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On the equipartition law in quantum statistical mechanics

M Fannes†, Ph Martin‡ and A Verbeure

Instituut voor Theoretische Fysica, Universiteit Leuven, B-3030 Leuven, Belgium

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Abstract. We prove that the fluctuations of the total momentum of a system of quantum mechanical particles at equilibrium obey the classical equipartition law whenever the correlation functions have an integrable clustering. The result holds for a large class of translation invariant two-body potentials and for arbitrary statistics. We also discuss higher moments of the total momentum and position. Finally the behaviour in models with broken symmetry is analysed.

1. Introduction

In classical statistical mechanics it is well known that the kinetic energy per particle is equal to $3kT/2$. This law of equipartition yields a direct and intrinsic method for the definition of the absolute temperature, irrespective of the interaction or the phase state.

It is also well known that the kinetic energy of a quantum mechanical system in equilibrium does not follow the equipartition law. For interacting particles and to second order in Planck's constant this quantity is always strictly larger than the classical value (Landau and Lifshitz 1967). This also holds for quantum particles without statistics confined by external forces (Martens and Verbeure 1979). The statistics, however, does change this result, indeed e.g. a free Bose gas (respectively Fermi gas) has a kinetic energy strictly smaller (respectively larger) than $3kT/2$. Therefore the temperature of a quantum system cannot be determined by a measure of its kinetic energy independently of the interactions and of the statistics.

However, let us continue with the free Bose (Fermi) gas at equilibrium in a cubic box of side L with periodic boundary conditions. The density $\rho_{\mp}(\beta, z)$ in the thermodynamic limit is given by

$$\rho_{\mp}(\beta, z) = \int \mathrm{d}^3p\, f_{\mp}(p, \beta, z)$$

where

$$f_{\mp}(p, \beta, z) = (2\pi)^{-3}\, z/[\exp(\beta p^2/2m) \mp z] \tag{1}$$

is the Bose (resp Fermi) distribution, z is the activity and taken to be larger than one in the Bose case (i.e. without condensation; for the case $z = 1$, see § 4). Then if P_L is

† Bevoegdverklaard Navorser NFWO.

‡ On leave of absence from the Institut de Physique Théorique, Ecole Polytechnique Fédérale Lausanne, Switzerland.

the total momentum observable for the gas in the box, one finds

$$\lim_{L\to\infty}\frac{\langle|P_L|^2\rangle}{2m\rho L^3}=\frac{1}{\rho(\beta,z)}\int d^3p\,\frac{p^2}{2m}(1\pm(2\pi)^3f_\mp(p,\beta,z))f_\pm(p,\beta,z)$$
$$=-(\partial/\partial\beta)\ln\rho_\mp(\beta,z)=\tfrac{3}{2}kT \qquad (2)$$

which shows that the fluctuations of the total momentum in the thermodynamic limit follow the classical law independently of the statistics.

The point of this paper is to give a rigorous proof of the fact that under fairly general clustering conditions, for non-trivial translation invariant interactions between the particles and a large class of boundary conditions, the fluctuations of the total momentum are still given by their classical values. Such a result has been known for a long time (Blatt *et al* 1955). The demonstration relied on an argument for finite systems disregarding the boundary conditions. The main idea was based on the following heuristic considerations.

Since the total momentum is nothing but the momentum of the centre of mass of the whole system it decouples from the relative coordinates. It will behave as the momentum of an independent macroscopic free system and hence by the computation above in a classical way.

It is clear that this argument can only hold asymptotically in the thermodynamic limit and not for a finite volume quantum system. In the latter case the transformation of the particle coordinates to the centre of mass and relative coordinates is not canonical because of the presence of boundary conditions. Therefore the motion of the centre of mass is neither independent of the other degrees of freedom nor of the choice of the boundary conditions. It was indeed noted that different choices may lead to different results (Lebowitz and Onsager 1957). Clearly in order to obtain the result even in the thermodynamic limit, one needs cluster properties strong enough to eliminate the effects of the boundary conditions of the finite system.

Technically we take the following point of view. We assume that we are given an infinite system in an equilibrium state ω (i.e. positive linear normalised functional on a suitable quasi-local algebra), characterised by the energy–entropy balance correlation inequality (Fannes and Verbeure 1977, 1978). Then for any sphere of radius R and volume V we define the bulk momentum P_R of the particles in this sphere; it represents a local approximation of the momentum of the infinite system. We prove that $\omega(|P_R|^2)/2m\rho V$ converges to $3kT/2$ as R tends to infinity when the state ω has integrable clustering properties. This result is also formulated as an exact sum rule for the kinetic energy per particle and the integral of the two-particle momentum correlation per particle which add up to $3kT$.

The paper is organised as follows. In § 2 we bring together the necessary preparatory material and pay special attention to a statistics independent formulation of a quantum many-body system. In particular we construct the quasi-local algebra of observables generated by the one-particle momentum and position observables.

Our main point mentioned above is given and proved in § 3. We also show that when the clustering is integrable the suitably scaled pair momentum position obeys a classical central limit theorem: all the joint moments are those of the Gaussian distribution which we would obtain for the corresponding classical quantities.

We do not expect that these results will remain true in phases which spontaneously break a continuous symmetry: in such phases the clustering is too weak (non-integrable) (Martin 1982, Fannes *et al* 1982) and our theorem will not apply. We investigate this situation in § 4 by means of the free Bose gas and the BCS model. Indeed, both models violate our result at high density (Bose gas) or low temperature (BCS).

2. General setting

As in this paper we aim at a result for infinite quantum systems independent of the statistics, we first describe the relevant algebra of observables in terms of its n-particle components. It will show much similarity with the classical algebra of observables (see e.g. Ruelle 1969).

For simplicity of presentation we take $\mathscr{H}=L^2(\mathbb{R}^\nu)$, where ν is the dimension, as configuration space of one particle disregarding internal degrees of freedom. The local algebra $\mathscr{A}_1$ of observables per particle is the *-algebra generated by the operators $R(p)f(q)$, where R runs through the polynomials, f belongs to the set of infinitely differentiable functions with compact support in $\mathbb{R}^\nu$, q and p stand for the canonical observables of multiplication and differentiation (i.e. $[q^\alpha, p^\beta]=\mathrm{i}\delta_{\alpha\beta}$).

The algebra of observables $\mathscr{A}$ for the infinite system consists of the sequences $A=\{A_j\}_{j=0}^{\infty}$ with only a finite number of the A_i different from zero, and where the A_i belong to the symmetrised tensor product of n copies of $\mathscr{A}_1$; the component A_n of A is the n-particle component, and A_0 is a scalar. $\mathscr{A}$ becomes a vector space for the usual summation, and an algebra for the following product rule. As $\mathscr{A}$ is generated by elements of the type

$$A=(0,\ldots,0,S_n(a_1\otimes\ldots\otimes a_n),0,\ldots), \qquad a_i\in\mathscr{A}_1,$$

$$B=(0,\ldots,0,S_m(b_1\otimes\ldots\otimes b_m),0,\ldots), \qquad b_j\in\mathscr{A}_1,$$

where S_k denotes the projection on the permutation symmetric operators on $(\otimes\mathscr{H})^k$, it is sufficient to define the product for these elements. We set

$$AB=\{(AB)_j\}_{j=0}^{\infty} \tag{3}$$

where

$$(AB)_j=0 \qquad \text{if} \qquad j>m+n \qquad \text{or} \qquad j<\max(n,m),$$

$$(AB)_j=\frac{j!}{n!m!(j-n)!(j-m)!(m+n-j)!}S_j\sum_\pi\sum_\sigma a_{\pi(1)}\otimes\ldots\otimes a_{\pi(j-m)}\otimes a_{\pi(j-m+1)}b_{\sigma(1)}$$
$$\otimes\ldots\otimes a_{\pi(n)}b_{\sigma(m+n-j)}\otimes b_{\sigma(m+n-j+1)}\otimes\ldots\otimes b_{\sigma(m)}$$
$$\text{if } \max(n,m)\leqslant j\leqslant m+n;$$

π and σ run in the permutation groups of n and m elements.

It is clear that this product extends to, say, the set $\tilde{\mathscr{A}}=(\tilde{\mathscr{A}}_1,\tilde{\mathscr{A}}_2,\ldots)$ where the $\tilde{\mathscr{A}}_n$ are suitable closures of $(\otimes\mathscr{A}_1)^n$. The *-operation is the usual operation of taking the adjoint.

The above presentation of the algebra of observables is nothing but a more abstract form of what is usually done with Bose or Fermi creation and annihilation operators $a^{\pm}(x)$. In this language the n-body operator corresponding to the kth component A_k of the observable A is represented by

$$(1/k!)\int \mathrm{d}x_1\ldots\mathrm{d}x_k\,\mathrm{d}y_1\ldots\mathrm{d}y_k(x_1\ldots x_k|A_k|y_1\ldots y_k)$$
$$\times a^+(x_1)\ldots a^+(x_k)a(y_k)\ldots a(y_1).$$

The product rule (3) is a result of the Wick ordering in the product of such n- and m-body operators.

A state of the infinite quantum system is a normalised linear functional ω of $\mathscr{A}$ such that for all $A=\{A_n\}_{n=0}^{\infty}$, $\omega(A^*A)\geq 0$ (positivity of ω). Denote by $\omega_n (n=0,1,\ldots)$ the n-particle restriction of ω, i.e. $\omega(A)=\Sigma_{n=0}^{\infty}\omega_n(A_n)$. We assume furthermore that the states under consideration are described in terms of a family of reduced density matrices $\{\rho^{(n)}\}_{n=0}^{\infty}$, where the $\rho^{(n)}$ are positive linear operators on $(\otimes\mathscr{H})^n$ with an infinitely differentiable kernel $(y|\rho^{(n)}|x)$ such that

$$\omega_n(A_n)=\frac{1}{n!}\int \mathrm{d}^n x\, \mathrm{d}^n y\, (x|A_n|y)(y|\rho^{(n)}|x)=\frac{1}{n!}\int \mathrm{d}^n x\, (x|A_n\rho^{(n)}|x).$$

In the following we are interested in properties of equilibrium states of a system of particles interacting via a translation invariant two-body potential V.

By now there are many ways to characterise an equilibrium state. For the purpose of this paper it will turn out that the most convenient way is by means of correlation inequalities. Therefore we call ω an equilibrium state at inverse temperature β if for all $A\in\mathscr{A}$ (Fannes and Verbeure 1977)

$$\beta\omega(A^*\delta(A))\geq\omega(A^*A)\ln[\omega(A^*A)/\omega(AA^*)] \tag{4}$$

holds, where $\delta(A)$ is given by the commutator $[H, A]$ with the formal Hamiltonian

$$H=(0, p^2/2, V, 0, \ldots)$$

(corresponding to the usual second quantised form of the Hamiltonian). The two-body potential V is a multiplication operator by $v(x_1-x_2)$ on $\mathscr{H}\otimes\mathscr{H}$, where the function v satisfies

(i) $x\in\mathbb{R}^{\nu}\to v(x)\in\mathbb{R}$ is differentiable AE;

(ii) $v(x)=v(-x)$ and rotation symmetric;

(iii) there exists an $\eta>0$ such that $\int(1+|x|^{\eta})|\nabla v(x)|\,\mathrm{d}x<\infty$.

In writing the equilibrium condition (4) we have implicitly assumed that the state ω extends to all observables of the form $\delta(A)$, $A\in\mathscr{A}$. There are some technical reasons why in general $\delta(A)\notin\mathscr{A}$, in particular if v is not of finite range $\delta(A)$ is not strictly local; however, it is reasonable to expect on the basis of condition (iii) on the potential V that the equilibrium states indeed do share the assumed extension property.

Finally we shall deal only with equilibrium states ω which are Euclidean invariant and time reversal invariant. Therefore in particular let τ be the homomorphism of the space translation group $\mathbb{R}^{\nu}$ into the *-automorphisms of $\mathscr{A}$. Then one has $\omega(\tau_x(A))=\omega(A)$ for all $x\in\mathbb{R}^{\nu}$, $A\in\mathscr{A}$. Let σ be the time reversal anti-automorphism of $\mathscr{A}$ defined by $\sigma(p)=-\sigma(p)$, $\sigma(q)=q$; then $\omega(\sigma(A))=\omega(A^*)$ for all $A\in\mathscr{A}$.

In addition we remark that any state ω satisfying (4) is stationary, i.e. $\omega(\delta(B))=0$, $B\in A$. This follows by substituting $A=1+\lambda B$, $B=B^*\in\mathscr{A}$, $\lambda\in\mathbb{R}$ in the inequality (4).

3. Fluctuations of the bulk position and momentum

For infinite systems quantities like total momentum, total mean position, total number of particles, etc are ill defined; instead one should consider the corresponding local densities. In particular one introduces the following local approximations. Consider the sequence $(f_R)_{R\in\mathbb{R}^+}$ of real functions on $\mathbb{R}^\nu$ such that

$$f_R \in C_0^\infty, \qquad 0 \le f_R \le 1, \qquad \|\nabla^\alpha f_R\|_\infty < \infty \text{ uniformly in } R,$$

$$f_R(x) = \begin{cases} 1, & |x| \le R, \\ 0, & |x| \ge R+1. \end{cases} \tag{5}$$

We denote by $P^\alpha(f_R)$ the observable corresponding to the bulk momentum located in the support of f_R, where in general

$$P^\alpha(f) = (0, \tfrac{1}{2}(p^\alpha f(q) + f(q)p^\alpha), 0, \ldots), \qquad \alpha = 1, \ldots, \nu, \qquad \text{for any } f \in C_0^\infty(\mathbb{R}^\nu),$$

and the corresponding position operator is $Q^\alpha(f_R)$ where

$$Q^\alpha(f) = (0, q^\alpha f(q), 0, \ldots.), \qquad \alpha = 1, \ldots, \nu, \qquad \text{for any } f \in C_0^\infty.$$

It is clear that both $P^\alpha(f)$ and $Q^\alpha(f)$ belong to $\mathscr{A}$.

For notational convenience we introduce for any Euclidean invariant state ω the following quantities: the density $\rho = (x|\rho^{(1)}|x)$ and the density and momentum correlations

$$\langle \rho^{(n)} p_{i_1}^{\alpha_1} \ldots p_{i_m}^{\alpha_m} \rangle (x_1, \ldots, x_{n-1}, 0) = (x_1, \ldots, x_{n-1}, 0|\rho^{(n)} p_{i_1}^{\alpha_1} \ldots p_{i_m}^{\alpha_m}|x_1, \ldots, x_{n-1}, 0).$$

Due to rotation invariance of the state one has

$$\langle \rho^{(1)} p^\alpha \rangle = 0, \qquad \langle \rho^{(1)} p^\alpha p^\beta \rangle = \delta_{\alpha\beta} \langle \rho^{(1)} (p^\alpha)^2 \rangle. \tag{6a, b}$$

First we derive expressions for the momentum and position fluctuations in terms of the one- and two-body correlations.

Lemma 3.1. Let ω be a Euclidean and time reversal invariant state with density ρ and the cluster properties

$$\int dx |\langle \rho^{(2)} p_1^\alpha p_2^\gamma \rangle (x)| < \infty, \qquad \alpha, \gamma = 1, \ldots, \nu,$$

$$\int dx |\langle \rho^{(2)} \rangle (x) - \rho^2| < \infty.$$

Denoting by Σ_ν the volume of the unit ball in ν dimensions, then

(i) $$\lim_{R\to\infty} \frac{\omega(P^\alpha(f_R)^2) - \omega(P^\alpha(f_R))^2}{\Sigma_\nu R^\nu} = \langle \rho^{(1)} (p^\alpha)^2 \rangle + \int dx \langle \rho^{(2)} p_1^\alpha p_2^\alpha \rangle (x),$$

(ii) $$(\nu+2) \lim_{R\to\infty} \frac{\omega(Q^\alpha(f_R)^2) - \omega(Q^\alpha(f_R))^2}{\Sigma_\nu R^{\nu+2}} = \rho + \int dx (\langle \rho^{(2)} \rangle (x) - \rho^2) = \rho^2 \beta^{-1} \chi,$$

where χ is the compressibility. The last equality holds if ω is an equilibrium state at inverse temperature β.

Proof. Using the product rule (3), the only non-zero components of $P^\alpha(f)^2$ are

$$[P^\alpha(f)^2]_1 = (p^\alpha)^2 f^2 + \mathrm{i} p^\alpha \nabla^\alpha (f^2) - \tfrac{1}{4} \nabla^\alpha (f \nabla^\alpha f) - \tfrac{1}{4} f \Delta_\alpha f,$$

$$[P^\alpha(f)^2]_2 = 2 p_1^\alpha f_1 p_2^\alpha f_2 + \tfrac{1}{2}\mathrm{i}(p_1^\alpha f_1 \nabla^\alpha f_2 + p_2^\alpha f_2 \nabla^\alpha f_1) - \tfrac{1}{4}(\nabla^\alpha f_1)(\nabla^\alpha f_2),$$

where $f_i = f(q_i)$, $i = 1, 2$.

Then using (6*a*) and integration by parts

$$\omega_1([p^\alpha(f)^2]_1) = \langle\rho^{(1)}(p^\alpha)^2\rangle \int \mathrm{d}x\, f^2(x) + \tfrac{1}{4}\rho \int (\nabla^\alpha f(x))^2\,\mathrm{d}x.$$

About the two-particle contribution using the time reversal invariance one gets

$$\begin{aligned}\omega_2(p_1^\alpha f_1\nabla^\alpha f_2 + p_2^\alpha f_2\nabla^\alpha f_1) &= -\omega_2(\sigma(p_1^\alpha f_1\nabla^\alpha f_2 + p_2^\alpha f_2\nabla^\alpha f_1))\\ &= -\omega_2(f_1 p_1^\alpha\nabla^\alpha f_2 + f_2 p_2^\alpha\nabla^\alpha f_1).\end{aligned}$$

Hence

$$\omega_2(p_1^\alpha f_1\nabla^\alpha f_2 + p_2^\alpha f_2\nabla^\alpha f_1) = -\mathrm{i}\omega_2((\nabla^\alpha f_1)(\nabla^\alpha f_2))$$

and after a change of variables

$$\begin{aligned}\omega_2([P^\alpha(f)^2]_2) &= \int \mathrm{d}u\,\langle\rho^{(2)}p_1^\alpha p_2^\alpha\rangle(u)\int \mathrm{d}x\, f(u+x)f(x)\\ &\quad + \tfrac{1}{4}\int \mathrm{d}u\,\langle\rho^{(2)}\rangle(u)\int \mathrm{d}x\,\nabla^\alpha f(u+x)\nabla^\alpha f(x).\end{aligned} \tag{7}$$

Taking $f = f_R$ as in (5), we have clearly

$$\lim_{R\to\infty}\frac{\int f_R^2(x)\,\mathrm{d}x}{\Sigma_\nu R^\nu} = 1 \qquad\text{and}\qquad \lim_{R\to\infty}\frac{\int(\nabla^\alpha f_R)^2(x)\,\mathrm{d}x}{\Sigma_\nu R^\nu} = 0$$

since $\int(\nabla^\alpha f_R)^2(x)\,\mathrm{d}x = \mathrm{O}(R^{\nu-1})$, due to the presence of the derivative and the special choice of f_R (5).

About the two-particle contribution, the quantity

$$(\Sigma_\nu R^\nu)^{-1}\int f_R(u+x)f_R(u)\,\mathrm{d}x$$

is uniformly bounded ($R > 1$) and converges to one for each fixed u. Hence using the momentum cluster condition, the first term of (7) converges to the desired result as a consequence of the dominated convergence theorem. For the second term of (7), since now

$$\frac{1}{\Sigma_\nu R^\nu}\left|\int \mathrm{d}x\,\nabla^\alpha f_R(u+x)\nabla^\alpha f_R(x)\right| \leqslant \frac{\|\nabla^\alpha f_R\|_\infty}{\Sigma_\nu R^\nu}\int \mathrm{d}x\,|\nabla^\alpha f_R(x)| = \mathrm{O}\left(\frac{1}{R}\right)$$

uniformly in u, using the density cluster condition and again dominated convergence

$$\begin{aligned}&\lim_{R\to\infty}\frac{1}{\Sigma_\nu R^\nu}\int \mathrm{d}u\,\langle\rho^{(2)}\rangle(u)\int \mathrm{d}x\,\nabla^\alpha f_R(u+x)\nabla^\alpha f_R(x)\\ &\quad = \lim_{R\to\infty}\frac{1}{\Sigma_\nu R^\nu}\int \mathrm{d}u\,(\langle\rho^{(2)}\rangle(u)-\rho^2)\int \mathrm{d}x\,\nabla^\alpha f_R(u+x)\nabla^\alpha f_R(x) = 0.\end{aligned}$$

This proves (i).

To prove (ii), remark that

$$\begin{aligned}&\omega(Q^\alpha(f_R)^2) - \omega(Q^\alpha(f_R))^2\\ &\quad = \rho\int \mathrm{d}x\,(x^\alpha f_R(x))^2 + \int \mathrm{d}u\,(\langle\rho^{(2)}\rangle(u)-\rho^2)\int \mathrm{d}x\,(x+u)^\alpha f_R(x+u)x^\alpha f_R(x)\end{aligned}$$

and the result follows by computing the limit $R\to\infty$ in the same way as above.

The main point of the paper consists in calculating the value of the momentum fluctuations in an equilibrium state ω defined by (4). We do not need this strong inequality but the following weakened form,

$$\beta\omega(A^*\delta(A)) \geqslant \omega([A^*, A]), \qquad A \in \mathscr{A}, \tag{8}$$

which follows from (4) and $a \ln(a/b) \geqslant a - b$; $(a, b > 0)$.

In order to make an optimal use of (8) it is important to choose for A a non-normal operator with a simple commutator $[A^*, A]$. This is realised by the choices

$$A^\alpha_\varepsilon = P^\alpha(f) + i\varepsilon Q^\alpha(g), \qquad \alpha = 1, \ldots, \nu; \qquad \varepsilon \in \mathbb{R}, \tag{9}$$

where f and g are appropriate cut-off functions.

Theorem 3.2. Let ω be a Euclidean and time reversal invariant equilibrium state satisfying the cluster properties stated in the lemma. Then the bulk momentum density fluctuations are given by

$$\langle \rho^{(1)}(p^\alpha)^2\rangle + \int \mathrm{d}x\, \langle \rho^{(2)} p_1^\alpha p_2^\alpha\rangle(x) = \rho kT, \qquad \alpha = 1, \ldots, \nu.$$

Proof. Substituting the operators A^α_ε (9) in (8) and using the time invariance of the state in the form

$$0 = \omega(\delta(Q^\alpha(g)P^\alpha(f))) = \omega(\delta(Q^\alpha(g))P^\alpha(f)) + \omega(Q^\alpha(g)\delta(P^\alpha(f)))$$

we get

$$\begin{aligned} &\beta[\omega(P^\alpha(f)\delta(P^\alpha(f))) + \varepsilon^2\omega(Q^\alpha(g)\delta(Q^\alpha(g))) \\ &\qquad + i\varepsilon\omega(P^\alpha(f)\delta(Q^\alpha(g))) + i\varepsilon\omega(\delta(Q^\alpha(g))P^\alpha(f)) \\ &\qquad \geqslant -2i\varepsilon\omega([Q^\alpha(g), P^\alpha(f)]). \end{aligned} \tag{10}$$

We choose for f a spherically symmetric function f_R in the class (5) and for g a real function g_R defined by

$$g_R(x) = h(|x|/R)$$

with $h \in C_0^\infty(\mathbb{R}^+)$, $h(r) = 1$ for $0 \leqslant r \leqslant 1$, $h(r) = 0$ for $r \geqslant 2$. We shall prove consecutively the following steps:

(a) $\omega(P^\alpha(f_R)\delta(P^\alpha(f_R))) = O(R^{\nu-\eta}) + O(R^{\nu-1})$;

(b) $\omega(Q^\alpha(g_R)\delta(Q^\alpha(g_R)) = O(R^\nu)$;

(c) $(\Sigma_\nu R^\nu)^{-1}\omega(P^\alpha(f_R)\delta(Q^\alpha(g_R)) + \delta(Q^\alpha(g_R))P^\alpha(f_R))$ is proportional to the momentum fluctuations and converges as $R \to \infty$ to $-2i(\langle \rho^{(1)}(p^\alpha)^2\rangle + \int \langle \rho^{(2)} p_1^\alpha p_2^\alpha\rangle(x)\,\mathrm{d}x)$;

(d) $(\Sigma_\nu R^\nu)^{-1}\omega([Q^\alpha(g_R), P^\alpha(f_R)])$ converges to $i\rho$ as $R \to \infty$.

Now the main argument is the following. Divide the inequality (10) by $\Sigma_\nu R^\nu$, and suppose that (a)–(d) are proved; letting $R \to \infty$, as ε is arbitrary one gets the result of the theorem.

Now we proceed to the proof of the points (a)–(d).

Proof of (a). According to the definition of δ (4) one finds that the non-zero components of $\delta(P^\alpha(f_R))$ are

$$[\delta(P^\alpha(f_R))]_1 = -ip^\alpha p\cdot\nabla f_R + \tfrac{1}{2}p^\alpha\Delta f_R + \tfrac{1}{2}p\cdot\nabla\,\nabla^\alpha f_R + \tfrac{1}{4}i\Delta\nabla^\alpha f_R, \tag{11a}$$

$$[\delta(P^\alpha(f_R))]_2 = i(f_R(q_1) - f_R(q_2))(\nabla_1^\alpha V)(q_1 - q_2) \equiv i\phi_R(q_1, q_2), \tag{11b}$$

where ∇_1^α stands for the derivative with respect to the variable indexed by 1.

According to (11) and the product rule (3) $\omega_1([P^\alpha(f_R)\delta(P^\alpha(f_R))]_1)$ is a linear combination of terms of the type

$$\langle\rho^{(1)}(p^{\alpha_1})^{n_1}\dots(p^{\alpha_\nu})^{n_\nu}\rangle\int \mathrm{d}x\,K_R(x)$$

$(n_1+\dots n_\nu\leqslant 3)$ where $K_R(x)$ contains as a factor a derivative of f_R of first or higher order. Therefore the support of K_R is contained in the domain $R\leqslant|x|\leqslant R+1$ and as $K_R(x)$ is uniformly bounded in x and R, we have $\int \mathrm{d}x\,K_R(x)=\mathrm{O}(R^{\nu-1})$.

Furthermore, using time reversal invariance and a change of variables we find

$$\begin{aligned}\omega_2([P^\alpha(f_R)\delta(P^\alpha(f_R))]_2)&=\tfrac{1}{2}\mathrm{i}\int \mathrm{d}u\,(\langle\rho^{(2)}p_1^\alpha\rangle(u)-\langle\rho^{(2)}p_2^\alpha\rangle(u))(\nabla^\alpha V)(u)\\&\quad\times\int \mathrm{d}x\,(f_R(x)-f_R(x-u))f_R(x)-\tfrac{1}{4}\int \mathrm{d}u\,\langle\rho^{(2)}\rangle(u)(\nabla^\alpha V)(u)\\&\quad\times\int \mathrm{d}x\,(\nabla^\alpha f_R(x)+\nabla^\alpha f_R(x-u))(f_R(x)-f_R(x-u)).\end{aligned}\tag{12}$$

For the first term we can use the bounds

$$\begin{aligned}\int \mathrm{d}x\,|f_R(x)-f_R(x-u)|&\leqslant C_1|u|R^{\nu-1}, &&|u|\leqslant R,\\&\leqslant C_2R^\nu, &&|u|\geqslant R,\end{aligned}$$

$$|\langle\rho^{(2)}p_1^\alpha\rangle(u)|\leqslant C_3,$$

where C_j $(j=1, 2, 3)$ are constants independent of u and R. Hence

$$\begin{aligned}&\left|\int \mathrm{d}u\,(\langle\rho^{(2)}p_1^\alpha\rangle(u)-\langle\rho^{(2)}p_2^\alpha\rangle(u))(\nabla^\alpha V)(u)\int \mathrm{d}x\,(f_R(x)-f_R(x-u))f_R(x)\right|\\&\qquad\leqslant 2C_3C_1R^{\nu-1}\int_{|u|\leqslant R}\mathrm{d}u|(\nabla^\alpha V)(u)||u|+2C_3C_2R^\nu\int_{|u|\geqslant R}\mathrm{d}u\,|\nabla^\alpha V(u)|\\&\qquad\leqslant 2C_3C_1R^{\nu-\eta}\int_{|u|\leqslant R}\mathrm{d}u\,|u^\eta\nabla^\alpha V(u)|\\&\qquad\quad+2C_3C_2R^{\nu-\eta}\int_{|u|\geqslant R}\mathrm{d}u\,|u^\eta\nabla^\alpha V(u)|\\&\qquad=\mathrm{O}(R^{\nu-\eta}).\end{aligned}$$

The second term of (12) handled by the bound $\int \mathrm{d}x\,|\nabla^\alpha f_R(x)|=\mathrm{O}(R^{\nu-1})$ is itself $\mathrm{O}(R^{\nu-1})$.

The three-particle contribution is of the form

$$\omega_3([P^\alpha(f_R)\delta(P^\alpha(f_R))]_3)=\omega_3(\tfrac{1}{2}(p_1^\alpha f_R(q_1)+f_R(q_1)p_1^\alpha)\phi_R(q_2,q_3)+\text{perm symm})$$

where $\phi_R(q_2,q_3)$ is a real function (see (11*b*)). This contribution vanishes by time reversal invariance. All this proves (a).

Proof of (*b*). According to the definition of δ (4) one finds

$$\delta(Q^\alpha(g_R))=\{0,-\tfrac{1}{2}\mathrm{i}\,(p\cdot\nabla(q^\alpha g_R)+\nabla(q^\alpha g_R)\cdot p),0,\dots\}\tag{13a}$$

$$=-\mathrm{i}\,P\cdot\nabla(x^\alpha g_R)=-\mathrm{i}\sum_\gamma P^\gamma(\nabla^\gamma(x^\alpha g_R)).\tag{13b}$$

Using (13b) and time reversal invariance of the state one gets

$$\begin{aligned}
\omega(Q^\alpha(g_R)\delta(Q^\alpha(g_R)))
&= -\mathrm{i}\omega(Q^\alpha(g_R)P\cdot\nabla(x^\alpha(g_R)))\\
&= \mathrm{i}\omega(P\cdot\nabla(x^\alpha g_R)Q^\alpha(g_R)) = -\tfrac{1}{2}\mathrm{i}\omega([Q^\alpha(g_R), P\cdot\nabla(x^\alpha g_R)])\\
&= \tfrac{1}{2}\rho\int \mathrm{d}x\, |\nabla(x^\alpha g_R(x))|^2 = \tfrac{1}{2}\rho R^\nu \int \mathrm{d}x\, |\nabla(x^\alpha h(x))|^2\\
&= \mathrm{O}(R^\nu).
\end{aligned}$$

Proof of (c). According to (13b), the product rule (3) and (6a) the one-particle contribution to

$$\omega(P^\alpha(f_R)\delta(Q^\alpha(g_R))) + \omega(\delta(Q^\alpha(g_R))P^\alpha(f_R))$$

is given by

$$-2\mathrm{i}\langle\rho^{(1)}(p^\alpha)^2\rangle \int \mathrm{d}x\, f_R(x)\nabla^\alpha(x^\alpha g_R(x)) - \tfrac{1}{2}\mathrm{i}\rho \int \mathrm{d}x\, \nabla^\alpha f_R(x)\Delta(x^\alpha g_R(x)). \tag{14}$$

Since $|\Delta(x^\alpha g_R(x))| \leq C_4/R$ the second term of (14) is clearly $\mathrm{O}(R^{\nu-2})$. As far as the first term of (14) is concerned, one finds

$$\lim_{R\to\infty} \frac{1}{R^\nu} \int \mathrm{d}x\, f_R(x)\nabla^\alpha(x^\alpha g_R(x)) = \lim_{R\to\infty} \int \mathrm{d}y\, f_R(yR)(h(y) + y^\alpha\nabla^\alpha h(y)) = \Sigma_\nu. \tag{15}$$

This follows by dominated convergence from the fact that $f_R(yR) = h(y) + y^\alpha\nabla^\alpha h(y) = 1$ when $0 \leq |y| < 1$ and $\lim_{R\to\infty} f_R(yR) = 0$ when $|y| > 1$.

The two-particle contribution becomes, after having applied time reversal invariance and rotation invariance of the state,

$$\begin{aligned}
-2\mathrm{i}\sum_\gamma \int \mathrm{d}u\, \langle\rho^{(2)}p_1^\alpha p_2^\gamma\rangle(u) \int \mathrm{d}x\, f_R(x+u)\nabla^\gamma(x^\alpha g_R(x))&\\
-\tfrac{1}{2}\mathrm{i}\int \mathrm{d}u\, (\langle\rho^{(2)}\rangle(u) - \rho^2) \int \mathrm{d}x\, (\nabla^\alpha f_R)(x+u)\Delta(x^\alpha g_R(x)).&
\end{aligned} \tag{16}$$

Using again $|\Delta(x^\alpha g_R(x))| \leq C_4/R$ and the cluster condition, the second term of (16) is clearly $\mathrm{O}(R^{\nu-2})$.

The first term of (16) gives a contribution because

$$\begin{aligned}
\lim_{R\to\infty} \frac{1}{R^\nu} \int \mathrm{d}x\, f_R(x+u)\nabla^\gamma(x^\alpha g_R(x)) &= \lim_{R\to\infty} \int \mathrm{d}y\, f_R(u+yR)(h(y)\delta_{\alpha\gamma} + y^\alpha\nabla^\gamma h(y))\\
&= \Sigma_\nu\delta_{\alpha\gamma}
\end{aligned}$$

by the same argument as in (15), the above integral being uniformly bounded with respect to u.

Proof of (d). A direct computation of the commutator and an argument as for the first term of (14) yields immediately

$$\begin{aligned}
\lim_{R\to\infty} \frac{1}{R^\nu}\omega([P^\alpha(f_R), Q^\alpha(g_R)]) &= \lim_{R\to\infty} \frac{1}{R^\nu}\mathrm{i}\rho \int \mathrm{d}x\, f_R(x)\nabla^\alpha(x^\alpha g_R(x))\\
&= \mathrm{i}\rho\Sigma_\nu.
\end{aligned}$$

This concludes the proof of the theorem.

In the main theorem we studied the second moment of the momentum. Now we show that under the conditions of L^1-clustering for the higher-order correlations the suitably scaled pair momentum-position becomes classical with the same distribution as one would obtain from classical statistical mechanics.

The L^1-clustering condition is defined in terms of the fully truncated expectation values defined as follows. If we denote by X either $P^\alpha(f)$ or $Q^\gamma(g)$ for $f, g \in C_0^\infty(\mathbb{R}^\nu)$, we define $\omega_{\mathrm{T}}(X) = \omega(X)$, and recursively

$$\omega(X_1 \ldots X_n) = \omega_{\mathrm{T}}(X_1, \ldots, X_n) + \sum \omega_{\mathrm{T}}(X_{i_1}, \ldots, X_{i_a}) \ldots \omega_{\mathrm{T}}(X_{i_{k+1}}, \ldots, X_{i_n})$$

where the sum extends over all partitions

$$(i_1 \ldots i_a) \ldots (i_{k+1} \ldots i_n)$$

of $(1 \ldots n)$ into p parts, $p \geq 2$, writing in each part the indices in their natural order.

We require that for all choices X_j and $n = 3, 4, \ldots$

$$\int \mathrm{d}x_1 \ldots \mathrm{d}x_{n-1} \left|\omega_{\mathrm{T}}(\tau_{x_1}(X_1), \ldots, \tau_{x_{n-1}}(X_{n-1}), X_n)\right| < \infty \tag{17}$$

where τ_x is the space translation automorphism. Let l be a spherically symmetric positive function in $C_0^\infty(\mathbb{R}^\nu)$ such that $\int l(x)\, \mathrm{d}(x) = 1$, $l(x) = 0$ for $|x| > \frac{1}{2}$. Denote

$$P_R^\alpha(l) = \{0, \tfrac{1}{2}(p^\alpha f_R(q) + f_R(q) p^\alpha), 0, \ldots\} \tag{18a}$$

where $f_R(x) = \int_{|y| \leq R} \mathrm{d}y\, l(y+x)$ and

$$Q_R^\alpha(l) = \left\{0, \int_{|y| \leq R} \mathrm{d}y\, y^\alpha l(y+x), 0, \ldots\right\} = \int_{|x| \leq R} \mathrm{d}x\, x^\alpha \tau_x(Q^\alpha(l)). \tag{18b}$$

Notice that $Q_R^\alpha(l)$ is also of the form $Q^\alpha(\tilde{f}_R)$ where $\tilde{f}_R$ is within the class of functions defined in (5).

Corollary 3.3. Let ω be a state satisfying the hypotheses of theorem 3.2 supplemented by the condition (17), and let q^α, p^γ ($\alpha, \gamma = 1, \ldots, \nu$) be the classical random variables with Gaussian distribution

$$r(q^\alpha, p^\gamma) = \left(\frac{\beta}{2\pi}\right)^\nu \left(\frac{1}{\chi\rho^3}\right)^{\nu/2} \exp -\beta \left(\frac{p^2}{2\rho} + \frac{q^2}{2\rho^2\chi}\right); \tag{19}$$

then if Y_R is an arbitrary monomial in the operator $P_R^\alpha(l)/(\Sigma_\nu R^\nu)^{1/2}$ and/or $(\nu+2)^{1/2} Q_R^\alpha(l)/R(\Sigma_\nu R^\nu)^{1/2}$ (see (18)), and if $Y_{\mathrm{cl}}(q^\alpha, p^\gamma)$ is the corresponding classical monomial, then

$$\lim_{R\to\infty} \omega(Y_R) = \int \mathrm{d}^\nu p\, \mathrm{d}^\nu q\, Y_{\mathrm{cl}}(q^\alpha, p^\gamma) r(q^\alpha, p^\gamma). \tag{20}$$

Proof. Remark that $\omega(P_R^\alpha(l)) = 0$ because of (6a) and also

$$\omega(Q_R^\alpha(l)) = \rho \int \mathrm{d}x \int_{|y| \leq R} \mathrm{d}y\, l(x+y) y^\alpha = \rho \int_{|y| \leq R} \mathrm{d}y\, y^\alpha = 0.$$

Therefore in order to prove (20) as a consequence of lemma 3.1 and theorem 3.2 it is sufficient to prove

$$\text{(i)} \qquad \lim_{R\to\infty} \frac{\omega_{\mathrm{T}}(P_R^\alpha(l), Q_R^\gamma(l))}{R^{\nu+1}} = 0, \qquad \alpha, \gamma = 1, \ldots, \nu,$$

and

$$\text{(ii)} \qquad \lim_{R\to\infty} \omega_{\mathrm{T}}(Y_R) = 0,$$

where Y_R is a monomial of order n in $P_R^\alpha(l)/(\Sigma_\nu R^\nu)^{1/2}$ and of order m in $Q_R^\alpha(l)(\nu+2)^{1/2}/(\Sigma_\nu R^\nu)^{1/2}R$ for $n+m \geq 3$.

To prove (i) we use time reversal invariance yielding

$$\begin{aligned}\omega_{\mathrm{T}}&(P_R^\alpha(l), Q_R^\gamma(l))\\ &= \tfrac{1}{2}\omega([P_R^\alpha(l), Q_R^\gamma(l)])\\ &= -\tfrac{1}{2}\mathrm{i}\rho \int \mathrm{d}x \int_{|y|\leq R} \mathrm{d}y\, l(y+x)\nabla_x^\alpha \int_{|y|\leq R} \mathrm{d}z\, z^\gamma l(z+x) = \mathrm{O}(R^\nu).\end{aligned}$$

Now we check (ii). It is sufficient to consider

$$\lim_{R\to\infty} \frac{1}{R^{m+(m+n)\nu/2}} \int_{|x_i|\leq R} \mathrm{d}x_1 \ldots \mathrm{d}x_{n+m}\, x_{i_1}^{\alpha_{i_1}} \ldots x_{i_m}^{\alpha_{i_m}}\, \omega_{\mathrm{T}}(\tau_{x_1}(X_1) \ldots \tau_{x_{n+m}}(X_{n+m}))$$

where $X_i = Q^\alpha(l)$ for $i = i_1, \ldots, i_m$ and $X_i = P^\alpha(l)$ otherwise.

Note that $|x_i^\alpha|/R \leq 1$. Using the translation invariance and the cluster condition (17) one concludes that for $n+m \geq 3$ the expression tends to zero. This proves (ii).

For notational convenience we have performed the proofs for the case where there is only one type of particle in the system. The formalism and the proofs of the results are straightforwardly extended to the case where different species of particles with different masses are present. In this case we define the algebra of observables with the different particle structure built in it; in particular, the canonical momentum and position operators are equipped with a supplementary index $k \in [1, \ldots, N]$ referring to the type of particles. Also a state ω is now described by the reduced density matrices $\rho_{k_1,\ldots,k_n}^{(n)}$ for n particles of the type $k_1, \ldots, k_n$.

Let $P^\alpha(f_R)$ be the local approximation of the infinitesimal generator of the translations of the infinite system, in terms of our notations

$$P^\alpha(f_R) = \left\{0, \sum_{k=1}^N \tfrac{1}{2}(p_k f_R(q_k^\alpha) + f_R(q_k)p_k^\alpha), 0, \ldots\right\}$$

and

$$Q^\alpha(f_R) = \left\{0, \sum_{k=1}^N m_k q_k^\alpha f_R(q_k), 0, \ldots\right\}$$

where m_k is the mass of the particle of type k. Then one gets as in lemma 3.1 and theorem 3.2

$$\lim_{R\to\infty} \frac{\omega(P^\alpha(f_R)^2)}{\Sigma_\nu(\nu)R^\nu} = \sum_k \langle \rho_k^{(1)}(p^\alpha)^2\rangle + \sum_{k,k'} \int du\, \langle \rho_{kk'}^{(2)} p_1^\alpha p_2^\alpha\rangle(u) = kT\sum_k \rho_k m_k$$

where $\rho_k = \langle \rho_k^{(1)}\rangle$ is the density of the particles of type k.

4. Discussion

It is instructive to investigate the momentum fluctuations in a couple of simple models showing phase transitions. This might give a better insight into the effect of these phenomena on the fluctuations.

First we consider the condensed state of the three-dimensional free Bose gas. The particle density is given by (Lewis and Pulé 1974)

$$\rho = \rho_c + \rho_0 = \int dp\, f(p, \beta) + \rho_0 \tag{21}$$

where

$$\rho_c = \int dp\, f(p,\beta), \qquad f(p,\beta) = (2\pi)^{-3}[\exp(\beta p^2/2) - 1]^{-1},$$

ρ_c is the critical density, ρ_0 is the condensate density, and ρ is the total density. As in the introduction (2) one calculates

$$\langle \rho^{(1)} p^2\rangle + \int dx\, \langle \rho^{(2)} p_1 p_2\rangle(x) = \int dp\, p^2(1 + (2\pi)^3 f(p,\beta)) f(p,\beta) = 3kT\rho_c. \tag{22}$$

Hence for $\rho > \rho_c$ we find the same result as at $\rho = \rho_c$, i.e. the condensed particles do not contribute to the expression (22) and therefore theorem 3.2 does not hold. This is obviously due to the weak clustering in the condensed phase. In fact the momentum fluctuations $\langle \rho^{(2)} p_1^\alpha p_2^\gamma\rangle(x) = O(1/|x|^4)$ are still integrable but the density fluctuations have the asymptotic behaviour

$$\langle \rho^{(2)}\rangle(x) - \rho^2 = (\rho_0/\pi\beta)|x|^{-1} + O(|x|^{-2}).$$

As a consequence surface contributions will not vanish as R tends to infinity; e.g. the second term of (7) gives now a non-zero contribution to the computation of $\lim_{R\to\infty}\langle p^\alpha(f_R)^2\rangle/R^3$.

Indeed, after integration by parts, using the rotation invariance and the asymptotic expansion of $\langle \rho^{(2)}\rangle(x) - \rho^2$, one gets

$$\begin{aligned}
&\lim_{R\to\infty} -\frac{1}{3\Sigma_3 R^3}\int dx \left[\frac{\rho_0}{\pi\beta}\frac{1}{|x|} + O\left(\frac{1}{|x|^2}\right)\right]\int dy\, f_R(y+x) f_R(x) \\
&\quad = \lim_{R\to\infty}\left[-\frac{1}{3\Sigma_3 R^3}\int dx \frac{\rho_0}{\pi\beta}\Delta\left(\frac{1}{|x|}\right)\left(\int dy\, f_R(y+x) f_R(x) + O(1)\right)\right] \\
&\quad = \tfrac{4}{3}kT\rho_0
\end{aligned}$$

and thus for the ideal Bose gas

$$\lim_{R\to\infty} \frac{\langle P(f_R)^2\rangle}{\Sigma(3)R^3} \neq \langle \rho^{(1)} p^2\rangle + \int \mathrm{d}x\, \langle \rho^{(2)} p_1 \cdot p_2\rangle(x).$$

In fact this limit will depend on the type of local approximation of the total momentum.

Remark that by the Goldstone theorem (Martin 1982, Fannes *et al* 1982) the $1/|x|$ behaviour of the clustering is the onset of the breaking of a continuous symmetry. Therefore we expect that the phenomenon described for the ideal Bose gas is of a general nature.

Another type of phase transition is provided by the BCS model (Haag 1967). Strictly speaking this model does not fit into our scheme because of the non-local character of the interaction. The one- and two-body correlations for the superconducting phase are given by an extremal invariant quasi-free state ω_β determined by the following two-point functions. Let $a_i^{\mp}$ $(i=1,2)$ be the creation and annihilation operators of the fermions with spin index i $(i=1,2)$; then the only non-vanishing two-point functions are

$$\rho_i = \omega_\beta(a_i^+(x)a_i^-(x)) = (2\pi)^{-3} \int \mathrm{d}p\, \tfrac{1}{2}(1-(E_p/\Omega_p)\tanh \tfrac{1}{2}\beta\Omega_p), \qquad i=1,2, \tag{23}$$

$$\omega_\beta(a_1^-(x)a_2^-(y)) = (2\pi)^{-3} \int \mathrm{d}p\, (\delta_\beta S_p/2\Omega_p) \tanh(\tfrac{1}{2}\beta\Omega_p)\, \mathrm{e}^{\mathrm{i}p(x-y)}, \tag{24}$$

where

$$E_p = |\tfrac{1}{2}p^2 - \mu|, \qquad \Omega_p = (E_p^2 + |\delta_\beta S_p|^2)^{1/2}, \qquad S_p = 0 \quad \text{for } |p| > |p_0|$$

and δ_β is a constant determined by the 'gap equation'

$$1 = \tfrac{1}{2}(2\pi)^{-3} \int \mathrm{d}p\, (|S_p|^2/\Omega_p) \tanh \tfrac{1}{2}\beta\Omega_p.$$

From (23), (24) one calculates

$$\langle \rho^{(1)} p^2\rangle + \int \mathrm{d}x\, \langle \rho^{(2)} p_1\cdot p_2\rangle(x) = \frac{1}{(2\pi)^3} \int \mathrm{d}p\, p^2\left(1 - \frac{E_p}{\Omega_p}\tanh\frac{\beta}{2}\Omega_p\right) + \frac{1}{(2\pi)^3}\int \mathrm{d}p\, p^2 \frac{|\delta_\beta S_p|^2}{2\Omega_p^2}\tanh^2\frac{\beta}{2}\Omega_p. \tag{25}$$

If $\delta_\beta = 0$, ω_β is the free fermion state, the normal phase and (25) yields $3kT\rho$ with $\rho = \rho_1 + \rho_2$.

If $\delta_\beta \neq 0$ then as (25) is a continuous function of the temperature tending to

$$\frac{1}{(2\pi)^3}\left[\int \mathrm{d}p\, p^2\left(1 - \frac{E_p}{\Omega_p}\right) + \int \mathrm{d}p\, p^2 \frac{|\delta_\beta S_p|^2}{2\Omega_p^2}\right]$$

for $T \to 0(\beta \to \infty)$, and as this expression is strictly positive, theorem 3.2 does not hold.

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