QUANTUM MECHANICS OF INFINITE SYSTEMS AND MACROSCOPIC EVOLUTION EQUATIONS

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The quantum mechanics of infinite systems is formulated. The state of an infinite medium is defined in terms of a set of expectation values of products of ψ-operators. For noninteracting systems this reduces to prescribing a small number of functions which describe irreducible correlations and are expressible in terms of macroscopic quantities. The peculiarities of the dynamics of infinite systems are discussed briefly. The following adiabatic theorem is proved: If one removes the divergences that occurring at the interaction switch-on time $t_0 \to -\infty$ by means of renormalization of some quantities on which the initial state depends, then there exists a closed evolution equation for these quantities. This equation can be derived in a unique manner from the renormalization equations. The renormalized expressions represent states of the system with the interaction switched on. It is shown that this is true in the case of a nonideal gas and a Markovian kinetic equation is derived for the momentum-space density $n_{\mathbf{k}}$, valid in all orders of perturbation theory. This equation, as well as the expressions of the expectation values in states with given $n_{\mathbf{k}}$ are written in the form of sums over a certain class of diagrams.

THE problem of the relation between exact macroscopic equations of motion and macroscopic evolution equations is discussed in the present paper with the kinetic equations as an example. Although decisive progress has been achieved in the understanding of this problem, mainly related to the names Bogolyubov, van Hove, Prigogine, and others (cf. the review[1]), there still remain a few unclear questions. In particular, the kinetic equations derived by van Hove and Prigogine are Markovian only up to second order in the coupling constant, and in Bogolyubov's method[2] (to which our approach is closest in all respects) the higher approximations are hard to survey.

The approach to be developed below is based on taking explicitly into account two circumstances (which were stressed with full clarity already by van Hove[3]): a) equations in closed form for quantities describing the average behavior exist only for infinite systems, in the limits $N \to \infty$ and $V \to \infty$ (N is the number of particles and V is the volume); b) such equations are valid only for a selected class of states, but not for an arbitrary state. Our approach yields a complete characterization of this class of states. Thus, kinetic equations are valid only for those states of a nonideal gas which can be obtained from states of an ideal gas by means of adiabatic switching-on of the interaction. Our derivation of the kinetic equations is based upon an adiabatic theorem, the formulation and proof of which the author considers to be the fundamental result of this paper. It should be remarked that the use of this approach allows one to derive Markovian equations in any order of perturbation theory, and for the formalisms of Prigogine and van Hove. Moreover, this approach could be extended almost to all problems related to the derivation of equations in closed form for quantities which give an incomplete description.

Circumstance a) is explicitly taken into account by taking the limits $N \to \infty$, $V \to \infty$ already in the formulation of the problem. This is achieved by formulating quantum mechanics for the limiting case of an infinite system (with infinite N and V). Mathematical objects that describe such limiting concepts are often used in physics; it is hard to imagine how much more complicated scattering problems would become, for example, if we tried to avoid functions like e^{ikx}, $\delta(x)$ etc. (which do not belong to the Hilbert space), and would solve such problems for a finite V, letting V go to infinity only at the end of the computations.

It is natural to think that if one introduces a mathematical scheme for a limiting concept—like the concept of an infinite medium—the concepts and behavior characteristic for a many-particle system should appear in the most natural manner. Such a formulation is sketched in Sec. 1, where answers

to the following questions can be found: i) How should physical quantities and states of an infinite medium be described? ii) How should one formulate equations of motion for these quantities? Of course, our formulations will only formalize mathematically concepts which have arisen as a result of work carried out over the past decades. However, an analysis of the consequences of these definitions (on which, unfortunately, we cannot dwell here) leads to a series of curious results (which do not seem to be general knowledge). (For instance, the fact that for an infinite system there is no distinction between pure states, described by a state vector, and mixtures, described by a density matrix; the distinction gets lost in the limiting process $N \to \infty$, $V \to \infty$.)

The definitions to be introduced also allow to formulate clearly all other problems (which are not discussed in this paper) of the quantum mechanics of infinite media (e.g. the problem of excited states and their energy spectrum, transition probabilities, etc.). Thus, for example, one-particle excitations are described by the function $\rho(\mathbf{r}_1, \mathbf{r}_2; t)$ (the density matrix of the added particle), which in the presence of damping cannot be reduced to a product $\psi^+(\mathbf{r}, t)\psi(\mathbf{r}, t)$, transition probabilities cannot be reduced to matrix elements, etc. The author hopes to return to these problems in the future.

1. DESCRIPTION OF STATES AND THE DYNAMICS OF AN INFINITE MEDIUM

1. We first discuss the nature of the mathematical objects which define the state of an infinite medium.

We denote the operators of second quantization by $\psi_\pm(\mathbf{r})$, where $\psi_-(\mathbf{r})$ is the destruction operator (usually denoted by $\psi(\mathbf{r})$), and $\psi_+(\mathbf{r})$ is its adjoint, the creation operator. Let p denote the variable which takes on the two values + and −; we use the notation

$$\psi_p(\mathbf{r}) = \begin{cases} \psi_+(\mathbf{r}) & \text{for } p = + \\ \psi_-(\mathbf{r}) & \text{for } p = - \end{cases}$$

In these notations a general operator can be written in the form

$$\hat{A} = \sum_{(n)} \sum_{p_1 \dots p_n} \int \dots \int \alpha_{p_1 \dots p_n}(\mathbf{r}_1, \dots, \mathbf{r}_n) \times \psi_{p_1}(\mathbf{r}_1) \dots \psi_{p_n}(\mathbf{r}_n)\, d\mathbf{r}_1 \dots d\mathbf{r}_n. \tag{1}$$

We call local those physical quantities for which the values depend only on the state of the system in a bounded region of space surrounding a point. Obviously, such quantities are described by operators of the form (1), where the functions $\alpha_{p_1 \dots p_n}(\mathbf{r}_1, \dots, \mathbf{r}_n)$ are either functions of compact support (i.e., vanishing identically outside a bounded region), or functions which vanish sufficiently rapidly as $|\mathbf{r}_i| \to \infty$. Such functions will be called rapidly decreasing and the fact that $\alpha(\mathbf{r}_1, \dots, \mathbf{r}_n)$ is a rapidly decreasing function will be denoted in the following manner

$$\alpha(\mathbf{r}_1, \dots, \mathbf{r}_n) \to 0 \quad (\mathbf{r}_1, \dots, \mathbf{r}_n \to \infty). \tag{2}$$

Operators (1) for which condition (2) is satisfied will be called local operators.

The density matrix of an infinite system must be capable of describing the properties of a real (finite) system insofar as measurements are concerned which are carried out far from the boundaries of the finite system. Such measurements reduce to the determination of expectation values of local physical quantities. Therefore one can assume that if the sequence of density matrices ρ_m describing the finite systems (with finite particle number N_m and volume V_m) approximates the state of an infinite system with definite properties, then for any local operator there exists the limit

$$\lim_{m \to \infty} \mathrm{Sp}(\hat{A}\hat{\rho}_m) = \langle \hat{A} \| \rho \rangle \quad (N_m \to \infty, \quad V_m \to \infty) \tag{3}$$

(the limiting procedure must be described unequivocally).

The limit (3) can be treated as the expectation value of the operator A in a state of the infinite system. Obviously, if the expectation values for every A are given, the state of the infinite system will be completely determined. It is sufficient to define the functions

$$\langle \psi_{p_1}(\mathbf{r}_1) \dots \psi_{p_n}(\mathbf{r}_n) \| \rho \rangle \tag{4}$$

or rules for the computation of these functions; then the expectation value (3) becomes

$$\langle \hat{A} \| \rho \rangle = \sum_{(n)} \sum_{p_1 \dots p_n} \int \dots \int \alpha_{p_1 \dots p_n}(\mathbf{r}_1, \dots, \mathbf{r}_n) \times \langle \psi_{p_1}(\mathbf{r}_1) \dots \psi_{p_n}(\mathbf{r}_n) \| \rho \rangle\, d\mathbf{r}_1, \dots, d\mathbf{r}_n \tag{5}$$

(the integrals converge by virtue of (2)).

The expectation values (5) must satisfy certain conditions (compatibility with the commutation relations and nonnegativity of the expectation values of operators of the form $\hat{A}^+\hat{A}$, where $\hat{A}^+$ is the adjoint of $\hat{A}$). The limits (3) satisfy these conditions, and conversely, one may assume that any linear functional (5) defined on the local operators $\hat{A}$ (of the form (1), (2)) and satisfying these additional conditions represents a state of the infinite system, i.e., is a limit of the type (3) for some sequence of density matrices $\hat{\rho}_m$. Such positive linear functionals will be called quantum-mechanical distri-

butions, or simply distributions;* we assume that these mathematical objects can serve for the definition of a density matrix of the infinite system.

2. We consider an example of distributions with which we deal throughout this paper. We define the distributions $\|n_{\mathbf{k}}\rangle = \|\mathbf{n}\rangle$, depending on a function of the wave vector $\mathbf{k}$ which we denote either by $n_{\mathbf{k}}$ or, omitting the independent variable, by $\mathbf{n}$ (in boldface and without the argument)[1]. We call this function the momentum-space density. The distributions $\|\mathbf{n}\rangle$ are described by the following W($\mathbf{n}$) rule, which is a generalization of Wick's rule:

The W($\mathbf{n}$) rule: The expectation values

$$\langle \psi_{p_1}(\mathbf{r}_1)\dots\psi_{p_n}(\mathbf{r}_n)\|\mathbf{n}\rangle \tag{6}$$

are nonzero only for such products of ψ-operators which can be split up into pairs consisting of one ψ_+ and one ψ_-. In this case one must list all possible partitions and associate to each partition a contribution equal to the product of functions obtained by replacing each pair $\psi_{\pm}(\mathbf{r}_i)\psi_{\mp}(\mathbf{r}_j)$ by a function of $\mathbf{r}_i$ and $\mathbf{r}_j$ called the pairing function (contraction). Then (6) is the sum of contributions from all partitions, and in the case of fermion operators the contribution from each partition must be taken with the appropriate sign, as in the usual Wick rules.

The pairing functions (pairings, or contractions) have the form[2]

$$\overline{\psi_+(\mathbf{r})\psi_-(\mathbf{r}')} = \int e^{-i\mathbf{k}(\mathbf{r}-\mathbf{r}')}\,\overline{\psi_+\psi_-}(\mathbf{k})\,d\mathbf{k},$$
$$\overline{\psi_-(\mathbf{r})\psi_+(\mathbf{r}')} = \int e^{i\mathbf{k}(\mathbf{r}-\mathbf{r}')}\,\overline{\psi_-\psi_+}(\mathbf{k})\,d\mathbf{k} \tag{7}$$

(the operators in the pairing appear in the same order as in (6)). In (7) we adopt the notations

$$\overline{\psi_+\psi_-}(\mathbf{k}) = n_{\mathbf{k}}, \quad \overline{\psi_-\psi_+}(\mathbf{k}) = 1 + \gamma n_{\mathbf{k}}, \tag{8}$$

and also (henceforth to be used throughout)

$$\gamma = \begin{cases} +1 & \text{for Bose-statistics} \\ -1 & \text{for Fermi-statistics,} \end{cases} \tag{9}$$

$$d\mathbf{k} = \frac{dk_x\,dk_y\,dk_z}{(2\pi)^3}. \tag{10}$$

One can show that the expectation values with respect to the distribution $\|\mathbf{n}\rangle$ are obtained from the expectation values for states of an ideal gas by means of a limiting procedure. Let $|\Phi_m\rangle$ denote a sequence of states of an ideal gas, obtained by filling the one-particle levels in a volume V_m. We denote by $L(V_m, \mathbf{k}, \Delta k) = V(2\pi)^{-3}\Delta k$ the number of such levels per volume Δk of the momentum space, and by $N_m(k, \Delta k)$ the number of particles which are in the state $|\Phi_m\rangle$ and are situated on these levels. We now consider such sequences of $|\Phi_m\rangle$ which for $m \to \infty$ have a definite limit, equal to $n_{\mathbf{k}}d\mathbf{k}$, for the number of particles per unit volume with momenta between $\mathbf{k}$ and $\mathbf{k} + d\mathbf{k}$, i.e.,

$$\lim_{m\to\infty}[N_m(\mathbf{k};\Delta k)/L(V_m;\mathbf{k},\Delta k)] = n_{\mathbf{k}}$$

or

$$\lim_{m\to\infty}[N_m(\mathbf{k},\Delta k)/V_m] = n_{\mathbf{k}}\Delta k/(2\pi)^3. \tag{11}$$

Here $n_{\mathbf{k}}$ is a function of $\mathbf{k}$ which is integrable for $|\mathbf{k}| \to \infty$ without non-integrable singularities (the density $\lim(N/V) = n_{\mathbf{k}}d\mathbf{k}$ must be finite); $n_{\mathbf{k}} \geq 0$ for a boson gas and $1 \geq n_{\mathbf{k}} \geq 0$ for a fermion gas. Then one can show that for sequences $|\Phi_m\rangle$ satisfying the conditions (11), the expectation value of any local operator $\hat{A}$ in the states $|\Phi_m\rangle$ converges to a well-defined limit for $m \to \infty$, and this limit is the expectation value of the operator $\hat{A}$ with respect to the distribution $\|n_{\mathbf{k}}\rangle$:

$$\lim_{m\to\infty}\langle\Phi_m|\hat{A}|\Phi_m\rangle = \langle A\|n_{\mathbf{k}}\rangle. \tag{12}$$

In other words, in the limit $N \to \infty$, $V \to \infty$ Wick's theorem is valid for the expectation values in each state of an ideal gas, whereas for a finite volume the theorem holds only for expectation values with respect to the Gibbs distribution (ensemble) (cf.[4]).

In order to exhibit the significance of $n_{\mathbf{k}}$ as a momentum space density, without resorting to a limiting process, it is necessary to define the momentum space density for an arbitrary distribution $\|\rho\rangle$ and to show that for the distribution $\|n_{\mathbf{k}}\rangle$ it turns out to be equal to $n_{\mathbf{k}}$. If $\|\rho\rangle$ is a spatially homogeneous (translation-invariant) state, the functions (4) will be translation invariant). In particular, $\langle\psi_+(\mathbf{r}_1)\psi_-(\mathbf{r}_2)\|\rho\rangle$ will depend only on the difference $\mathbf{r}_1 - \mathbf{r}_2$ and can be represented in the form

$$\langle\psi_+(\mathbf{r}_1)\psi_-(\mathbf{r}_2)\|\rho\rangle = \int d\mathbf{k}\,\nu(\mathbf{k})\exp\{-i\mathbf{k}(\mathbf{r}_1-\mathbf{r}_2)\}.$$

The function $\nu(\mathbf{k})$ is easily seen to be the momentum-space density corresponding to the distribution $\|\rho\rangle$; for a spatially-inhomogeneous state one must take the Fourier transform with respect to $\mathbf{r}_1 - \mathbf{r}_2$ of the function

$$\nu(\mathbf{r}_1 - \mathbf{r}_2) = \lim_{\mathbf{r}\to\infty}\langle\psi_+(\mathbf{r}_1+\mathbf{r})\psi_-(\mathbf{r}_2+\mathbf{r})\|\rho\rangle.$$

*Not to be confused with "distributions" in the sense of L. Schwartz, i.e. generalized functions. The term "ensemble" would be more usual. (Translator's note).

[1] This notation will be used whenever it is convenient to consider the function $n_{\mathbf{k}}$ as a vector in an infinite-dimensional function space.

[2] For simplicity we omit the spin indices.

Thus, the momentum-space density of the distribution $\|\rho\rangle$ equals

$$\int d(\mathbf{r}_1-\mathbf{r}_2)\exp\{i\mathbf{k}(\mathbf{r}_1-\mathbf{r}_2)\}\lim_{\mathbf{r}\to\infty}\langle\psi_+(\mathbf{r}_1+\mathbf{r})\psi_-(\mathbf{r}_2+\mathbf{r})\|\rho\rangle. \tag{13}$$

This expression can be rewritten (in a rather formal way) as the expectation value of the "momentum-space density operator":

$$\mathbf{n}=n_{\mathbf{k}}-\int d(\mathbf{r}_1-\mathbf{r}_2)\exp\{i\mathbf{k}(\mathbf{r}_1-\mathbf{r}_2)\}\lim_{\mathbf{r}\to\infty}\psi_+(\mathbf{r}_1+\mathbf{r})\psi_-(\mathbf{r}_2+\mathbf{r}). \tag{14}$$

Obviously, for the distributions $\|\mathbf{n}\rangle$ we have $\langle n_{\mathbf{k}}\|\mathbf{n}\rangle = n_{\mathbf{k}}$.

Here are some other examples of distributions.

A. Spatially-inhomogeneous states of a nonideal gas are described by distributions $\|\rho_1(\mathbf{r}, \mathbf{r}')\rangle$ depending on a function $\rho_1(\mathbf{r}, \mathbf{r}')$ which can be interpreted as a one-particle density matrix. The expectation values (4) with respect to such distributions are given by the same Wick rules with the following pair correlation functions

$$\begin{aligned}\overline{\psi_+(\mathbf{r})\psi_-(\mathbf{r}')}&=\rho_1(\mathbf{r},\mathbf{r}'),\\ \overline{\psi_-(\mathbf{r})\psi_+(\mathbf{r}')}&=\delta(\mathbf{r}-\mathbf{r}')-\gamma\rho_1(\mathbf{r},\mathbf{r}').\end{aligned} \tag{15}$$

B. States with pair-correlations (such as are encountered in the theory of superconductivity) can be described by means of distributions $\|n_{\mathbf{k}}, \varphi_{\mathbf{k}}\rangle$ depending on the functions $\mathbf{n} = n_{\mathbf{k}}$, and $\varphi = \varphi_{\mathbf{k}}$. The rules for the computation of expectation values (7) for such states differ from the W(n)-rules by the presence of nonvanishing pairings between two ψ_+ or two ψ_-:

$$\begin{aligned}\overline{\psi_+(\mathbf{r})\psi_+(\mathbf{r}')}&=\int d\mathbf{k}\varphi_{\mathbf{k}}{}^* e^{-i\mathbf{k}(\mathbf{r}-\mathbf{r}')},\\ \overline{\psi_-(\mathbf{r})\psi_-(\mathbf{r}')}&=\int d\mathbf{k}\varphi_{\mathbf{k}} e^{i\mathbf{k}(\mathbf{r}-\mathbf{r}')}.\end{aligned} \tag{16}$$

We do not consider further examples. One can show (making use of Schwinger's equations for the generating functional of the functions (4)) that the pairings (contractions) can be used to define any distribution, but in the general case there may occur irreducible pairings involving an arbitrary number of ψ-operators.

3. We now discuss the time evolution of the states of an infinite system. The equation of motion for distributions must relate expectation values of the operator $\hat{A}$ in a state ρ_t at time t with the expectation values with respect to the initial state $\rho_{t=0}$. It is natural to define this relation by means of the formula

$$\langle\hat{A}\|\rho_t\rangle=\langle e^{iHt}\hat{A}e^{-iHt}\|\rho_{t=0}\rangle=\langle\hat{A}^H(t)\|\rho_{t=0}\rangle, \tag{17}$$

where $\hat{A}^H(t)$ is the Heisenberg operator corresponding to $\hat{A}$ for the motion determined by the Hamiltonian H:

$$\hat{A}^H(t)=e^{iHt}\hat{A}e^{-iHt}. \tag{18}$$

The Heisenberg operator $\hat{A}^H(t)$ corresponding to the operator $\hat{A}$ in (1) is

$$\hat{A}^H(t)=\sum_{(n)}\sum_{p_1\dots p_n}\int\dots\int\alpha_{p_1\dots p_n}(\mathbf{r}_1,\dots,\mathbf{r}_n)\times\psi_{p_1}{}^H(\mathbf{r},t)\dots\psi^H_{p_n}(\mathbf{r}_n,t)\,d\mathbf{r}_1\dots d\mathbf{r}_n, \tag{19}$$

where $\alpha_{p_1\dots p_n}(\mathbf{r}_1, \dots, \mathbf{r}_n)$ are the same functions as in (1). Therefore it is sufficient to know how to express $\psi^H_\pm(\mathbf{r}, t)$ in terms of $\psi_\pm(\mathbf{r})$. This can be achieved either by means of Eq. (18) (with $\hat{A} = \psi_\pm(\mathbf{r})$), or by solving the Heisenberg equation of motion

$$i\frac{\partial}{\partial t}\psi_\pm{}^H(\mathbf{r},t)=[\psi_\pm{}^H(\mathbf{r},t);H]\ \text{with}\ \psi_\pm{}^H(\mathbf{r},t=0)=\psi_\pm(\mathbf{r}). \tag{20}$$

For an infinite medium it is necessary to make more precise the meaning of (18), since the Hamiltonian is not a local operator for the majority of problems. For example, if the potentials $h_{p_1\dots p_n}(\mathbf{r}_1, \dots, \mathbf{r}_n)$ in the expression of the Hamiltonian

$$H=\sum_{(n)}\sum_{p_1\dots p_n}\int\dots\int h_{p_1\dots p_n}(\mathbf{r}_1,\dots,\mathbf{r}_n)\times\psi_{p_1}(\mathbf{r}_1)\dots\psi_{p_n}(\mathbf{r}_n)\,d\mathbf{r}_1\dots d\mathbf{r}_n \tag{21}$$

are translation-invariant functions, the operator H cannot be local. In our formalism the use of such operators encounters the following obstruction: their expectation values may diverge. We assume henceforth that the potentials $h(\mathbf{r}_1, \dots, \mathbf{r}_n)$ are functions which differ appreciably from zero only if the points $\mathbf{r}_1, \dots, \mathbf{r}_n$ are all sufficiently close to each other, and that they vanish rapidly as the distance between any pair of points increases:

$$h(\mathbf{r}_1,\dots,\mathbf{r}_n)\to 0\quad(|\mathbf{r}_i-\mathbf{r}_j|\to\infty;\ i,j=1,\dots,n;\quad j\neq i); \tag{22}$$

such functions will be called "short-range" potentials.

We shall call operators of the form (21) extensive if the functions $h_{p_1\dots p_n}(\mathbf{r}_1, \dots, \mathbf{r}_n)$ are short-range; their expectation values with respect to the distributions $\|\mathbf{n}\rangle$, for instance, diverge proportionally to the volume, and the expectation values of e^{iHt} will contain terms having any degree of divergence. One can show, however, that in the case of an extensive H these divergences cancel mutually in the expression (18), so that for a local operator $\hat{A}$, the Heisenberg operator $\hat{A}^H(t)$ will also be local. This can be seen from the Heisenberg equation, since the commutator $[\psi_\pm(\mathbf{r}), H]$ (for fixed $\mathbf{r}$) will be a local operator if H is an extensive operator. This can also be seen from the well-known expansion of (18) as a commutator series. The Heisenberg equation of motion and the commutator series

are inconvenient for writing down perturbation expansions, therefore we select another way of making expressions of type (18) well-defined, namely by means of a limiting procedure.

We associate with each extensive H an operator H_L:

$$H_L = \sum_{(n)} \sum_{p_1 \dots p_n} \int \dots \int h_{p_1 \dots p_n}(\mathbf{r}_1, \dots, \mathbf{r}_n) \times \exp\{-|\mathbf{r}_1|/L\} \dots \exp\{-|\mathbf{r}_n|/L\} \cdot \times \psi_{p_1}(\mathbf{r}_1) \dots \psi_{p_n}(\mathbf{r}_n) d\mathbf{r}_1 \dots d\mathbf{r}_n, \quad (23)$$

introducing the cut-off factors $\exp(-|\mathbf{r}|/L)$ into the integrals. For $L > 0$ the operator H_L in (23) is a local operator, and for $L \to \infty$ it converges to H, Eq. (21). Therefore for an extensive H the expression (18) and analogous expressions can be considered as limits of the corresponding expressions for H_L as $L \to \infty$ (the preceding considerations make it plausible that such limits exist). In particular, it can be seen from this mode of defining H, that the expressions (18) satisfy the same type of relations as those for a local H, e.g.,

$$e^{iHt_2}(e^{iHt_1}\hat{A}e^{-iHt_1})e^{-iHt_2} = e^{iH(t_1+t_2)}\hat{A}e^{-iH(t_1+t_2)}. \quad (24)$$

Thus (18) is a formal expression for a transformation group which maps the operator $\hat{A}$ into an operator $\hat{A}^H(t)$ which is also local, and for the corresponding transformation law of the distributions. The dynamics we have described should reflect the peculiarities characteristic for the limiting case of an infinite system. We now discuss these peculiarities.

According to well-known concepts, the evolution of a macroscopic system can be pictured as consisting of a "rapid" passage to a partial equilibrium, followed by a "slow" relaxation of the macroscopic quantities which describe this state of partial equilibrium. If these concepts are valid, the equations of motion of an infinite medium must possess a family of solutions which describe the behavior of the system after the partial equilibrium is already established, and only the relaxation of the macroscopic quantities which characterize this equilibrium occurs, leading to a more perfect state of equilibrium. Then the description of dynamics reduces to two problems: a) the description of states of partial equilibrium, i.e., determination of the density matrix as a function of the macroscopic parameters which describe this partial equilibrium, and b) derivation of equations describing the variation of these macroscopic parameters in the course of time.

One purpose of the present paper is to show that the dynamics of an infinite medium described above does indeed admit a representation of this kind. In order to clarify the fundamental idea we show that this is indeed so using as an example a non-ideal gas, and only in the spatially-homogeneous case. In particular, for a nonideal gas with coupling constant g, we show that there exists a family of distributions $\|g, \mathbf{n}\rangle$ with momentum space density $\mathbf{n}$, such that: i) for $g \to 0$ the distributions $\|g, \mathbf{n}\rangle$ become the distributions $\|\mathbf{n}\rangle$ discussed above, and ii) that with the evolution of time each of the distributions of the family $\|g, \mathbf{n}\rangle$ goes over into another distribution belonging to the same family (i.e., one with different $\mathbf{n}$).

To express these assertions mathematically we denote the Hamiltonian of the nonideal gas by

$$H_g = H_0 + gH' \quad (25)$$

(gH′ is the interaction energy, g is the coupling constant) and also introduce the following notation:

We denote by $\tilde{R}$, $\tilde{B}$, etc. the (generally nonlinear) functional transformations which transform one function $\mathbf{n} = \mathbf{n}_\mathbf{k}$ into another $\mathbf{n}' = \mathbf{n}'_\mathbf{k}$:

$$\mathbf{n}' = \tilde{R}\mathbf{n}, \quad (26)$$

which can be written in more detail in the form

$$n_\mathbf{k}' = \sum_{(m)} \int \dots \int R^{(m)}(\mathbf{k}; \mathbf{k}_1, \dots, \mathbf{k}_m) n_{\mathbf{k}_1} \dots n_{\mathbf{k}_m} d\mathbf{k}_1 \dots d\mathbf{k}_m. \quad (26')$$

For the transformations (26) we use the usual notations: the product and inverse are defined by

$$(\tilde{P}\tilde{Q})\mathbf{n} = \tilde{P}(\tilde{Q}\mathbf{n}), \quad \tilde{R}^{-1}\tilde{R}\mathbf{n} = \tilde{R}\tilde{R}^{-1}\mathbf{n} = \tilde{I}\mathbf{n} = \mathbf{n}. \quad (27)$$

We shall call the transformations (26) ($\mathbf{n} \to \mathbf{n}$) transformations.

With this notation we can formulate our fundamental assertion in the following form:

Fundamental assertion. There exists a family of distributions $\|g, \mathbf{n}\rangle$, such that $\langle \hat{\mathbf{n}}_\mathbf{k} \| g, \mathbf{n}\rangle = \mathbf{n}_\mathbf{k}$ and $\lim \langle \hat{A} \| g, \mathbf{n}\rangle$ for $g \to 0$ equals $\langle \hat{A} \| \mathbf{n}\rangle$ and the following relation holds

$$\langle e^{iHt}\hat{A}e^{-iHt} \| g, \mathbf{n}\rangle = \langle \hat{A} \| g, \tilde{R}_g^t \mathbf{n}\rangle, \quad t \geqslant 0, \quad (28)$$

where $\tilde{R}_g^t$ is a semigroup of ($\mathbf{n} \to \mathbf{n}$)-transformations:

$$\tilde{R}_g^{t_2}\tilde{R}_g^{t_1} = \tilde{R}_g^{t_1+t_2}, \quad t_1, t_2 \geqslant 0. \quad (29)$$

In particular, defining the infinitesimal transformation (generator) B_g of the semigroup (29):

$$\tilde{B}_g = \lim_{\Delta t \to 0} \frac{1}{\Delta t}(\tilde{R}_g^{\Delta t} - \tilde{I}), \quad \tilde{R}_g^{t+dt} = (\tilde{I} + \tilde{B}_g dt)\tilde{R}_g^t, \quad (30)$$

we can rewrite (28) in differential form:

$$\frac{\partial}{\partial t}\|g, \mathbf{n}\rangle = \|g; \tilde{B}_g\mathbf{n}\rangle,$$

so that the momentum space density obeys a Boltzmann equation (kinetic equation):

$$\frac{\partial}{\partial t}\mathbf{n} = \tilde{B}_g\mathbf{n}. \tag{31}$$

A proof of the fundamental assertion is given in Sec. 2. The existence of the limit (45), on which the proof is based, is demonstrated in Sec. 3, by means of an analysis of diagrams.

2. PROOF OF THE ADIABATIC THEOREM

We now come to the proof of our fundamental assertion. We select the Hamiltonian of the ideal gas in the form

$$\begin{aligned} H_0 &= \int \varepsilon_0(\mathbf{r}-\mathbf{r}')\psi_+(\mathbf{r})\psi_-(\mathbf{r}')\,d\mathbf{r}\,d\mathbf{r}', \\ \varepsilon_0(\mathbf{r}-\mathbf{r}') &= \int \varepsilon_{\mathbf{k}}{}^0 \exp\{-i\mathbf{k}(\mathbf{r}-\mathbf{r}')\}\,d\mathbf{k}. \end{aligned} \tag{32}$$

The Heisenberg equations are easily integrated and yield

$$\begin{aligned} \psi_\pm{}^{H_0}(\mathbf{r},t) &= \int g_\pm(\mathbf{r}-\mathbf{r}',t)\psi_\pm(\mathbf{r}')\,d\mathbf{r}', \\ g_\pm(\mathbf{r}-\mathbf{r}',t) &= \int d\mathbf{k} \exp\{\pm i\varepsilon_{\mathbf{k}}{}^0 t \mp i\mathbf{k}(\mathbf{r}-\mathbf{r}')\}. \end{aligned} \tag{33}$$

It can be seen from here that the distributions $\|\mathbf{n}\rangle$ are the stationary distribution functions of an ideal gas. Indeed, from (33) it is easy to obtain for arbitrary $\hat{A}$

$$\langle \hat{A}^{H_0}(t)\|\mathbf{n}\rangle = \langle e^{iH_0t}\hat{A}e^{-iH_0t}\|\mathbf{n}\rangle = \langle \hat{A}\|\mathbf{n}\rangle. \tag{34}$$

We consider a nonideal gas with the Hamiltonian (25), where H′ is an extensive interaction Hamiltonian of the form (21), (22). Assume that up to time t_0 we have an ideal gas in a state $\rho_{in} = \|\mathbf{n}\rangle$, and at t_0 we switch on the interaction H′ and the Hamiltonian becomes (25). Then the expectation value in the state ρ_t is defined by

$$\langle \hat{A}\|\rho_t\rangle = \langle S_g{}^+(t,t_0)\hat{A}^{H_0}(t)S_g(t,t_0)\|\mathbf{n}\rangle, \tag{35}$$

where $S_g(t, t_0)$ is the S-matrix for the interaction gH′, defined by

$$S_g(t,t_0) = T\exp\left\{-i\int_{t_0}^{t} gH'^{H_0}(t')\,dt'\right\} \quad (t > t_0), \tag{36}$$

where $H'^{H_0}(t)$ is the interaction Hamiltonian expressed in terms of the Heisenberg operators of the unperturbed motion

$$\begin{aligned} H'^{H_0}(t) = \sum_{(n)}\sum_{p_1\ldots p_n} \int\ldots\int h'_{p_1\ldots p_n}(\mathbf{r}_1,\ldots,\mathbf{r}_n) \\ \times\ \psi_{p_1}^{H_0}(\mathbf{r}_1,t)\ldots\psi_{p_n}^{H_0}(\mathbf{r}_n,t)\,d\mathbf{r}_1,\ldots,d\mathbf{r}_n. \end{aligned} \tag{37}$$

We list the properties of the S-matrix which will be of use in the sequel:

$$S_g{}^+(t,t_0)S_g(t,t_0) = 1, \tag{38}$$

$$S_g(t_2,t_1)S_g(t_1,t_0) = S_g(t_2,t_0), \tag{39}$$

$$S_g(t_1+\tau,\ t_0+\tau) = \exp\{iH_0\tau\}\,S_g(t_1,t_0)\exp\{-iH_0\tau\}, \tag{40}$$

$$\exp\{-iH_0t\}\,S_g(t,0) = \exp\{-iH_gt\}. \tag{41}$$

Regarding the operators on both sides of Eqs. (38)—(41), it should be stressed again that in the case of an extensive H the only meaningful expressions are those in which a local operator $\hat{A}$ is multiplied on the right by one of these operators, and on the left by its adjoint. For example, (41) is an abbreviated notation for the equation

$$\begin{aligned} S_g{}^+(t,0)\,(\exp\{iH_0t\}\hat{A}\exp\{-iH_0t\})\,S_g(t,0) \\ = \exp\{iH_gt\}\hat{A}\exp\{-iH_gt\}. \end{aligned}$$

As already indicated, Eq. (35) expresses the expectation value in a state of the gas at time t, if the interaction was switched on at time t_0. If the limit of (35) for $t_0 \to -\infty$ would exist, this limit would obviously represent the expectation value in the actual state of the nonideal gas. However, the limit of (35) for $t_0 \to -\infty$ does not exist in general, due to the presence of macroscopic transitions involving modifications of the momentum space density. We show in Sec. 3 that these divergences can be removed by means of a t, t_0-dependent renormalization of the momentum space density.

In order to formulate this assertion in a more precise manner, we define the transformations $\tilde{R}_g(t, t_0)$ by means of the formula

$$\tilde{R}_g(t,t_0)\mathbf{n} = \langle S_g{}^+(t,t_0)\hat{\mathbf{n}}S_g(t,t_0)\|\mathbf{n}\rangle, \tag{42}$$

where $\hat{\mathbf{n}} = \hat{\mathbf{n}}_{\mathbf{k}}$ is the momentum space density operator (14). (In other words, $\tilde{R}_g(t, t_0)$ is that $(\mathbf{n} \to \mathbf{n})$-transformation which maps the momentum space density before the interaction is switched on into the momentum space density at time t).

With the aid of (42) we introduce the distribution $\|t, t_0; g; \mathbf{n}\rangle$ defining the expectation value with respect to it by the equation

$$\langle \hat{A}\|t,t_0;g;\mathbf{n}\rangle = \langle S_g{}^+(t,t_0)\hat{A}^{H_0}(t)S_g(t,t_0)\,\|\tilde{R}_g{}^{-1}(t,t_0)\mathbf{n}\rangle. \tag{43}$$

This definition can be rewritten in a different equivalent form, making in both sides of Eq. (43) the substitution $\mathbf{n} \to \tilde{R}_g(t, t_0)\mathbf{n}$. We obtain then

$$\langle S_g{}^+(t,t_0)\hat{A}^{H_0}(t)S_g(t,t_0)\|\mathbf{n}\rangle = \langle \hat{A}\|t,t_0;g;\tilde{R}_g(t,t_0)\mathbf{n}\rangle; \tag{44}$$

in other words, the expectation value (43) is obtained by expressing the expectation value in terms of $\tilde{R}_g(t, t_0)\mathbf{n}$ (i.e., the momentum space density at time t) instead of in terms of $\mathbf{n}$ (i.e., the momentum space density before the interaction is switched on), and then relabel the former variable again by $\mathbf{n}$.

Our assertion can now be formulated in the following manner: for the expectation value (43) there exists the limit for $t_0 \to -\infty$, defining the asymptotic distribution $\|t; g; \mathbf{n}\rangle$:

$$\langle\hat{A}\|t; g; \mathbf{n}\rangle = \lim_{t_0\to-\infty}\langle\hat{A}\|t, t_0; g; \mathbf{n}\rangle. \quad (45)$$

This assertion will be proved in Sec. 3, where the expectation values (43) will be represented as a sum of contributions from diagrams of a definite type. The existence of the limits (45) will follow from this representation. In the present section we show that if the limits (45) exist, then they are independent of t and satisfy the fundamental relation (28), so that they can be considered as expectation values in a state of a nonideal gas with momentum space density $\mathbf{n}$.

The proof is based on two lemmas.

Lemma 1. The following relations hold: a) for (42):

$$\tilde{R}_g(t+\tau,\ t_0+\tau) = \tilde{R}_g(t, t_0); \quad (46)$$

and b), for (45):

$$\langle\hat{A}\|t+\tau; g; \mathbf{n}\rangle = \langle\hat{A}\|t; g; \mathbf{n}\rangle. \quad (47)$$

Proof. From the property (40) of the S-matrix and Eq. (24) it follows that

$$\begin{aligned}&\langle S_g^+(t+\tau, t_0+\tau)\hat{A}^{H_0}(t+\tau)S_g(t+\tau, t_0+\tau)\|\mathbf{n}\rangle\\ &\quad= \langle e^{iH_0\tau}S_g^+(t, t_0)e^{-iH_0\tau}(e^{iH_0\tau}\hat{A}^{H_0}(t)e^{-iH_0\tau})\\ &\quad\times e^{iH_0\tau}S_g(t, t_0)e^{-iH_0\tau}\|\mathbf{n}\rangle\\ &\quad= \langle e^{iH_0\tau}(S_g^+(t, t_0)\hat{A}^{H_0}(t)S_g(t, t_0))e^{-iH_0\tau}\|\mathbf{n}\rangle.\end{aligned}$$

The latter expression can be subjected to the transformation (34), where the role of $\hat{A}$ is played by the operator in parentheses. It follows that

$$\begin{aligned}&S_g^+(t+\tau, t_0+\tau)\hat{A}^{H_0}(t+\tau)S_g(t+\tau, t_0+\tau)\|\mathbf{n}\rangle\\ &\quad= \langle S_g^+(t, t_0)\hat{A}^{H_0}(t)S_g(t, t_0)\|\mathbf{n}\rangle.\end{aligned} \quad (48)$$

In particular, setting here $\hat{A} = \hat{\mathbf{n}}$, we obtain on the basis of (42)

$$\tilde{R}_g(t+\tau, t_0+\tau)\mathbf{n} = \tilde{R}_g(t, t_0)\mathbf{n},$$

which proves (46).

On the other hand, transforming both sides of (48) by means of (44) we obtain

$$\begin{aligned}&\langle\hat{A}\|t+\tau, t_0+\tau; g; \tilde{R}_g(t+\tau, t_0+\tau)\mathbf{n}\rangle\\ &\quad= \langle\hat{A}\|t, t_0; g; \tilde{R}_g(t, t_0)\mathbf{n}\rangle.\end{aligned}$$

Making the substitution $\mathbf{n} \to \tilde{R}_g^{-1}(t+\tau, t_0+\tau)\mathbf{n}$ in the left hand side, and the substitution $\mathbf{n} \to \tilde{R}_g^{-1}(t, t_0)\mathbf{n}$ in the right hand side (these substitutions are equivalent in view of the already proved relation (46)), we obtain

$$\langle\hat{A}\|t+\tau, t_0+\tau; g; \mathbf{n}\rangle = \langle\hat{A}\|t, t_0; g; \mathbf{n}\rangle;$$

taking the limit $t_0 \to -\infty$ in this equality we obtain (47). Thus the lemma is proved.

It follows from (47) that the distribution (45) does not depend on t, therefore t can be omitted from its expression:

$$\langle\hat{A}\|t; g; \mathbf{n}\rangle = \langle\hat{A}\|0; g; \mathbf{n}\rangle = \langle\hat{A}\|g; \mathbf{n}\rangle. \quad (49)$$

We now consider our expression (35) and transform it making use of the property (39) of the S-matrix. We have

$$\begin{aligned}&\langle S_g^+(t, t_0)\hat{A}^{H_0}(t)S_g(t, t_0)\|\mathbf{n}\rangle\\ &\quad= \langle S_g^+(0, t_0)(S_g^+(t, 0)\hat{A}^{H_0}(t)S_g(t, 0))S_g(0, t_0)\|\mathbf{n}\rangle.\end{aligned} \quad (50)$$

We rewrite the right hand side of (50) making use of (44), with the operator $\hat{A}$ replaced by the expression in parentheses. This yields

$$\begin{aligned}&\langle S_g^+(t, t_0)A^{\hat{H}_0}(t)S_g(t, t_0)\|\mathbf{n}\rangle\\ &\quad= \langle S_g^+(t, 0)\hat{A}^{H_0}(t)S_g(t, 0)\|0, t_0; g; \tilde{R}_g(0, t_0)\mathbf{n}\rangle.\end{aligned} \quad (51)$$

We first apply this relation to the operator $\hat{A} = \hat{\mathbf{n}}$:

$$\tilde{R}_g(t, t_0)\mathbf{n} = \langle S_g^+(t, 0)\hat{\mathbf{n}}^{H_0}(t)S_g(t, 0)\|0, t_0; g; \tilde{R}_g(0, t_0)\mathbf{n}\rangle$$

Making a substitution $\mathbf{n} \to \tilde{R}_g^{-1}(0, t)\mathbf{n}$ in this expression we obtain

$$\tilde{R}_g(t, t_0)\tilde{R}_g^{-1}(0, t_0)\mathbf{n} = \langle S_g^+(0, t_0)\hat{\mathbf{n}}^{H_0}(t)S_g(t, 0)\|0, t_0; g; \mathbf{n}\rangle \quad (52)$$

Since one can take the limit $t_0 \to -\infty$ in the right hand side of (52) we obtain the following lemma from this last equation:

Lemma 2. The limit

$$\lim_{t_0\to-\infty}\tilde{R}_g(t, t_0)\tilde{R}_g^{-1}(0, t_0) = \tilde{R}_g^t \quad (53)$$

exists and can be computed from the expression

$$\tilde{R}_g^t = \langle S_g^+(t, 0)\hat{\mathbf{n}}^{H_0}(t)S_g(t, 0)\|g; \mathbf{n}\rangle. \quad (54)$$

We now rewrite the left hand side of (51), making use of (44). This yields

$$\begin{aligned}&\langle\hat{A}\|t, t_0; g; \tilde{R}_g(t, t_0)\mathbf{n}\rangle\\ &\quad= \langle S_g^+(t, 0)\hat{A}^{H_0}(t)S_g(t, 0)\|t, t_0; g; \tilde{R}_g(0; t_0)\mathbf{n}\rangle.\end{aligned}$$

Here we make the substitution $\mathbf{n} \to \tilde{R}_g^{-1}(0, t_0)\mathbf{n}$ and take into account the fact that according to the property (41) of the S-matrix

$$\begin{aligned}&S_g^+(t, 0)\hat{A}^{H_0}(t)S_g(t, 0)\\ &\quad= S_g(t, 0)(e^{iH_0t}\hat{A}e^{-iH_0t})S_g(t, 0) = e^{iH_gt}\hat{A}e^{-iH_gt};\end{aligned}$$

therefore

$$\langle\hat{A}\|t, t_0; g; \tilde{R}_g(t, t_0)\tilde{R}_g^{-1}(0, t_0)\mathbf{n}\rangle = \langle e^{iH_gt}\hat{A}e^{-iH_gt}\|t, t_0; g; \mathbf{n}\rangle. \quad (55)$$

We now take the limit $t_0 \to -\infty$ in (55), making use of (45), (49), and (53). This results in

$$\langle\hat{A}\|g; \tilde{R}_g^t\mathbf{n}\rangle = \langle e^{iH_gt}\hat{A}e^{-iH_gt}\|g; \mathbf{n}\rangle, \quad (56)$$

which in fact is the content of our fundamental assertion.

It remains only to be shown that the transformations $\tilde{R}_g^t$ form a semigroup. This follows from the

definition (53) and from (46). Indeed:

$$\tilde{R}_g(t_2+t_1,t_0)\tilde{R}_g^{-1}(0,t_0)$$
$$=(\tilde{R}_g(t_2+t_1,t_0)\tilde{R}_g^{-1}(t_1,t_0))\,(\tilde{R}_g(t_1,t_0)\tilde{R}_g^{-1}(0,t_0))=$$
$$=(\tilde{R}_g(t_2,t_0-t_1)\tilde{R}_g^{-1}(0,t_0-t_1))\,(\tilde{R}_g(t_1,t_0)\tilde{R}_g^{-1}(0,t_0)) \tag{57}$$

(in the last equation we made use of (46) with $t = t_2 + t_1$, $\tau = -t_1$). Going to the limit $t_0 \to -\infty$ in (57) we obtain from the definition (57)

$$\tilde{R}_g^{t_2+t_1}=\tilde{R}_g^{t_2}\tilde{R}_g^{t_1}, \tag{58}$$

as required.

From (58) it follows for infinitesimal $t_2 = dt$ that

$$\frac{\partial}{\partial t}\tilde{R}_g^t=\tilde{B}_g\tilde{R}_g^t, \tag{59}$$

where the operator $\tilde{B}_g$, resulting from (54) for infinitesimal t, obeys the equation

$$\tilde{B}_g\mathbf{n}=-i\langle[gH',\hat{\mathbf{n}}]\|g;\mathbf{n}\rangle, \tag{60}$$

i.e.,

$$\frac{\partial n_{\mathbf{k}}}{dt}=(\tilde{B}_g\mathbf{n})_{\mathbf{k}}=-i\int d(\mathbf{r}_1-\mathbf{r}_2)\exp\{i\mathbf{k}(\mathbf{r}_1-\mathbf{r}_2)\}$$
$$\times\langle[gH',\psi_+(\mathbf{r}_1)\psi_-(\mathbf{r}_2)]\|g;\mathbf{n}\rangle.$$

3. ANALYSIS OF PERTURBATION-THEORY DIAGRAMS

We show that the representation (44) for the expectation values (35) and the existence of the limit (45), facts which were essential for our proof in Section 2, are valid to all orders of perturbation theory. For this purpose we define the S-matrix $S_{g,L}(t, t_0)$ for a perturbation H'_L which is obtained from H′ by means of cut-off factors, in the same manner as (23) is derived from (21). We define:

$$\langle S_g^+(t,t_0)\hat{A}^{H_0}(t)S_g(t,t_0)\|\mathbf{n}\rangle$$
$$=\lim_{L\to\infty}\langle S_{g,L}^+(t,t_0)\hat{A}^{H_0}(t)S_{g,L}(t,t_0)\|\mathbf{n}\rangle. \tag{61}$$

In order to compute (61) one must be able to evaluate expectation values of the form

$$\left\langle T_a\left(\prod_i\psi^0_{p_i}(\mathbf{r}_i,t_i)\right)\left(\prod_j\psi^0_{p_j}(\mathbf{r}_j,t)\right)T_c\left(\prod_k\psi^0_{p_k}(\mathbf{r}_k,t_k)\right)\|\mathbf{n}\right\rangle \tag{62}$$

(we write $\psi^0_\pm(\mathbf{r}, t)$ in place of $\psi^{H_0}_\pm(\mathbf{r}, t)$; T_c denotes the chronological (time-ordered) product and T_a is the anti-chronological product. The operators under the T_c sign refer to $S_g(t, t_0)$, the operators under the T_a sign refer to $S_g^+(t, t_0)$, and the operators in the middle parentheses belong to $\hat{A}^{H_0}(t)$. The expressions for the expectation values (62) are easily obtained in the following manner: since the operators $\psi^{H_0}_\pm(\mathbf{r}, t)$ are expressed in terms of $\psi_\pm(\mathbf{r})$ by means of Eq. (33), the expectation values (62) reduce to the expectation values (6), which can be computed according to the W(n) rules.

Thus, starting from (33) and the W(n) rules, we obtain the following rules for the computation of the expectation values (62): The expectation values (62) equal the sum of contribution from all possible pairings, and there exist three types of pairings:

1) chronological pairings, i.e., contractions of pairs of ψ-operators which in (62) both occur under the T_c sign (i.e. both refer to $S_g(t, t_0)$;

2) antichronological pairings, i.e., contractions of pairs of operators which both occur under the T_a sign in (62) (i.e. both refer to $S_g^+(t, t_0)$;

3) mixed pairings—for all other pairs of operators (i.e., one coming from $S_g(t, t_0)$ and the other from $S_g^+(t, t_0)$, or when one or both of the contracted operators occur in $\hat{A}^{H_0}(t)$).

All pairings (contractions) have the form

$$\overline{\psi^0_\pm(\mathbf{r},t)\psi^0_\mp(\mathbf{r}',t')}^{c,a,m}$$
$$=\int\exp\{\pm i\varepsilon_{\mathbf{k}}^0(t-t')\mp i\mathbf{k}(\mathbf{r}-\mathbf{r}')\}$$
$$\times\,\overline{\psi_\pm\psi_\pm}^{c,a,m}(\mathbf{k},t-t')\,d\mathbf{k}, \tag{63}$$

where the superscripts c, a, m refer, respectively to chronological, antichronological and mixed pairings. For mixed pairings we have

$$\overline{\psi_+\psi_-}^m(\mathbf{k},t-t')=\overline{\psi_+\psi_-}(\mathbf{k}),\quad \overline{\psi_-\psi_+}^m(\mathbf{k},t-t')=\overline{\psi_-\psi_+}(\mathbf{k}) \tag{64}$$

(for the right-hand side cf. (7)). For chronological pairings

$$\overline{\psi_+\psi_-}^c(\mathbf{k},t-t')=\overline{\psi_+\psi_-}(\mathbf{k})\eta^a(t-t')+\overline{\psi_-\psi_+}(\mathbf{k})\eta^c(t-t'), \tag{64′}$$

and the other (anti)chronological pairings are obtained from (64′) by changing the upper and lower indices into their opposites (i.e., $\pm$ into $\mp$ and c, a into a, c). Here

$$\eta^a(t-t')=\begin{cases}1 & \text{for } t>t'\\ 0 & \text{for } t<t'\end{cases},\quad \eta^c(t-t')=\begin{cases}0 & \text{for } t>t'\\ 1 & \text{for } t<t'\end{cases}. \tag{65}$$

As we shall see in the sequel, a different notation for the expressions (64′) will turn out to be convenient; it is obtained by separating in (64) a term proportional to $\eta^c(t - t')$ by means of the identity $\eta^a(t - t') = 1 - \eta^c(t - t')$. We thus obtain (taking into account (7)) the following identity for chronological pairings

$$\begin{aligned}\overline{\psi_+\psi_-}^c(\mathbf{k},t-t')&=\gamma\eta^c(t-t')+n_{\mathbf{k}},\\ \overline{\psi_-\psi_+}^c(\mathbf{k},t-t')&=-\eta^c(t-t')+(1+\gamma n_{\mathbf{k}}),\end{aligned} \tag{66}$$

and for antichronological pairings

$$\begin{aligned}\overline{\psi_+\psi_-}^a(\mathbf{k},t-t')&=-\gamma\eta^c(t-t')+\gamma(1+\gamma n_{\mathbf{k}}),\\ \overline{\psi_-\psi_+}^a(\mathbf{k},t-t')&=\eta^c(t-t')+\gamma n_{\mathbf{k}}.\end{aligned} \tag{66′}$$

Note that (64) coincides with the second term in (66).

According to (63), the decompositions (66) lead to decompositions of the chronological and anti-chronological pairings into two terms each, which we shall designate as an R-pairing and an S-pairing:

$$\overline{\psi_{\pm}^{0}(\mathbf{r},t)\psi_{\mp}^{0}(\mathbf{r}',t')}=\overline{R\psi_{\pm}^{0}(\mathbf{r},t)\psi_{\mp}(\mathbf{r}',t')}+\overline{S\psi_{\pm}^{0}(\mathbf{r},t)\psi_{\mp}(\mathbf{r}',t')}. \tag{67}$$

The following properties of this decomposition will be important for us: 1) the R-pairings are proportional to $\eta^{c}(t-t')$ and do not depend on $n_{\mathbf{k}}$; 2) the total dependence on $n_{\mathbf{k}}$ is contained in the S-pairing. Note that the decomposition (67) can be applied to mixed pairings also, if for the latter one considers the R-pairings to vanish, so that they consist of an S-pairing only.

The representation of the expectation values (62) in terms of the pairings (63) allows one to represent the terms of the series for (61) by means of diagrams, where the lines correspond to the pairings (contractions) (63) and the vertices represent the functions $h_{p_1 \dots p_n}(\mathbf{r}_1 \dots \mathbf{r}_n)$ in (21) and the functions $\alpha_{p_1 \dots p_n}(\mathbf{r}_1 \dots \mathbf{r}_n)$ in (19). The latter vertices will be designated as A-vertices, and the corresponding points will be called A-points. The term "diagram" will be used in the sequel to represent not only the graph, but also the integrand represented by it. This integrand is the product of vertex functions (briefly—vertices) and pairings, and also contains cut-off factors $\exp(-|\mathbf{r}|/L)$. For the space-time points and exponents in (63) we use the standard abbreviations:

$$x=(\mathbf{r},t),\quad k=(\mathbf{k};\varepsilon_{\mathbf{k}}^{0}),\quad (k,x)=\varepsilon_{\mathbf{k}}^{0}t-\mathbf{kr}.$$

We now analyze the diagrams. The diagrams are classified in the usual manner according to the topological properties of their graphical representations. First of all, an arbitrary diagram is represented as the product of its connected components (for a definition of the latter cf., e.g.,[5]). Our diagrams have distinguished vertices, namely the A-points. All A-points refer to one vertex function $\alpha_{p_1 \dots p_n}(\mathbf{r}_1 \dots \mathbf{r}_n)$ and are connected into one node, therefore they all belong to one connected component, which will be called the connected A-component of the diagram. An arbitrary diagram D for (61) can be represented as a product $D = D_1 D'_A$, where D'_A is the connected A-component and D_1 is the product of the remaining connected components of the diagram (not containing A-vertices).

We note that D_1 is exactly equal to some diagram for the expression

$$\langle S_g^{+}(t,t_0)S_g(t,t_0)\|\mathbf{n}\rangle \tag{68}$$

and all diagrams D of (61) can be obtained forming the products of their connected A-components with all possible diagrams for the expression (68). Based on this it is easy to show that the sum of the contributions to the expression (61) from all the diagrams equals the product of the sum of the contributions of all A-connected components by the sum of the contributions of all diagrams for the expressions (68), i.e.,

$$\langle S_g^{+}(t,t_0)\hat{A}^{H_0}(t)S_g(t,t_0)\|\mathbf{n}\rangle \tag{69}$$
$$=\langle S_g^{+}(t,t_0)\hat{A}^{H_0}(t)S_g(t,t_0)\|\mathbf{n}\rangle_{\text{conn}}'\langle S_g^{+}(t,t_0)S_g(t,t_0)\|\mathbf{n}\rangle,$$

where $\langle \dots \|\mathbf{n}\rangle'_{\text{conn}}$ denotes the sum of the contributions from the A-connected components only. However, owing to (38), i.e., unitarity, the expectation value of (68) is one, so that one can write:

$$\langle S_g^{+}(t,t_0)\hat{A}^{H_0}(t)S_g(t,t_0)\|\mathbf{n}\rangle \tag{70}$$
$$=\langle S_g^{+}(t,t_0)\hat{A}^{H_0}(t)S_g(t,t_0)\|\mathbf{n}\rangle_{\text{conn}}'.$$

Thus the expression (61) equals the sum of contributions from connected A-components only. The contributions of all other diagrams cancel.

This also demonstrates the existence of the limit (61) for $L\to\infty$. Indeed a connected A-component contains a rapidly decreasing factor: the A-vertex function $\alpha(\mathbf{r}_1, \dots, \mathbf{r}_n)$ and the other factors (vertex functions and pairings) are short-range functions. Owing to connectedness the total diagram will then be a rapidly decreasing function, and its integral over space points converges even in the absence of the cut-off factors $\exp(-|\mathbf{r}|/L)$. On the contrary, for connected components which do not contain A-vertices, this integral will diverge proportionally to the volume, but the contributions of all those diagrams cancel in (61).

In the sequel we assume that the limit is already taken, and the term "diagram" will always designate a connected A-component. In addition we assume that all pairings in the diagram are represented, according to (67), as a sum of R-pairings and S-pairings. Then the diagram will decompose into a sum of "split" diagrams in which either the R-component, or the S-component is left over from each pairing. Then the expectation value (70) will consist of a sum of contributions from all such "split" diagrams. Thus, starting from this point, we consider only connected A-components with two types of pairings: R-pairings and S-pairings, and the mixed R-pairings vanish.

We now consider the behavior of (69) for $t_0\to-\infty$. It was already noted that whenever the switching-on of the interaction leads to macroscopic changes, this manifests itself in a definite manner in perturbation theory: contributions from diagrams

a b c

Diagrams corresponding to the renormalization of the momentum space density: a – a diagram with a singular $\mathfrak{R}$-part; b – the contracted diagram (with respect to this $\mathfrak{R}$-part); c – the corresponding diagram for the renormalization $\Delta n_{\mathbf{k}}(t,t_0)$. In the case a the central part is at left, the $\mathfrak{R}$-part is to the right. The shaded part represents an A-vertex, the heavy dots represent A-points; the heavy line represents a reduced pairing.

containing certain vertex parts become divergent (these are vertex parts connected to the remainder of the diagram by a certain number of incoming or outgoing lines). This also happens with our diagrams; the modification of each macroscopic quantity leads to divergences related to the form of the corresponding vertex parts. In particular, as will be shown below, the modification of the momentum space density corresponds to vertex parts connected to the diagram by two lines: one incoming and one outgoing.

Let us consider such a diagram (cf. fig., case a). More precisely, we have in mind diagrams which can be decomposed into two parts, connected to each other by two lines with opposite relative orientations, and all A-points are contained only in one of the two parts. This part (containing the A-points) will be called the central part, or the A-part, and the other part (which does not contain A-points) will be called the $\mathfrak{R}$-part. The contractions corresponding to the lines connecting the $\mathfrak{R}$-part with the A-part will be called the external pairings of the $\mathfrak{R}$-part, the vertices in which these lines originate and terminate will be called the external vertices of the $\mathfrak{R}$-part, and will be denoted by x_1', x_2' and the remaining (internal) vertices of the $\mathfrak{R}$-part will be denoted by $x' \dots x'$. The function describing the $\mathfrak{R}$-part will be denoted by $\mathfrak{R}(x_1', x_2'; x' \dots x')$. For the A-part the corresponding notations are $x_2, x_1; x \dots x$ and $A(x \dots x; x_1, x_2)$. A diagram with an $\mathfrak{R}$-part can then be written as:

$$D(x \dots x, x_1, x_2; x_1', x_2'; x' \dots x') = A(x \dots x; x_1, x_2)\overline{\psi_+(x_1)\psi_-(x_1')}\,\overline{\psi_-(x_2)\psi_+(x_2')} \times \mathfrak{R}(x_1', x_2'; x' \dots x') \tag{71}$$

(each external pairing can be either an R-pairing or an S-pairing). Integrating (71) over the internal vertices of the $\mathfrak{R}$-part we obtain an expression which differs from the original (71) by replacing the $\mathfrak{R}$-part by its integral over the internal points:

$$\int \dots \int \mathfrak{R}(x_1', x_2'; x' \dots x')\,dx' \dots dx' = \mathfrak{R}(x_1', x_2' | t, t_0) = \int \exp\{-ik(\mathbf{r}_1' - \mathbf{r}_2')\}\,\mathfrak{R}_{\mathbf{k}}(t_1', t_2' | t, t_0)\,d\mathbf{k} \tag{72}$$

(we have explicitly written out the dependence of t and t_0 and have introduced the Fourier transform with respect to $\mathbf{r}_1' - \mathbf{r}_2'$, having here in mind the spatially-homogeneous case only, as already mentioned).

We now call an $\mathfrak{R}$-part where both external pairings are S-pairings a singular part (briefly s-part), and show that the integration over the times of the external points of the s-part

$$\int_{t_0}^{t}\int_{t_0}^{t} dt_1'\,dt_2'$$

lead to a divergence for $t_0 \to -\infty$.

It is sufficient to prove this for such s-parts (to be called simple s-parts) for which no pair of internal points is external for another s-part. Then for non-simple s-parts (72) is already divergent. For simple s-parts we can assume that (72) has a limit for $t_0 \to -\infty$. It is easy to see that if it exists, this limit must depend asymptotically, for $t_1' \to -\infty$, $t_2' \to -\infty$, only on the difference $t_2' - t_1'$:

$$\lim_{t_0 \to -\infty} \mathfrak{R}_{\mathbf{k}}(t_1', t_2' | t, t_0) = \mathfrak{R}_{\mathbf{k}}(t_1', t_2' | t) \underset{t_1' \to -\infty,\ t_2' \to -\infty}{\longrightarrow} \mathfrak{R}_{\mathbf{k}}(t_1' - t_2'). \tag{73}$$

It follows that if even one of the external pairings is an R-pairing, the integral over the domain $t < t_1' < +\infty$, $t < t_2' < +\infty$ converges since the factor $\eta^c(t_1 - t_1')$ effectively reduces the integration region to $t < t_1' < t_1$, $t < t_2' < +\infty$, and similarly for the factor $\eta^c(t_2 - t_2')$ (the times t_1 and t_2 refer to the A-part and remain fixed in this integration). On the contrary, if both external pairings are S-pairings, the integral over the external points of the $\mathfrak{R}$-part diverges for $t_0 \to -\infty$. For instance, if both external pairings are chronological, this integral has the form

$$\int d\mathbf{k}\,A(x \dots x; x_1, x_2)\exp\{i(k, x_1 - x_2)\} \times \int_{t_0}^{t}\int_{t_0}^{t} dt_1'\,dt_2' \exp\{i\varepsilon_{\mathbf{k}}^0(t_1' - t_2')\} \times n_{\mathbf{k}}(1 + \gamma n_{\mathbf{k}})\mathfrak{R}_{\mathbf{k}}(t_1', t_2' | t, t_0); \tag{74}$$

and the divergence of this expression for $t_0 \to -\infty$ is an obvious consequence of (72).

The cases when both external pairings are antichronological, or when one is chronological and the other is mixed, etc. are completely analogous, and we refrain from writing them out explicitly.

Let us consider in more detail the expressions (74). One can associate with each diagram which has a singular $\mathfrak{R}$-part a simpler diagram, by re-

placing this s-part and its external pairings by one S-pairing (cf. the figure, case b). Then the diagram (71) will be replaced by the diagram

$$\bar{D}(x\dots x; x_1, x_2) = A(x\dots x; x_1, x_2)\overline{S\psi_+(x_1)\psi_-(x_2)}, \quad (75)$$

where the A-part A(x ... x; x_1, x_2) is identical with the one in (71). We call this diagram the contraction of the initial one, and the pairing which replaces the s-part and its external pairings is called the reduced pairing of the contracted diagram.

For the case (74) (both external S-pairings are chronological) the contracted diagram has the form

$$\int d\mathbf{k} A(x\dots x; x_1, x_2)\exp\{i(k(x_1 - x_2)\}\, n_{\mathbf{k}} \quad (76)$$

Comparing this with (74) we see that both are of the same form, only the momentum space density $n_{\mathbf{k}}$ belonging to the reduced S-pairing is replaced by $n_{\mathbf{k}}(t, t_0)$, with

$$\Delta n_{\mathbf{k}}(t, t_0) = \int_{t_0}^{t}\int_{t_0}^{t} dt_1' dt_2' \exp\{i\varepsilon_{\mathbf{k}}^0(t_1' - t_2')\} \times n_{\mathbf{k}}(1 + \gamma n_{\mathbf{k}})\mathfrak{N}_{\mathbf{k}}(t_1', t_2'|t, t_0). \quad (77)$$

If one adds (74) and the contracted diagram (76) the sum will be the expression which is obtained if one replaces the reduced S-pairing in the contracted diagram by an S-pairing with the momentum space density $n_{\mathbf{k}} + \Delta n_{\mathbf{k}}(t, t_0)$, leaving $n_{\mathbf{k}}$ unchanged in all other S-pairings.

On the other hand, the replaced part of the initial diagram, i.e., the $\mathfrak{R}$-part and its external pairings can be uniquely associated with a diagram :D for the expression

$$\langle S_g^+(t, t_0)\hat{n}_{\mathbf{k}}^{H_0}(t) S_g(t, t_0)\|\mathbf{n}\rangle = \langle S_g^+(t, t_0)\hat{n}_{\mathbf{k}} S_g(t, t_0)\|\mathbf{n}\rangle \quad (78)$$

($\hat{n}_{\mathbf{k}}$ is the momentum space density operator (14)). This is done (cf. figure, case c) by associating with the replaced part of the initial diagram (71) the expression

$$:D(\mathbf{r}_1, \mathbf{r}_2; t; x_1'; x_2'; x\dots x) = \overline{S\psi_+^0(\mathbf{r}_1, t)\psi_-^0(x_1')} \times \overline{S\psi_-^0(\mathbf{r}_2, t)\psi_+^0(x_2')}\ \mathfrak{R}(x_1', x_2'; x'\dots x'), \quad (79)$$

where $\mathfrak{R}(x_1', x_2'; x\dots x)$ is the same function as in (71). Obviously, (79) is one of the possible diagrams for (78); its relation to the corresponding s-part consists in expressing the appropriate renormalization $\Delta n_{\mathbf{k}}(t, t_0)$ in terms of the contribution from the diagram (79). Indeed, one can rewrite Eq. (77) in the form

$$\Delta n_{\mathbf{k}}(t, t_0) = \int d(\mathbf{r}_1 - \mathbf{r}_2)\exp\{-i\mathbf{k}(\mathbf{r}_1 - \mathbf{r}_2)\}\cdot \left(\int \dots \int dx_1' dx_2' dx \dots dx : D(\mathbf{r}_1, \mathbf{r}_2, t; x_1' x_2'; x\dots x)\right) = \langle S_g^+(t, t_0)\hat{n}_{\mathbf{k}} S_g(t, t_0)\|\mathbf{n}\rangle_{:D}. \quad (80)$$

This notation signifies that one should consider in (78) only the contribution from the diagram (79) (which corresponds to the contracted s-part).

It follows from all this that the contribution from diagrams which have an s-part (we call such diagrams $\mathfrak{R}$-singular diagrams) reduces to a renormalization of the momentum space density in diagrams which do not have an s-part (such diagrams will be called $\mathfrak{R}$-regular). This is done by taking an $\mathfrak{R}$-singular diagram and separating in it the maximal s-parts (i.e., s-parts which are not contained in any other s-parts of the same diagram). The separation of maximal s-parts is unique, and they can be successively contracted out by means of the procedure outlined above. As a result the contribution of the original $\mathfrak{R}$-singular diagram is reduced to a renormalization of the momentum space density in the reduced pairings of the completely contracted diagram. The latter is obtained from the initial diagram by replacing each maximal s-part together with its external pairings by one reduced S-pairing. Then the renormalization $\Delta n_{\mathbf{k}}(t, t_0)$ of the reduced S-pairing will be expressed in the form (80) in terms of the contribution of the diagram which corresponds to the contracted maximal s-part.

It is easy to see that not only does each $\mathfrak{R}$-singular diagram yield a unique completely contracted diagram, but also conversely, to an arbitrary $\mathfrak{R}$-regular diagram and given contracted s-parts for definite S-pairings of this diagram one can reconstruct the initial $\mathfrak{R}$-singular diagram in a unique manner. It follows that the sum of the contributions from all diagrams can be computed in the following manner: one calculates the sum of the contributions from all $\mathfrak{R}$-regular diagrams and in the resulting expression one carries out the following substitution on the momentum space density

$$n_{\mathbf{k}} \to n_{\mathbf{k}}'(t, t_0) = \langle S_g^+(t, t_0)\hat{n}_{\mathbf{k}}^0(t) S_g(t, t_0)\|\mathbf{n}\rangle = (\bar{R}_g(t, t_0)\mathbf{n})_{\mathbf{k}}. \quad (81)$$

The sum of the contributions from all $\mathfrak{R}$-regular diagrams can be considered as an expectation value with respect to a distribution which we denote by $\|t, t_0; g, \mathbf{n}\rangle$, in the following manner

$$\langle S_g^+(t, t_0)\hat{A}^{H_0}(t) S_g(t, t_0)\|\mathbf{n}\rangle_{\text{conn}},\ \mathfrak{R}_{\text{reg}} = \langle\hat{A}\|t, t_0; g, \mathbf{n}\rangle. \quad (82)$$

(The left hand side defines a notation for the sum of contributions of the $\mathfrak{R}$-regular diagrams.) Then the assertion we have proved can be written in the form

$$\langle S_g^+(t, t_0)\hat{A}^{H_0}(t) S_g(t, t_0)\|\mathbf{n}\rangle = \langle\hat{A}\|t, t_0; g; n_{\mathbf{k}}'(t, t_0)\rangle = \langle\hat{A}\|t, t_0; g; \bar{R}_g(t, t_0)\mathbf{n}\rangle, \quad (83)$$

and comparing this equation with (44) shows that (82) defines the same distribution as (43). Thus the

expectation value with respect to the distribution $\|t, t_0; g, \mathbf{n}\rangle$, discussed in Sec. 2, is represented as the sum of contributions from all $\mathfrak{R}$-regular diagrams.

We now assume that the only divergences for $t_0 \to -\infty$ are those related to the presence of singular $\mathfrak{R}$-parts. Then, since the distribution (83) is a sum of contributions from diagrams with no singular $\mathfrak{R}$-parts, a limit for $t_0 \to -\infty$ will exist for the expectation values (82), i.e. (45) will hold. The existence of this limit, which according to (82) can be written in the form:

$$\langle \hat{A} \| g; \mathbf{n} \rangle = \langle S_g^+(0, -\infty) \hat{A} S_g(0, -\infty) \| \mathbf{n} \rangle'_{\text{conn}, \mathfrak{R}-\text{reg}}, \tag{84}$$

it follows rigorously that this limit, i.e. (84), is the expectation value in quasi-equilibrium states of a non-ideal gas with momentum space density $n_{\mathbf{k}}$, as was shown in Sec. 2. Here $n_{\mathbf{k}}$ varies with time according to the kinetic equation (60), i.e. according to (84)

$$\frac{\partial n_k}{dt} = -i\langle S_g^+(0, -\infty) [g\hat{H}', \hat{n}_k] S_g(0, -\infty) \| \mathbf{n} \rangle_{\text{conn}, \mathfrak{R}-\text{reg}} \tag{85}$$

Thus, the existence of evolution equations in closed form for $n_{\mathbf{k}}$ is equivalent to the absence for $t_0 \to -\infty$ of other divergences than those related to singular $\mathfrak{R}$-parts. These latter divergences are the only ones which are always present (for any Hamiltonian), but in concrete cases there may exist in addition other singularities (in particular, such will be the case for systems with Coulomb interactions). In these cases the quantities $n_{\mathbf{k}}$ do not suffice for the description of quasi-equilibrium situations; one must add other macroscopic quantities, and evolution equations in closed form will exist only for this enlarged set. The approach developed in the present paper can be generalized in an obvious manner to the derivation of such equations, and to all analogous cases. Thus, considering the switching-on of the interaction for states of the form $\|n_{\mathbf{k}}, \varphi_{\mathbf{k}}\rangle$ (cf. (16)) we obtain evolution equations for $n_{\mathbf{k}}$ and $\varphi_{\mathbf{k}}$, which describe the kinetics of superconducting states. For spatially nonhomogeneous states (15) we obtain an equation for $\rho_1(\mathbf{r}, \mathbf{r}', t)$; in the latter case one can also derive an ordinary kinetic equation for $n_{\mathbf{k}}(\mathbf{r})$ if one generalizes our approach, considering a switching-on of the interaction not only as a function of time, but also of space. The author hopes to discuss this in another place.

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