the matrix multiplication by Born, who remembered the lectures delivered by Jakob Rosanes at the Breslau University when reading the Heisenberg manuscript. Definition (2.20) has become the cornerstone of the *matrix mechanics* of Heisenberg—it means that a quantum abservable $\hat{x}(t)$ is the *matrix of an operator* with the *matrix entries* $x_{mn}(t)$.

It is worth noting that the classical observables (2.8) correspond to particular case of the *Töplitz matrices*

$$\hat{x}(t) = \left(x_{m-n}e^{i\omega(m-n)t}\right), \qquad \hat{p}(t) = \left(p_{m-n}e^{i\omega(m-n)t}\right) \qquad (2.21)$$

which are Hermitian, since the functions $x(t)$ and $p(t)$ are real. Respectively, the corresponding quantum observables (2.15) are postulated to be Hermitian.

Now *the quantum equations* (2.16) are well-defined at least for any polynomial function f.

Dynamical Equations

Dynamical equations for $\hat{x}(t)$ and $\hat{p}(t)$ follow by differentiating (2.15): using the key Bohr's relation (1.52), we obtain

$$\partial_t \hat{x}(t) = i\frac{E_m - E_n}{\hbar}x_{mn}e^{i\omega_{mn}t}, \qquad \partial_t \hat{p}(t) = i\frac{E_m - E_n}{\hbar}p_{mn}e^{i\omega_{mn}t}. \qquad (2.22)$$

In the matrix form, the equations are known as the *Heisenberg equations*,

$$i\hbar\partial_t \hat{x}(t) = \left[\hat{x}(t), \hat{E}\right], \qquad i\hbar\partial_t \hat{p}(t) = \left[\hat{p}(t), \hat{E}\right], \qquad (2.23)$$

in which $\hat{E}$ is the diagonal matrix $E_{mn} = E_m\delta_{mn}$. The next crucial step was the identification

$$\hat{E} = H\left(\hat{x}(t), \hat{p}(t)\right). \qquad (2.24)$$

Now the Heisenberg equations (2.23) take the form

$$i\hbar\partial_t \hat{x}(t) = \left[\hat{x}(t), H\left(\hat{x}(t), \hat{p}(t)\right)\right], \qquad i\hbar\partial_t \hat{p}(t) = \left[\hat{p}(t), H\left(\hat{x}(t), \hat{p}(t)\right)\right]. \quad (2.25)$$

From these equations it follows that the dynamics of *any polynomial observable* $M(\hat{x}(t), \hat{p}(t))$ should be described by the similar equation

$$i\hbar\partial_t M\left(\hat{x}(t), \hat{p}(t)\right) = \left[M\left(\hat{x}(t), \hat{p}(t)\right), H\left(\hat{x}(t), \hat{p}(t)\right)\right] \qquad (2.26)$$

(by the Jacobi identity for commutators). In particular,

$$i\hbar\partial_t H\left(\hat{x}(t), \hat{p}(t)\right) = \left[H\left(\hat{x}(t), \hat{p}(t)\right), H\left(\hat{x}(t), \hat{p}(t)\right)\right] = 0, \qquad (2.27)$$

which means the *conservation of quantum energy* and justifies identification (2.24).

Commutation Relations

Comparing (2.25) with the postulate (2.16), it follows that

$$i\hbar\hat{p}(t) = \left[\hat{x}(t), H(\hat{x}, \hat{p})\right], \qquad i\hbar f\left(\hat{x}(t)\right) = \left[\hat{p}(t), H(\hat{x}, \hat{p})\right]. \qquad (2.28)$$

Applying to a particular Hamilton function $H = p^2/2 + x$, which corresponds to $f(x) = -1$, this establishes

$$i\hbar\hat{p}(t) = \left[\hat{x}(t), \hat{p}^2(t)/2\right], \qquad -i\hbar = \left[\hat{p}(t), \hat{x}(t)\right]. \qquad (2.29)$$

Here the first identity follows from the second one; the latter is known to be the fundamental *commutation relation* obtained first in the Born and Jordan's paper [18]:

$$\left[\hat{x}(t), \hat{p}(t)\right] = i\hbar. \qquad (2.30)$$

Example 2.1 The examples of linear operators in $C_0^\infty(\mathbb{R})$ satisfying (2.30) are as follows:

$$\hat{x}\psi(x) = x\psi(x), \qquad \hat{p}\psi(x) = -i\hbar\frac{d}{dx}\psi(x), \quad \psi \in C_0^\infty(\mathbb{R}). \qquad (2.31)$$

Exercise 2.2 Prove the formulas

$$\left[\hat{x}(t), \hat{p}^N(t)\right] = i\hbar N\hat{p}^{N-1}(t), \qquad \left[\hat{p}(t), \hat{x}^N(t)\right] = -i\hbar N\hat{x}^{N-1}(t) \qquad (2.32)$$

for any $N = 1, 2, \ldots$. **Hint:** Use (2.30).

2.2 Early Applications of Heisenberg Theory

Heisenberg's theory was immediately applied in [19, 148] to atoms with the energy-matrix

$$\hat{E} = \frac{1}{2\mathrm{m}}\hat{p}^2 + V(\hat{x}), \qquad (2.33)$$

where $V(x)$ is a nucleus potential defined for $x \in \mathbb{R}^3$, and $\hat{x}$, $\hat{p}$ are subject to commutation relations

$$[\hat{x}_j, \hat{p}_k] = i\hbar\delta_{jk}, \qquad [\hat{x}_j, \hat{x}_k] = [\hat{p}_j, \hat{p}_k] = 0, \quad j, k = 1, 2, 3, \qquad (2.34)$$

which 'follow' similarly to (2.29). Next triumph of Heisenberg's theory was the quantization of a Maxwell field by Dirac [44], who automatically implied the Planck's spectral law (1.24). Up to now, Heisenberg approach's has great value in quantum field theory (see [13, 33, 77, 138, 158, 159, 163, 189, 195, 196]).

2.2.1 Eigenvalue Problem

The main advantage of Heisenberg's theory was the identification of the spectral terms E_n with eigenvalues of the Hermitian operator $\hat{E}$. Namely, the matrix $\hat{E}$ in (2.23) is diagonal by definition, and E_n are its eigenvalues. To obtain E_n, one

should find such dynamical variables $\hat{x}$ and $\hat{p}$ that the commutation relations (2.34) hold, and at the same time, the corresponding matrix (2.24) should be diagonal.

However, the dynamical variables $\hat{x}$ and $\hat{p}$ are not specified uniquely by (2.34). For example, we can choose operators (2.31) and make the transformation $\hat{x} \mapsto T^{-1}\hat{x}T$, $\hat{p} \mapsto T^{-1}\hat{p}T$, under which the commutation relations (2.34) are invariant. Then operator (2.24) transforms as follows: $\hat{E} \mapsto T^{-1}\hat{E}T$. The matrix $\hat{E}$ from (2.24) is Hermitian, like $\hat{p}$ and $\hat{x}$. Hence, one could expect to reduce $\hat{E}$ to the diagonal form:

$$
T^{-1}\hat{E}T = \begin{pmatrix}
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\cdots & E_2 & 0 & 0 & 0 & 0 & \cdots \\
\cdots & 0 & E_1 & 0 & 0 & 0 & \cdots \\
\cdots & 0 & 0 & E_0 & 0 & 0 & \cdots \\
\cdots & 0 & 0 & 0 & E_{-1} & 0 & \cdots \\
\cdots & 0 & 0 & 0 & 0 & E_{-2} & \cdots \\
\cdots & 0 & 0 & 0 & 0 & 0 & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots
\end{pmatrix}.
\tag{2.35}
$$

The existence of the transformation T was known at that time (1925) for bounded Hermitian operators with discrete and continuous spectrum in Hilbert spaces [86, 88]. The authors [19] suggested the existence also for unbounded operators—this was proved later by J. von Neumann [142].

Reduction (2.35) is obviously equivalent to the eigenvalue problem. In fact, (2.35) reads

$$
\sum_n \hat{E}_{mn} T_{nk} = T_{mk} E_k, \quad m, k = 0, \pm 1, \ldots.
\tag{2.36}
$$

In other words, the columns $e_k = (T_{mk} : m = 0, \pm 1, \ldots)$ of the matrix T are the eigenvectors of $\hat{E}$:

$$
\hat{E}e_k = E_k e_k, \quad k = 0, \pm 1, \ldots.
\tag{2.37}
$$

The eigenvectors can be normalized: for the discrete eigenvalues,

$$
\langle e_k, e_l \rangle = \delta_{kl},
\tag{2.38}
$$

where $\langle \cdot, \cdot \rangle$ stands for the inner product in the Hilbert space l^2, and similarly for the eigenfunctions of continuous spectrum. Then the matrix T is orthogonal.

For the Hydrogen atom with the Coulomb potential $V(x)$, the spectrum E_n was obtained in this way by Pauli [148], who had obtained the Balmer formula (1.2) with $\omega_n = E_n/\hbar$.

Example: Quantization of Harmonic Oscillator

The solution of the eigenvalue problem (2.37) for one-dimensional harmonic oscillator was a cornerstown for further development of quantum mechanics and quan-

tum field theory. In this case, the Hamilton function reads: $H = \frac{1}{2}p^2 + \frac{1}{2}\omega^2 x^2$, and

$$\hat{E} = \frac{1}{2}\hat{p}^2 + \frac{1}{2}\omega^2 \hat{x}^2, \quad [\hat{x}, \hat{p}] = i\hbar. \tag{2.39}$$

The following proposition will be proved in Sect. 14.8.

Proposition 2.1 *Eigenvalues of $\hat{E}$ are given by* $E_n = \hbar\omega(n + \frac{1}{2})$, $n = 0, 1, \ldots$.

2.2.2 Intensity of Spectral Lines

The key observation in the celebrated 'three-man paper' [19] was that the matrix element $\hat{x}_{nn'} = \langle e_n, \hat{x}e_{n'} \rangle$ of the transformed matrix $T^*\hat{x}T$ should be responsible for intensity of the corresponding spectral line $\omega_{nn'} = \omega_n - \omega_{n'}$:

$$I_{nn'} = \frac{2e^2}{3c^3}\hat{x}_{nn'}^2\omega_{nn'}^4. \tag{2.40}$$

This expression is suggested by the Hertz formula (12.127) for radiation of the dipole with the moment

$$\mathbf{p} = e\hat{x}_{nn'}. \tag{2.41}$$

This identification was motivated by the following facts:

 (i) $\mathbf{p} = e\mathbf{x}$ in the classical theory;
 (ii) Formula (12.127) for radiation of a harmonic dipole $\mathbf{p}(t) = ex_{m-n}\cos\omega(m-n)t$ was used previously by Heisenberg and Kramers for calculation of the dispersion formula [123];
 (iii) The correspondence principle suggests that the Fourier coefficient $x_{n-n'}$ and the frequency $\omega(n - n')$ of the classical dipole should be substituted by the matrix element $\hat{x}_{nn'}$ and the frequency $\omega_{nn'}$ respectively.

2.2.3 The Normal Zeeman Effect

Formula (2.40) was applied in [19] for the derivation of selection rules and intensity of spectral lines in the normal Zeeman effect (see (9.14)). Calculation of the corresponding intensities (2.40) relies on the following arguments:

 (i) The commutation relations

$$[\hat{M}_1, \hat{M}_2] = -i\hbar\hat{M}_3 \tag{2.42}$$

hold for the components of quantum angular momentum $\hat{M} := \hat{p} \times \hat{x}$ (cf. (6.39)).

(ii) Operators $\hat{E}$, $\hat{M}^2$ and $\hat{M}_3$ commute and hence can be simultaneously diagonalized (cf. Lemma 6.10(ii)). Therefore, the eigenvectors of $\hat{E}$ can be numbered by the corresponding eigenvalues E, m and m_3 of the operators $\hat{E}$, $\sqrt{\hat{M}^2}$ and $\hat{M}_3$, respectively.

The selection rules mean that the matrix elements $\hat{x}_{nn'} = \langle e_n, \hat{x} e_{n'} \rangle$ and intensities (2.40) vanish if $m'_3 \neq m_3, m_3 \pm \hbar$. Here, the eigenvector e_n corresponds to the triple (E, m, m_3), and $e_{n'}$, to the triple (E', m', m'_3). In terms of Bohr's postulate, *the transitions $(E, m, m_3) \rightarrow (E', m', m'_3)$ are forbidden if $m'_3 \neq m_3, m_3 \pm \hbar$.* In short, the selection rule $m_3 \rightarrow m'_3, m'_3 \pm \hbar$ holds.

2.2.4 Quantization of Maxwell Field and Planck's Law

Dirac [44] was first to quantize a Maxwell field by representing it as the system of independent harmonic oscillators (1.32). The system is Hamiltonian with the Hamilton function (1.33) and the canonical variables $q_{\mathbf{k}\alpha}$, $p_{\mathbf{k}\alpha}$. Therefore, the commutation relations for the corresponding Heisenberg matrices should be

$$\begin{cases} \left[\hat{q}_{\mathbf{k}\alpha}(t), \hat{p}_{\mathbf{k}'\alpha'}(t)\right] = i\hbar\delta_{\mathbf{k}\alpha,\mathbf{k}'\alpha'}, \\ \left[\hat{q}_{\mathbf{k}\alpha}(t), \hat{q}_{\mathbf{k}'\alpha'}(t)\right] = \left[\hat{p}_{\mathbf{k}\alpha}(t), \hat{p}_{\mathbf{k}'\alpha'}(t)\right] = 0, \end{cases} \quad \mathbf{k}, \mathbf{k}' \in \Gamma, \; \alpha, \alpha' = 1, 2, \quad (2.43)$$

which is suggested by (2.34). Further, (1.33) implies that the corresponding energy operator reads:

$$\hat{\mathcal{E}} = \sum_{\alpha=1,2} \sum_{\mathbf{k}\in\Gamma} \hat{\mathcal{E}}_{\mathbf{k}\alpha} \tag{2.44}$$

where $\hat{\mathcal{E}}_{\mathbf{k}\alpha} = \frac{\omega(\mathbf{k})}{2}[\hat{q}_{\mathbf{k}\alpha}^2 + \hat{p}_{\mathbf{k}\alpha}^2]$. Finally, Proposition 2.1 with $\omega = 1$ implies that eigenvalues of $\hat{\mathcal{E}}_{\mathbf{k}\alpha}$ equal $E_{\mathbf{k}\alpha n} = \hbar\omega(\mathbf{k})(n + \frac{1}{2})$ with $n = 0, 1, \ldots$. Therefore, eigenvalues of $\hat{\mathcal{E}}$ are given by finite sums of $E_{\mathbf{k}\alpha, n(\mathbf{k}\alpha)}$, since $\hat{\mathcal{E}}_{\mathbf{k}\alpha}$ all commute, and hence can be simultaneously diagonalized. Hence, the Boltzmann distribution (1.65) implies that the eigenvalues of $\hat{\mathcal{E}}_{\mathbf{k}\alpha}$ are independent for different $\mathbf{k}\alpha$.

Application of the Boltzmann distribution (1.65) to the quantized Maxwell field immediately implies Planck's low (1.24). First, the probabilities (1.65) of the eigenvalues $E_{\mathbf{k}\alpha n}$ are given by

$$p(E_{\mathbf{k}\alpha n}) = \frac{1}{Z_{\mathbf{k}\alpha}} e^{-\frac{E_{\mathbf{k}\alpha n}}{kT}}, \quad Z_{\mathbf{k}\alpha} := \sum_n e^{-\frac{E_{\mathbf{k}\alpha n}}{kT}}. \tag{2.45}$$

This means that we have a discretization of the Einstein type (1.42) for the energy distribution of each field oscillator. Further arguments mainly repeat those of (1.43)–(1.44) and (1.36)–(1.37). In fact, the mean value of $E_{\mathbf{k}\alpha}$ is as follows:

$$\bar{E}_{\mathbf{k}\alpha} = \sum_n E_{\mathbf{k}\alpha n}\, p(E_{\mathbf{k}\alpha n}) = -\left[\frac{d}{d\beta}\log\sum_{n=0}^{\infty}e^{-\beta\hbar\omega(\mathbf{k})(n+\frac{1}{2})}\right]_{\beta=1/kT}$$

$$= -\left[\frac{d}{d\beta}\log\frac{e^{-\beta\hbar\omega(\mathbf{k})/2}}{1-e^{-\beta\hbar\omega(\mathbf{k})}}\right]_{\beta=1/kT} = \hbar\omega(\mathbf{k})/2 + \frac{\hbar\omega(\mathbf{k})e^{-\frac{\hbar\omega(\mathbf{k})}{kT}}}{1-e^{-\frac{\hbar\omega(\mathbf{k})}{kT}}};\quad (2.46)$$

this coincides with (1.44) up to the additional term $\hbar\omega(\mathbf{k})/2$, which makes the total energy infinite after summation in $\mathbf{k}$. We will drop this term, since the energy is defined up to an additive constant and should vanish at $T = 0$. Then we obtain (1.44):

$$\bar{E}_{\mathbf{k}\alpha} = \bar{E}(\omega(\mathbf{k})) := \frac{\hbar\omega(\mathbf{k})e^{-\frac{\hbar\omega(\mathbf{k})}{kT}}}{1-e^{-\frac{\hbar\omega(\mathbf{k})}{kT}}}. \tag{2.47}$$

Therefore, repeating the arguments of (1.36)–(1.37), we arrive at (1.38) and (1.24).

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