Einstein Condensation in a Macroscopic Field

Rainer Brendle *
Institut für Theoretische Physik, Universität Tübingen

Z. Naturforsch. **40 a**, 1189–1198 (1985); received October 3, 1985

A new kind of thermodynamic limit is given for the model of an ideal Boson gas which scales the supports of the local Weyl operators into infinitesimal regions leaving the external potential fixed. A technical assumption in a paper of Davies on this subject is derived from geometrical arguments. The spatial distribution of the condensate density is calculated for an arbitrary potential being bounded from below. This is used for a simple qualitative explanation of the Helium film effect.

§ 1 Introduction

Einstein condensation, that is the phase transition occurring in an interaction free quantum gas consisting of Boson particles, has always been considered as a first explanation for the superfluid properties of liquid ^{4}He as well as for the related field of superconductivity. Einstein's arguments were very intuitive and simple, mainly based on the existence of an upper bound for the particle density, if one uses the common Bose-Einstein-distribution. Mathematically convincing investigations of the problem, however, were performed much later [1–4].

In this paper, a condensing Boson gas in the presence of macroscopic inhomogeneities is studied, and arguments are supplied which are missing in the literature on the Einstein condensation.

We will imagine that the macroscopic inhomogeneity of the system is caused by a potential field V, for which we assume that it varies so slowly that from a microscopic point of view it can be considered to be almost constant. A slight generalization allowing for infinite energy values includes a special spatial inhomogeneity, namely the vessel holding the gas.

Basic concepts in the description of Boson systems are the creation and annihilation operators $a^*(f)$ and $a(f)$ as operator valued distributions over an appropriate complex test function space E with scalar product $\langle f, g\rangle$, $f, g \in E$, fulfilling the canonical commutation relations (CCR):

$$[a(f), a(g)] = [a^*(f), a^*(g)] = 0$$

and

$$[a(f), a^*(g)] = \langle f, g\rangle \quad \forall f, g \in E\,. \tag{1}$$

The Hilbert space the operators act on, however, is unknown at first and all one really knows are the above algebraic relations.

To avoid the problems caused by the unboundedness of those operators one can introduce the field operators $\Phi(f) := (1/\sqrt{2})\,(a(f) + a^*(f))$ and then use them to construct the unitary Weyl operators

$$W(f) := \exp\{i\Phi(f)\}\,.$$

They fulfill the so-called Weyl relation

$$W(f)\,W(g) = \exp\{-(i/2)\,\mathrm{Im}\langle f, g\rangle\}\,W(f+g) \tag{2}$$

for all $f, g \in E$ as a consequence.

Manuceau [5] and independently Slawny [6] showed that for every complex inner product space E (which may not be complete) there exists a unique C*-algebra CCR(E) – the CCR algebra or Weyl algebra over E – which is generated by non-zero elements $W(f)$, $f \in E$, satisfying $W(f)^* = W(-f)$ and (2).

The choice of an appropriate Hilbert space will be done by the construction of a representation of the CCR algebra. It should be noted that the algebra is simple and thus has only faithful representations.

Given a representation $(\mathscr{H}, \pi)$ of the CCR(E) every physical state defined by a density operator ϱ

* Present adress: Max-Planck-Institut für Festkörperforschung, D-7000 Stuttgart 80.

Reprint requests to Doz. Dr. A. Rieckers, Institut für Theoretische Physik der Universität Tübingen, Auf der Morgenstelle 14, D-7400 Tübingen.

0340-4811 / 85 / 1200-1189 $ 01.30/0. – Please order a reprint rather than making your own copy.

on $\mathscr{H}$ generates a state of the algebra, that is to say a positive, normalized, linear functional

$$\omega : \mathrm{CCR}(E) \mapsto \mathbb{C}, \quad A \mapsto \omega(A) = \mathrm{tr}(\varrho \pi(A)) .$$

Since the algebra is generated by the $W(f)$, every state is uniquely defined by the expectation values of the Weyl operators $\omega(W(f))$, which as a functional of f is called the state's generating functional. On the other hand, via the GNS construction, one obtains a cyclic representation of the algebra from every state.

A state of the CCR algebra is called gauge invariant, if

$$\omega(W(f)) = \omega(W(e^{i\varphi} f)) , \quad \forall \varphi \in \mathbb{R} . \tag{3}$$

A state ω is called quasifree and gauge invariant, if

$$\omega(W(f)) = \exp\{-\tfrac{1}{4} \| f \|^2\} \exp\{-\tfrac{1}{2} n_\omega(f)\} , \quad \forall f \in E . \tag{4}$$

The quantity $n_\omega(f)$ is a positive quadratic form on E. It is called the state's two point form and it has the meaning of the occupation number expectation value of the "single particle state" f. A special quasifree and gauge invariant state is the Fock space vacuum ω_0 with the two point form $n_0 = 0$.

We will generally assume that we have a system consisting of spinless, non-interacting Boson particles being confined to a vessel – mathematically described by an open, bounded set Λ in $\mathbb{R}^n$, $n = 1, 2, 3, \ldots$, and Dirichlet boundary conditions of the kinetic energy operator (the physical space dimension is of course $n = 3$, but the following calculations do not require this).

The system shall be exposed to an external potential field – mathematically described by a piecewise continuous function V on $\mathbb{R}^n$ (or Λ). What we are searching for is the state the system assumes in equilibrium. To avoid complicated formulas we will choose V so that $\min\{V(y); y \in \Lambda\} = 0$. Thus the potential can and shall always be taken positive.

The original hamiltonian of the system is the second quantization $\mathrm{d}\Gamma(H)$ of

$$H := T_\Lambda + V , \tag{5}$$

where $T_\Lambda = -1/2m\,\Delta$ with the Dirichlet Laplacian in Λ and with m the single particle mass.

In order to formulate the thermodynamic limit we will use as the test function space of the Weyl algebra the space of square integrable functions on $\mathbb{R}^n$ with essentially compact support. The space shall be denoted by $L_0^2(\mathbb{R}^n)$. The CCR algebra over $L_0^2(\mathbb{R}^n)$ becomes a quasilocal algebra; the CCR $(L^2(\Omega))$ with bounded and open subsets Ω form a generating net. We will call the CCR (L_0^2) the quasilocal CCR or Weyl algebra.

To give a precise meaning to what we mean by a microscopic or macroscopic point of view we need a very special kind of thermodynamic limit. We want to keep the notion of the vessel and the potential field even in the limit of an infinite system and, therefore, the usual inflation of the basic region has to be replaced by a spatial "contraction" of the CCR-algebra.

To that end we define the contraction and shift automorphism groups

$$c_\lambda(W(f)) = W(C_\lambda f) \quad \text{and} \quad s_x(W(f)) = W(S_x f)$$

of the quasilocal CCR algebra as Bogoliubov transformations generated by the single particle unitarities

$$(C_\lambda f)(y) := \lambda^{n/2} f(\lambda y)$$

and

$$(S_x f)(y) := f(y - x) , \tag{6}$$

where $x \in \mathbb{R}^n$, $\lambda > 0$ and $f \in L_0^2(\mathbb{R}^n)$.

Moreover, we define new single particle hamiltonians

$$H^\lambda := \lambda^{-2} T_\Lambda + V - \varepsilon_{\lambda 0} \tag{7}$$

as well as the corresponding grand canonical Gibbs states $\omega_{\beta\varrho}^\lambda$ defined as Fock normal states with density operators

$$\frac{1}{\gamma} \Gamma(z\, e^{\beta H^\lambda}) = \frac{1}{\gamma} e^{\beta \mathrm{d}\Gamma(H^\lambda - \mu)} . \tag{8}$$

$\varepsilon_{\lambda 0}$ shall be the lowest eigenvalue of the operator $\lambda^{-2} T_\Lambda + V$, β is the inverse temperature (in units, where $k_B = 1$), μ the chemical potential, z the activity $z = \exp(\beta\mu)$, γ the partition function and ϱ the particle concentration expectation value

$$\varrho = \frac{1}{\lambda^n |\Lambda|} \frac{1}{\gamma} \mathrm{tr}(\Gamma(z\, e^{\beta H^\lambda}) N) ,$$

where $|\Lambda|$ is the volume of Λ. z shall be understood as a function of ϱ (and λ, β).

The $\omega_{\beta\varrho}^\lambda$ are quasifree and gauge invariant states:

$$\omega_{\beta\varrho}^\lambda(W(f)) = \exp\{-\tfrac{1}{4} \| f \|^2\} \exp\{-\tfrac{1}{2} n_{\beta\varrho}^\lambda(f)\}$$

with

$$n^{\lambda}_{\beta\varrho}(f) = \langle f, z\,(e^{\beta H^{\lambda}} - z)^{-1} f \rangle \tag{9}$$

(see Bratteli and Robinson [7], for instance). The renormalization of the hamiltonians by the $\varepsilon_{\lambda 0}$ is chosen so that the values of z are independently of λ restricted to $0 < z < 1$.

So defined, the $\omega^{\lambda}_{\beta\varrho}$ are just states of the CCR $(L^2(\Lambda))$. To get a state of the quasilocal algebra we can set it equal to the (Fock space) vacuum outside the vessel. This can be done by assuming an infinite energy of the gas particles when being in a state outside Λ.

Mathematically more precise, let us assign a projection valued measure (p.v.m.) P_{A} on $[0, +\infty]$ to every positive operator A (like H^{λ}) on a domain D, not necessarily dense in $L^2(\mathbb{R}^n)$, where in $[0, +\infty]$ P_{A} is the usual p.v.m. of A as a selfadjoint operator on D and $P_{\mathrm{A}}(\{+\infty\})$ is the projector on $D^{\perp}$. Via functional calculus we then can give sense to $\exp(-\beta A)$ or $(A+1)^{-1}$ as bounded operators on $L^2(\mathbb{R}^n)$. One should note that $\exp(-O A)$ may not be the identity and that $(A+1)^{-1}$ may not be an inverse in the usual sense in general. Operators originally defined on subspaces of $L^2(\mathbb{R}^n)$ shall in the following always be extended in this manner.

The thermodynamic limit shall be performed by letting the parameter λ go to infinity. With growing λ the Bogoliubov transformations c_{λ} concentrate the CCR algebra at the origin of the coordinate system. The origin itself can be changed by the shift automorphisms s_x. The second effect of the growth of λ is the change of the hamiltonians and the corresponding Gibbs states.

The scaling of the hamiltonians is chosen so that the geometry of space is kept fixed on one side, but on the other side (infinitesimal) spatial distances (which occur in differential operators) are assumed to be linearly growing with λ. So, in the thermodynamic limit macroscopically different points get infinitely far away from each other from a microscopic point of view.

The local equilibrium state of the system in the macroscopic point x then will be the state $\omega^{x}_{\beta\varrho}$ with generating functional

$$\omega^{x}_{\beta\varrho}(W(f)) = \lim_{\lambda\to\infty} \omega^{\lambda}_{\beta\varrho}(s_x\, c_{\lambda}(W(f)))\,,$$

i.e. the state

$$\omega^{x}_{\beta\varrho} = \omega^{*} - \lim_{\lambda\to\infty} c^{*}_{\lambda}\, s^{*}_{x}\, \omega^{\lambda}_{\beta\varrho} = w^{*} - \lim_{\lambda\to\infty} \omega_{\beta\varrho\lambda x}\,, \tag{10}$$

where $\omega_{\beta\varrho\lambda x} := c^{*}_{\lambda}\, s^{*}_{x}\, \omega^{\lambda}_{\beta\varrho}$. In the same way the two point form of $\omega_{\beta\varrho\lambda x}$ shall be denoted by $n_{\beta\varrho\lambda x}$. The activity in the states $\omega_{\beta\varrho\lambda x}$ shall be chosen so that the expectation value of the particle number is $\lambda^n\,|\,\Lambda\,|\,\varrho$.

What is the relation of this procedure to the usual thermodynamic limit? Here one keeps the region Λ (the vessel) fixed all the time and varies the dynamics and the corresponding Gibbs state. In the usual formulation one assigns Gibbs states to a great class of regions (a subset of the set of all bounded, open sets) and then looks at their limit state for increasing volume.

But this is exactly represented by the states $c^{*}_{\lambda}\,\omega^{\lambda}_{\beta\varrho}$, $\lambda \in \mathbb{R}_{+}$. The additional transformations s^{*}_{x}, however, change the considered set of regions and if $\omega^{x}_{\beta\varrho}$ is not independent of $x \in \mathbb{R}^n$, the states $\omega^{x}_{\beta\varrho}$ form a set of accumulation points of the traditional thermodynamic limit.

The operators $\lambda^{-2} T_{\Lambda} + V - \varepsilon_{\lambda 0}$ are transformed by C_{λ} and S_x into

$$H_{\lambda x} := S^{*}_{x}\, C^{*}_{\lambda}\, H^{\lambda}\, C_{\lambda}\, S_x = T_{\lambda(\Lambda - x)} + V\left(\frac{\cdot}{\lambda} + x\right) - \varepsilon_{\lambda 0} \tag{11}$$

which are similar to the operators used in the work of Davies [2].

Besides some technical advantages the new approach makes it clear that the nonuniqueness of the usual thermodynamic limit can be used to create a macroscopic space scale described by the parameter x in addition to the microscopic space, which is described by the spatial coordinate of the test functions in $L^2_0(\mathbb{R}^n)$. Thus we can get a precise meaning of the expressions microscopic and macroscopic.

Now, some facts about the operators H^{λ} and $H_{\lambda x}$ shall be listed.

1. If $A \gg 0$ means the operator A is positively preserving, i.e. $Af \geqq 0$, $\forall f \geqq 0$, $f \in L^2(\mathbb{R}^n)$, then we have

$$0 \ll e^{-\beta(T_{\Omega} + V)} \ll e^{-\beta T_{\Omega}} \ll e^{-\beta T_0}\,, \tag{12}$$

where Ω is a bounded, open subset and $T_0 = -1/2m\Delta$ the free hamiltonian in $\mathbb{R}^n$. The semigroup $\exp\{-\beta T_0\}$ has the integral kernel

$$G_0(\beta; x, y) = \left(\frac{m}{2\pi\beta}\right)^{n/2} \exp\left\{-\frac{m}{2\beta}\,\|x - y\|^2\right\}. \tag{13}$$

The relation $\ll$ implies corresponding expressions for the operator norm, the Hilbert-Schmidt norm

and the trace of positive operators. ((12) can be proved by using the techniques of Davies [8] together with Kato's [9] extension of the Trotter product formula.)

2. An important estimation is

$$\| e^{-\beta(T_\Omega + V)} \psi \|_\infty \leqq \left(\frac{m}{4\pi\beta}\right)^{n/4} \| \psi \|_2 ,$$

if ψ is any L^2 function. If ψ is an eigenvector of $T_\Omega + V$ with eigenvalue ε, then we can even conclude

$$\| \psi \|_\infty \leqq \left(\frac{e\, m\, \varepsilon}{\pi n}\right)^{n/4} . \tag{14}$$

The above relations can also be found in [8].

3. For the strong graph limit of $H_{\lambda x}$, when λ goes to infinity, one gets, if V is continuous in x,

$$\operatorname{str.gr.lim}_{\lambda \to \infty} H_{\lambda x} = T_0 + V(x)\, \mathbb{1} . \tag{15}$$

As a consequence one has

$$\operatorname{s-lim}_{\lambda \to \infty} e^{-\beta H_{\lambda x}} = e^{-\beta V(x)}\, e^{-\beta T_0} . \tag{16}$$

4. The lowest eigenvalue $\varepsilon_{\lambda 0}$ of H^λ is non-degenerate. The corresponding eigenvector shall be denoted by Φ^λ and its spectral projector by P_λ. $H_{\lambda x}$ has the same spectrum as H^λ; the ground state eigenvector and projector shall be called $\Phi_{\lambda x}$ and $P_{\lambda x}$. Moreover we have $\lim_{\lambda \to \infty} \varepsilon_{\lambda 0} = 0$.

§2 The Constant Concentration Condition

From a mathematical point of view this chapter is rather a better review of Davies' article [2].

It is well known, that for elaborating the phase transition in a condensing Bose gas one needs control on the relationship between the activity and the particle concentration (density). We assumed the activity z as a function of the concentration ϱ and the parameter λ, which describes the thermodynamic limit. For an explicit calculation, however, we prefer keeping the activity fixed and computing ϱ as a function of z and λ (and β).

Since the two point form of a quasifree and gauge invariant state corresponds to the occupation number of the inserted single particle state, one gets the total particle number in the region Ω with volume 1 by

$$\varrho^{\lambda x}_{\beta z}(\Omega) = \sum_i n_{\beta \varrho \lambda x}(f_i) = \sum_{\nu=1}^{\infty} z^\nu \operatorname{tr}\left(e^{-\nu \beta H_{\lambda x}} P_\Omega\right) ,$$

if the f_i form an orthonormal basis of $L^2(\Omega)$. The last equality follows by a geometric series expansion of the two point form.

The mean particle concentration in the vessel then is

$$\begin{aligned} \varrho^{\lambda}_{\beta z} &= \frac{1}{|\lambda(\Lambda - x)|} \sum_{\nu=1}^{\infty} z^\nu \operatorname{tr}\left(e^{-\nu\beta H_{\lambda x}}\right) \\ &= \frac{1}{\lambda^n |\Lambda|} \sum_{\nu=1}^{\infty} z^\nu \operatorname{tr}\left(e^{-\nu\beta H^\lambda}\right) . \end{aligned}$$

Using the Green's functions (the integral kernels) of the semigroups $\exp(-\beta H^\lambda)$ and Fubini's theorem one easily derives

$$\varrho^{\lambda}_{\beta z} = \frac{1}{|\Lambda|} \int \varrho^{\lambda x}_{\beta z}(\Omega)\, \mathrm{d}^n x \quad \forall \Omega .$$

If we set

$$\varrho_{\beta z} := \lim_{\lambda \to \infty} \varrho^{\lambda}_{\beta z} \quad \text{and} \quad \varrho_{\beta z}(x) := \lim_{\lambda \to \infty} \varrho^{\lambda x}_{\beta z}(\Omega) ,$$

then we get

$$\varrho_{\beta z} = \frac{1}{|\Lambda|} \int \varrho_{\beta z}(x)\, \mathrm{d}^n x$$

if we use the estimation

$$\operatorname{tr}\left(e^{-\beta H_{\lambda x}} P_\Omega\right) \leqq \operatorname{tr}\left(e^{-\beta T_0} P_\Omega\right) = \left(\frac{m}{2\pi\beta}\right)^{n/2} ,$$

the boundedness of the Jonquière function

$$g_{n/2}(z) = \sum_{\nu=1}^{\infty} \frac{z^\nu}{\nu^{n/2}} ; \quad 0 \leqq z < 1 ,$$

as well as Lebesgue's dominated convergence theorem.

So it remains to compute $\varrho_{\beta z}(x)$, which will be called the local particle concentration in the macroscopic point x. The reason for this name will soon become clear.

Lemma 1 (Davies)

Let $0 < z < 1$ and V be continuous in the point x, then

$$\varrho_{\beta z}(x) = \left(\frac{m}{2\pi\beta}\right)^{n/2} g_{n/2}\left(e^{-\beta V(x)} z\right) .$$

Especially the limit is independent of Ω.

The proof can be found in [2]. It mainly rests on the validity of (16).

Since the $\varrho^{\lambda}_{\beta z}$ are strict monotonically increasing as functions of z and since $\varrho^{\lambda}_{\beta z}|_{z\to 0} = 0$ and $\varrho^{\lambda}_{\beta z}|_{z\to\infty} = +\infty$, we can find for every given concentration ϱ a unique value of $z(\lambda)$. Also $\varrho_{\beta z}$ is a strict monotonically increasing function of z, but in general it is bounded. Its lowest upper bound is the so called critical concentration

$$\varrho_c(\beta) = \frac{1}{|\Lambda|}\left(\frac{m}{2\pi\beta}\right)^{n/2} \int g_{n/2}(e^{-\beta V(x)})\, \mathrm{d}^n x\,,$$

which is always finite if $n \geqq 3$.

Because of the monotony the convergence of $\varrho^{\lambda}_{\beta z}$ to $\varrho_{\beta z}$ is uniform, and so one gets the following theorem:

Theorem 2 (Davies)

Let the critical concentration be the expression

$$\varrho_c(\beta) = \frac{1}{|\Lambda|}\left(\frac{m}{2\pi\beta}\right)^{n/2} \int g_{n/2}(e^{-\beta V(x)})\, \mathrm{d}^n x\,.$$

Let $\varrho > 0$ be given and let $z(\lambda)$ be the solution of the equation

$$\varrho^{\lambda}_{\beta z(\lambda)} = \varrho\,.$$

1) If $0 < \varrho < \varrho_c(\beta)$, then

$$\lim_{\lambda\to\infty} z(\lambda) = z\,,$$

where z is given by the condition $\varrho_{\beta z} = \varrho$.

2) If $\varrho_c(\beta) \leqq \varrho < \infty$, then

$$\lim_{\lambda\to\infty} z(\lambda) = 1\,.$$

§3 The Local Limit States

Now the limit states $\omega^x_{\beta\varrho}$ shall be computed. Since they are of course also quasifree and gauge invariant, it is enough to look at their two point form, which shall be called $n^x_{\beta\varrho}$.

Below the critical concentration one gets the following result:

Lemma 3 (Davies)

Let $0 < \varrho < \varrho_c(\beta)$ and let V be continuous in x. Then the local equilibrium state in the point x is given by

$$n^x_{\beta\varrho}(f) = \sum_{\nu=1}^{\infty} z^{\nu} e^{-\nu\beta V(x)} \langle f, e^{-\nu\beta T_0} f\rangle$$
$$= \langle f, z(e^{\beta(T_0+V(x))} - z)^{-1} f\rangle\,,$$

where z is the solution of the equation $\varrho_{\beta z} = \varrho$.

Proof: Let $\hat{z}$ be so that $z < \hat{z} < 1$ and let $z(\lambda)$ be the solution of $\varrho_{\beta z(\lambda)} = \varrho$.

Then $0 < z(\lambda) < \hat{z}$, if λ is big enough. The estimation

$$\left|\sum_{\nu=1}^{\infty} z(\lambda)^{\nu} \langle f, e^{-\nu\beta H_{\lambda x}} f\rangle\right|$$
$$\leqq \sum_{\nu=1}^{\infty} \hat{z}^{\nu} \| e^{-\nu\beta H_{\lambda x}}\| \, \|f\|^2 = \|f\|^2 \sum_{\nu=1}^{\infty} \hat{z}^{\nu}$$

gives a dominating, convergent series. This together with (16) proves the lemma.

If the system has a mean particle concentration which is lying above the critical concentration, it is useful to decompose the two point form into a normal and a super part, where the latter describes the contribution of the single particle ground state:

$$n^{\lambda x}_{\beta\varrho} = N^{\lambda x}_{\beta\varrho} + S^{\lambda x}_{\beta\varrho}$$

with

$$S^{\lambda x}_{\beta\varrho}(f) := \frac{z(\lambda)}{1 - z(\lambda)} |\langle \Phi_{\lambda x}, f\rangle|^2$$
$$= \frac{z(\lambda)}{1 - z(\lambda)} |\langle \Phi^{\lambda}, S_x C_{\lambda} f\rangle|^2$$

and

$$N^{\lambda x}_{\beta\varrho}(f) := \sum_{\nu=1}^{\infty} z(\lambda)^{\nu} \langle f, (e^{-\nu\beta H_{\lambda x}} - P_{\lambda x}) f\rangle\,.$$

Let us start with the normal part. There to the following lemma also being derived by Davies [2].

Lemma 4 (Davies)

Let $n \geqq 3$. If $\varepsilon_{\lambda 0}$ and $\varepsilon_{\lambda 1}$ are the two lowest eigenvalues of $\lambda^{-2} T_{\Lambda} + V$ and if they fulfil the condition

$$\exists\, \alpha\ \forall\, \lambda\ \frac{\varepsilon_{\lambda 0}}{\varepsilon_{\lambda 1}} \leqq \alpha < 1\,,$$

then

$$\lim_{\lambda\to\infty} \sum_{\nu=1}^{\infty} z^{\nu} \langle f, (e^{-\nu\beta H_{\lambda x}} - P_{\lambda x}) f\rangle$$
$$= \sum_{\nu=1}^{\infty} z^{\nu} e^{-\nu\beta V(x)} \langle f, e^{-\nu\beta T_0} f\rangle$$

uniformly for $0 \leqq z \leqq 1$, if V is continuous in x.

However, Davies did not succeed in giving his condition on the eigenvalues a physical meaning. The proof of the next theorem will show that under realistic physical conditions Davies' assumption is almost always true.

Theorem 5

Let $n \geqq 3$. Let $\Lambda_0 := \{y \in \Lambda; V(y) = 0\}$ be the set of global minimas of the potential V. If Λ_0 is a Borel set with volume $|\Lambda_0| > 0$, and its shape is so, that T_{Λ_0}, the kinetic energy operator with Dirichlet boundary conditions in Λ_0, has a non degenerate lowest eigenvalue, then

$$N^x_{\beta\varrho}(f) := \lim_{\lambda\to\infty} N^{\lambda x}_{\beta\varrho}(f) = \sum_{\nu=1}^{\infty} e^{-\nu\beta V(x)} \langle f, e^{-\nu\beta T_0} f\rangle$$
$$= \langle f, (e^{\beta T_0} e^{\beta V(x)} - 1)^{-1} f\rangle ,$$

if V is continuous in x. If $x \in \Lambda_0$, the last scalar product has to be understood as a closed quadratic form.

Proof: The uniform convergence of lemma 4 implies the theorem, if one can make sure the eigenvalue condition there. Let us look at the operator $T_\Lambda + \lambda^2 V$ and let $E_{\lambda i}$, $i = 0, 1, \ldots$ be its eigenvalues, increasingly ordered and repeated after multiplicity. Of course, we have $E_{\lambda i} = \lambda^2 \varepsilon_{\lambda i}$, with $\varepsilon_{\lambda i}$ the corresponding eigenvalues of $\lambda^{-2} T_\Lambda + V$ and therefore $E_{\lambda 0}/E_{\lambda 1} = \varepsilon_{\lambda 0}/\varepsilon_{\lambda 1}$. The operators $T_\Lambda + \lambda^2 V$ are monotonically increasing with respect to the ordering induced by the cone of positive operators and therefore by the minimax theorem the same is true for the $E_{\lambda i}$.

Let q be the quadratic form

$$q(f) := \sup_{\lambda} \{\| T_\Lambda^{1/2} f\|^2 + \lambda^2 \langle f, Vf\rangle\}$$

on the domain

$$Q(q) := \{f \in C_0(\Lambda); q(f) < \infty\} .$$

Obviously $Q(q) = C_0(\Lambda_0)$, which is a form core of T_{Λ_0} and so the closure of q corresponds to the self-adjoint operator T_{Λ_0}.

If the E_i, $i = 0, 1, \ldots$, form the increasingly ordered eigenvalues of T_{Λ_0}, repeated after multiplicity, then again by the minimax theorem [10] we get

$$\sup_\lambda E_{\lambda i} = \sup_\lambda \sup_{\varphi_1,\ldots,\varphi_i} \inf_{\substack{f \in Q(T_\Lambda + V) \\ \|f\| = 1 \\ f \perp \varphi_j, j = 1,\ldots,i}} \| T_\Lambda^{1/2} f\|^2$$
$$+ \lambda^2 \| V^{1/2} f\|^2 = \sup_{\varphi_1,\ldots,\varphi_i} \inf_{\substack{f \in Q(T_{\Lambda_0}) \\ \|f\| = 1 \\ f \perp \varphi_j, j = 1,\ldots,i}} \sup_\lambda \| T_\Lambda^{1/2} f\|^2$$
$$+ \lambda^2 \| V^{1/2} f\|^2 = E_i ,$$

where $Q(T_\Lambda + V)$ and $Q(T_{\Lambda_0})$ shall mean the form domains of $T_\Lambda + V$ or T_{Λ_0}.

Because of the monotony we also get

$$\lim_{\lambda\to\infty} E_{\lambda i} = E_i .$$

But if $E_0 \neq E_1$, then there exists a $\varkappa > 0$, so that

$$E_{\lambda 1} - E_0 \geqq \varkappa E_0$$

if λ is big enough, and therefore

$$E_{\lambda 1} - E_{\lambda 0} \geqq E_{\lambda 1} - E_0 \geqq \varkappa E_0 \geqq \varkappa E_{\lambda 0}$$

and

$$E_{\lambda 1}/E_{\lambda 0} - 1 \geqq \varkappa > 0 .$$

If then we set $\alpha := (\varkappa + 1)^{-1} < 1$, we just get the desired condition

$$E_{\lambda 0}/E_{\lambda 1} = \varepsilon_{\lambda 0}/\varepsilon_{\lambda 1} \leqq \alpha < 1 .$$

Lemma 4 then implies the validity of the expression for $N^x_{\beta\varrho}$. Since 1 lies in the spectrum of $\exp(\beta T_0)$, the operator in the last scalar product in the theorem is unbounded, if $x \in \Lambda_0$. Implicitly lemma 4 showed, that every $f \in L^2_0(\mathbb{R}^n)$ lies in the form domain of $(\exp(\beta T_0) - 1)^{-1}$. Then $\langle f, (\exp(\beta T_0) - 1)^{-1} f\rangle$ has to be extended into a closed quadratic form. □

It should be noted, that T_{Λ_0} always has a non degenerate ground state, if the region Λ_0 is connected. If this is not the case, both is possible. For example, if Λ_0 consists of two connected parts Λ_0^1 and Λ_0^2, the ground state is degenerate, if the two parts coincide under euklidean rotations and shifts. On the other hand, if by rotations and shifts one of the parts can be made into a proper subset of the other and the volumes of the two regions are not the same, the ground state of T_{Λ_0} is never degenerate.

So the above theorem covers almost all physical relevant situations. The case, where Λ_0 consists of single points, which is not covered, leads to infinitely occupied ground states. The corresponding local equilibrium state in the minima will be the trace state of the algebra. An example can be found in Davies' paper [2]. Because of this unphysical solu-

tion this case shall not be considered further here. So in the following it shall be generally assumed, that Λ_0 is a non-negligible Borel set and that the lowest eigenvalue of T_{Λ_0} is non-degenerate.

Let us now come to the super part of the two point form, where Davies could not derive a convincing result. It is given by

$$S^X_{\beta\varrho}(f) := \lim_{\lambda\to\infty} S^{\lambda X}_{\beta\varrho}(f)$$

$$= \lim_{\lambda\to\infty} \frac{z(\lambda)}{1-z(\lambda)} |\langle C^*_\lambda S^*_x \Phi^\lambda, f\rangle|^2$$

$$= \lim_{\lambda\to\infty} \frac{1}{\lambda^n} \frac{z(\lambda)}{1-z(\lambda)}$$

$$\cdot \lim_{\lambda\to\infty} \left| \int \Phi^\lambda\left(\frac{y}{\lambda}+x\right) \overline{f(y)}\, \mathrm{d}^n y \right|^2 .$$

On the condition of the existence of the "mean condensate concentration"

$$\varrho_s := \lim_{\lambda\to\infty} \frac{1}{\lambda^n |\Lambda|} \frac{z(\lambda)}{1-z(\lambda)},$$

i.e. the mean concentration of particles in the ground state, the first limit is $|\Lambda|\,\varrho_s$.

The eigenvectors Φ^λ are only fixed up to a phase. But if you have got a net of functions Φ^λ which are uniformly converging to a function $\Psi(x) = \lim_\lambda \Phi^\lambda(x)$ locally around x, then in virtue of the continuity and the uniform boundedness

$$\|\Phi^\lambda\|_\infty \leqq \text{const.} \cdot E_0^{n/4}$$

of the Φ^λ, the super part in the thermodynamic limit is

$$S^X_{\beta\varrho}(f) = |\Lambda|\,\varrho_s\,|\Psi(x)|^2\,|\hat{f}(0)|^2,$$

where $\hat{f}(0) = \int f(y)\,\mathrm{d}^n y$ is the zero Fourier component of f.

Let us first consider ϱ_s.

Lemma 6

Let $n \geqq 3$, $\varrho_c(\beta) \leqq \varrho < \infty$, $|\Lambda_0| > 0$ and let the ground state of T_{Λ_0} be non degenerate. Then

$$\varrho_s = \varrho - \varrho_c(\beta).$$

This lemma can easily be proved by using the technique of Robinson in (Bratteli and Robinson [7], Theorem 5.2.30) together with the characteristics of the $\varepsilon_{\lambda i}$ developed in the proof of Theorem 5. Also there exists a proof of the above lemma using a Dirichlet-Neumann bracketing technique in a publication of Pulè [11]. So the somewhat lengthy proof can be ommitted here.

To look for a converging eigenvector family Φ^λ, we will first prove that the operators $T_\Lambda + \lambda^2 V$ converge to T_{Λ_0} in the strong resolvent sense. This can be done by using the Feynman-Kac formula

$$(e^{-\beta(T_\Lambda+\lambda^2 V)}\Phi)(y)$$

$$= \int_{\Omega_\beta} \exp\left\{-\lambda^2 \int_0^\beta V(\omega(t))\,\mathrm{d}t\right\} \chi_\Lambda(\omega)\,\Phi(\omega(\beta))\,\chi\mu(\omega),$$

where $\chi_\Lambda(\omega)$ is 1, if the total path ω lies in Λ and 0 elsewhere. Ω_β means the set of paths $\Omega_\beta = \bigtimes_{0\leqq t\leqq\beta} \dot{\mathbb{R}}^n$.

If Φ is any L^2 function, then we get by the monotone convergence theorem

$$\lim_{\lambda\to\infty} (e^{-\beta(T_\Lambda+\lambda^2 V)}\Phi)(y)$$

$$= \int_{\Omega_\beta} \lim_{\lambda\to\infty} \exp\left(-\lambda^2 \int_0^\beta V(\omega(t))\,\mathrm{d}t\right)$$

$$\cdot \chi_\Lambda(\omega)\,\Phi(\omega(\beta))\,\mathrm{d}\mu_y(\omega)$$

$$= \int_{\Omega_\beta} \chi_{\Lambda_0}(\omega)\,\chi_\Lambda(\omega)\,\Phi(\omega(\beta))\,\mathrm{d}\mu_y(\omega)$$

$$= \int_{\Omega_\beta} \chi_{\Lambda_0}(\omega)\,\Phi(\omega(\beta))\,\mathrm{d}\mu_y(\omega) = (e^{-\beta T_{\Lambda_0}}\Phi)(y),$$

because $\exp\left(-\lambda^2 \int_0^\beta V(\omega(t))\,\mathrm{d}t\right)$ is monotonically decreasing with λ. From the pointwise convergence we get – via the boundedness

$$\|e^{-\beta T_{\Lambda_0}}\Phi\|_\infty \leqq \left(\frac{m}{4\pi\beta}\right)^{n/4} \|\Phi\|_2 \;\forall \beta > 0 -$$

also L^2-convergence and therefore

$$\text{s-lim}_{\lambda\to\infty}\, e^{-\beta(T_\Lambda+\lambda^2 V)} = e^{-\beta T_{\Lambda_0}}.$$

Laplace transform and functional calculus imply

$$(T_{\Lambda_0}+1)^{-1} = \int_0^\infty e^{-\beta} e^{-\beta T_0}\,\mathrm{d}\beta,$$

and so we also have

$$\text{s-lim}_{\lambda\to\infty}\, (T_\Lambda + \lambda^2 V + 1)^{-1} = (T_{\Lambda_0}+1)^{-1}.$$

The positively of T_{Λ_0} and $T_\Lambda + \lambda^2 V$ as well as the analyticity of the resolvent then proves

$$\text{str.Res.lim}_{\lambda\to\infty}\, T_\Lambda + \lambda^2 V = T_{\Lambda_0}.$$

On the general conditions described in Theorem 5 there exists a $\delta > 0$ so that eventually

$$|\lambda^2 \varepsilon_{\lambda 0} - E_0| < \delta$$

and

$$|\lambda^2 \varepsilon_{\lambda i} - E_0| > \delta \qquad \forall i > 0 .$$

Then from Cauchy's formula and again functional calculus

$$P_\lambda = -\frac{1}{2\pi i} \oint_{|E-E_0|=\delta} (T_\Lambda + \lambda^2 V - E)^{-1} \, \mathrm{d}E$$

is the projector on the ground state of $T_\Lambda + \lambda^2 V$, if λ is big enough. In virtue of the strong resolvent convergence P_λ is converging strongly to the ground state projector of T_{Λ_0}. If Ψ is the eigenvector of T_{Λ_0} to the eigenvalue E_0, then

$$\Phi^\lambda := \frac{1}{\| P_\lambda \Psi \|} P_\lambda \Psi$$

is a family of ground state eigenvectors of the operators $T_\Lambda + \lambda^2 V$ or $\lambda^{-2} T_\Lambda + V$ converging to Ψ in the L^2-topology. The wanted locally uniform convergence finally one can get by the aid of the continuity of the functions and the Egorov theorem (cf. Halmos [11] for instance).

Now we have all informations needed to write down the local equilibrium states of the system.

Theorem 7

Let $\omega^x_{\beta\varrho} = \mathrm{w}^*\text{-}\lim_{\lambda \to \infty} \omega_{\beta\varrho\lambda x}$ be the local equilibrium state of the system in the macroscopic point x.

1) If $0 < \varrho < \varrho_c(\beta)$, the almost everywhere with respect to x, $\omega^x_{\beta\varrho}$ is given by the two point from

$$n^x_{\beta\varrho}(f) = \langle f, z\,(e^{\beta T_0} \mathrm{e}^{\beta V(x)} - z)^{-1} f \rangle ,$$

where z is the solution of the equation $\varrho_{\beta z} = \varrho$.

2) If $\varrho_c(\beta) \leqq \varrho < \infty$, if $n \geqq 3$, if the set Λ_0 of global minima of V is a non negligible Borel set and if the lowest eigenvalue of T_{Λ_0} is non degenerate, then (a.e.) $\omega^x_{\beta\varrho}$ is given by the two point form

$$n^x_{\beta\varrho}(f) = |\Lambda|\, \varrho_s\, |\Psi(x)|^2\, |\hat{f}(0)|^2 + \langle f, (e^{\beta T_0} e^{\beta V(x)} - 1)^{-1} f \rangle ,$$

where $\varrho_s = \varrho - \varrho_c(\beta)$ and Ψ is the ground state eigenvector of T_{Λ_0}.

The two point form is a quadratic form in the test functions f, and so we can compute its integral kernel, the real two point function. Especially the particle concentration in the state is given by the diagonal part of the two point function. Below the critical concentration we have

$$\begin{aligned} n^x_{\beta\varrho}(y,y) &= \frac{1}{(2\pi)^n} \sum_{\nu=1}^{\infty} z^\nu e^{-\nu\beta V(x)} \int e^{-\frac{\nu\beta}{2m} k^2} \mathrm{d}^n k \\ &= \frac{1}{(2\pi)^n} \sum_{\nu=1}^{\infty} z^\nu e^{-\nu\beta V(x)} \left(\frac{2\pi m}{\beta \nu}\right)^{n/2} \\ &= \left(\frac{m}{2\pi\beta}\right)^{n/2} \sum_{\nu=1}^{\infty} \nu^{-n/2} z^\nu e^{-\nu\beta V(x)} \\ &= \left(\frac{m}{2\pi\beta}\right)^{n/2} g_{n/2}(z\, e^{-\beta V(x)}) = \varrho_{\beta z}(x) , \end{aligned}$$

which is the previously defined local concentration, so that its name now becomes clear. It should be noted that the expression is independent of the microscopic point y and so a local state describes a homogeneous system.

When condensation occurs, the particle concentration is

$$\begin{aligned} n^x_{\beta\varrho}(y,y) &= \left(\frac{m}{2\pi\beta}\right)^{n/2} g_{n/2}(e^{-\beta V(x)}) \\ &\quad + |\Lambda|\, \varrho_s\, |\Psi(x)|^2\, |\hat{\delta}_y(0)|^2 \\ &= \varrho_{\beta 1}(x) + |\Lambda|\, \varrho_s\, |\Psi(x)|^2 . \end{aligned}$$

So one can interprete $\varrho_s(x) := |\Lambda|\, \varrho_s\, |\Psi(x)|^2$ as the local condensate concentration. Since Ψ is an eigenvector of T_{Λ_0}, it must lie in the domain of T_{Λ_0}, and so it must vanish outside Λ_0. As a consequence, no condensate can exist there in equilibrium.

The original parameter ϱ can be obtained by averaging the local concentration with respect to the microscopic points x:

$$\begin{aligned} \frac{1}{|\Lambda|} \int n^x_{\beta\varrho}(y,y)\, \mathrm{d}^n x &= \varrho_c(\beta) + \varrho_s \int |\Psi(x)|^2 \mathrm{d}^n x \\ &= \varrho_c(\beta) + \varrho_s = \varrho . \end{aligned}$$

Although we started with a fixed concentration ϱ and an inhomogeneous structure given by V, the limit states do describe a spatially homogeneous system with particle concentration $\varrho_{\beta z}(x)$ or $\varrho_{\beta 1}(x) + |\Lambda|\, \varrho_s\, |\Psi(x)|^2$, respectively.

One can say that the states $\omega^x_{\beta\varrho}$ locally approximate an inhomogeneous system by a homogeneous

one, may be similar to the approximation of a non linear manifold by its tangent space. So the kind of limit used regards the macroscopically inhomogeneous structure as irrelevant from a microscopic point of view.

On the other hand, however, the inhomogeneity manifests in the existence of a class of many different limit states, one for each macroscopic point x. This family of states has been used to calculate the particle concentration as a function of x.

The normal part $\varrho_{\beta z}(x)$ behaves quite natural. Namely, the external field $V(x)$ can be inserted just like an additional chemical potential of the same value. But this is not true for the condensed particles.

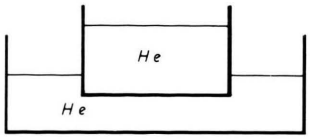

Fig. 1. The helium-film-experiment.

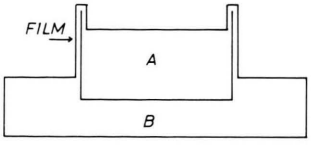

Fig. 2. The model for its explanation.

§4 A Superfluid Cannot be Locked In

Above the critical concentration the local concentration of the condensate $\varrho_s(x) := \varrho_s |\Lambda| \, |\Psi(x)|^2$ has to be used as an additional order parameter describing the equilibrium besides the chemical potential and the temperature. It has a remarkable property. Only in the global (!) minima of the potential V it can assume a nonvanishing value.

But then a condensate in a physical vessel, which has no infinitely high walls, is never in its equilibrium, if there exists a region outside, which is energetically more favorable.

This may serve for an explanation of an interesting effect of superfluid helium discovered by Rollin and Simon in 1939, the so called helium film effect. They found that bringing two vessels filled with superfluid helium into an arrangement like in Fig. 1 will cause an immediate adjustment of the two fluid levels.

The fluid surface forms a barrier for the particles of the fluid, which has to be introduced into the ideal gas model as an additional wall. Within the fluid the gravitational force is almost neutralized by the hydrostatic pressure and so we can set the potential V equal to the gravitational potential at the surface there.

Of course, to derive more than qualitative results, one has to consider superfluid helium as an interacting fluid. But the main reason for the superfluid phase transition is believed to be the Einstein condensation, and so a simple model using an ideal gas may serve.

If we imagine we have two at first independent systems A and B with respectively constant potentials V_A and V_B in disjoint regions Λ_A and Λ_B, and if we assume that a thin film of particles on the walls of the vessels is caused by bringing together the two systems, then

$$\Lambda_A \cup \Lambda_B \cup \text{FILM}$$

forms a connected region and the above results can be applied.

Let $V_A > V_B$. If the mean concentration in A and B lies above the critical one, the condensate in A will flow to B, when the systems are brought into contact. In a fluid the thereby caused changings of the concentrations are compensated by a raising and lowering of the surface. Therefore the concentrations remain supercritical and new condensate is formed, which again flows from A to B as long as V_A and V_B (i.e. the levels of the liquids) differ.

Acknowledgement

This work would not have been possible without the help and support by Dr. A. Rieckers. Also I am grateful to Prof. S. Ruijsenaars for his helpful advice.

[1] H. Araki and E. J. Woods, J. Math. Phys. **4,** 637 (1963).
[2] E. B. Davies, Comm. Math. Phys. **30,** 229 (1973).
[3] J. T. Lewis and J. V. Pulè, Comm. Math. Phys. **36,** 1 (1974), using ideas of M. Kac. Also cf. R. M. Ziff, G. E. Uhlenbeck, and M. Kac, Phys. Rep. **32C,** 169 (1977).
[4] M. Van den Berg and J. T. Lewis, Comm. Math. Phys. **81,** 475 (1981).
[5] J. Manuceau, Ann. Inst. H. Poincaré **8,** (2) 139 (1968).
[6] J. Slawny, Comm. Math. Phys. **24,** 151 (1972).
[7] O. Bratteli and D. W. Robinson, Operator Algebras and Quantum Statistical Mechanics II, Springer, New York 1981.
[8] E. B. Davies, J. Lond. Math. Soc. (2) **7,** 483 (1973).
[9] T. Kato, pp. 185–195 in I. Gohberg and M. Kac (eds.), Topics in Functional Analysis, Academic Press, New York 1978.
[10] M. Reed and B. Simon, Methods of Modern Mathematical Physics, Vol. IV: Analysis of Operators, Academic Press, New York 1978.
[11] J. V. Pulè, J. Math. Phys. **24,** 138 (1983).
[12] P. R. Halmos, Measure Theory, Van Nostrand, Princeton 1950.