

ASPECTS OF POLARON THEORY

Equilibrium and Nonequilibrium Problems

N. N. BOGOLUBOV

N. N. BOGOLUBOV JR.



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Introduction

It is well known that a local change in the electronic state in a crystal leads to corresponding local changes in the interactions between individual atoms of the crystal, and hence to the excitation of atomic oscillations, i.e. the excitation of phonons. And vice versa, any local change in the state of the lattice ions alters the local electronic state. It is common in this situation to talk about an “electron–phonon interaction”. This interaction manifests itself even at the absolute zero of temperature, and results in a number of specific microscopic and macroscopic phenomena. When an electron moves through the crystal, this state of polarization can move together with it. This combined quantum state, of “moving electron + accompanying polarization”, may be considered as a sort of a quasiparticle with its own particular characteristics, such as effective mass, total momentum, energy, and maybe other quantum numbers describing the internal state of the quasiparticle in the presence of an external magnetic field presence or in the case of a very strong lattice polarization that causes self-localization of the electron in the polarization well with the appearance of discrete energy levels. Such a quasiparticle is usually called a “polaron state” or simply a “polaron”. Polaron formation is a consequence of dynamic electron-lattice interaction which is also responsible for scattering of charge carriers, phonon frequency renormalization as well as screening of interaction between charge carriers in solids.

The concept of the polaron was introduced first by S.I. Pekar [1], who investigated the most essential properties of stationary polaron in the limiting case of very intense electron-phonon interaction, so that the polaron behavior could be analyzed in the so-called adiabatic approximation. Such famous researchers as L.D. Landau, S.I. Pekar, H. Fröhlich and R. Feynman have contributed to the development of polaron theory [1–5].

Despite the apparent simplicity of the formulation, the polaron problem has not yet been solved, and continues to attract much attention. It plays an important role in statistical mechanics and quantum field theory because it can be considered as the simplest example of a nonrelativistic quantum particle interacting with a quantum field. Therefore many sophisticated mathematical techniques have been tested for the first time using this problem as a model. A shining example of this is Feynman’s functional integration method, which was applied first to the polaron problem, before becoming one of the main methods used in statistical mechanics and quantum field theory. Moreover, polaron theory is an expanding field of investigation in solid state physics because polarons are

not only theoretical constructs but practically observable physical objects (see e.g. [6]).

One of the most important contributions to polaron theory, made by N.N. Bogolubov, is the rigorous adiabatic perturbation theory [7] created in 1950, in which the kinetic energy of the phonon field was treated as a small perturbation. The theory is translationally invariant (which is important for the development of the strong coupling theory), and reproduced at zeroth order the results for large values of the interaction constant that had already been derived. Despite a systematic attempt to calculate higher orders of the perturbation theory, these have not yet been derived, although much effort has been devoted to the problem.

Bogolubov returned to the polaron problem in 1980, when he developed and applied the well-known method of chronological or T-products [8]. This method appeared to be effective for the theory of the large-radius polarons for all strengths (weak, intermediate and strong) of electron-phonon interaction and also for the derivation of higher terms of the perturbation series in the weak-coupling limit. Like the functional integration formalism, the T-product method has various applications in many fields of quantum physics.

Interest to the polaron problem is growing: in addition to earlier fields of research dealing mostly with spatially homogeneous systems, investigation of charged-particle interactions with elementary excitations in spatially inhomogeneous low-dimensional systems, such as quantum wells, wires and boxes, is gaining significance. Experimental techniques have had great success in producing such systems with well-controlled parameters, thus allowing the manufacturing of structures with predictable characteristics. Electron-phonon interactions of the polaron type play a very important role in the properties of low-dimensional quantum systems. Thus, much efforts has been devoted to the investigation of surface polarons (see [9, 10] and references therein).

Of course, it is impossible to cover all off the numerous aspects of polaron theory in this short introduction or even in a far larger text. The main purpose of the present book is to acquaint the reader with methods of modern mathematical physics developed in connection with polaron theory.

The book is organized in the following way. Chapter 1 is an introduction to the T-product approach in the theory of a particle interacting with bosonic fields. As an example, this method is applied to the linearized polaron model and Feynman's two-body oscillator model, for which all calculations can be carried out explicitly. Feynman's well-known inequality in polaron theory is also reproduced as a particular case. The rest of the chapter is devoted to one version of finite-temperature perturbation theory for the polaron partition function and the ground-state energy developed on the basis of the T-product formalism. Adiabatic perturbation theory for the polaron ground-state energy, which is valid for the strong-coupling case, is also highlighted.

Chapter 2 deals with the equilibrium-state investigation for the Fröhlich polaron model. The main objective of this chapter is to derive Bogolubov's inequality for the reduced free energy of the polaron. This inequality allows one to obtain various upper bounds for the polaron ground-state energy relevant for different values of the particle-field interaction strength.

Chapter 3 touches on some problems related to nonequilibrium polaron theory including polaron kinetics. An exact evolution equation for a particle interacting with a bosonic field is derived here. It is shown that in the weak-coupling case this equation can be reduced to the Boltzmann equation in the polaron theory. Special attention is paid to the investigation of the nonequilibrium properties of the linearized polaron model. The main characteristics of this system, such as the impedance and the admittance, are calculated explicitly. It is also shown that the equilibrium momentum distribution function in the weak coupling limit can be derived by means of the T-product formalism without having recourse to the Boltzmann-equation approach.

Investigation of the dynamics in a “small” system weakly coupled to a “large” system (the heat bath) is one of the essential problems of statistical mechanics. The work by N.N. Bogolubov and N.M. Krylov [49] laid theoretical foundation for studies in this field. In this work the problem of possibility of a stochastic process in a dynamic system being under the influence of a large system was considered. The behavior of a classical system was studied on the basis of the Liouville equation for the probability distribution function in the phase space while for a quantum system the equivalent von Neuman equation for the statistical operator was employed. In [49] a method was developed allowing to derive the Fokker-Planck equation already in the first order approximation. In [50] a concrete model was studied in detail, the dynamics of which could be described by integrable equations. This property allowed rigorous critical analysis of various approximations to this model dynamics which had been derived earlier. Similar results for quantum mechanical systems were obtained in [51].

In lectures given by N. N. Bogolubov in 1974 while visiting the Rockefeller University, a modified version of the method, developed in [49], was outlined and its relation to the theory of two-time Green functions was discussed [52].

It is worth noticing that the notions of the “small” system and the “large” system are to be comprehended in the sense that the number of degrees of freedom of the former is much less than this number for the latter one.

Further development of ideas outlined in [49–52] provided an opportunity to formulate, on the basis of a model polaron problem, a method of derivation of exact system of hierarchic equations for time-dependent averages [35]. Bose-variables elimination from operator dynamic equations being averaged with respect to the initial statistical operator represents

the cornerstone of the method. Special lemmas proved for the case of adiabatic switching on of the interaction between the “small” and the “large” systems played significant role in this elimination procedure [35]. If the “large” system is in the thermodynamically equilibrium state (being the heat bath in effect), the method allows to describe approach to equilibrium for the distribution of probabilities in the “small” system.

The above mentioned method proved itself very useful in studies of superradiant generation processes [53–55]. The phenomenon of superradiance reveals itself in appearance of spontaneous coherence of electromagnetic radiation due to photon exchange between atoms of active medium taking place under some additional conditions [56].

Here, in Chapter 3, an approach to derive an exact equation for the evolution of a particle interacting with bosonic field is proposed. It is shown that in the case of weak interaction this equation can be reduced to the Boltzmann equation in the polaron theory. Particular attention is paid to investigation of nonequilibrium properties of the linearized polaron model. Principle characteristics of this model, such as impedance and admittance, are calculated explicitly. It is also shown that the equilibrium function of momentum distribution in the limiting case of weak interaction can be derived within the frame of the T-product formalism without any recourse to approximate Boltzmann equation.

Polaron Model: General Discussion

Let us consider a slow electron in a dielectric crystal, interacting with the lattice ions through long-range electrostatic forces. This electron will be permanently surrounded by a region of lattice polarization. Moving through the crystal, the electron carries the lattice distortion with it. The electron together with the accompanying self-consistent polarization field can be treated as a quasiparticle called a “polaron”. Its effective mass is larger than that of a Bloch electron. Polaron formation is a consequence of the dynamical electron–phonon interaction.

One may speak about a “cloud of phonons” accompanying the electron. Thus a polaron can be also thought of as a compound system: “electron + accompanying phonons”. The polaron problem was initially formulated in the context of solid state physics, where this concept has some direct applications [6, 11, 12]. On the other hand, this problem is of great theoretical interest quite apart from its particular solid-state interpretation, since it provides a very simple example of a particle interacting with a quantum field, and is thus a suitable model to probe the methods of quantum field theory and quantum statistics, and to formulate intuitive ideas about the properties of a particle moving through a fluctuating quantum medium. A detailed discussion on the physical origins and basic features of the polaron model can be found in old papers [11].

In this text we should like to give an introduction to a new method in the equilibrium polaron theory based on the T-product operator

technique. Here and below we follow mainly the ideas outlined in our lectures [8].

Let us analyse in more detail the polaron Hamiltonian and its properties. From a general point of view, the polaron model may be considered as a particular case of a “small” subsystem S interacting with a “large” bosonic reservoir Σ . Let S be the electron and Σ be the phonon field of a crystal. Denote by X_S the set of arguments of the electron wave function and denote by $X_\Sigma = (\dots n_f \dots)$ the set of occupation numbers of the phonon modes.

The dynamical states of the polaron $S + \Sigma$ are then characterized by wave functions $\Psi(X_S, X_\Sigma)$ forming the space $\mathcal{H}_{S+\Sigma} = \mathcal{H}_S \otimes \mathcal{H}_\Sigma$, where $\mathcal{H}_S$ is the state space of the free electron while $\mathcal{H}_\Sigma$ is the phonon Fock space. We shall use below the notation $A(S)$, $A(\Sigma)$ and $A(S, \Sigma)$ for the operators acting correspondingly on the variables X_S , X_Σ and (X_S, X_Σ) of the wave function $\Psi(X_S, X_\Sigma)$. Note that the operators $A(S)$ and $A(\Sigma)$ will always commute with each other. The polaron Hamiltonian may be written as follows:

$$H_P = H(S) + H(\Sigma) + H_{\text{int}}(S, \Sigma), \quad (0.1)$$

with

$$H(S) = \frac{\mathbf{p}^2}{2m}, \quad (0.1a)$$

$$H(\Sigma) = \frac{1}{2} \sum_{(f)} (p_f p_{-f} + \omega_f^2 q_f q_{-f}), \quad (0.1b)$$

$$H_{\text{int}}(S, \Sigma) = \frac{1}{V^{1/2}} \sum_{(f)} L_f q_f e^{i\mathbf{f} \cdot \mathbf{r}}, \quad (0.1c)$$

where the three operator terms correspond respectively to the Hamiltonian of the free band electron $H(S)$ with effective mass m , the Hamiltonian of the optical lattice phonons $H(\Sigma)$ with wave vectors $\mathbf{f}$ and frequencies ω_f , and the Hamiltonian of the electron–phonon interaction $H_{\text{int}}(S, \Sigma)$. The electron–phonon interaction is characterized by the coupling parameter L_f , which is assumed to be a real and spherically symmetric function:

$$L_f = L_f^* = L(|f|),$$

$\mathbf{r}$, $\mathbf{p}$ are quantum operators satisfying the usual commutation relations:

$$r_\alpha p_\beta - p_\beta r_\alpha = i\hbar \delta_{\alpha\beta} \quad (\alpha, \beta = x, y, z).$$

the phonon amplitudes p_f , and q_f are also quantum operators satisfying analogous relations:

$$\begin{aligned} q_f p_{f'} - p_{f'} q_f &= i\hbar \delta_{ff'}, \\ p_f^\dagger &= p_{-f}, \quad q_f^\dagger = q_{-f}. \end{aligned}$$

As usually, the phonon wave vector $\mathbf{f}$ runs over a quasidiscrete set of values:

$$\mathbf{f} = \left(\frac{2\pi n_1}{L}, \frac{2\pi n_2}{L}, \frac{2\pi n_3}{L} \right),$$

where $L^3 = V$ is the volume of the system and n_1, n_2, n_3 are integers.

In most articles the so-called Fröhlich polaron (also known as a large-radius polaron) is considered. For the Fröhlich polaron, the electron is supposed to interact with a dielectric continuum by means of long-range Coulomb forces. This assumption is adequate if the polaron, composed of the electron and the polarization well, which is induced by the electron itself, spreads over a range large compared with the lattice constant. Then, the polarization field $P(\mathbf{r})$ will be a smooth function of $\mathbf{r}$ and the polarization of the medium can be characterized by macroscopic dielectric constants ε_∞ and ε_0 . The continuous approximation for the polarization field and hence the Fröhlich Hamiltonian itself would lose their meaning if the polaron size were comparable to the lattice constant.

The interaction parameter for the Fröhlich polaron model is determined in the following way:

$$L_f = \frac{g_0}{|\mathbf{f}|}, \quad g_0 = e \left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon} \right), \quad (0.2)$$

where e is the electron charge, ε_∞ and ε_0 are high-frequency and low-frequency dielectric constants. In the case of the usual Fröhlich model, one deals with the optical phonon branch, for which

$$\omega_f \rightarrow \omega > 0 \quad \text{when} \quad f \rightarrow 0,$$

and the dispersion is neglected, i.e. $\omega_f \equiv \omega$.

It is generally accepted that the strength of the interaction in this standard model can be characterized by a dimensionless coupling constant:

$$\alpha = \frac{g_0^2}{2\pi\hbar\omega^2} \left(\frac{m}{2\hbar\omega} \right)^{1/2}. \quad (0.3)$$

One usually distinguishes the cases of weak ($\alpha \ll 1$), strong ($\alpha > 10$) and intermediate ($\alpha \approx 3 - 6$) coupling.

It should be noted that when investigating the polaron problem in the general case, one should take into account the dependencies of ω_f and L_f on $\mathbf{f}$. In particular, one or other modification of the Coulomb case (0.2) might be analyzed. There are some physical reasons, for example, to introduce some kind of damping of the interaction for large $|\mathbf{f}|$. The simplest way to do this is to supplement the conditions (0.2) with the following restriction:

$$L_f \equiv 0, \quad (0.2a)$$

for $|\mathbf{f}| > f_0$, preserving old definition (0.2) for $|\mathbf{f}| < f_0$ at the same time. A natural value for the cut-off wave vector f_0 is $2\pi/a$, where a is the reciprocal lattice vector, since phonons with $|\mathbf{f}| > 2\pi/|\mathbf{a}|$ are not

represented correctly in (0.1c) and thus can be omitted. Nevertheless, later we shall consider the standard Fröhlich polaron without any cut-off. And all calculations will be carried out, wherever possible, for an arbitrary functional dependence of the interaction parameter L_f .

Symmetries and Quantum Properties

It must be stressed that the polaron problem is essentially quantum in character. It may easily be shown, for instance, that for a “classical” electron the interaction (0.1c) is not important and reduces simply to some additive constant in the equivalent Hamiltonian.

Let us introduce in (0.1) instead of p_f and q_f the phonon creation and annihilation operators $b_f^\dagger$ and b_f :

$$\begin{aligned} q_f &= \left(\frac{\hbar}{2\omega_f} \right)^{1/2} (b_f + b_{-f}^\dagger), \\ p_f &= i \left(\frac{\hbar\omega_f}{2} \right)^{1/2} (b_f^\dagger - b_{-f}) \end{aligned} \quad (0.4)$$

satisfying the commutation relations

$$b_f b_{f'}^\dagger - b_{f'}^\dagger b_f = \delta_{f,f'}, \quad b_f b_{f'} - b_{f'} b_f = 0, \quad b_f^\dagger b_{f'}^\dagger - b_{f'}^\dagger b_f^\dagger = 0. \quad (0.4a)$$

Then the Hamiltonian (0.1) reads

$$H_P = \frac{\mathbf{p}^2}{2m} + \sum_{(f)} \hbar\omega_f \left(b_f^\dagger b_f + \frac{1}{2} \right) + \frac{1}{V^{1/2}} \sum_{(f)} L_f \left(\frac{\hbar}{2\omega_f} \right)^{1/2} (b_f + b_{-f}^\dagger) e^{i\mathbf{f}\cdot\mathbf{r}}, \quad (0.5)$$

It may also be rewritten as

$$H_P = \frac{\mathbf{p}^2}{2m} + \sum_{(f)} \hbar\omega_f \left(B_f^\dagger B_f + \frac{1}{2} \right) - \frac{1}{V} \sum_{(f)} \frac{L_f^2}{2\omega_f^2}, \quad (0.6)$$

where

$$\begin{aligned} B_f &= b_f e^{-i\mathbf{f}\cdot\mathbf{r}} + \frac{1}{V^{1/2}} \frac{L_f}{\hbar\omega_f} \left(\frac{\hbar}{2\omega_f} \right)^{1/2}, \\ B_f^\dagger &= b_f^\dagger e^{i\mathbf{f}\cdot\mathbf{r}} + \frac{1}{V^{1/2}} \frac{L_f}{\hbar\omega_f} \left(\frac{\hbar}{2\omega_f} \right)^{1/2}. \end{aligned} \quad (0.6a)$$

The new operators B_f and $B_f^\dagger$ satisfy the same standard commutation relations as the Bose operators, (0.4a). If we assume that position and momentum operators $\mathbf{r}$ and $\mathbf{p}$ are commuting C -functions in the classical case then the operators B_f and $B_f^\dagger$ in (0.6) commute with the term $\mathbf{p}^2/2m$. In this case the relations (0.6a) can be interpreted as a canonical transformation to new Bose operators B_f and $B_f^\dagger$. Comparing (0.5) and (0.6), we conclude that for a classical electron the interaction is ineffective, being reduced to an additive constant term in the Hamiltonian.

On the contrary, in the quantum case, the “quasibosonic” amplitudes B_f and $B_f^\dagger$ do not commute with $\mathbf{p}^2/2m$ because of the factors $\exp(\pm i\mathbf{f} \cdot \mathbf{r})$, and hence the electronic and the quasibosonic parts of the Hamiltonian (0.6) are not independent of each other.

The difference between the classical and quantum situations may be clarified further by performing a unitary transformation on the Hamiltonian. To this end, let us introduce unitary operators

$$U = \exp\left(i \sum_{(f)} \mathbf{f} \cdot \mathbf{r} b_f^\dagger b_f\right), \quad (0.7)$$

compensating for the exponential phase factors in B_f and $B_f^\dagger$:

$$UB_f U^\dagger = b_f + \frac{L_f}{\hbar\omega_f} \left(\frac{\hbar}{2\omega_f}\right)^{1/2} \equiv \tilde{b}_f, \quad (0.8)$$

$$UB_f^\dagger U^\dagger = b_f^\dagger + \frac{L_f}{\hbar\omega_f} \left(\frac{\hbar}{2\omega_f}\right)^{1/2} \equiv \tilde{b}_f^\dagger. \quad (0.9)$$

On the other hand the operator U transforms the electron momentum as follows:

$$U\mathbf{p}U^\dagger = \mathbf{p} - \sum_{(f)} \hbar\mathbf{f} b_f^\dagger b_f. \quad (0.10)$$

The second term on the right-hand side here is obviously the total momentum of phonons. Thus we get, after U -transformation of the polaron Hamiltonian,^a

$$H'_P = UH_P U^\dagger = \frac{1}{2m} \left(\mathbf{p} - \sum_{(f)} \hbar\mathbf{f} b_f^\dagger b_f \right)^2 + \sum_{(f)} \hbar\omega_f \left(\tilde{b}_f^\dagger \tilde{b}_f + \frac{1}{2} \right) - \sum_{(f)} \frac{|L_f|^2}{2\omega_f^2} \quad (0.10a)$$

$$= \frac{1}{2m} \left(\mathbf{p} - \sum_{(f)} \hbar\mathbf{f} b_f^\dagger b_f \right)^2 + \sum_{(f)} \hbar\omega_f b_f^\dagger b_f + \sum_{(f)} L_f \left(\frac{\hbar}{2\omega_f} \right)^{1/2} (b_f + b_{-f}^\dagger). \quad (0.10b)$$

Comparing (0.5) and (0.10b) and bearing in mind that the factors $\exp(\pm i\mathbf{f} \cdot \mathbf{r})$ in (0.5) are unimportant phase factors that are negligible in the classical case (in fact, they can be included in the operators $b_f^\dagger$ and b_f), we see that the quantum effect in polaron theory manifests itself in replacing the electron momentum $\mathbf{p}$ by the relative momentum of the electron with respect to the total momentum of phonons. It is interesting to note that the only important feature here is the quantum nature of the model itself but not the strength of the interaction.

^a It is known that a unitary transformation of a Hamiltonian does not change the energy spectrum, and hence does not affect thermodynamic properties, ground-state energy, and so on.

Incidentally, it is possible to obtain some consequences of the representation (0.10) by observing that the momentum $\mathbf{p}$ is an integral of motion for the transformed Hamiltonian:

$$\mathbf{p}H'_P - H'_P\mathbf{p} \equiv 0.$$

On performing the inverse transformation, one finds that the corresponding integral of motion for the initial Hamiltonian is the sum of the electron momentum and the momentum of phonons:

$$\mathbf{P} = \mathbf{p} + \sum_{(f)} \hbar \mathbf{f} b_f^\dagger b_f, \quad \mathbf{P}H_P - H_P\mathbf{P} \equiv 0. \quad (0.11)$$

The latter identity can easily be verified by direct calculation. Note that the total momentum $\mathbf{P}$ is the generator of the translational symmetry group of the original Hamiltonian (0.5):

$$\begin{aligned} \mathbf{r} &\rightarrow \mathbf{r} + \mathbf{a} & (\mathbf{a} = \text{const}), \\ b_f &\rightarrow b_f e^{-i\mathbf{a}\cdot\mathbf{f}}, & b_f^\dagger \rightarrow b_f^\dagger e^{i\mathbf{a}\cdot\mathbf{f}}. \end{aligned} \quad (0.12)$$

The unitary transformations (0.7)–(0.12) were first introduced by Bogolubov [7] and Lee, Low and Pines [13] in order to develop appropriate approximate methods for the polaron problem.

Problems and Methods of Polaron Theory

One can distinguish two basic directions in polaron studies: the first deals with kinetic and transport properties, while the second investigates equilibrium properties, including quantum-mechanical phenomena at zero temperature.

In the kinetic theory one studies time-dependent phenomena in non-equilibrium or quasi-equilibrium situations such as relaxation processes (described by a Boltzmann-type equation) or the motion of an electron under given external forces, etc.

The equilibrium theory deals with the properties of the system at a given temperature. Of considerable interest are different averages related to the electron or to the polaron as a whole: the average kinetic and average total energies, the effective mass, the effective radius, etc. An interesting problem is to study the equilibrium distribution function of the electron momentum and its deviations from a Maxwellian form. Analogous problems can be formulated for the polaron ground state, which can also be considered as the limiting zero-temperature state (when $T \rightarrow 0$).

The basic function at equilibrium is the free energy (the logarithm of the partition function), which may be considered as a generating functional in order to compute the average energy and the ground-state energy. And, after introducing the corresponding fields (some additional terms) into the Hamiltonian, the free energy may be used to compute one

or another average, the effective mass, etc.^b The equilibrium free energy of a polaron will be the main quantity considered in the following sections.

Many important papers devoted to various aspects of the polaron problem have been published. For the standard papers of the first period of polaron studies one may consult [11] and references cited therein. Further progress in the field is described in [6, 15, 37, 38, 59–61] and the numerous references therein.

The general trend of developments can be seen from the titles of the articles reproduced in the list of references, so we shall not review here all the aspects of the polaron problem, making only some specific comments. Examples of basic review articles are [6, 11, 17, 18].

Since the polaron Hamiltonian does not admit an exact solution, various approximate methods have been proposed in order to obtain numerical results. These methods usually involve elements of perturbation theory, canonical transformations and variational principles.

At zero temperature the polaron problem is a quantum-mechanical problem (see [11] and references therein). In the weak-coupling case $\alpha \ll 1$ one can apply a more or less standard perturbation approach. Some improvements of the perturbation scheme can be achieved by appropriate canonical transformation of the Hamiltonian and a proper choice of the trial (variational) wave function (see [7, 11, 13, 19–24]). Special forms of perturbation theory have also been developed for the strong-coupling case [2, 7, 11, 20, 25–27].

The problem becomes more complicated when one investigates polaron equilibrium properties at finite temperature [5, 28].

Analogous investigations have also been performed for the nonequilibrium situation in [29–32].

A new general method in the polaron theory has been proposed by N.N. Bogolubov and N.N. Bogolubov, Jr. in [8, 33–35], which is based on the elimination of the phonon degrees of freedom by means of the

^b For an arbitrary system at equilibrium, with the temperature $\vartheta = kT = \beta^{-1}$ and Hamiltonian H , the free energy is given by

$$f[H, \beta] = -\frac{1}{\beta} \ln \text{Tr } e^{-\beta H},$$

where $\beta = \vartheta^{-1}$ is the inverse temperature. Here $\text{Tr } e^{-\beta H}$ is the so-called partition function. An arbitrary average $\langle A \rangle_{\beta, H}$ can be obtained, in particular, by differentiating the free energy with respect to the corresponding source term introduced into the Hamiltonian:

$$\langle A \rangle_{\beta, H} = -\frac{\partial}{\partial x} f[\beta, H - xA]_{x=0}.$$

For instance, the average energy is

$$\langle H \rangle_{\beta, H} = \frac{\partial}{\partial \beta} \{\beta f[H, \beta]\}.$$

averaged T-product operator technique. This technique may be considered as an analog of the path-integration approach. However, it seems to be much more transparent and rigorous from the mathematical point of view, and more convenient for practical calculations. For instance, when treating equilibrium aspects of a polaron below, we shall deal in all cases with proper quantum Gibbs averages over quadratic bosonic Hamiltonians instead of cumbersome path integral analysis.

A generalized approximation scheme for the free energy (partition function) has been developed in [8], based on a “linear-model” trial Hamiltonian. The linear model can be considered as a natural generalization of Feynman’s two-body approximation (0.13) to the case of a continuum of “heavy particles” coupled with the electron. All of the characteristics of the linear-model Hamiltonian can be evaluated exactly in terms of the spectral representation, thus providing the basis for a systematic variational approach in a general form. In [36] a perturbation theory for the free energy (partition function) has been considered within the framework of the T-product approach. The T-product approach has also been developed for the nonequilibrium case. In [33, 34] a generalized kinetic equation with eliminated phonons has been derived. After simple approximations this equation yields the standard Boltzmann equation for a polaron, and may be used to obtain its generalizations. Some other applications of the generalized kinetic equation with eliminated phonons can be found in [35]. We should also mention that in [35], the expression for the impedance and the admittance of a polaron, derived earlier in [29] by path integration, are reproduced on the basis of the linear-model Hamiltonian in a simpler and more rigorous manner.

In [59] a linear polaron model in constant uniform magnetic field was considered at zero temperature. An approach based on the model Hamiltonian diagonalization by means of the Bogolubov u - v transformation was proposed. The ground state energy was studied in the simplest case of equal frequencies for all the phonons involved in the interaction. Joint effect of the magnetic field and the electron-phonon interaction on the energy spectrum was studied too. It was also shown that the usage of the linear model as a trial model results in the action functional commonly employed in treatment of polarons in external constant uniform magnetic field [57, 58].

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Chapter 1

LINEAR POLARON MODEL

This chapter is mainly a pedagogical introduction to a modern method in equilibrium finite-temperature polaron theory based on the T-product operator technique. As an example of the application of this method, Bogolubov's exactly solvable linearized polaron model, as well as Feynman's two-body oscillator model, are considered.

1.1. Introduction to the Linear Polaron Model

Here we consider the so-called linear polaron model described by a Hamiltonian that consists of the well-known oscillator Hamiltonian H_S , the phonon field Hamiltonian H_Σ and the interaction Hamiltonian $H_{S\Sigma}$, i.e.

$$H_{S+\Sigma} = H_S + H_\Sigma + H_{S\Sigma}, \quad (1.1)$$

where

$$H_S = \frac{\mathbf{p}^2}{2m} + \frac{K^2 \mathbf{r}^2}{2}, \quad H_\Sigma = \frac{1}{2} \sum_{(f)} \{p_f p_f^* + \nu^2(f) q_f q_f^*\},$$

$$H_{S\Sigma} = \frac{1}{V^{1/2}} \sum_{(f)} S(f) \mathbf{f} \cdot \mathbf{r} q_f.$$

Here $\mathbf{r}$ and $\mathbf{p}$ are respectively the position and the momentum of the electron and $S(f) = S(|f|)$ is a real radially symmetric function:

$$\nu(f) = \nu(|f|) > 0,$$

$$q_{-f} = q_f^*, \quad p_{-f} = p_f^*.$$

Summation over f is over the range of quasidiscrete values

$$f = \left(\frac{2\pi n_1}{L}, \frac{2\pi n_2}{L}, \frac{2\pi n_3}{L} \right),$$

where $L^3 = V$ is the volume of the system and n_1, n_2, n_3 are integers covering the whole space of integers from $-\infty$ to $+\infty$. The total number of oscillators N is assumed to be finite for any finite volume V (later we should take the so-called thermodynamic limit as usual; that is, we must put $N \rightarrow \infty$, $V \rightarrow \infty$, imposing the additional condition $N/V = \text{const}$).

It should be noted that the following identity holds:

$$\begin{aligned} \frac{1}{2} \sum_{(f)} \nu^2(f) \left\{ q_f - \frac{i \mathbf{f} \cdot \mathbf{r}}{\nu^2(f)} \frac{S(f)}{V^{1/2}} \right\} \left\{ q_f^* + \frac{i \mathbf{f} \cdot \mathbf{r}}{\nu^2(f)} \frac{S(f)}{V^{1/2}} \right\} &= \frac{1}{2} \sum_{(f)} \nu^2(f) q_f q_f^* \\ &+ \frac{1}{2} \sum_{(f)} \frac{1}{\nu^2(f)} \frac{S^2(f)}{V} (\mathbf{f} \cdot \mathbf{r})^2 + \frac{i}{2} \sum_{(f)} (\mathbf{f} \cdot \mathbf{r} q_f - \mathbf{f} \cdot \mathbf{r} q_f^*) \frac{S(f)}{V^{1/2}}. \end{aligned}$$

It is obvious that

$$-i \sum_{(f)} \mathbf{f} \cdot \mathbf{r} q_f^* \frac{S(f)}{\sqrt{V}} = -\frac{i}{V^{1/2}} \sum_{(f)} \mathbf{f} \cdot \mathbf{r} q_{-f} S(-f) = \frac{1}{V^{1/2}} \sum_{(f)} \mathbf{f} \cdot \mathbf{r} q_f S(f),$$

where the property $q_{-f} = q_f^*$ has been taken into account.

Because of the radial symmetry, the following identity holds for an arbitrary function $F(|f|)$:

$$\sum_{(f)} F(|f|) f_\alpha f_\beta = \delta_{\alpha\beta} \frac{1}{3} \sum_{(f)} F(|f|) f^2,$$

where

$$|f| = (f_1^2 + f_2^2 + f_3^2)^{1/2}, \quad f^2 = |f|^2.$$

Therefore

$$\frac{1}{2V} \sum_{(f)} \frac{S^2(f)}{\nu^2(f)} (\mathbf{f} \cdot \mathbf{r})^2 = \frac{\mathbf{r}^2}{6V} \sum_{(f)} \frac{S^2(f) f^2}{\nu^2(f)}.$$

Therefore the potential energy can be represented in the form

$$\begin{aligned} U &= \frac{K^2 \mathbf{r}^2}{2} + \frac{1}{2} \sum_{(f)} \nu^2(f) q_f q_f^* + \frac{i}{V^{1/2}} \sum_{(f)} S(f) \mathbf{f} \cdot \mathbf{r} q_f = \frac{(K^2 - K_0^2) \mathbf{r}^2}{2} \\ &+ \frac{1}{2} \sum_{(f)} \nu^2(f) \left\{ q_f - \frac{i \mathbf{f} \cdot \mathbf{r}}{\nu^2(f)} \frac{S(f)}{V^{1/2}} \right\} \left\{ q_f^* + \frac{i \mathbf{f} \cdot \mathbf{r}}{\nu^2(f)} \frac{S(f)}{V^{1/2}} \right\}, \quad (1.2) \end{aligned}$$

where

$$K_0^2 = \frac{1}{3V} \sum_{(f)} \frac{S^2(f) f^2}{\nu^2(f)}.$$

Consider the case $K^2 = K_0^2$. For this case, $U \geq 0$, with $U = 0$ if

$$q_f = \frac{i \mathbf{f} \cdot \mathbf{r}}{\nu^2(f)} \frac{S(f)}{V^{1/2}}.$$

We write down the kinetic energy which is obviously positive:

$$\frac{\mathbf{p}^2}{2m} + \frac{1}{2} \sum_{(f)} |p_f|^2.$$

Let us introduce normal variables Q_λ . Then $\mathbf{r}$ and q_f are linear combinations of the new variables Q_λ . It will be noted that for $K = K_0$ the system (1.1) is described by the Hamiltonian $H = T + U$, where both quadratic forms are positive-definite. It can be shown by purely linear algebraic methods that these can be reduced to the diagonal form simultaneously, and the Hamiltonian reads as

$$H = \sum_{\lambda} \left(\dot{Q}_\lambda^2 + \Omega_\lambda^2 Q_\lambda^2 \right).$$

if written in the new normal variables Q_λ . In this case each Q_λ satisfies the following equation:

$$\ddot{Q}_\lambda + \Omega_\lambda^2 Q_\lambda = 0.$$

For $K = K_0$, it follows from (1.2) that U becomes zero if and only if all q_f belong to the three-dimensional set

$$q_f = \frac{i\mathbf{f} \cdot \mathbf{r}}{\nu^2(f)} \frac{S(f)}{V^{1/2}}.$$

In other words, for $K = K_0$ the Hamiltonian H is translation-invariant with respect to the three-dimensional group of translations:

$$\mathbf{r} \rightarrow \mathbf{r} + \mathbf{R}, \quad q_f \rightarrow q_f + \frac{i\mathbf{f} \cdot \mathbf{R}}{\nu^2(f)} \frac{S(f)}{V^{1/2}}.$$

Hence exactly three components among the whole set of Ω_λ^2 are equal to zero, while the other Ω_λ^2 are positive. So, there are three modes of collective evolution, such that

$$\ddot{Q}_\alpha = 0,$$

which correspond to inertial motion. Therefore $\mathbf{r}(t)$ describes uniform inertial motion in the case $K = K_0$, on which harmonic vibrations are superimposed.

Note also that when $K < K_0$, the form U is not positive, so that some values Ω_λ^2 must be negative, and the motion is unstable and can be characterized by the exponentially increasing function of t .

Later we will be interested especially in the case $K = K_0$, but it is more convenient for technical reasons to consider the more general expression

$$K^2 = K_0^2 + \eta^2, \quad (1.3)$$

having in mind a future passage to the limit $\eta \rightarrow 0$ (which must be taken before the usual limit $V \rightarrow \infty$).

It is worth stressing that, with the above choice for K , the form U is positive-definite because $\eta^2 > 0$ by definition. So, all values Ω_λ^2 are positive too. Therefore all of the functions $\mathbf{r}(t)$, $\mathbf{p}(t)$, $q_f(t)$ and $p_f(t)$ can be represented as corresponding sums of harmonic vibrations.

1.2. Equations of Motion

Let us introduce Bose amplitudes b_f and $b_f^\dagger$ by means of the relations

$$q_f = \left(\frac{\hbar}{2\nu(f)} \right)^{1/2} (b_f + b_{-f}^\dagger), \quad p_f = i \left(\frac{\hbar\nu(f)}{2} \right)^{1/2} (b_f^\dagger - b_{-f}).$$

These amplitudes satisfy the usual commutation relations

$$b_f b_f^\dagger - b_f^\dagger b_f = 1.$$

One can see from here that

$$q_{-f} = q_f^*, \quad p_{-f} = p_f^*,$$

and also

$$[q_f, p_f] = \frac{q_f p_f - p_f q_f}{i\hbar} = 1.$$

Therefore the Hamiltonian (1.1) can be rewritten in the form

$$\begin{aligned} H = \frac{\mathbf{p}^2}{2m} + \frac{1}{2} (K_0^2 + \eta^2) \mathbf{r}^2 + i \sum_{(f)} \frac{1}{V^{1/2}} S(f) \left(\frac{\hbar}{2\nu(f)} \right)^{1/2} \mathbf{f} \cdot \mathbf{r} (b_f + b_{-f}^\dagger) \\ + \sum_{(f)} \hbar\nu(f) b_f^\dagger b_f + \frac{1}{2} \sum_{(f)} \hbar\nu(f). \end{aligned} \quad (1.4)$$

The equations of motion for this Hamiltonian are

$$\begin{aligned} \frac{d\mathbf{r}}{dt} &= \frac{\partial H}{\partial \mathbf{p}}, & \frac{d\mathbf{p}}{dt} &= -\frac{\partial H}{\partial \mathbf{r}}, \\ i\hbar \frac{db_f}{dt} &= b_f H - H b_f, & i\hbar \frac{db_{-f}^\dagger}{dt} &= b_{-f}^\dagger H - H b_{-f}^\dagger. \end{aligned}$$

Transforming the right-hand sides of these equations, we see that

$$m \frac{d\mathbf{r}}{dt} = \mathbf{p},$$

$$\begin{aligned}
\frac{d\mathbf{p}}{dt} &= -(K_0^2 + \eta^2)\mathbf{r} - \frac{i}{V^{1/2}} \sum_{(f)} S(f) \left(\frac{\hbar}{2\nu(f)} \right)^{1/2} \mathbf{f}(b_f + b_{-f}^\dagger), \\
i\hbar \frac{db_f}{dt} &= \hbar\nu(f)b_f - \frac{i}{V^{1/2}} \left(\frac{\hbar}{2\nu(f)} \right)^{1/2} S(f)\mathbf{f} \cdot \mathbf{r}, \\
i\hbar \frac{db_{-f}^\dagger}{dt} &= -\hbar\nu(f)b_{-f}^\dagger + \frac{i}{V^{1/2}} \left(\frac{\hbar}{2\nu(f)} \right)^{1/2} S(f)\mathbf{f} \cdot \mathbf{r}.
\end{aligned} \tag{1.5}$$

Later we are going to convert the system of equations (1.5) into a system of equations for Green functions. This step allows us to calculate explicitly such Green functions as $\langle\langle r_\alpha, r_\beta \rangle\rangle$ and $\langle\langle p_\alpha, p_\beta \rangle\rangle$, the spectral function $J_{p_\alpha p_\beta}$, and hence the equilibrium correlation functions $\langle p_\alpha(t)p_\beta(\tau) \rangle$ calculated with respect to the Hamiltonian (1.4).

It is appropriate to recall the definition of the two-time correlation and Green functions [40, 41]. For any two operators $A(t)$ and $B(\tau)$ taken in the Heisenberg representation, two-time equilibrium correlation functions are usually defined in the following way:

$$\begin{aligned}
\langle A(t)B(\tau) \rangle_{\text{eq}} &= \int_{-\infty}^{+\infty} J_{A,B}(\omega) e^{-i\omega(t-\tau)} d\omega, \\
\langle B(\tau)A(t) \rangle_{\text{eq}} &= \int_{-\infty}^{+\infty} J_{A,B}(\omega) e^{-\beta\omega\hbar} e^{-i\omega(t-\tau)} d\omega,
\end{aligned} \tag{1.6}$$

where

$$\beta = \frac{1}{\vartheta} = \frac{1}{K_\beta T},$$

and K_β is Boltzmann's constant and T the absolute temperature. Retarded and advanced Green functions can be introduced in the usual manner [41]:

$$\begin{aligned}
\langle\langle A(t), B(\tau) \rangle\rangle_{\text{ret}} &= \vartheta(t-\tau) \langle [A(t), B(\tau)] \rangle_{\text{eq}} \\
&= \vartheta(t-\tau) \frac{\langle A(t)B(\tau) - B(\tau)A(t) \rangle_{\text{eq}}}{i\hbar}, \\
\langle\langle A(t)B(\tau) \rangle\rangle_{\text{adv}} &= -\vartheta(\tau-t) \langle [A(t), B(\tau)] \rangle_{\text{eq}}.
\end{aligned} \tag{1.7}$$

Here $\langle \dots \rangle_{\text{eq}}$ denotes the statistical-equilibrium average value calculated with respect to the Hamiltonian (1.4):

$$\langle \dots \rangle_{\text{eq}} = \frac{\text{Tr } e^{-H/\vartheta} (\dots)}{\text{Tr } e^{-H/\vartheta}}.$$

Introduce a function of the complex variable Ω , $\text{Im } \Omega \neq 0$:

$$\langle\langle A, B \rangle\rangle_\Omega = \frac{1}{\hbar} \int_{-\infty}^{+\infty} J_{A,B}(\nu) \frac{1 - e^{-\beta\nu\hbar}}{\Omega - \nu} d\nu. \tag{1.8}$$

Then the spectral densities for the advanced and retarded Green functions can be introduced by means of the relations

$$\begin{aligned}\langle\langle A(t), B(\tau) \rangle\rangle_{\text{adv}} &= \frac{1}{2\pi} \int_{-\infty}^{+\infty} \langle\langle A, B \rangle\rangle_{\omega-i0} e^{-i\omega(t-\tau)} d\omega, \\ \langle\langle A(t), B(\tau) \rangle\rangle_{\text{ret}} &= \frac{1}{2\pi} \int_{-\infty}^{+\infty} \langle\langle A, B \rangle\rangle_{\omega+i0} e^{-i\omega(t-\tau)} d\omega.\end{aligned}\quad (1.9)$$

Taking into account the well-known formula

$$\frac{1}{\omega - \nu \pm i\varepsilon} = \mathcal{P} \left(\frac{1}{\omega - \nu} \right) \mp i\pi\delta(\omega - \nu), \quad (1.10)$$

we arrive at the important relation

$$\langle\langle A, B \rangle\rangle_{\omega+i0} - \langle\langle A, B \rangle\rangle_{\omega-i0} = -\frac{2\pi i}{\hbar} J_{A,B}(\omega)(1 - e^{-\beta\hbar\omega}). \quad (1.11)$$

Our aim is to derive a system of equations for the Green functions (1.7). From a formal point of view,

$$\frac{d}{dt} \vartheta(t) = \delta(t), \quad \frac{d}{dt} \vartheta(-t) = -\delta(t).$$

These relations allows us to differentiate formally both sides of (1.7), thus leading to the desired equations for the Green functions:

$$\begin{aligned}i \frac{d}{dt} \langle\langle A(t), B(\tau) \rangle\rangle_{\text{ret, adv}} \\ = \frac{1}{\hbar} \delta(t - \tau) \langle AB - BA \rangle + \left\langle \left\langle i \frac{dA(t)}{dt}, B(\tau) \right\rangle \right\rangle_{\text{ret, adv}}.\end{aligned}\quad (1.12)$$

From these equations one has, in the “ Ω -representation”

$$\Omega \langle\langle A, B \rangle\rangle_{\Omega} = \frac{1}{\hbar} \langle AB - BA \rangle + \left\langle \left\langle i \frac{dA}{dt}, B \right\rangle \right\rangle_{\Omega}, \quad (1.13)$$

or equivalently, in a slightly different form,

$$-i\Omega \langle\langle A, B \rangle\rangle_{\Omega} = \frac{1}{i\hbar} \langle AB - BA \rangle + \left\langle \left\langle \frac{dA}{dt}, B \right\rangle \right\rangle_{\Omega}.$$

We should note one more useful identity^c:

$$\langle B(\tau)A(t) \rangle_{\text{eq}} = \int_{-\infty}^{+\infty} J_{B,A}(\omega) e^{-i\omega(\tau-t)} d\omega = \int_{-\infty}^{+\infty} J_{B,A}(-\omega) e^{-i\omega(t-\tau)} d\omega,$$

where

$$J_{B,A}(-\omega) = J_{A,B}(\omega) e^{-\beta\omega\hbar} \quad (\text{cf. (1.6)}),$$

From (1.8), one has, after the permutation

$$\begin{pmatrix} A \rightarrow B \\ B \rightarrow A \end{pmatrix},$$

the following equation:

$$\begin{aligned} \langle\langle B, A \rangle\rangle_{\Omega} &= \frac{1}{\hbar} \int_{-\infty}^{+\infty} J_{A,B}(\nu) \frac{1 - e^{-\beta\nu\hbar}}{\Omega - \nu} d\nu = \frac{1}{\hbar} \int_{-\infty}^{+\infty} J_{B,A}(-\nu) \frac{1 - e^{\beta\nu\hbar}}{\Omega + \nu} d\nu \\ &= \frac{1}{\hbar} \int_{-\infty}^{+\infty} J_{A,B}(\nu) e^{-\beta\nu\hbar} \left(\frac{1 - e^{\beta\nu\hbar}}{\Omega + \nu} \right) d\nu = -\frac{1}{\hbar} \int_{-\infty}^{+\infty} J_{A,B}(\nu) \frac{1 - e^{-\beta\nu\hbar}}{\Omega + \nu} d\nu. \end{aligned}$$

Thus we have proved the property

$$\langle\langle B, A \rangle\rangle_{\Omega} = \langle\langle A, B \rangle\rangle_{-\Omega}, \quad \text{Im } \Omega \neq 0. \quad (1.14)$$

1.3. Two-time Correlation Functions and Green Functions for the Linear Polaron Model

Starting from (1.5) and (1.13), we construct a system of equations for Green functions in the case of the linear polaron model^d:

$$-im\Omega \langle\langle r_{\alpha}, r_{\beta} \rangle\rangle_{\Omega} = \langle\langle p_{\alpha}, r_{\beta} \rangle\rangle_{\Omega}, \quad (1.15)$$

^c Clarification: Let us write the equality

$$\langle A(t)B(\tau) \rangle_{\text{eq}} = \int_{-\infty}^{+\infty} J_{A,B}(\omega) e^{-i\omega(t-\tau)} d\omega.$$

Making the substitutions

$$A \rightarrow B, \quad t \rightarrow \tau, \quad B \rightarrow A, \quad \tau \rightarrow t,$$

we arrive at the following result:

$$\langle B(\tau)A(t) \rangle_{\text{eq}} = \int_{-\infty}^{+\infty} J_{B,A}(\omega) e^{-i\omega(\tau-t)} d\omega = \int_{-\infty}^{+\infty} J_{B,A}(-\omega) e^{-i\omega(t-\tau)} d\omega.$$

^d Here: $\mathbf{r} = (r_1, r_2, r_3)$, $\mathbf{p} = (p_1, p_2, p_3)$ and $p_{\alpha}r_{\beta} - r_{\beta}p_{\alpha} = -i\hbar\delta_{\alpha\beta}$.

$$\begin{aligned}
-i\Omega\langle\langle p_\alpha, r_\beta \rangle\rangle_\Omega &= -\delta_{\alpha,\beta} - (K_0^2 + \eta^2)\langle\langle r_\alpha, r_\beta \rangle\rangle_\Omega \\
&\quad - \frac{i}{V^{1/2}} \sum_f S(f) \left(\frac{\hbar}{2\nu(f)} \right)^{1/2} f_\alpha \langle\langle b_f + b_{-f}^\dagger, r_\beta \rangle\rangle_\Omega, \quad (1.16)
\end{aligned}$$

$$\begin{aligned}
\hbar\Omega\langle\langle b_f, r_\beta \rangle\rangle_\Omega &= \hbar\nu(f)\langle\langle b_f, r_\beta \rangle\rangle_\Omega - \frac{i}{V^{1/2}} \left(\frac{\hbar}{2\nu(f)} \right)^{1/2} S(f)\langle\langle \mathbf{f} \cdot \mathbf{r}, r_\beta \rangle\rangle_\Omega, \\
\hbar\Omega\langle\langle b_{-f}, r_\beta \rangle\rangle_\Omega &= -\hbar\nu(f)\langle\langle b_{-f}^\dagger, r_\beta \rangle\rangle_\Omega \\
&\quad + \frac{i}{V^{1/2}} \left(\frac{\hbar}{2\nu(f)} \right)^{1/2} S(f)\langle\langle \mathbf{f} \cdot \mathbf{r}, r_\beta \rangle\rangle_\Omega. \quad (1.17)
\end{aligned}$$

From (1.17), we have

$$\begin{aligned}
\langle\langle b_f, r_\beta \rangle\rangle_\Omega &= -\frac{i}{V^{1/2}} \frac{1}{\Omega - \nu(f)} \left(\frac{1}{2\hbar\nu(f)} \right)^{1/2} S(f)\langle\langle \mathbf{f} \cdot \mathbf{r}, r_\beta \rangle\rangle_\Omega, \\
\langle\langle b_{-f}^\dagger, r_\beta \rangle\rangle_\Omega &= \frac{i}{\sqrt{V}} \frac{1}{\Omega + \nu(f)} \left(\frac{1}{2\hbar\nu(f)} \right)^{1/2} S(f)\langle\langle \mathbf{f} \cdot \mathbf{r}, r_\beta \rangle\rangle_\Omega.
\end{aligned}$$

Thus

$$\begin{aligned}
&\langle\langle b_f + b_{-f}^\dagger, r_\beta \rangle\rangle_\Omega \\
&= \frac{i}{\sqrt{V}} \left(\frac{1}{\Omega + \nu(f)} - \frac{1}{\Omega - \nu(f)} \right) \left(\frac{1}{2\hbar\nu(f)} \right)^{1/2} S(f)\langle\langle \mathbf{f} \cdot \mathbf{r}, r_\beta \rangle\rangle_\Omega.
\end{aligned}$$

Inserting this formula into (1.15) and (1.16), we find that

$$\begin{aligned}
-m\Omega^2\langle\langle r_\alpha, r_\beta \rangle\rangle_\Omega &= -(K_0 + \eta^2)\langle\langle r_\alpha, r_\beta \rangle\rangle_\Omega - \delta_{\alpha,\beta} \\
&\quad + \frac{1}{V} \sum_f \frac{S^2(f)}{2\nu(f)} f_\alpha \left(\frac{1}{\Omega + \nu(f)} - \frac{1}{\Omega - \nu(f)} \right) \langle\langle \mathbf{f} \cdot \mathbf{r}, r_\beta \rangle\rangle_\Omega.
\end{aligned}$$

Since

$$\sum_f F(|f|) f_\alpha f_\beta = \delta_{\alpha\beta} \frac{1}{3} \sum_f F(|f|) f^2$$

and

$$K_0^2 = \frac{1}{3V} \sum_f \frac{S^2(f) f^2}{\nu^2(f)},$$

the following equation results:

$$-m\Omega^2\langle\langle r_\alpha, r_\beta \rangle\rangle_\Omega = -\eta^2\langle\langle r_\alpha, r_\beta \rangle\rangle_\Omega - \frac{1}{3V} \sum_f \frac{S^2(f) f^2}{\nu^2(f)} \langle\langle r_\alpha, r_\beta \rangle\rangle_\Omega$$

$$+ \frac{1}{V} \sum_f \frac{S^2(f)}{6\nu(f)} f^2 \left(\frac{1}{\Omega + \nu(f)} - \frac{1}{\Omega - \nu(f)} \right) \langle\langle r_\alpha, r_\beta \rangle\rangle_\Omega - \delta_{\alpha\beta}. \quad (1.18)$$

However,

$$\begin{aligned} \frac{1}{\Omega + \nu(f)} - \frac{1}{\nu(f)} + \frac{1}{\nu(f) - \Omega} - \frac{1}{\nu(f)} \\ = -\Omega \left(\frac{1}{\nu(f)\{\Omega + \nu(f)\}} + \frac{1}{\{\Omega - \nu(f)\}\nu(f)} \right). \end{aligned}$$

Taking account of this transformation, (1.18) can be represented as

$$\begin{aligned} \delta_{\alpha,\beta} &= \langle\langle r_\alpha, r_\beta \rangle\rangle_\Omega \\ &\times \left\{ m\Omega^2 - \eta^2 - \frac{\Omega}{V} \sum_{(f)} \frac{S^2(f)}{6\nu^2(f)} f^2 \left(\frac{1}{\Omega + \nu(f)} + \frac{1}{\Omega - \nu(f)} \right) \right\}. \end{aligned} \quad (1.19)$$

Let us define

$$\Delta(\Omega) = -\frac{1}{V} \sum_{(f)} \frac{S^2(f)}{6\nu^2(f)} f^2 \left(\frac{1}{\Omega + \nu(f)} + \frac{1}{\Omega - \nu(f)} \right) \quad (1.20)$$

and note that

$$\Delta(-\Omega) = -\Delta(\Omega). \quad (1.21)$$

Then (1.19) can be rewritten in the form

$$\langle\langle r_\alpha, r_\beta \rangle\rangle_\Omega = \frac{\delta_{\alpha,\beta}}{m\Omega^2 - \eta^2 + \Omega\Delta(\Omega)}. \quad (1.22)$$

Taking (1.15) into account, we have also

$$\langle\langle p_\alpha, r_\beta \rangle\rangle_\Omega = \frac{-im\Omega\delta_{\alpha,\beta}}{m\Omega^2 - \eta^2 + \Omega\Delta(\Omega)}. \quad (1.23)$$

Recalling (1.14), we get

$$\langle\langle r_\beta, p_\alpha \rangle\rangle_\Omega = \frac{im\Omega\delta_{\alpha,\beta}}{m\Omega^2 - \eta^2 + \Omega\Delta(\Omega)}. \quad (1.24)$$

Using (1.5) and (1.13), we have further

$$-i\Omega m \langle \langle r_\beta, p_\alpha \rangle \rangle_\Omega = \frac{m}{i\hbar} \langle r_\beta p_\alpha - p_\alpha r_\beta \rangle + \langle \langle p_\beta, p_\alpha \rangle \rangle_\Omega,$$

so that

$$\langle \langle p_\beta, p_\alpha \rangle \rangle_\Omega = -m\delta_{\alpha,\beta} + \frac{(m\Omega)^2 \delta_{\alpha,\beta}}{m\Omega^2 - \eta^2 + \Omega\Delta(\Omega)} = -\delta_{\alpha,\beta} \frac{m(\Omega\Delta(\Omega) - \eta^2)}{m\Omega^2 - \eta^2 + \Omega\Delta(\Omega)}. \quad (1.25)$$

For $|\text{Im } \Omega| > 0$ we can take the limit $\eta \rightarrow 0$, in (1.22) to (1.25). Then

$$\begin{aligned} \langle \langle r_\alpha, r_\beta \rangle \rangle_\Omega &= \frac{\delta_{\alpha,\beta}}{m\Omega^2 + \Omega\Delta(\Omega)}, \\ \langle \langle p_\alpha, r_\beta \rangle \rangle_\Omega &= -\langle \langle r_\beta, p_\alpha \rangle \rangle_\Omega = -\frac{im\delta_{\alpha,\beta}}{m\Omega + \Delta(\Omega)}, \\ \langle \langle p_\alpha, p_\beta \rangle \rangle_\Omega &= -\delta_{\alpha,\beta} \frac{m\Delta(\Omega)}{m\Omega + \Delta(\Omega)}. \end{aligned} \quad (1.26)$$

It should be stressed that when calculating a spectral intensity $J_{A,B}(\omega)$, for example $J_{p_\alpha, p_\beta}(\omega)$, we have to use (1.25), which contains $\eta > 0$, and only after this can we take the limit $\eta \rightarrow 0$.

By means of (1.11), we arrive at the following spectral density:

$$\begin{aligned} J_{p_\alpha, p_\beta}(\omega) &= \delta_{\alpha,\beta} \frac{i\hbar}{2\pi} (1 - e^{-\beta\hbar\omega})^{-1} \frac{(m\Omega)^2}{m\Omega^2 - \eta^2 + \Omega\Delta(\Omega)} \Big|_{\omega-i0}^{\omega+i0} \\ &= -m\delta_{\alpha,\beta} \frac{i\hbar}{2\pi(1 - e^{-\beta\hbar\omega})} \left(\frac{\Omega\Delta(\Omega) - \eta^2}{m\Omega^2 - \eta^2 + \Omega\Delta(\Omega)} \right) \Big|_{\omega-i0}^{\omega+i0}. \end{aligned} \quad (1.27)$$

Here we have introduced the notation

$$F(\Omega) \Big|_a^b = F(b) - F(a).$$

It must be kept in mind that division by $(1 - e^{-\beta\hbar\omega})^{-1}$ in (1.27) may lead to a delta function $K\delta(\omega)$ with some unknown coefficient K . However, when $\eta^2 > 0$, the expression

$$\dots \Big|_{\omega-i0}^{\omega+i0}$$

in (1.27) is equal to zero in the vicinity of the point $\omega = 0$. On the other hand, we know that in this case (namely for $\eta^2 > 0$), function $p_\alpha(t)$ can be represented as a sum of harmonic oscillations with nonzero frequencies. Therefore the corresponding spectral intensity

$$J_{p_\alpha p_\beta}(\omega) = 0$$

in a neighborhood of the point $\omega = 0$ that does not contain the harmonic-oscillator frequencies. Therefore we have to calculate (1.27) first of all under the condition $\eta^2 > 0$, and only after this can we take the limit $\eta \rightarrow 0$.

Let us consider in detail the simplest example when

$$\nu(f) = \nu = \text{const} > 0. \quad (1.28)$$

In this case (1.20) if one takes into account that

$$K_0^2 = \frac{1}{3V} \sum_{(f)} \frac{S^2(f)}{\nu^2(f)} f^2$$

can be rewritten as

$$\Delta(\Omega) = -\frac{K_0^2}{2} \left(\frac{1}{\Omega + \nu} + \frac{1}{\Omega - \nu} \right) = -\frac{K_0^2 \Omega}{\Omega^2 - \nu^2}. \quad (1.29)$$

From (1.27), we derive

$$J_{p_\alpha p_\beta}(\omega) = \delta_{\alpha, \beta} \frac{i\hbar}{2\pi} (1 - e^{-\beta\hbar\omega})^{-1} \frac{(m\Omega)^2 (\Omega^2 - \nu^2)}{m\Omega^4 - \Omega^2(K_0^2 + \eta^2 + m\nu^2) + \nu^2\eta^2} \Big|_{\omega-i0}^{\omega+i0}. \quad (1.30)$$

Here the denominator has two roots with respect to Ω^2 :

$$\omega_1^2 = \frac{\nu^2\eta^2}{K_0^2 + \nu^2m} + O(\eta^4), \quad \omega_2^2 = \frac{K_0^2 + \nu^2m}{m} + O(\eta^2). \quad (1.31)$$

Hence

$$m\Omega^4 - \Omega^2(K_0^2 + \eta^2 + \nu^2m) + \nu^2\eta^2 = m(\Omega^2 - \omega_1^2)(\Omega^2 - \omega_2^2).$$

Therefore

$$\begin{aligned} & \frac{m^2\Omega^2(\Omega^2 - \nu^2)}{m\Omega^4 - \Omega^2(K_0^2 + \eta^2 + \nu^2m) + \nu^2\eta^2} \\ &= \frac{m\omega_1^2(\omega_1^2 - \nu^2)}{\omega_1^2 - \omega_2^2} \frac{1}{\Omega^2 - \omega_1^2} + \frac{m\omega_2^2(\omega_2^2 - \nu^2)}{\omega_2^2 - \omega_1^2} \frac{1}{\Omega^2 - \omega_2^2} + \mathcal{E}, \end{aligned}$$

where the expression $\mathcal{E}$ is regular and does not have singularities on the real axis. On the other hand,

$$\frac{1}{\Omega^2 - \omega_j^2} = \frac{1}{2\omega_j} \left(\frac{1}{\Omega - \omega_j} - \frac{1}{\Omega + \omega_j} \right), \quad j = 1, 2,$$

and

$$\frac{1}{\Omega^2 - \omega_j^2} \Big|_{\omega-i0}^{\omega+i0} = \frac{\pi i}{\omega_j} \{ \delta(\omega - \omega_j) - \delta(\omega + \omega_j) \}.$$

Hence it follows from (1.30) that

$$\begin{aligned}
 J_{p_\alpha p_\beta}(\omega) &= \frac{1}{2} \delta_{\alpha,\beta} \frac{m(\nu^2 - \omega_1^2)}{\omega_2^2 - \omega_1^2} \left(\frac{\hbar\omega_1}{1 - e^{-\beta\hbar\omega_1}} \delta(\omega - \omega_1) + \frac{\hbar\omega_1}{e^{\beta\hbar\omega_1} - 1} \delta(\omega + \omega_1) \right) \\
 &\quad + \frac{1}{2} \delta_{\alpha,\beta} \frac{m(\omega_2^2 - \nu^2)}{\omega_2^2 - \omega_1^2} \left(\frac{\hbar\omega_2}{1 - e^{-\beta\hbar\omega_2}} \delta(\omega - \omega_2) + \frac{\hbar\omega_2}{e^{\beta\hbar\omega_2} - 1} \delta(\omega + \omega_2) \right). \quad (1.32)
 \end{aligned}$$

Keeping in mind (1.31), one has $\omega_1 \rightarrow 0$, when $\eta \rightarrow 0$, and at the same time

$$\begin{aligned}
 \frac{\hbar\omega_1}{1 - e^{-\beta\hbar\omega_1}} &\rightarrow \frac{1}{\beta} = \vartheta, & \frac{\hbar\omega_1}{e^{\beta\hbar\omega_1} - 1} &\rightarrow \frac{1}{\beta} = \vartheta, \\
 \omega_2 &\rightarrow \mu = \left(\frac{K_0^2}{m} + \nu^2 \right)^{1/2}.
 \end{aligned}$$

Taking the limit $\eta \rightarrow 0$ in (1.32), we find that

$$\begin{aligned}
 J_{p_\alpha p_\beta}(\omega) &= \delta_{\alpha,\beta} \frac{m^2 \nu^2 \vartheta}{K_0^2 + m\nu^2} \delta(\omega) \\
 &\quad + \frac{K_0^2 \delta_{\alpha,\beta}}{2\mu} \left(\frac{\hbar}{1 - e^{-\beta\hbar\mu}} \delta(\omega - \mu) + \frac{\hbar}{e^{\beta\hbar\mu} - 1} \delta(\omega + \mu) \right). \quad (1.33)
 \end{aligned}$$

If one knows the spectral intensity, one can easily calculate two-time correlation functions:

$$\begin{aligned}
 \langle p_\alpha(t) p_\beta(\tau) \rangle_{\text{eq}} &= 0, \quad \alpha \neq \beta, \\
 \langle p_\alpha(t) p_\alpha(\tau) \rangle_{\text{eq}} &= \frac{m^2 \nu^2 \vartheta}{K_0^2 + m\nu^2} + \frac{K_0^2}{2\mu} \left(\frac{\hbar}{1 - e^{-\beta\hbar\mu}} e^{-i\mu(t-\tau)} + \frac{\hbar}{e^{\beta\hbar\mu} - 1} e^{i\mu(t-\tau)} \right). \quad (1.34)
 \end{aligned}$$

Now we consider the more general case when $\nu(f)$ possesses a continuous spectrum in the limit $V \rightarrow \infty$. Let us return to (1.27) and transform this formula into a new one:

$$J_{p_\alpha p_\beta}(\omega) = m \delta_{\alpha,\beta} \frac{i\hbar\omega}{2\pi(1 - e^{-\beta\hbar\omega})} \frac{1}{\omega} f_\eta(\Omega) \Big|_{\omega-i0}^{\omega+i0}, \quad (1.35)$$

where

$$-f_\eta(\Omega) = \frac{\Omega \Delta(\Omega) - \eta^2}{m\Omega^2 - \eta^2 + \Omega \Delta(\Omega)}.$$

We can see that

$$f_\eta(0) = -1 \quad \text{and} \quad f_\eta(\Omega) \Big|_{\omega-i0}^{\omega+i0} = 0$$

for small enough ω . Hence, for small enough ω

$$\frac{1}{\Omega} f_{\eta}(\Omega) \Big|_{\omega-i0}^{\omega+i0} = f_{\eta}(\omega) \left(\frac{1}{\omega+i\varepsilon} - \frac{1}{\omega-i\varepsilon} \right) = -2\pi i f_{\eta}(\omega) \delta(\omega) = 2\pi i \delta(\omega). \quad (1.36)$$

It should be stressed that the function $1/\Omega$ has only one singular point $\Omega = 0$. So, for arbitrary real ω

$$\frac{1}{\Omega} f_{\eta}(\Omega) \Big|_{\omega-i0}^{\omega+i0} = 2\pi i \delta(\omega) + \frac{1}{\omega} f_{\eta}(\Omega) \Big|_{\omega-i0}^{\omega+i0}$$

or

$$\frac{1}{\omega} f_{\eta}(\Omega) \Big|_{\omega-i0}^{\omega+i0} = -2\pi i \delta(\omega) + \frac{1}{\Omega} f_{\eta}(\Omega) \Big|_{\omega-i0}^{\omega+i0}.$$

Therefore it follows from (1.35) that

$$J_{p_{\alpha}p_{\beta}}(\omega) = \delta_{\alpha,\beta} \frac{i\hbar\omega m}{2\pi(1 - e^{-\beta\hbar\omega})} \left(-2\pi i \delta(\omega) + \frac{1}{\Omega} f_{\eta}(\Omega) \Big|_{\omega-i0}^{\omega+i0} \right).$$

But the function

$$\frac{\Omega}{1 - e^{-\beta\hbar\Omega}}$$

is regular in the vicinity of the real axis, and so

$$\frac{\hbar\omega}{1 - e^{-\beta\hbar\omega}} \frac{1}{\Omega} f_{\eta}(\Omega) \Big|_{\omega-i0}^{\omega+i0} = \frac{\hbar}{1 - e^{-\beta\hbar\Omega}} f_{\eta}(\Omega) \Big|_{\omega-i0}^{\omega+i0}.$$

Thus

$$J_{p_{\alpha}p_{\beta}}(\omega) = 0 \quad \text{if} \quad \alpha \neq \beta,$$

and

$$J_{p_{\alpha}p_{\alpha}}(\omega) = m\vartheta\delta(\omega) - \frac{i\hbar m}{2\pi(1 - e^{-\beta\hbar\Omega})} \frac{\Omega\Delta(\Omega) - \eta^2}{m\Omega^2 - \eta^2 + \Omega\Delta(\Omega)} \Big|_{\omega-i0}^{\omega+i0}.$$

As a result, we have

$$\langle p_{\alpha}(t)p_{\beta}(\tau) \rangle_{\text{eq}} = 0 \quad \text{for} \quad \alpha \neq \beta,$$

$$\langle p_{\alpha}(t)p_{\alpha}(\tau) \rangle_{\text{eq}} = m\vartheta - \int_{-\infty}^{+\infty} \frac{i\hbar m e^{-i\Omega(t-\tau)}}{2\pi(1 - e^{-\beta\hbar\Omega})} \frac{\Omega\Delta(\Omega) - \eta^2}{m\Omega^2 - \eta^2 + \Omega\Delta(\Omega)} \Big|_{\omega-i0}^{\omega+i0} d\omega.$$

Consider the function

$$\begin{aligned} f_{\eta}(\Omega) &= -\frac{\Omega\Delta(\Omega) - \eta^2}{m\Omega^2 - \eta^2 + \Omega\Delta(\Omega)} = -1 + \frac{m\Omega^2}{m\Omega^2 - \eta^2 + \Omega\Delta(\Omega)} \\ &= -1 + \frac{m\Omega}{m\Omega + \Delta(\Omega) - \eta^2/\Omega} \end{aligned}$$

for $\Omega = i\varepsilon + \omega$ and $\Omega = -i\varepsilon + \omega$; $\varepsilon > 0$. Taking account of (1.20), we have

$$-\text{Im } \Delta(\omega + \varepsilon) = \frac{\varepsilon}{V} \sum_{(f)} \frac{S^2(f)}{6\nu^2(f)} f^2 \left(\frac{1}{\{\nu(f) + \omega\}^2 + \varepsilon^2} + \frac{1}{\{\nu(f) - \omega\}^2 + \varepsilon^2} \right) > 0.$$

Then it is obvious that

$$\text{Im } \frac{-\eta^2}{\Omega} = + \frac{\eta^2 \varepsilon}{\omega^2 + \varepsilon^2} > 0, \quad \Omega = \omega + i\varepsilon.$$

Hence

$$\text{Im} \left(m\Omega + \Delta(\Omega) - \frac{\eta^2}{\Omega} \right) > \varepsilon m, \quad \Omega = \omega + i\varepsilon$$

and

$$\left| m\Omega + \Delta(\Omega) - \frac{\eta^2}{\Omega} \right| > \varepsilon m. \quad (1.37)$$

In the same way, it can be proved that, for $\varepsilon = -\text{Im } \Omega > 0$

$$\left| m\Omega + \Delta(\Omega) - \frac{\eta^2}{\Omega} \right| > \varepsilon.$$

Therefore the function $f_\eta(\Omega)$ is a regular function of the complex variable Ω on the two half-planes

$$\text{Im } \Omega > 0 \quad \text{and} \quad \text{Im } \Omega < 0. \quad (1.38)$$

Then we note that the poles of the function

$$\frac{1}{1 - e^{-\beta \hbar \Omega}}$$

in the domain (1.38) in the vicinity of the real axis are

$$\Omega = \frac{2\pi i}{\hbar \beta} \quad \text{and} \quad \Omega = -\frac{2\pi i}{\hbar \beta}.$$

in the domain (1.38) in the vicinity of the real axis are

$$0 < \text{Im } \Omega < \frac{2\pi}{\hbar \beta}$$

or in the region

$$0 > \text{Im } \Omega > -\frac{2\pi}{\hbar \beta}.$$

Then

$$\int_{\mathcal{L}} \frac{e^{-i\Omega(t-\tau)}}{1 - e^{-\beta \hbar \Omega}} f_\eta(\Omega) d\Omega = 0.$$

We recall (1.20),

$$\Delta(\Omega) = -\frac{1}{V} \sum_{(f)} \frac{S^2(f)}{6\nu^2(f)} f^2 \left(\frac{1}{\nu(f) + \Omega} + \frac{1}{\Omega - \nu(f)} \right), \quad (1.39)$$

which contains only a finite number (f) , of terms if the volume V is fixed. Therefore, for large enough $|\Omega|$,

$$\begin{aligned} |\Omega \Delta(\Omega)| &= \text{const}, & |\text{Im } \Omega| &\geq \varepsilon > 0 \\ |\Delta(\Omega)| &\leq \frac{\text{const}}{|\Omega|}. \end{aligned} \quad (1.40)$$

As a result, one can choose for the contour $\mathcal{L}$ an infinite contour (see Fig. 1):

$$\begin{aligned} i\varepsilon_1 - \infty < \vec{\omega} < i\varepsilon_1 + \infty, & \quad i\varepsilon - \infty < \overleftarrow{\omega} < i\varepsilon + \infty, \\ 0 < \varepsilon < \varepsilon_1 < \frac{2\pi}{\hbar\beta} \end{aligned}$$

Fig. 1.1.

and obtain the expression

$$\begin{aligned} -\frac{im\hbar}{2\pi} \int_{i\varepsilon_1 - \infty}^{i\varepsilon_1 + \infty} \frac{e^{-i\Omega(t-\tau)}}{1 - e^{-\beta\hbar\Omega}} \frac{\Omega\Delta(\Omega) - \eta^2}{m\Omega^2 - \eta^2 + \Omega\Delta(\Omega)} d\Omega \\ = +\frac{im\hbar}{2\pi} \int_{i\varepsilon - \infty}^{i\varepsilon + \infty} \frac{e^{-i\Omega(t-\tau)}}{1 - e^{-\beta\hbar\Omega}} \frac{\Omega\Delta(\Omega) - \eta^2}{m\Omega^2 - \eta^2 + \Omega\Delta(\Omega)} d\Omega = 0, \end{aligned}$$

from which it follows that the integral

$$-\frac{im\hbar}{2\pi} \int_{i\varepsilon - \infty}^{i\varepsilon + \infty} \frac{e^{-i\Omega(t-\tau)}}{1 - e^{-\beta\hbar\Omega}} \frac{\Omega\Delta(\Omega) - \eta^2}{m\Omega^2 - \eta^2 + \Omega\Delta(\Omega)} d\Omega$$

does not depend on the magnitude of ε , when ε belongs to the domain

$$0 < \varepsilon < \frac{2\pi}{\hbar\beta}. \quad (1.41)$$

In full analogy with the previous consideration, one can prove that the same integral, calculated along the closed contour $(-i\varepsilon - \infty, -i\varepsilon + \infty)$, situated on the lower half-plane, does not depend on the precise value of ε , if ε belongs to the region (1.41). We can write (1.36) in the form

$$\begin{aligned} \langle p_\alpha(t)p_\alpha(\tau) \rangle_{\text{eq}} = m\vartheta - \frac{im\hbar}{2\pi} \int_{i\varepsilon-\infty}^{i\varepsilon+\infty} \frac{e^{-i\Omega(t-\tau)}}{1 - e^{-\beta\hbar\Omega}} \frac{\Omega\Delta(\Omega) - \eta^2}{m\Omega^2 - \eta^2 + \Omega\Delta(\Omega)} d\Omega \\ + \frac{im\hbar}{2\pi} \int_{-i\varepsilon-\infty}^{-i\varepsilon+\infty} \frac{e^{-i\Omega(t-\tau)}}{1 - e^{-\beta\hbar\Omega}} \frac{\Omega\Delta(\Omega) - \eta^2}{m\Omega^2 - \eta^2 + \Omega\Delta(\Omega)} d\Omega. \end{aligned}$$

Here, owing to (1.37) and (1.40), we may pass to the limit $\eta \rightarrow 0$ and write

$$\begin{aligned} \langle p_\alpha(t)p_\alpha(\tau) \rangle_{\text{eq}} = m\vartheta - \frac{im\hbar}{2\pi} \int_{i\varepsilon-\infty}^{i\varepsilon+\infty} \frac{e^{-i\Omega(t-\tau)}}{1 - e^{-\beta\hbar\Omega}} \frac{\Delta(\Omega)}{m\Omega + \Delta(\Omega)} d\Omega \\ + \frac{im\hbar}{2\pi} \int_{-i\varepsilon-\infty}^{-i\varepsilon+\infty} \frac{e^{-i\Omega(t-\tau)}}{1 - e^{-\beta\hbar\Omega}} \frac{\Delta(\Omega)}{m\Omega + \Delta(\Omega)} d\Omega. \quad (1.42) \end{aligned}$$

Consider now the standard limit $V \rightarrow \infty$. It follows from (1.20) that

$$\Delta(\Omega) = - \int_{-\infty}^{+\infty} E_V(\nu) \frac{d\nu}{\Omega - \nu},$$

where

$$\begin{aligned} E_V(\omega) = \frac{1}{V} \sum_{(f)} \frac{S^2(f)}{6\nu^2(f)} f^2 \{ \delta(\nu(f) + \omega) + \delta(\nu(f) - \omega) \}, \\ E_V \geq 0, \quad E_V(-\omega) = E_V(\omega). \end{aligned}$$

Let us suppose that this generalized function $E_V(\omega)$ has the behavior

$$E_V(\omega) \rightarrow E(\omega) = \frac{1}{(2\pi)^3} \int \frac{S^2(f)}{6\nu^2(f)} f^2 \{ \delta(\nu(f) + \omega) + \delta(\nu(f) - \omega) \} df$$

if $V \rightarrow \infty$ in such a way that the convergence of the function:
(1°) is uniform on any finite interval

$$+i\varepsilon - \infty < \omega < i\varepsilon + \infty, \quad \varepsilon > 0 \quad (1.43)$$

(on the upper half-plane) and

$$-i\varepsilon - \infty < \omega < -i\varepsilon + \infty, \quad \varepsilon > 0 \quad (1.44)$$

(on the lower half-plane):

$$\int_{-\infty}^{+\infty} E_V(\nu) \frac{d\nu}{\Omega - \nu} \rightarrow -\Delta_\infty(\Omega) = \int_{-\infty}^{+\infty} \frac{E(\nu) d\nu}{\Omega - \nu};$$

(2°) for $|\operatorname{Im} \Omega| \geq \varepsilon$

$$|\Omega \Delta(\Omega)| \leq K_\varepsilon,$$

where K_ε — is some constant independent of the volume V .

Under these conditions, we can go to the limit $V \rightarrow \infty$ in (1.42) and write

$$\begin{aligned} \langle p_\alpha(t) p_\alpha(\tau) \rangle_{\text{eq}} &= m\vartheta - \frac{im\hbar}{2\pi} \int_{i\varepsilon-\infty}^{i\varepsilon+\infty} \frac{e^{-i\Omega(t-\tau)}}{1 - e^{-\beta\hbar\Omega}} \frac{\Delta_\infty(\Omega)}{m\Omega + \Delta_\infty(\Omega)} d\Omega + \\ &+ \frac{im\hbar}{2\pi} \int_{-i\varepsilon-\infty}^{-i\varepsilon+\infty} \frac{e^{-i\Omega(t-\tau)}}{1 - e^{-\beta\hbar\Omega}} \frac{\Delta_\infty(\Omega)}{m\Omega + \Delta_\infty(\Omega)} d\Omega = \\ &= m\vartheta - \frac{im\hbar}{2\pi} \int_{i\varepsilon-\infty}^{i\varepsilon+\infty} \frac{e^{-i\Omega(t-\tau)}}{1 - e^{-\beta\hbar\Omega}} \frac{\Delta_\infty(\Omega)}{m\Omega + \Delta_\infty(\Omega)} d\omega \Big|_{\omega-i\varepsilon}^{\omega+i\varepsilon}, \quad (1.45) \end{aligned}$$

where

$$\Delta(\Omega) = - \int_{-\infty}^{+\infty} \frac{E(\nu)}{\Omega - \nu} d\nu, \quad E(\nu) = E(-\nu) \geq 0, \quad (1.46)$$

and, from (2°)

$$|\Omega \Delta_\infty(\Omega)| \leq K_\varepsilon \quad \text{for} \quad |\operatorname{Im} \Omega| \geq \varepsilon. \quad (1.47)$$

The right-hand side of (1.45) is independent of the value of ε , if ε is positive and small enough. Owing to this fact, we can take the passage to the limit $\varepsilon \rightarrow 0$, $\varepsilon > 0$ in (1.45). The result is^e

$$\langle p_\alpha(t) p_\alpha(\tau) \rangle_{\text{eq}} = m\vartheta - \frac{im\hbar}{2\pi} \int_{-\infty}^{+\infty} \frac{\omega e^{-i\omega(t-\tau)}}{1 - e^{-\beta\hbar\omega}} \frac{1}{\Omega} \frac{\Delta_\infty(\Omega)}{m\Omega + \Delta_\infty(\Omega)} d\omega \Big|_{\omega-i0}^{\omega+i0}.$$

Since

$$-\frac{\Delta_\infty(\Omega)}{m\Omega + \Delta_\infty(\Omega)} = -1 + \frac{m\Omega}{m\Omega + \Delta_\infty(\Omega)}$$

and

$$-\frac{i\hbar m}{2\pi} \frac{\omega}{1 - e^{-\beta\hbar\omega}} \frac{1}{\Omega} \Big|_{\omega-i0}^{\omega+i0} = -\frac{m}{\beta} \delta(\omega) = -m\vartheta \delta(\omega),$$

we come at last to the expression

$$\langle p_\alpha(t) p_\alpha(\tau) \rangle_{\text{eq}} = \int_{-\infty}^{+\infty} J(\omega) e^{-i\omega(t-\tau)} d\omega, \quad (1.48)$$

^e Here we assume that discontinuities of the expression

$$\frac{1}{\Omega} \frac{\Delta_\infty(\Omega)}{m\Omega + \Delta_\infty(\Omega)} \Big|_{\omega-i0}^{\omega+i0}$$

are of the first order, so that if $F(\Omega)$ — is an analytic function in the vicinity of the real axis, such as the function

$$F(\Omega) = \frac{\Omega}{1 - e^{-\beta\hbar\omega}}, \quad \text{then} \quad \{F(\Omega) - F(\omega)\} \frac{1}{\Omega} \frac{\Delta_\infty(\Omega)}{m\Omega + \Delta_\infty(\Omega)} \Big|_{\omega-i0}^{\omega+i0} = 0.$$

where

$$J(\omega) = \frac{i\hbar m^2}{2\pi} \frac{\omega}{1 - e^{-\beta\hbar\omega}} \frac{1}{m\Omega + \Delta_\infty(\Omega)} \Big|_{\omega-i0}^{\omega+i0}.$$

From (1.46), one can derive

$$\Delta_\infty(\omega \pm i0) = -\int E(\nu) \mathcal{P}\left(\frac{1}{\omega - \nu}\right) d\nu \pm i\pi E(\omega).$$

It follows from this equation that

$$i \frac{1}{m\Omega + \Delta_\infty(\Omega)} \Big|_{\omega-i0}^{\omega+i0} \geq 0.$$

Because, in addition,

$$\frac{\omega}{1 - e^{-\beta\hbar\omega}} \geq 0,$$

it is easy to find that

$$J(\omega) \geq 0. \quad (1.49)$$

It should be noted that if we put $E(\omega)$ equal to

$$E(\omega) = \frac{K_0^2}{2} \{\delta(\omega - \nu_0) + \delta(\omega + \nu_0)\},$$

we get from (1.48) our previous (1.34) that we derived earlier.

1.4. Free Energy Calculation for the Linear Polaron Model

We now proceed with the calculation of the free energy for the dynamical system under consideration. The free energy is defined as

$$F = -\vartheta \ln \text{Tr } e^{\beta H}, \quad (H = H_{\text{linear model}}).$$

The free energy for a single free particle of mass m that does not interact with the phonon bath is

$$F_s = -\vartheta \ln \text{Tr} \exp\left(-\frac{\mathbf{p}^2 \beta}{2m}\right) = -\vartheta \lim_{\eta \rightarrow 0} \ln \text{Tr} \exp\left\{-\left(\frac{\mathbf{p}^2}{2m} + \frac{\eta^2}{2} \mathbf{r}^2\right) \beta\right\}.$$

The free energy of the free-phonon field Σ is

$$F_\Sigma = -\vartheta \ln \text{Tr } e^{-H_\Sigma \beta}, \quad H_\Sigma = \frac{1}{2} \sum_{(f)} \{p_f p_f^* + \nu(f)^2 q_f q_f^*\}.$$

Because explicit expressions for these energies are well known, we need calculate only that part of the total free energy that is due to the interaction between the phonon field and the particle, i.e.

$$F_{\text{int}} = F - F_s - F_\Sigma.$$

For technical reasons, we introduce an auxiliary parameter λ ($0 \leq \lambda \leq 1$) into the total Hamiltonian $H = H_{\text{linear model}}$:

$$H(\lambda) = \frac{\mathbf{p}^2}{2m} + \frac{\eta^2 \mathbf{r}^2}{2} + \frac{\lambda^2}{V} \sum_{(f)} \frac{S^2(f)}{6\nu^2(f)} f^2 \mathbf{r}^2 + \frac{i}{V^{1/2}} \sum_{(f)} \lambda S_f q_f \mathbf{f} \cdot \mathbf{r} + H_{\Sigma}.$$

We see that

$$H(0) = H_S + H_{\Sigma}, \quad H(1) = H.$$

Thus

$$\begin{aligned} F_{\text{int}} &= \int_0^1 d\lambda \frac{\partial F(\lambda)}{\partial \lambda} = -\vartheta \int_0^1 d\lambda \frac{\partial}{\partial \lambda} \ln \text{Tr} e^{-\beta H(\lambda)} = \\ &= \int_0^1 d\lambda \frac{\text{Tr}[\{\partial H(\lambda)/\partial \lambda\} e^{-\beta H(\lambda)}]}{\text{Tr} e^{-\beta H(\lambda)}} = \int_0^1 d\lambda \left\langle \frac{\partial H}{\partial \lambda} \right\rangle_{\lambda, \text{eq}}, \end{aligned} \quad (1.50)$$

i. e.

$$F_{\text{int}} = \int_0^1 d\lambda \left\langle \frac{\partial H}{\partial \lambda} \right\rangle_{\lambda, \text{eq}}. \quad (1.51)$$

In this formula the subscript λ indicates that the averaging is with respect to the Hibbs equilibrium statistical operator corresponding to the Hamiltonian $H(\lambda)$:

$$\rho(H(\lambda)) = e^{-\beta H(\lambda)} / \text{Tr}(e^{-\beta H(\lambda)}).$$

But

$$\frac{\partial H(\lambda)}{\partial \lambda} = \frac{\lambda}{3V} \sum_{(f)} \frac{S^2(f)}{\nu^2(f)} f^2 \mathbf{r}^2 + \frac{i}{V^{1/2}} \sum_{(f)} S_f q_f \mathbf{f} \cdot \mathbf{r}.$$

From another point of view, we can write the equations of motion (1.5) for the Hamiltonian $H(\lambda)$:

$$-m \frac{d^2 \mathbf{r}}{dt^2} - \eta^2 \mathbf{r} = \frac{\lambda^2}{3} \sum_{(f)} \frac{S^2(f)}{\nu^2(f)} f^2 \mathbf{r} + \frac{i}{\sqrt{V}} \sum_{(f)} \lambda S_f q_f \mathbf{f}.$$

Therefore

$$\lambda \left\langle \frac{\partial H(\lambda)}{\partial \lambda} \right\rangle_{\lambda, \text{eq}} = - \left\langle \left(m \frac{d^2 \mathbf{r}}{dt^2} + \eta^2 \mathbf{r} \right) \cdot \mathbf{r} \right\rangle_{\lambda, \text{eq}}. \quad (1.52)$$

Taking (1.6), (1.11) and (1.22) into account, we have

$$\langle r_{\alpha}(t) r_{\beta}(\tau) \rangle_{\lambda, \text{eq}} = 0 \quad \text{for} \quad \alpha \neq \beta,$$

$$\langle r_{\alpha}(t) r_{\alpha}(\tau) \rangle_{\lambda, \text{eq}} = \frac{i\hbar}{2\pi} \int_{-\infty}^{+\infty} \frac{e^{-i\omega(t-\tau)}}{1 - e^{-\beta\hbar\omega}} \frac{1}{m\Omega^2 - \eta^2 + \lambda^2 \Omega \Delta(\Omega)} \Big|_{\omega-i0}^{\omega+i0} d\omega. \quad (1.53)$$

.....

Here we have not forgotten that on changing from the Hamiltonian H to the Hamiltonian $H(\lambda)$, we have introduced the parameter λ into S_f , which results in the necessity to change $\Delta(\Omega)$ into $\lambda^2\Delta(\Omega)$. So

$$\begin{aligned} & \left\langle \left(-m \frac{d^2 r_\alpha(t)}{dt^2} - \eta^2 r_\alpha(t) \right) r_\alpha(\tau) \right\rangle_{\lambda, \text{eq}} \\ &= \frac{i\hbar}{2\pi} \int_{-\infty}^{+\infty} \frac{m\omega^2 - \eta^2}{1 - e^{-\beta\hbar\omega}} e^{-i\omega(t-\tau)} \frac{1}{m\Omega^2 - \eta^2 + \lambda^2\Omega\Delta(\Omega)} \Big|_{\omega-i0}^{\omega+i0} d\omega \\ &= \frac{i\hbar}{2\pi} \int_{-\infty}^{+\infty} \frac{e^{-i\omega(t-\tau)}}{1 - e^{-\beta\hbar\omega}} \frac{m\Omega^2 - \eta^2}{m\Omega^2 - \eta^2 + \lambda^2\Omega\Delta(\Omega)} \Big|_{\omega-i0}^{\omega+i0} d\omega, \end{aligned}$$

if $\Omega \rightarrow \omega$, and, inserting this result into (1.51) we see that

$$\lambda \left\langle \frac{\partial H(\lambda)}{\partial \lambda} \right\rangle_{\lambda, \text{eq}} = 3 \frac{i\hbar}{2\pi} \int_{-\infty}^{+\infty} \frac{1}{1 - e^{-\beta\hbar\omega}} \frac{m\Omega^2 - \eta^2}{m\Omega^2 - \eta^2 + \lambda^2\Omega\Delta(\Omega)} \Big|_{\omega-i0}^{\omega+i0} d\omega.$$

Let us note that

$$\begin{aligned} \frac{m\Omega^2 - \eta^2}{m\Omega^2 - \eta^2 + \lambda^2\Omega\Delta(\Omega)} &= 1 - \frac{\Omega\lambda^2\Delta(\Omega)}{m\Omega^2 - \eta^2 + \lambda^2\Omega\Delta(\Omega)}, \\ \frac{m\Omega^2 - \eta^2}{m\Omega^2 - \eta^2 + \lambda^2\Omega\Delta(\Omega)} \Big|_{\omega-i0}^{\omega+i0} &= - \frac{\Omega\lambda^2\Delta(\Omega)}{m\Omega^2 - \eta^2 + \lambda^2\Omega\Delta(\Omega)} \Big|_{\omega-i0}^{\omega+i0}. \end{aligned}$$

Hence (1.51) gives us

$$\begin{aligned} \left\langle \frac{\partial H(\lambda)}{\partial \lambda} \right\rangle_{\lambda, \text{eq}} &= -3 \frac{i\hbar}{2\pi} \int_{-\infty}^{+\infty} \frac{1}{1 - e^{-\beta\hbar\omega}} \frac{\Omega\lambda\Delta(\Omega)}{m\Omega^2 - \eta^2 + \lambda^2\Omega\Delta(\Omega)} \Big|_{\omega-i0}^{\omega+i0} d\omega \\ &= -3 \frac{i\hbar}{2\pi} \int_{-\infty}^{+\infty} \frac{\Omega}{1 - e^{-\beta\hbar\omega}} \frac{\lambda\Delta(\Omega)}{m\Omega^2 - \eta^2 + \lambda^2\Omega\Delta(\Omega)} \Big|_{\omega-i0}^{\omega+i0} d\omega. \quad (1.54) \end{aligned}$$

Using a similar approach for the calculation of the correlation function

$$\langle p_\alpha(t) p_\alpha(\tau) \rangle_{\text{eq}},$$

we find in the limit $\eta \rightarrow 0$, $V \rightarrow \infty$ that

$$\left\langle \frac{\partial H(\lambda)}{\partial \lambda} \right\rangle_{\lambda, \text{eq}} = -\frac{3i\hbar}{2\pi} \int_{-\infty}^{+\infty} \frac{\Omega}{1 - e^{-\beta\hbar\omega}} \frac{1}{\Omega} \frac{\lambda\Delta_\infty(\Omega)}{m\Omega + \lambda^2\Delta_\infty(\Omega)} \Big|_{\omega-i0}^{\omega+i0} d\omega. \quad (1.55)$$

The right-hand side of this equation does not depend on ε when $0 < \varepsilon < 2\pi/\hbar\beta$. Thus, assuming $\varepsilon > 0$, $\varepsilon \rightarrow 0$, we derive from (1.50)

$$F_{\text{int}} = -\frac{3i\hbar}{2\pi} \int_0^1 d\lambda \int_{-\infty}^{+\infty} \frac{\Omega}{1 - e^{-\beta\hbar\omega}} \frac{1}{\Omega} \frac{\lambda\Delta_\infty(\Omega)}{m\Omega + \lambda^2\Delta_\infty(\Omega)} \Big|_{\omega-i0}^{\omega+i0} d\omega. \quad (1.56)$$

Consider now the special “single-frequency” case

$$E(\omega) = \frac{K_0^2}{2} \{ \delta(\omega - \nu_0) + \delta(\omega + \nu_0) \}. \quad (1.57)$$

Then

$$\Delta_\infty(\Omega) = -\frac{K_0^2 \Omega}{\Omega^2 - \nu_0^2},$$

and

$$-\frac{1}{\Omega} \frac{\lambda \Delta_\infty(\Omega)}{m\Omega + \lambda^2 \Delta_\infty(\Omega)} = \frac{1}{\Omega} \frac{\lambda K_0^2}{m\Omega^2 - (m\nu_0^2 + \lambda^2 K_0^2)}.$$

This expression has three poles:

$$\Omega = 0, \quad \Omega = \mu(\lambda), \quad \Omega = -\mu(\lambda),$$

where

$$\mu(\lambda) = \left(\nu_0^2 + \lambda^2 \frac{K_0^2}{m} \right)^{1/2}.$$

Let us notice that

$$\frac{1}{\Omega^2 - \mu^2(\lambda)} = \frac{1}{2\mu(\lambda)} \left(\frac{1}{\Omega - \mu(\lambda)} - \frac{1}{\Omega + \mu(\lambda)} \right).$$

Because of the obvious identity

$$\begin{aligned} & -\frac{1}{\Omega} \frac{\lambda \Delta_\infty(\Omega)}{m\Omega + \lambda^2 \Delta_\infty(\Omega)} \Big|_{\omega-i0}^{\omega+i0} \\ &= \frac{2\pi i \delta(\omega) \lambda K_0^2}{m\nu_0^2 + \lambda^2 K_0^2} - \frac{2\pi i \lambda K_0^2}{2\mu^2(\lambda)m} \{ \delta(\omega - \mu(\lambda)) + \delta(\omega + \mu(\lambda)) \} \end{aligned}$$

and

$$\begin{aligned} & -\frac{3i\hbar}{2\pi} \int_{-\infty}^{+\infty} \frac{\Omega}{1 - e^{-\beta\hbar\Omega}} \frac{1}{\Omega} \frac{\lambda \Delta_\infty(\Omega)}{m\Omega + \lambda^2 \Delta_\infty(\Omega)} \Big|_{\omega-i0}^{\omega+i0} d\omega \\ &= -3\vartheta \frac{\lambda K_0^2}{m\nu_0^2 + \lambda^2 K_0^2} + \frac{3\lambda K_0^2 \hbar}{2m\mu(\lambda)} \left(\frac{1}{1 - e^{-\beta\hbar\mu(\lambda)}} + \frac{e^{-\beta\hbar\mu(\lambda)}}{1 - e^{-\beta\hbar\mu(\lambda)}} \right) \\ &= \frac{d}{d\lambda} \left(-\frac{3\vartheta}{2} \ln(m\nu_0^2 + \lambda^2 K_0^2) + \frac{3}{2} \vartheta \ln(1 - e^{-\beta\hbar\mu(\lambda)}) + \frac{3}{2} \vartheta \ln(e^{\beta\hbar\mu(\lambda)} - 1) \right). \end{aligned}$$

Therefore^f

$$F_{\text{int}} = -3\vartheta \ln \left(\frac{m + K_0^2/\nu_0^2}{m} \right)^{1/2} + \frac{3\hbar}{2} (\mu - \nu_0) - 3\vartheta \ln \frac{1 - e^{-\beta\hbar\nu_0}}{1 - e^{-\beta\hbar\mu}}, \quad (1.58)$$

where

$$\mu = \left(\nu_0^2 + \frac{K_0^2}{m} \right)^{1/2} \equiv \mu(\lambda = 1).$$

As we have seen by now, all considered Green functions and correlation functions relating to the particle S , as well as the free energy F_{int} , are determined by one and the same function $E(\nu)$. The influence of the phonon field upon these quantities depends exclusively on this spectral intensity $E(\nu)$.

Thus, if we had two different systems of oscillators interacting with the given particle S (in the manner considered), for which the function $E(\nu)$ was one and the same, then all relevant quantities, mentioned above, would remain unchanged.

To illustrate this statement, it is worth considering a two-body problem, for example

$$H = \frac{\mathbf{p}^2}{2m} + \frac{K_0^2}{2} (\mathbf{r} - \mathbf{R})^2 + \frac{\mathbf{P}^2}{2M} = \sum_{\alpha=1}^3 H_{\alpha}, \quad (1.59)$$

where

$$H_{\alpha} = \frac{p_{\alpha}^2}{2m} + \frac{K_0^2}{2} (r_{\alpha} - R_{\alpha})^2 + \frac{P_{\alpha}^2}{2M},$$

and the corresponding “one-body” free Hamiltonians are:

$$H_S = \frac{\mathbf{p}^2}{2m} = \frac{1}{2m} \sum_{\alpha=1}^3 p_{\alpha}^2,$$

$$H_{\Sigma} = \frac{\mathbf{P}^2}{2M} + \frac{K_0^2}{2} \mathbf{R}^2 = \sum_{\alpha=1}^3 \left(\frac{P_{\alpha}^2}{2M} + \frac{K_0^2}{2} R_{\alpha}^2 \right).$$

^f Here we have used the fact that

$$\begin{aligned} & \frac{3}{2} \vartheta \int_0^1 d\lambda \frac{d}{d\lambda} \left\{ \ln(1 - e^{-\beta\hbar\mu(\lambda)}) + \ln(e^{\beta\hbar\mu(\lambda)} - 1) \right\} \\ &= \frac{3}{2} \vartheta \left(\ln \frac{e^{\beta\hbar\mu} - 1}{e^{\beta\hbar\nu_0} - 1} + \ln \frac{e^{\beta\hbar\mu} - 1}{e^{\beta\hbar\nu_0} - 1} \right) \\ &= \frac{3}{2} \vartheta \left(\ln \frac{1 - e^{-\beta\hbar\mu}}{1 - e^{-\beta\hbar\nu_0}} + \ln \frac{e^{\beta\hbar\mu} e^{-\beta\hbar\nu_0} (1 - e^{-\beta\hbar\mu})}{1 - e^{-\beta\hbar\nu_0}} \right) \\ &= -3\vartheta \ln \frac{1 - e^{-\beta\hbar\nu_0}}{1 - e^{-\beta\hbar\mu}} + \frac{3\hbar}{2} (\mu - \nu_0). \end{aligned}$$

We shall calculate explicitly the free energy

$$F_{\text{int}} = -\vartheta \ln \frac{\text{Tr } e^{-\beta H}}{\text{Tr}_{(S)} e^{-\beta H_S} \text{Tr}_{(\Sigma)} e^{-\beta H_\Sigma}} = -3\vartheta \ln \frac{\text{Tr } e^{-\beta \mathcal{H}}}{\text{Tr}_{(S)} e^{-\beta \mathcal{H}_S} \text{Tr}_{(\Sigma)} e^{-\beta \mathcal{H}_\Sigma}},$$

where the one-dimensional Hamiltonians $\mathcal{H}$, $\mathcal{H}_S$ and $\mathcal{H}_\Sigma$ are given by the following expressions:

$$\begin{aligned} \mathcal{H} &= \frac{p^2}{2m} + \frac{K_0^2}{2} (x - X)^2 + \frac{1}{2M} P^2, \\ \mathcal{H}_S &= \frac{p^2}{2m}, \quad \mathcal{H}_\Sigma = \frac{P^2}{2M} + \frac{K_0^2}{2} X^2. \end{aligned}$$

To diagonalize the one-dimensional Hamiltonian $\mathcal{H}$, we introduce normal coordinates q , Q and corresponding normal momentum variables y , Y :

$$q = \frac{mx + MX}{m + M}, \quad Q = x - X. \quad (1.58a)$$

Noting that

$$\frac{\partial}{\partial x} = \frac{m}{m + M} \frac{\partial}{\partial q} + \frac{\partial}{\partial Q}, \quad (1.58b)$$

$$\frac{\partial}{\partial X} = \frac{M}{m + M} \frac{\partial}{\partial q} - \frac{\partial}{\partial Q},$$

we put

$$p = \frac{m}{m + M} y + Y, \quad P = \frac{M}{m + M} y - Y. \quad (1.58c)$$

Substituting these results into (1.57), we arrive at the canonically transformed Hamiltonian

$$H = \frac{1}{2(m + M)} y^2 + \frac{1}{2} \frac{M + m}{Mm} Y^2 + \frac{K_0^2}{2} Q^2 = H_{\text{in}} + H_{\text{osc}}, \quad (1.61)$$

where

$$H_{\text{in}} = \frac{y^2}{2(m + M)}, \quad H_{\text{osc}} = \frac{1}{2} \frac{M + m}{Mm} Y^2 + \frac{K_0^2}{2} Q^2.$$

Thus

$$F_{\text{int}} = -3\vartheta \ln \frac{\text{Tr } e^{-\beta H_{\text{in}}}}{\text{Tr } e^{-\beta H_S}} - 3\vartheta \ln \frac{\text{Tr } e^{-\beta H_{\text{osc}}}}{\text{Tr } e^{-\beta H_\Sigma}}.$$

It is well known that the free energy of the oscillator H_Σ with the frequency $\nu_0 = (K_0^2/M)^{1/2}$ in the one-dimensional case is^g

$$F_\Sigma = \frac{\hbar\nu_0}{2} - \vartheta \ln \frac{1}{1 - e^{-\beta\hbar\nu_0}},$$

and because the oscillator H_{osc} has frequency

$$\mu = \left(\frac{K_0^2(M+m)}{Mm} \right)^{1/2} = \nu_0 \left(1 + \frac{M}{m} \right)^{1/2},$$

then F_{osc} is

$$F_{\text{osc}} = \frac{\hbar\mu}{2} - \vartheta \ln \frac{1}{1 - e^{-\beta\hbar\mu}}.$$

Therefore

$$F_{\text{int}} = -3\vartheta \ln \frac{\text{Tr } e^{-\beta H_{\text{in}}}}{\text{Tr } e^{-\beta H_S}} - 3\vartheta \ln \frac{1 - e^{-\beta\hbar\nu_0}}{1 - e^{-\beta\hbar\mu}} + \frac{3}{2} \hbar(\mu - \nu_0).$$

Because the position x belongs to the interval $-L/2 < x < L/2$, the corresponding momentum variable p can take only discrete values

$$\frac{2\pi}{L} n\hbar, \quad n = 0, \pm 1, \pm 2, \dots,$$

and

$$\begin{aligned} \frac{\text{Tr } e^{-\beta H_{\text{in}}}}{\text{Tr } e^{-\beta H_S}} &= \frac{\sum_{(n)} \exp \left\{ - \left(\frac{2\pi}{L} n\hbar \right)^2 \frac{\beta}{2(M+m)} \right\}}{\sum_{(n)} \exp \left\{ - \left(\frac{2\pi}{L} n\hbar \right)^2 \frac{\beta}{2m} \right\}} \\ &\xrightarrow{L \rightarrow \infty} \frac{\frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} \exp \left(- \frac{\beta p^2}{2(M+m)} \right) dp}{\frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} \exp \left(- \frac{\beta p^2}{2m} \right) dp} = \left(\frac{m+M}{m} \right)^{1/2}. \end{aligned}$$

Finally, we obtain the expression for the free energy:

$$F_{\text{int}} = -3\vartheta \ln \left(\frac{m+M}{m} \right)^{1/2} - 3\vartheta \ln \frac{1 - e^{-\beta\hbar\nu_0}}{1 - e^{-\beta\hbar\mu}} + \frac{3}{2} \hbar(\mu - \nu_0).$$

^gFor the Hamiltonian

$$H = \frac{P^2}{2m} + \frac{m\omega^2 X^2}{2}$$

the free energy is given by the expression

$$F = \frac{\hbar\omega}{2} - \vartheta \ln (1 - e^{-\beta\hbar\omega}), \quad \vartheta = K_\beta T.$$

This expression coincides with (1.56) if one puts

$$\frac{K_0^2}{\nu_0^2} = M.$$

Observation. It is easy to obtain (1.34) for the correlator starting from the Hamiltonian of the two-body problem (1.57). Put

$$Y = i(a^\dagger - a) \left(\frac{\hbar \mathcal{M} \mu}{2} \right)^{1/2}, \quad Q = (a^\dagger + a) \left(\frac{\hbar}{2 \mathcal{M} \mu} \right)^{1/2}, \quad (1.62)$$

where $a, a^\dagger$ are Bose-amplitudes,

$$\mathcal{M} = \frac{Mm}{M+m}.$$

and the mass parameter μ is determined by (1.59):

$$\mu^2 = \frac{K_0^2}{\mathcal{M}}.$$

Further, we proceed with the oscillator Hamiltonian rewritten in new terms:

$$H_{\text{osc}} = \frac{\hbar \mu}{2} + \hbar \mu a^\dagger a,$$

and

$$\begin{aligned} i\hbar \frac{da}{dt} &= \hbar \mu a, & i\hbar \frac{da^\dagger}{dt} &= -\hbar \mu a^\dagger, \\ a(t) &= e^{-i\mu t} a, & a^\dagger(t) &= e^{i\mu t} a^\dagger, \end{aligned}$$

since

$$\frac{dy}{dt} = 0, \quad y = \text{const.}$$

It follows from (1.58a) that

$$p_\alpha(t) = \frac{m}{m+M} y + i(a^\dagger e^{i\mu t} - a e^{-i\mu t}) \left(\frac{\hbar \mathcal{M} \mu}{2} \right)^{1/2}. \quad (1.63)$$

From this,

$$\langle p_\alpha(t) p_\alpha(\tau) \rangle_{\text{eq}} = \left(\frac{m}{m+M} \right)^2 \langle y^2 \rangle_{\text{eq}} + \frac{\hbar \mathcal{M} \mu}{2} (\langle a a^\dagger \rangle e^{-i\mu(t-\tau)} + \langle a^\dagger a \rangle e^{i\mu(t-\tau)}). \quad (1.64)$$

But

$$\begin{aligned} \langle y^2 \rangle_{\text{eq}} &= (m+M) \vartheta, \\ \langle a a^\dagger \rangle &= \frac{1}{1 - e^{-\beta \hbar \mu}}, & \langle a^\dagger a \rangle &= \frac{1}{e^{\beta \hbar \mu} - 1}, & \mathcal{M} \mu &= \frac{\mathcal{M} \mu^2}{\mu} = \frac{K_0^2}{\mu}, \end{aligned}$$

and we arrive at the same equation (1.34) as before.

Therefore we come to the conclusion that two-time equilibrium correlation functions of the particle S variables are the same for the Hamiltonian (1.1) in the single-frequency case to $\nu(f) = \nu_0$ and when

$$E(\omega) = \frac{K^2}{2} [\delta(\omega - \nu_0) + \delta(\omega + \omega_0)],$$

as in the case of the two-body problem Hamiltonian (1.57).

We now return to the expression for the free energy F_{int} in the single-frequency case and consider the passage to classical mechanics. By setting $\hbar \rightarrow 0$, in (1.56), we get the classical result for the free energy:

$$F_{\text{int}} = 0.$$

It is obvious that the part of the free energy that is due to interaction is always zero in classical mechanics for dynamical systems described by a Hamiltonian of the kind (1.1) in the case $K^2 = K_0^2 + \eta^2$. This statement can be proved starting from (1.53), which can be rewritten as

$$\left\langle \frac{\partial H(\lambda)}{\partial \lambda} \right\rangle_{\lambda, \text{eq}} = -\frac{3i\hbar}{2\pi} \int_{-\infty}^{+\infty} \frac{\Omega}{1 - e^{-\beta\hbar\Omega}} \frac{\lambda\Delta(\Omega)}{m\Omega^2 - \eta^2 + \lambda^2\Omega\Delta(\Omega)} \Big|_{\omega-i0}^{\omega+i0} d\omega, \quad (1.65)$$

where

$$0 < \varepsilon < \frac{2\pi}{\hbar\beta}.$$

In the classical limit,

$$\lim_{\hbar \rightarrow 0} \frac{\hbar\Omega}{1 - e^{-\beta\hbar\Omega}} = \frac{1}{\beta} = \vartheta.$$

Consequently, it is true for the classical mechanics that

$$\left\langle \frac{\partial H(\lambda)}{\partial \lambda} \right\rangle_{\lambda, \text{eq}} = -\frac{3i\vartheta}{2\pi} \left(\int_{i\varepsilon-\infty}^{i\varepsilon+\infty} F(\Omega) d\Omega - \int_{-i\varepsilon-\infty}^{-i\varepsilon+\infty} F(\Omega) d\Omega \right), \quad (1.66)$$

where

$$F(\Omega) = \frac{\lambda\Delta(\Omega)}{m\Omega^2 - \eta^2 + \lambda^2\Omega\Delta(\Omega)}. \quad (1.67)$$

It should be observed that $F(\Omega)$ is a regular analytic function on the half-plane

$$\text{Im}(\Omega) \geq \varepsilon > 0.$$

Thus

$$\int_{\mathcal{L}} F(\Omega) d\Omega = 0 \quad (1.68)$$

for any closed contour $\mathcal{L}$ lying in this half-plane. Let us take for $\mathcal{L}$ the contour composed of the interval $(i\varepsilon - L, i\varepsilon + L)$ and the half-circle C

Fig. 1.2.

Fig. 1.3.

with center at the point $i\varepsilon$ and of radius L (see Fig. 1.2). On this contour,

$$F(\Omega) = \mathcal{O}\left(\frac{1}{L^2}\right),$$

so we can see that

$$\int_C F(\Omega) d\Omega = \mathcal{O}\left(\frac{1}{L}\right) \rightarrow 0.$$

Therefore

$$\int_{i\varepsilon-\infty}^{i\varepsilon+\infty} F(\Omega) d\Omega = 0.$$

The same considerations may be applied to prove that

$$\int_{-i\varepsilon-\infty}^{-i\varepsilon+\infty} F(\Omega) d\Omega.$$

In fact, $F(\Omega)$ — is a regular analytic function on the lower half-plane

$$\text{Im } \Omega \leq -\varepsilon < 0.$$

Therefore it is sufficient to choose the proper contour (see Fig. 1.3) and to repeat all the previous reasoning.

Thus, taking (1.50) and (1.64) into account, we have

$$F_{\text{int}} = 0.$$

It should be stressed that this result follows entirely from the treatment of the dynamical system within the framework of classical mechanics.

In the opposite, quantum mechanical case, (1.63) indicates that the function

$$F(\Omega) = \frac{\hbar\Omega}{1 - e^{-\beta\hbar\Omega}} \frac{\lambda\Delta(\Omega)}{m\Omega^2 - \eta^2 + \lambda^2\Omega\Delta(\Omega)}$$

has an infinite number of poles on the imaginary axis:

$$\Omega = \frac{2\pi i n}{\hbar\beta}, \quad \text{for } n \text{ integer}, \quad (1.69)$$

and for this reason integrals of the type (1.66) are not equal to zero (they are equal to the sum of residues taken at the poles (1.67)).

1.5. Average Values of T-products

Consider now equilibrium averages of the operator products

$$\langle T \{ [r_\alpha(t) - r_\alpha(\tau)] [r_{\alpha'}(t) - r_{\alpha'}(\tau)] \} \rangle_{\text{eq}},$$

where T denotes the “T-product” (i.e. the product of operators ordered in time). By definition,

$$T\{A(t_1)B(t_2)\} = \begin{cases} A(t_1)B(t_2), & t_1 > t_2, \\ B(t_2)A(t_1), & t_2 > t_1. \end{cases} \quad (1.70)$$

Because

$$\begin{aligned} [r_\alpha(t) - r_\alpha(\tau)] [r_{\alpha'}(t) - r_{\alpha'}(\tau)] \\ = r_\alpha(t)r_{\alpha'}(t) - r_\alpha(\tau)r_{\alpha'}(t) - r_\alpha(t)r_{\alpha'}(\tau) + r_\alpha(\tau)r_{\alpha'}(\tau), \end{aligned}$$

the following relation holds:

$$\begin{aligned} T \{ [r_\alpha(t) - r_\alpha(\tau)] [r_{\alpha'}(t) - r_{\alpha'}(\tau)] \} \\ = \begin{cases} r_\alpha(t)r_{\alpha'}(t) - r_{\alpha'}(t)r_\alpha(\tau) - r_\alpha(t)r_{\alpha'}(\tau) + r_\alpha(\tau)r_{\alpha'}(\tau), & t > \tau, \\ r_\alpha(t)r_{\alpha'}(t) - r_\alpha(\tau)r_{\alpha'}(t) - r_{\alpha'}(\tau)r_\alpha(t) + r_\alpha(\tau)r_{\alpha'}(\tau), & t < \tau. \end{cases} \end{aligned}$$

Therefore, putting $\lambda = 1$ in (1.52), we get

$$\langle T \{ [r_\alpha(t) - r_\alpha(\tau)] [r_{\alpha'}(t) - r_{\alpha'}(\tau)] \} \rangle_{\text{eq}} = 0 \quad \text{if } \alpha \neq \alpha'$$

and

$$\begin{aligned} \langle T \{ [r_\alpha(t) - r_\alpha(\tau)]^2 \} \rangle_{\text{eq}} \\ = \frac{i\hbar}{2\pi} \int_{-\infty}^{+\infty} \frac{2(1 - e^{-i\omega(t-\tau)})}{1 - e^{-\beta\hbar\omega}} \frac{1}{m\Omega^2 - \eta^2 + \Omega\Delta(\Omega)} \Big|_{\omega-i0}^{\omega+i0} d\omega \quad \text{if } t > \tau, \end{aligned}$$

$$\begin{aligned} \langle T \{ [r_\alpha(t) - r_\alpha(\tau)]^2 \} \rangle_{\text{eq}} \\ = \frac{i\hbar}{2\pi} \int_{-\infty}^{+\infty} \frac{2(1 - e^{-i\omega(\tau-t)})}{1 - e^{-\beta\hbar\omega}} \frac{1}{m\Omega^2 - \eta^2 + \Omega\Delta(\Omega)} \Big|_{\omega-i0}^{\omega+i0} d\omega \quad \text{if } t < \tau. \end{aligned}$$

Thus

$$\begin{aligned} \langle T \{ [r_\alpha(t) - r_\alpha(\tau)]^2 \} \rangle_{\text{eq}} \\ = \frac{i\hbar}{2\pi} \int_{-\infty}^{+\infty} \frac{2(1 - e^{-i\omega|t-\tau|})}{1 - e^{-\beta\hbar\omega}} \frac{1}{m\Omega^2 - \eta^2 + \Omega\Delta(\Omega)} \Big|_{\omega-i0}^{\omega+i0} d\omega. \quad (1.71) \end{aligned}$$

For some applications it is helpful to be able to calculate the ordered products of operators depending on an “imaginary-time” argument.

Setting $t = -is$ and choosing real s to be the ordering parameter, we define the T-product as

$$T\{r_\alpha(-is)r_{\alpha'}(-i\sigma)\} = \begin{cases} r_\alpha(-is)r_{\alpha'}(-i\sigma) & \text{if } s > \sigma, \\ r_{\alpha'}(-i\sigma)r_\alpha(-is) & \text{if } \sigma > s. \end{cases}$$

Taking (1.52) into account under the condition $\lambda = 1$, one obtains

$$\langle T\{[r_\alpha(-is) - r_\alpha(-i\sigma)][r_{\alpha'}(-is) - r_{\alpha'}(-i\sigma)]\} \rangle_{\text{eq}} = 0 \quad (1.72)$$

if $\alpha \neq \alpha'$, and, in the opposite case,

$$\begin{aligned} & \langle T\{[r_\alpha(-is) - r_\alpha(-i\sigma)]^2\} \rangle_{\text{eq}} \\ &= \frac{i\hbar}{2\pi} \int_{-\infty}^{+\infty} \frac{2(1 - e^{-\omega|s-\sigma|})}{1 - e^{-\beta\hbar\omega}} \frac{1}{m\Omega^2 - \eta^2 + \Omega\Delta(\Omega)} \Big|_{\omega-i0}^{\omega+i0} d\omega. \end{aligned} \quad (1.73)$$

Consider the single-frequency case:

$$E(\omega) = \frac{K_0^2}{2} \{\delta(\omega - \nu_0) + \delta(\omega + \nu_0)\}.$$

Here we are not allowed to use (1.69) and (1.71) directly, observing from the very start that the final result would be just the same as in the case of the two-body model (1.57). Rigorously speaking, we mean that

$$\langle r_\alpha(t)r_\alpha(\tau) \rangle_{\text{eq}} = \langle x(t)x(\tau) \rangle_{\text{eq}}.$$

It follows from (1.58) that

$$x = q + \frac{M}{m+M} Q.$$

Since the time evolution of $q(t)$ and $Q(t)$ is generated by independent Hamiltonians H_{in} and H_{osc} respectively (see (1.59)), we have the equality

$$\langle x(t)x(\tau) \rangle_{\text{eq}} = \langle q(t)q(\tau) \rangle_{\text{eq}} + \frac{M^2}{(m+M)^2} \langle Q(t)Q(\tau) \rangle_{\text{eq}}.$$

From which

$$\begin{aligned} \langle T\{[r_\alpha(-is) - r_\alpha(-i\sigma)]^2\} \rangle_{\text{eq}} &= \langle T\{[q(-is) - q(-i\sigma)]^2\} \rangle_{\text{eq}} \\ &+ \frac{M^2}{(m+M)^2} \langle T\{(Q(-is) - Q(-i\sigma))^2\} \rangle_{\text{eq}} \end{aligned} \quad (1.74)$$

Thanks to (1.59),

$$\begin{aligned} q(t) - q(\tau) &= \frac{(t - \tau)}{(M + m)} y, \quad y = \text{const}, \\ \langle y^2 \rangle_{\text{eq}} &= (M + m)\vartheta. \end{aligned}$$

Hence

$$\langle [q(t) - q(\tau)]^2 \rangle_{\text{eq}} = \frac{(t - \tau)^2 \vartheta}{M + m}. \quad (1.75)$$

We also have

$$\begin{aligned} q(t)q(\tau) - q(\tau)q(t) &= \int_{\tau}^t \{q'(t)q(\tau) - q(\tau)q'(t)\} dt \\ &= \frac{1}{M+m} \int_{\tau}^t \{yq(\tau) - q(\tau)y\} dt = \frac{t-\tau}{M+m} (yq - qy) = -i\hbar \frac{t-\tau}{M+m}. \end{aligned} \quad (1.76)$$

Consequently,

$$\begin{aligned} \langle T\{[q(-is) - q(-i\sigma)]^2\} \rangle_{\text{eq}} &= \langle q^2(-is) - 2q(-is)q(-i\sigma) + q^2(-i\sigma) \rangle_{\text{eq}} \\ &= \langle [q(-is) - q(-i\sigma)]^2 \rangle_{\text{eq}} \\ &\quad + \langle -q(-is)q(-i\sigma) + q(-i\sigma)q(-is) \rangle_{\text{eq}} \quad \text{if } s > \sigma, \end{aligned}$$

and, thanks to (1.73) and (1.74),

$$\begin{aligned} \langle T\{[q(-is) - q(-i\sigma)]^2\} \rangle_{\text{eq}} &= -\frac{(s-\sigma)^2}{M+m} \vartheta + \frac{\hbar}{M+m} (s-\sigma) \quad \text{for } s > \sigma. \end{aligned}$$

Making the permutation $s \xrightarrow{\sim} \sigma$, it is easy to show that

$$\langle T\{[q(-is) - q(-i\sigma)]^2\} \rangle_{\text{eq}} = -\frac{(s-\sigma)^2}{M+m} \vartheta + \frac{\hbar}{M+m} |s-\sigma|. \quad (1.77)$$

We must now find an explicit expression for the ordered correlator

$$\langle T\{[Q(-is) - Q(-i\sigma)]^2\} \rangle_{\text{eq}},$$

in order to calculate the left-hand side of (1.72). Let us note that

$$Q(t) = (e^{i\mu t} a^{\dagger} + e^{-i\mu t} a) \left(\frac{\hbar}{2\mathcal{M}\mu} \right)^{1/2},$$

from which it follows that

$$\begin{aligned} \langle T\{[Q(-is) - Q(-i\sigma)]^2\} \rangle_{\text{eq}} &= \frac{\hbar}{2\mathcal{M}\mu} \{ (e^{\mu s} a^{\dagger} + e^{-\mu s} a)(e^{\mu s} a^{\dagger} + e^{-\mu s} a) \\ &\quad + (e^{\mu \sigma} a^{\dagger} + e^{-\mu \sigma} a)(e^{\mu \sigma} a^{\dagger} + e^{-\mu \sigma} a) - 2T(e^{\mu s} a^{\dagger} + e^{-\mu s} a)(e^{\mu \sigma} a^{\dagger} + e^{-\mu \sigma} a) \}. \end{aligned}$$

Hence

$$\begin{aligned} \langle T\{[Q(-is) - Q(-i\sigma)]^2\} \rangle_{\text{eq}} &= \frac{\hbar}{2\mathcal{M}\mu} (2\langle a^{\dagger} a \rangle + 2\langle a a^{\dagger} \rangle - 2e^{\mu|s-\sigma|} \langle a^{\dagger} a \rangle - 2e^{-\mu|s-\sigma|} \langle a a^{\dagger} \rangle). \end{aligned} \quad (1.78)$$

Here

$$\langle a^{\dagger} a \rangle = \frac{1}{e^{\beta\hbar\mu} - 1}, \quad \langle a a^{\dagger} \rangle = 1 + \frac{1}{e^{\beta\hbar\mu} - 1}.$$

Since

$$\frac{1}{m+M} = \frac{1}{Mm} \mathcal{M} = \frac{K_0^2}{\mu^2 M m} = \left(\frac{\nu_0}{\mu}\right)^2 \frac{1}{m}$$

(recalling that $\mathcal{M} = mM/(m+M)$) and

$$\frac{M^2}{(m+M)^2} \frac{1}{\mathcal{M}\mu} = \frac{\mathcal{M}^2}{m^2} \frac{1}{\mathcal{M}\mu} = \frac{\mathcal{M}}{m^2 \mu} = \frac{K_0^2}{m^2 \mu^3} = \frac{\mu^2 - \nu_0^2}{m\mu^3},$$

we find from (1.72), (1.75) and (1.76) that

$$\begin{aligned} \langle T\{[r_\alpha(-is) - r_\alpha(-i\sigma)]^2\} \rangle_{\text{eq}} \\ = - \left(\frac{\nu_0}{\mu}\right)^2 \frac{\vartheta}{m} (s - \sigma)^2 + \frac{\hbar}{m} \left(\frac{\nu_0}{m}\right)^2 |s - \sigma| \\ + \frac{\mu^2 - \nu_0^2}{m\mu^3} \hbar \left(\frac{1}{1 - e^{-\beta\hbar\mu}} (1 - e^{-\mu|s-\sigma|}) - \frac{1}{e^{\beta\hbar\mu} - 1} (e^{\mu|s-\sigma|} - 1) \right). \end{aligned} \quad (1.79)$$

It is interesting to note that

$$\langle T\{[r_\alpha(-is) - r_\alpha(-i\sigma)]^2\} \rangle_{\text{eq}} \geq 0 \quad \text{if} \quad |s - \sigma| \leq \beta\hbar = \hbar/\vartheta, \quad (1.80)$$

where $\beta = 1/\vartheta$ and $\vartheta = K_\beta T$.

1.6. Averaged Operator T-Product Calculus for Some Model Oscillatory Systems

Let the Hamiltonian Γ be a quadratic positive-definite form composed of Bose operators $b_\alpha, b_\alpha^\dagger$. We denote the statistical sum as

$$Z = \text{Tr } e^{-\beta\Gamma}$$

and consider linear forms composed of the Bose operators $b_\alpha, b_\alpha^\dagger$:

$$A_1, A_2, \dots, A_s,$$

and statistical averages consisting of the products of these linear forms:

$$\langle A_1 A_2 \cdots A_s \rangle_\Gamma = Z^{-1} e^{-\beta\Gamma} (A_1 A_2 \cdots A_s). \quad (1.81)$$

Let us apply to (1.79) the well-known Bloch–Dominicis theorem, which generalizes the Wick theorem. If we introduce couplings of the type

$$\overline{A_j A_l} = \langle A_j A_l \rangle_\Gamma,$$

we see that the expression (1.79) is equal to the sum of products of all possible couplings. For example,

$$\begin{aligned} \langle A_1 A_2 A_3 A_4 \rangle_\Gamma &= \langle \overline{A_1 A_2} \overline{A_3 A_4} \rangle_\Gamma + \langle \overline{A_1 A_2} \overline{A_3} \overline{A_4} \rangle_\Gamma + \langle \overline{A_1 A_2} \overline{A_3} \overline{A_4} \rangle_\Gamma \\ &= \langle A_1 A_2 \rangle_\Gamma \langle A_3 A_4 \rangle_\Gamma + \langle A_1 A_3 \rangle_\Gamma \langle A_2 A_4 \rangle_\Gamma + \langle A_1 A_4 \rangle_\Gamma \langle A_2 A_3 \rangle_\Gamma. \end{aligned} \quad (1.82)$$