

# The microcanonical ensemble of the ideal relativistic quantum gas

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**Abstract.** We derive the microcanonical partition function of the ideal relativistic quantum gas of spinless bosons in a quantum field framework as an expansion over fixed multiplicities. Our calculation generalizes well known expressions in the literature in that it does not introduce any large-volume approximation and it is valid at any volume. We discuss the issues concerned with the definition of the microcanonical ensemble for a free quantum field at volumes comparable with the Compton wavelength and provide a consistent prescription for calculating the microcanonical partition function that is finite at finite volume and yielding the correct thermodynamic limit. Besides an immaterial overall factor, the expression obtained turns out to be the same as in the non-relativistic multi-particle approach. This work is an introduction to the derivation of the most general expression of the microcanonical partition function fixing the maximal set of observables of the Poincaré group.

## 1 Introduction

The microcanonical ensemble of the relativistic gas is a subject that has not received much attention in the past. The reason of the scarce interest in this problem is the peculiarity of the physical applications, which have been essentially confined within statistical approaches to hadron production and the bag model [1]; these are indeed the only cases in which the volumes and particle numbers involved are so small that microcanonical corrections to average quantities become relevant. Otherwise, the involved energies or volumes are so large that canonical and grand-canonical ensembles are appropriate for most practical purposes (e.g. in relativistic heavy ion collisions). Recently [2], it has been pointed out that the equivalence, in the thermodynamic limit, between grand-canonical, canonical and microcanonical ensembles does not apply to fluctuations; or more in general: to moments of multiplicity distributions of order  $> 1$ . Indeed, the effects of the difference between statistical ensembles might be unveiled by studying multiplicity distributions in relativistic nuclear collisions [3]. In view of these phenomenological applications, it would be desirable to have an in-depth analysis of the microcanonical ensemble of a relativistic quantum gas.

The main difficulty in tackling this problem stems from the need of imposing a finite volume. This is necessary in order to have a correct thermodynamic limit because, the energy  $E$  being finite by construction, also  $V$  must be finite if the limit with  $E/V$  fixed is to be taken. Strange as it may seem, a full and rigorous treatment of the relativis-

tic microcanonical ensemble of an ideal gas at finite volume is still missing. In all previous works on the subject, at some point, the large-volume approximation is introduced; this is tacitly done, for instance, considering the single-particle level density as continuous, namely replacing sums over discrete quantum states with momentum space integrations [4]:

$$\sum_{\mathbf{k}} \rightarrow \int d^3p. \quad (1)$$

In a previous work [5], we have derived an expression of the microcanonical partition function of an ideal relativistic quantum gas with explicit finite-volume corrections (see (23) and (24)). However, that expression was obtained in an essentially multi-particle first-quantization framework, which, as pointed out in [6], should be expected to become inadequate at very low volumes, comparable with the Compton wavelength of particles. In this regime, underlying quantum field effects should become important, and pair creation due to localization is an unavoidable effect [7]. Indeed, there are several studies of the microcanonical ensemble of a free quantum field [8–10], but all of them, again, at some point invoke a large-volume approximation. In the limit of large volumes one obtains the same expressions of the microcanonical partition function and, consequently, of statistical averages as in the first-quantization multi-particle approach followed in [5].

The aim of this work is to derive a general expression for the microcanonical partition function in a full relativistic quantum field framework, valid for *any finite volume*, generalizing the results obtained in [5]. We will do this for

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the simplest case of an ideal gas of spinless bosons and postpone the treatment of particles with spin to a forthcoming publication [11]. We will show that the expression of the microcanonical partition function obtained in [5] in a non-relativistic multi-particle approach holds, provided that a consistent prescription of subtracting terms arising from field degrees of freedom outside the volume considered is introduced.

The paper is organized as follows: in Sects. 2 and 3 we will argue for general features of the microcanonical ensemble for a relativistic system and discuss several issues concerning a proper definition of the microcanonical partition function. In Sect. 4 we will cope with the further issues related to the definition of a microcanonical ensemble for a quantum field at finite volume. Sections 5 and 6 include the main body of this work, where the microcanonical partition function is worked out in a quantum field theoretical framework. In Sect. 7 we will give a summary and discuss the results.

## 2 On the definition of the microcanonical partition function

It is well known that the fundamental tool for the calculation of statistical averages in any ensemble is the partition function. For the microcanonical ensemble one has to calculate the *microcanonical partition function* (MPF), which is usually defined as the number of states with a definite value  $E$  of the total energy:

$$\Omega \equiv \sum_{\text{states}} \delta(E - E_{\text{state}}). \quad (2)$$

For a quantum system, the MPF is the trace of the operator  $\delta(E - \hat{H})$ :<sup>1</sup>

$$\Omega = \text{tr} \delta(E - \hat{H}), \quad (3)$$

with a proper normalization of the basis states. For instance, for one non-relativistic free particle, one has to calculate the trace summing over plane waves normalized so as to have  $\langle \mathbf{p} | \mathbf{p}' \rangle = \delta^3(\mathbf{p} - \mathbf{p}')$ :

$$\begin{aligned} \Omega &= \text{tr}(E - \hat{H}) = \sum_{\mathbf{p}} \delta\left(E - \frac{p^2}{2m}\right) \langle \mathbf{p} | \mathbf{p} \rangle \\ &= \frac{1}{(2\pi)^3} \int d^3x \int d^3p \delta\left(E - \frac{p^2}{2m}\right). \end{aligned} \quad (4)$$

Thereby, one recovers the well known classical expression implying that the MPF is the number of phase space cells with size  $h^3$  and given energy  $E$ . This number is infinite as the volume is unbounded and it is thus impossible to calculate a meaningful thermodynamic limit at finite energy density. Hence, one usually considers a system confined within a finite region by modifying the hamiltonian

$\hat{H}$  with the addition of infinite potential walls, i.e. setting  $\hat{H}' = \hat{H} + \hat{V}$ , where  $\hat{H}$  is the actual internal hamiltonian and  $\hat{V}$  an external potential implementing infinite walls. Classically, this leads to a finite  $\Omega$ , namely:

$$\Omega = \frac{V}{(2\pi)^3} \int d^3p \delta\left(E - \frac{p^2}{2m}\right), \quad (5)$$

where  $V$  is the volume of the region encompassed by the potential walls.<sup>2</sup> Also the corresponding quantum problem can easily be solved, and one has

$$\Omega = \text{tr}(E - \hat{H}') \equiv \sum_{\mathbf{k}} \delta\left(E - \frac{k^2}{2m}\right), \quad (6)$$

where the sum runs over all wave vectors  $\mathbf{k}$ , which, for a rectangular box with side  $L_i$  and periodic boundary conditions, are labeled by three integers  $(n_1, n_2, n_3)$  such that  $k_i = n_i\pi/L_i$ . The difficulty of the quantum expression (6) with respect to the classical one (5) is that, for a given energy  $E$ , a set of integers fulfilling the constraint imposed by the Dirac  $\delta$ ,

$$\frac{\pi^2}{2m} \left( \frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} + \frac{n_z^2}{L_z^2} \right) = E,$$

in general does not exist. Therefore, the MPF vanishes except for a discrete set of total energies, for which it is divergent. One has a finite result only for the integral number of states  $\int_0^{E'} dE \Omega(E)$ ; that is, the number of states with an energy less than a given  $E'$ , but this is clearly a stepwise and non-differentiable function of  $E'$ .

This holds for an ideal gas of any finite number of particles: strictly speaking, the MPF cannot be defined at finite energy and volume as a continuous function. Only in the thermodynamic limit  $E \rightarrow \infty$  and  $V \rightarrow \infty$  an expression like (6) becomes meaningful, because it is then possible to replace the sum over discrete levels with a phase space integration:

$$\sum_{\text{cells}} \xrightarrow{V \rightarrow \infty} \frac{V}{(2\pi)^3} \int d^3p. \quad (7)$$

Therefore, for a truly finite quantum system, one needs a better definition of the microcanonical partition function. A definition which does not suffer from the previous drawbacks is the following:

$$\Omega = \text{tr}_V \delta(E - \hat{H}) \equiv \sum_{h_V} \langle h_V | \delta(E - \hat{H}) | h_V \rangle, \quad (8)$$

where  $\hat{H}$  is the internal hamiltonian, without external confining potential, and the  $|h_V\rangle$  form a complete set of normalized *localized states*, i.e. a complete set of states for the wavefunctions vanishing outside the region  $V$ . It should be stressed that these states are not a basis of the full Hilbert

<sup>1</sup> Throughout this work quantum operators will be distinguished from ordinary numbers by the symbol  $\hat{\phantom{x}}$ .

<sup>2</sup> We will use the same symbol  $V$  to denote both the finite region and its volume.

space, because wavefunctions that do not vanish out of  $V$  cannot be expanded in this basis; therefore we have the notation  $\text{tr}_V$  instead of  $\text{tr}$ , meaning that the trace in (8) is not a proper one. The difference between (8) and a definition like (3) is that the  $|h_V\rangle$  are not eigenstates of the hamiltonian  $\hat{H}$  and the right hand side of (8) does not reduce to a discrete sum of  $\delta$ s. In fact, this is crucial to have a continuous function of  $E$ , unlike (6).

As an example, let us work out the definition (8) for the single free particle confined in a rectangular box by infinite potential walls and compare it to (4). A complete set of states for this problem is

$$|\mathbf{k}\rangle = \begin{cases} \frac{1}{\sqrt{V}} \exp(i\mathbf{k} \cdot \mathbf{x}) & \text{if } \mathbf{x} \in V, \\ \mathbf{k} = \pi n_x/L_x \hat{\mathbf{i}} + \pi n_y/L_y \hat{\mathbf{j}} + \pi n_z/L_z \hat{\mathbf{k}}, \\ 0 & \text{if } \mathbf{x} \notin V. \end{cases} \quad (9)$$

Therefore, the MPF definition (8) implies that

$$\begin{aligned} \Omega &= \sum_{\mathbf{k}} \langle \mathbf{k} | \delta(E - \hat{H}) | \mathbf{k} \rangle \\ &= \sum_{\mathbf{k}} \int d^3p |\langle \mathbf{k} | \mathbf{p} \rangle|^2 \delta\left(E - \frac{p^2}{2m}\right), \end{aligned} \quad (10)$$

where we have inserted a resolution of the identity by using a complete set of states for the full Hilbert space. The sum in (10) can be calculated and yields

$$\begin{aligned} \sum_{\mathbf{k}} |\langle \mathbf{k} | \mathbf{p} \rangle|^2 &= \sum_{\mathbf{k}} \frac{1}{V(2\pi)^3} \left| \int_V d^3x \exp[i(\mathbf{k} - \mathbf{p}) \cdot \mathbf{x}] \right|^2 \\ &= \sum_{\mathbf{k}} \frac{1}{V} \int_V d^3x \int_V d^3x' \exp[i\mathbf{k} \cdot (\mathbf{x} - \mathbf{x}')] \\ &\quad \times \exp[-i\mathbf{p} \cdot (\mathbf{x} - \mathbf{x}')] \\ &= \frac{1}{(2\pi)^3} \int_V d^3x \int_V d^3x' \delta^3(\mathbf{x} - \mathbf{x}') \\ &\quad \times \exp[-i\mathbf{p} \cdot (\mathbf{x} - \mathbf{x}')] = \frac{V}{(2\pi)^3}, \end{aligned} \quad (11)$$

where the completeness relation in  $V$ ,

$$\sum_{\mathbf{k}} \frac{1}{V} \exp[i\mathbf{k} \cdot (\mathbf{x} - \mathbf{x}')] = \delta^3(\mathbf{x} - \mathbf{x}'), \quad (12)$$

has been used. Thus, by using (11), (10) turns into

$$\Omega = \frac{V}{(2\pi)^3} \int d^3p \delta\left(E - \frac{p^2}{2m}\right); \quad (13)$$

that is, the same expression (5) as in the classical case.

The MPF (13) is now manifestly a continuous function of  $E$  and, remarkably, its thermodynamic limit  $V \rightarrow \infty$  is the same as the thermodynamic limit of the ‘‘pure’’ quantum expression (6) (because of (7)). Since the only strict requirement for a well defined MPF is that it reproduce the correct thermodynamic limit, for a quantum gas one can choose a definition like (8) instead of  $\Omega = \text{tr}\delta(E - \hat{H}')$

in (6). We emphasize again that in the passage from (6) to (8) the hamiltonian embodying an external confining potential is replaced by the internal hamiltonian while, at the same time, the localized eigenstates of the former hamiltonian are used to calculate the trace.

### 3 The microcanonical partition function of a relativistic system

In special relativity, the microcanonical ensemble must include momentum conservation beside energy conservation to fulfill Lorentz invariance. This means that the MPF definition (8) should be generalized to [5]

$$\Omega = \sum_{h_V} \langle h_V | \delta^4(P - \hat{P}) | h_V \rangle, \quad (14)$$

$P$  being the four-momentum of the system and  $\hat{P}$  the four-momentum operator. The MPF, now being a number of states per four-momentum cell, is a Lorentz-invariant quantity. The calculation of the MPF is easiest in the rest-frame of the system, where  $P = (M, \mathbf{0})$  and the four-volume  $Vu$ ,  $u$  being the four-velocity and  $V$  the proper volume of the system, reduces to  $(V, \mathbf{0})$ , according to the usual formulation of statistical relativistic thermodynamics [12, 13].

Equation (14) can be further generalized by enforcing the conservation of not only energy-momentum but of the maximal set of conserved quantities, i.e. a maximal set of commuting observables built with the generators of the Poincaré group. To achieve this, one has to replace  $\delta^4(P - \hat{P})$  in (14) with a generic projector  $\mathbf{P}_i$  over an irreducible state of the representation of the Poincaré group [5, 6], i.e.:

$$\Omega = \sum_{h_V} \langle h_V | \mathbf{P}_i | h_V \rangle. \quad (15)$$

This ensemble is still generally defined as a microcanonical ensemble and (15) as a microcanonical partition function.

In this work, we will confine ourselves to a microcanonical ensemble where only energy-momentum is fixed, i.e. our projector  $\mathbf{P}_i$  in (15) will be

$$\mathbf{P}_i = \delta^4(P - \hat{P}) \quad (16)$$

and to an ideal quantum gas, i.e. with  $\hat{P}$  being the free four-momentum operator. In fact, it should be stressed that  $\delta^4(P - \hat{P})$  is not a proper projector, because  $\mathbf{P}^2 = a\mathbf{P}$ , where  $a$  is a divergent constant. This is owing to the fact that normalized projectors onto irreducible representations cannot be defined for non-compact groups, such as the space-time translation group  $T(4)$ . Nevertheless, we will maintain this naming even for non-idempotent operators, relaxing mathematical rigor, because it will be favorable to adopt the projection formalism.

It is worth pointing out that the definition (8), involving only the internal (free) hamiltonian, is much better fit than (6) for a relativistic generalization. Besides the advantage of restoring continuity in  $E$ , discussed in the previous

section, this formulation can easily be extended to the full set of conservation laws without major conceptual difficulties. Conversely, had one tried to generalize (6), one should have defined a finite region and *afterwards* sought the observables commuting with the hamiltonian supplemented with an external confining potential. This would have not been an easy task, and, moreover, a maximal set of observables commuting with the modified  $\hat{H}$  would not, in general, define a Poincaré algebra. This is a well known problem in the static bag model, where the translational invariance is manifestly broken and momentum is thus not conserved. On the other hand, in the definition (15), we deal with the original Poincaré algebra of unmodified (free) operators and enforce the localization through the projector onto confined states.

Equation (15) can be recast as a full trace by inserting a complete set of states  $|f\rangle$  into (15):

$$\begin{aligned}\Omega &= \sum_{h_V} \langle h_V | \sum_f |f\rangle \langle f| \mathbf{P}_i |h_V\rangle \\ &= \sum_f \langle f| \mathbf{P}_i \sum_{h_V} |h_V\rangle \langle h_V|f\rangle \equiv \sum_f \langle f| \mathbf{P}_i \mathbf{P}_V |f\rangle \\ &= \text{tr} [\mathbf{P}_i \mathbf{P}_V],\end{aligned}\quad (17)$$

where

$$\mathbf{P}_V = \sum_{h_V} |h_V\rangle \langle h_V|,\quad (18)$$

is, by definition, the projector onto the Hilbert subspace  $H_V$  of confined states (i.e. of wavefunctions vanishing outside  $V$ ). Formula (17) is the starting point for carrying out a calculation of the MPF at finite volume. The first thing to do is to expand (17) as a sum of partition functions at fixed multiplicities,

$$\Omega = \sum_N \Omega_N\quad (19)$$

for a single species gas, and

$$\Omega = \sum_{\{N_j\}} \Omega_{\{N_j\}}\quad (20)$$

for a multi-species gas, where  $\{N_j\} = (N_1, \dots, N_K)$  is a set of particle multiplicities for each species  $j = 1, \dots, K$ , defining a *channel*.  $\Omega_N$  or  $\Omega_{\{N_j\}}$  are obtained by summing over all possible values of kinematical variables with fixed multiplicities. So, if  $|f\rangle \equiv |N, \{p\}\rangle$ , where  $\{p\}$  labels the set of kinematical variables of particles in the state  $|f\rangle$ ,  $\Omega_N$  reads

$$\Omega_N = \sum_{\{p\}} \langle N, \{p\} | \mathbf{P}_i \mathbf{P}_V | N, \{p\} \rangle.\quad (21)$$

Likewise, for a multi-species gas, the microcanonical partition function is expressed as an expansion over all possible channels:

$$\Omega_{\{N_j\}} = \sum_{\{p\}} \langle \{N_j\}, \{p\} | \mathbf{P}_i \mathbf{P}_V | \{N_j\}, \{p\} \rangle\quad (22)$$

and  $\Omega_{\{N_j\}}$  is defined as the *microcanonical channel weight*.

The microcanonical channel weights (22) have been calculated in [5] with energy-momentum conservation (i.e. using (16) in a multi-particle, first-quantization framework. For a single species ideal spinless gas:

$$\begin{aligned}\Omega_N &= \frac{1}{N!} \int d^3 p_1 \dots d^3 p_N \delta^4 \left( P - \sum_{n=1}^N p_n \right) \\ &\times \sum_{\rho \in S_N} \prod_{n=1}^N F_V(\mathbf{p}_{\rho(n)} - \mathbf{p}_n),\end{aligned}\quad (23)$$

while for a multi-species gas of  $K$  spinless bosons:

$$\begin{aligned}\Omega_{\{N_j\}} &= \left[ \prod_{j=1}^K \frac{1}{N_j!} \prod_{n_j=1}^{N_j} \int d^3 p_{n_j} \right] \delta^4 \left( P - \sum_{n=1}^N p_n \right) \\ &\times \prod_{j=1}^K \sum_{\rho_j \in S_{N_j}} \prod_{n_j=1}^{N_j} F_V(\mathbf{p}_{\rho_j(n_j)} - \mathbf{p}_{n_j}),\end{aligned}\quad (24)$$

where  $N = \sum_j N_j$ . In (23) and (24)  $\rho_j$  labels the permutation belonging to the permutation group  $S_{N_j}$ , and the  $F_V$  are Fourier integrals over the region  $V$ :

$$F_V(\mathbf{p} - \mathbf{p}') \equiv \frac{1}{(2\pi)^3} \int_V d^3 x e^{i(\mathbf{p} - \mathbf{p}') \cdot \mathbf{x}}.\quad (25)$$

If the volume is large enough so as to allow for the approximation

$$F_V(\mathbf{p} - \mathbf{p}') = \frac{1}{(2\pi)^3} \int_V d^3 x e^{i(\mathbf{p} - \mathbf{p}') \cdot \mathbf{x}} \simeq \delta^3(\mathbf{p} - \mathbf{p}'),\quad (26)$$

the microcanonical channel weights (24) can be resummed explicitly into the microcanonical partition function according to (20), and one obtains [5]

$$\begin{aligned}\Omega &= \frac{\lim_{\varepsilon \rightarrow 0}}{(2\pi)^4} \int_{-\infty - i\varepsilon}^{+\infty - i\varepsilon} dy^0 \int d^3 y e^{iP \cdot y} \\ &\times \exp \left[ \sum_j \frac{V}{(2\pi)^3} \int d^3 p \log(1 - e^{-ip \cdot y})^{-1} \right].\end{aligned}\quad (27)$$

A full analytical calculation of (27) is possible only for the limiting case of vanishing masses (e.g. microcanonical black body). For the massive case, four-dimensional integrations cannot be worked out analytically, and one has to resort to numerical computation.

Equation (27) was implicitly obtained in [4], where the first expression of the microcanonical partition function of a multi-species ideal relativistic quantum gas was derived as an expansion (20) over channels, by using the large-volume approximation (7) from the very beginning. This shows that the approximation (26) is indeed equivalent to (7), as also demonstrated in [5]. Noticeably, the MPF definition (14) without any large-volume approximation involves the appearance of Fourier integrals accounting for

Bose–Einstein and Fermi–Dirac correlations in the quantum gas, which do not show up in the large-volume approximation enforced in [4]. This approach also allows one to investigate further generalizations when the volume is so small that relativistic quantum field effects must be taken into account.

### 4 Microcanonical ensemble and field theory

The calculation of the partition function (14) in a quantum field framework brings in new difficulties with respect to the first-quantization scheme. This problem has been approached in the literature with a functional approach, inspired on the usual grand-canonical thermal field theory [8–10]. However, these calculations aim at the limit of large volumes and are therefore insensitive to the difficulties pertaining to the strict requirement of a finite volume, discussed in detail in Sect. 2. As a result, for a free field, the derived expressions are equivalent to (27).

Instead of starting with a functional integration from the very beginning, we calculate the microcanonical partition function of a free field by first expanding it at fixed multiplicities like in (19) and (21) (or channels, for a multi-species gas like in (20)), where the  $|N, \{p\}\rangle$  are Fock space states with a definite particle multiplicity and kinematical variables  $\{p\}$ . To carry out this calculation, we first need to find an expression of the *microcanonical state weight*:

$$\omega \equiv \langle N, \{p\} | \mathbf{P}_i \mathbf{P}_V | N, \{p\} \rangle . \tag{28}$$

By using (16) and choosing  $|N, \{p\}\rangle$  as an eigenstate of the four-momentum operator with eigenvalue  $P_f = \sum_i p_i$ , (28) becomes

$$\omega = \delta^4(P - P_f) \langle N, \{p\} | \mathbf{P}_V | N, \{p\} \rangle . \tag{29}$$

To calculate  $\omega$  and, by a further integration,  $\Omega_N$ , we need to know the projector  $\mathbf{P}_V$ . Since  $\mathbf{P}_V$  is defined as the projector onto the Hilbert subspace of localized states, it can easily be written down in a multi-particle non-relativistic quantum mechanical (NRQM) framework. As an example, for a non-relativistic spinless single particle, it reads (see also Sect. 2)

$$\mathbf{P}_V = \sum_{k_V} |k_V\rangle \langle k_V| , \tag{30}$$

where  $|k_V\rangle$  is a normalized state of the particle confined in a region  $V$ , with a corresponding wavefunction  $\psi_{k_V}(\mathbf{x})$  vanishing outside  $V$ . The symbol  $k_V$  stands for a set of three numbers labeling the kinematical modes of the confined states (e.g. discrete wave vectors, or energy and angular momenta), and the set  $|k_V\rangle$  form a complete set of states for the wavefunctions vanishing outside  $V$ . The projector (30) can easily be extended to the many-body case, and we have

$$\mathbf{P}_V = \sum_{\tilde{N}, \{k\}} |\tilde{N}, \{k_V\}\rangle \langle \tilde{N}, \{k_V\}| , \tag{31}$$

where the symbol  $\{k_V\}$  denotes a multiple set of kinematical modes of the confined states, while  $\tilde{N}$  is the integrated occupation number, i.e. the sum of occupation numbers over all single-particle kinematical modes. In the NRQM approach these numbers are simply particles multiplicities, implying

$$\langle N, \{p\} | \tilde{N}, \{k_V\} \rangle \neq 0 \quad \text{iff} \quad N = \tilde{N} . \tag{32}$$

To calculate the microcanonical state weight, and thence the MPF, the products  $\langle \tilde{N}, \{k_V\} | N, \{p\} \rangle$  can be worked out on the basis of (32) similarly to what has been done in Sect. 2 for a single particle, yielding for a scalar boson [5]

$$\langle N, \{p\} | \mathbf{P}_V | N, \{p\} \rangle = \sum_{\rho \in S_N} \prod_{n=1}^N F_V(\mathbf{p}_{\rho(n)} - \mathbf{p}_n) , \tag{33}$$

where  $\rho$  is a permutation of the integers  $1, \dots, N$ , and the  $F_V$  are the Fourier integrals (25) over the system region  $V$ . From the above equation the expression of the microcanonical channel weight in (23) follows. We will refer to the expression (33) as the NRQM one, meaning that it has been obtained in this first-quantized multi-particle NRQM framework, where, for instance, particles and antiparticles are simply considered as different species and their contributions factorize.

One could envisage that a projector like (31), written in terms of Fock space states, could simply be carried over to the relativistic quantum field case, where  $|\tilde{N}, \{k_V\}\rangle$  are states of the localized problem, obtained by solving the free field equations in a box with suitable boundary conditions. Yet, some difficulties soon arise. First of all, whilst in NRQM the single-particle localized wavefunction  $|k_V\rangle$  and the free plane wave state  $|\mathbf{p}\rangle$  live in the same Hilbert space, in quantum field theory the localized and the non-localized problem are associated with distinct Hilbert spaces. Thus, unlike in NRQM, it is not clear how to calculate a product like  $\langle \tilde{N}, \{k_V\} | N, \{p\} \rangle$ . Secondly, even if there was a definite prescription for it, it should be expected that *the integrated occupation numbers of the localized problem do not coincide with the actual particle multiplicities unless the volume is infinite*. To understand this point, one should keep in mind that particles, when these are properly so called, arise from solutions of the free field equations over the whole space and that the hamiltonian eigenstates of the localized problem are conceptually different. Consequently, the integrated particle number operators in the whole space should differ from integrated number operators within the finite region. Hence, unlike in NRQM, a state with definite integrated occupation numbers  $\tilde{N}$  (we purposely refrain from calling them particle numbers) should be expected to have non-vanishing components on *all* free states with different numbers of actual particles, namely

$$|\tilde{N}\rangle_V = \alpha_{0, \tilde{N}} |0\rangle + \alpha_{1, \tilde{N}} |1\rangle + \dots + \alpha_{\tilde{N}, \tilde{N}} |\tilde{N}\rangle + \dots , \tag{34}$$

where  $\alpha_{i,\tilde{N}}$  are non-trivial complex coefficients, and (32) no longer holds. Only in the large-volume limit one expects that the integrated occupation numbers coincide with the actual multiplicities and (32) applies. This kind of effect is pointed out in the introduction of Landau's book on quantum field theory [7]: when trying to localize an electron, an electron-positron pair unavoidably appears, meaning that the localized single "particle" is indeed a superposition of many true, asymptotic particle states. Another relevant manifestation of this difference which is probably more familiar, is the Casimir effect, which is related to the difference between the true vacuum state  $|0\rangle$  and the localized vacuum state  $|0\rangle_V$ . Hence, all formulae derived under the approximation (32) are asymptotic ones, valid in the limit  $V \rightarrow \infty$  but not at strictly finite volume. Thus, one should expect significant finite-volume corrections to (33) and the ensuing MPF (23) in a quantum field treatment.

If we want to give an expression like  $\langle \tilde{N}, \{k_V\} | N, \{p\} \rangle$  a precise meaning in a quantum field framework, we first need to map the Hilbert space  $H_V$  of the localized problem into the Hilbert space  $H$  of the free field over the whole space. This can be done by mapping the field eigenstates and operators of  $H$  into  $H_V$  in a natural way as follows:

$$\begin{aligned} \Psi(\mathbf{x})_{H_V} &\longrightarrow \Psi(\mathbf{x})_H \\ |\psi(\mathbf{x})\rangle_{H_V} &\longrightarrow |\psi(\mathbf{x})\rangle_H. \end{aligned} \quad (35)$$

This allows one to write linear, non-bijective, Bogoliubov relations, expressing the annihilation and creation operators of the finite region problem as a function of those of the whole (real scalar) field (see Appendix A for a derivation):

$$a_{\mathbf{k}} = \int d^3\mathbf{p} F(\mathbf{k}, \mathbf{p}) \frac{\varepsilon_{\mathbf{k}} + \varepsilon_{\mathbf{p}}}{2\sqrt{\varepsilon_{\mathbf{k}}\varepsilon_{\mathbf{p}}}} a_{\mathbf{p}} + F(\mathbf{k}, -\mathbf{p}) \frac{\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{p}}}{2\sqrt{\varepsilon_{\mathbf{k}}\varepsilon_{\mathbf{p}}}} a_{\mathbf{p}}^\dagger, \quad (36)$$

where  $\mathbf{k}$  are triplets of numbers labeling kinematical modes, just like the aforementioned  $k_V$ ,  $\varepsilon_{\mathbf{k}}$  is the associated energy,  $\varepsilon_{\mathbf{p}} = \sqrt{\mathbf{p}^2 + m^2}$ , and

$$F(\mathbf{k}, \mathbf{p}) = \frac{1}{(2\pi)^3} \int_V d^3\mathbf{x} u_{\mathbf{k}}^*(\mathbf{x}) e^{i\mathbf{p}\cdot\mathbf{x}}, \quad (37)$$

$u_{\mathbf{k}}$  being a complete set of orthonormal wavefunctions for the finite region. A remarkable feature of relativistic quantum fields is that, unlike in NRQM, the localized annihilation operators have non-vanishing components onto the creation operators in the whole space, as shown by (36). This confirms our expectation that a localized state with definite integrated occupation numbers is a non-trivial linear combination of states with different particle multiplicities. As expected, as the volume increases, these components become smaller and in the infinite volume limit one recovers  $a_{\mathbf{k}} = a_{\mathbf{p}}$  (see Appendix A).

Starting from the Bogoliubov relations (36), it should be possible, in principle, to calculate the coefficients in (34), and hence the microcanonical state weight (29) by using the expansion (31). In fact, we do not really need to do that. It is more advantageous, as pointed out in [6], to write the projector  $\mathbf{P}_V$  in terms of field states rather than

occupation numbers of field modes within the finite region. Indeed, in the general definition in (17),

$$\mathbf{P}_V = \sum_{h_V} |h_V\rangle \langle h_V|, \quad (38)$$

the states  $|h_V\rangle$  are a complete set of states of the Hilbert space of the localized problem  $H_V$ , where the degrees of freedom are values of the field in each point of the region  $V$ , i.e.  $\{\psi(\mathbf{x})\}_{\mathbf{x} \in V}$ . Therefore, the above projector is a resolution of the identity of the localized problem and can be written (for a real scalar field)

$$\mathbf{P}_V = \int_V \mathcal{D}\psi |\psi\rangle \langle \psi|, \quad (39)$$

where  $|\psi\rangle \equiv \otimes_{\mathbf{x}} |\psi(\mathbf{x})\rangle$  and  $\mathcal{D}\psi$  is the functional measure; the index  $V$  means that the functional integration must be performed over the field degrees of freedom in the region  $V$ ; that is,  $\mathcal{D}\psi = \prod_{\mathbf{x} \in V} d\psi(\mathbf{x})$ . The normalization of the states is chosen so as to have  $\langle \psi(\mathbf{x}) | \psi'(\mathbf{x}) \rangle = \delta(\psi(\mathbf{x}) - \psi'(\mathbf{x}))$  to ensure the idempotency of  $\mathbf{P}_V$ . If we now want to give a clear meaning to expressions like

$$\langle \{N_j\}, \{p\} | \mathbf{P}_V | \{N_j\}, \{p\} \rangle, \quad (40)$$

we should find a way of completing the tensor product in the projector (39) with the field states outside the region  $V$  in such a way that the scalar product can be performed unambiguously.

Unfortunately the answer to this question is not unique, and the projector can be extended to  $H$  in infinitely many ways. What is important is that the result of the calculation is independent of how the projector has been extended. Thus, at the end of the calculation, one has to check whether spurious terms appear, possibly divergent, depending explicitly on the chosen state of the field *outside*  $V$ , and these terms must be subtracted. In general, all terms depending on the degrees of freedom of the field outside  $V$  must be dropped from the final result.

In this work, we will extend the projector with eigenstates of the field, where the field function  $\psi(\mathbf{x})$  is some arbitrary function outside the region  $V$ . Thus, the projector  $\mathbf{P}_V$  (39) is mapped to

$$\mathbf{P}_V = \int_V \mathcal{D}\psi |\psi\rangle \langle \psi| \quad |\psi\rangle \equiv \otimes_{\mathbf{x} \in V} |\psi(\mathbf{x})\rangle \otimes_{\mathbf{x} \notin V} |\psi(\mathbf{x})\rangle, \quad (41)$$

where the index  $V$  still implies  $\mathcal{D}\psi = \prod_{\mathbf{x} \in V} d\psi(\mathbf{x})$ . We will see that, with the definition (41), spurious terms depending on the degrees of freedom outside  $V$  do arise indeed, but that they can be subtracted "by hand" in a consistent way.

## 5 Single particle channel

We will start calculating the expectation value  $\langle p | \mathbf{P}_V | p \rangle$  of a single-particle channel in the simple cases of neutral and charged scalar fields. This is preparatory to the general case of multiparticle states in Sect. 6.

### 5.1 Neutral scalar field

We consider a gas made of one type of spinless bosons described by the free real scalar field<sup>3</sup> (in the Schrödinger representation):

$$\Psi(\mathbf{x}) = \frac{1}{(2\pi)^{\frac{3}{2}}} \int \frac{d^3\mathbf{p}}{\sqrt{2\varepsilon}} (a(p)e^{i\mathbf{p}\cdot\mathbf{x}} + a^\dagger(p)e^{-i\mathbf{p}\cdot\mathbf{x}}), \quad (42)$$

where  $\varepsilon \equiv \sqrt{p^2 + m^2}$  is the energy,  $p$  is the modulus of the three-momentum, and the normalization has been chosen so as to have the following commutation rule between annihilation and creation operators:

$$[a(p), a^\dagger(p')] = \delta^3(\mathbf{p} - \mathbf{p}'). \quad (43)$$

We start writing the one-particle Fock state  $|p\rangle$  in terms of creation and annihilation operators acting on the vacuum:

$$\langle p | \mathbf{P}_V | p \rangle = \langle 0 | a(p) \mathbf{P}_V a^\dagger(p) | 0 \rangle. \quad (44)$$

Since  $\mathbf{P}_V$  is defined, according to (41), as a functional integral of eigenvectors of the field operator  $\Psi$ , it is convenient to express creation and annihilation operators in terms of the field operators. We shall use the following expressions, which are the most appropriate for our task:

$$\begin{aligned} \langle 0 | a(p) &= \langle 0 | \frac{1}{(2\pi)^{\frac{3}{2}}} \int d^3\mathbf{x} e^{-i\mathbf{p}\cdot\mathbf{x}} \sqrt{2\varepsilon} \Psi(\mathbf{x}) \\ a^\dagger(p) | 0 \rangle &= \frac{1}{(2\pi)^{\frac{3}{2}}} \int d^3\mathbf{x} e^{i\mathbf{p}\cdot\mathbf{x}} \sqrt{2\varepsilon} \Psi(\mathbf{x}) | 0 \rangle. \end{aligned} \quad (45)$$

These expressions can easily be checked by plugging, on the right hand side, the field operators in (42). By using (45) in (44) we have

$$\begin{aligned} \langle 0 | a(p) \mathbf{P}_V a^\dagger(p) | 0 \rangle &= \frac{1}{(2\pi)^3} \int d^3\mathbf{x} \int d^3\mathbf{x}' e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{x}')} \\ &\times 2\varepsilon \langle 0 | \Psi(\mathbf{x}') \mathbf{P}_V \Psi(\mathbf{x}) | 0 \rangle. \end{aligned} \quad (46)$$

It can easily be checked now that the rightmost factor in the above equation turns out to be (by using the definition (41)):

$$\langle 0 | \Psi(\mathbf{x}') \mathbf{P}_V \Psi(\mathbf{x}) | 0 \rangle = \int_V \mathcal{D}\psi | \langle \psi | 0 \rangle |^2 \psi(\mathbf{x}') \psi(\mathbf{x}), \quad (47)$$

where  $\psi(\mathbf{x})$  and  $\psi(\mathbf{x}')$  are field functions or the eigenvalues of the field operator relevant to the state  $|\psi\rangle$ ; that is,

$$\Psi(\mathbf{x}) |\psi\rangle = |\psi\rangle \psi(\mathbf{x}). \quad (48)$$

It is possible to find a solution of the functional integral (47) by first considering the infinite volume limit, when the projector  $\mathbf{P}_V$  reduces to the identity. In this limiting case, the functional integral in (41) is now performed over all possible field functions, and (41) becomes a resolution of

the identity;  $\langle 0 | \Psi(\mathbf{x}') \Psi(\mathbf{x}) | 0 \rangle$  is just the two-point correlation function that we write, according to (47), as

$$\langle 0 | \Psi(\mathbf{x}') \Psi(\mathbf{x}) | 0 \rangle = \int \mathcal{D}\psi | \langle \psi | 0 \rangle |^2 \psi(\mathbf{x}') \psi(\mathbf{x}). \quad (49)$$

The product  $\langle \psi | 0 \rangle$  is known as the *vacuum functional* and reads [14] for a scalar neutral field

$$\langle \psi | 0 \rangle = \mathcal{N} \exp \left\{ -\frac{1}{4} \int d^3\mathbf{x}_1 \int d^3\mathbf{x}_2 \psi(\mathbf{x}_1) K(\mathbf{x}_1 - \mathbf{x}_2) \psi(\mathbf{x}_2) \right\}, \quad (50)$$

where  $\mathcal{N}$  is a field-independent normalization factor that is irrelevant for our purposes. The function  $K(\mathbf{x}' - \mathbf{x})$  is called the *kernel* and fulfills the equation [14]

$$\int d^3\mathbf{x}' e^{-i\mathbf{p}\cdot\mathbf{x}'} K(\mathbf{x}' - \mathbf{x}) = 2\varepsilon e^{-i\mathbf{p}\cdot\mathbf{x}}, \quad (51)$$

whose solution is

$$K(\mathbf{x}' - \mathbf{x}) = \frac{1}{(2\pi)^3} \int d^3\mathbf{p} e^{-i\mathbf{p}\cdot(\mathbf{x}' - \mathbf{x})} 2\varepsilon. \quad (52)$$

The functional integral (49) is therefore a gaussian integral and can be solved by using the known formulae for multiple gaussian integrals of real variables [14]:

$$\begin{aligned} I_{2N} &= \int \mathcal{D}\psi \prod_{i=1}^{2N} \psi(\xi_i) \\ &\times \exp \left[ -\frac{1}{2} \int d^3\mathbf{x}_1 \int d^3\mathbf{x}_2 \psi(\mathbf{x}_1) K(\mathbf{x}_1 - \mathbf{x}_2) \psi(\mathbf{x}_2) \right] \end{aligned} \quad (53)$$

$$= I_0 \sum_{\substack{\text{pairings} \\ \text{of } \xi_1, \dots, \xi_{2N}}} \prod_{\text{pairs}} K^{-1}(\text{paired variables}),$$

where *paired variables* mean couples  $(\xi_i, \xi_j)$  whose difference  $\xi_i - \xi_j$  (or, what is the same,  $\xi_j - \xi_i$ , as  $K^{-1}$  is symmetric) is the argument of  $K^{-1}$ . The factor  $I_0$  is just the normalization of the vacuum state  $I_0 = \langle 0 | 0 \rangle$ , which is set to 1. The inverse kernel  $K^{-1}$  can be found from its definition:

$$\int d^3\mathbf{x}' K(\mathbf{y} - \mathbf{x}') K^{-1}(\mathbf{x}' - \mathbf{x}) = \delta^3(\mathbf{x} - \mathbf{y}) \quad \forall \mathbf{x}, \mathbf{y}, \quad (54)$$

leading to

$$\begin{aligned} K^{-1}(\mathbf{x}' - \mathbf{x}) &= \frac{1}{(2\pi)^3} \int \frac{d^3\mathbf{p}}{2\varepsilon} e^{-i\mathbf{p}\cdot(\mathbf{x}' - \mathbf{x})} \\ &= \langle 0 | \Psi(\mathbf{x}') \Psi(\mathbf{x}) | 0 \rangle. \end{aligned} \quad (55)$$

The last equality comes from (53) and (49) in the special case  $N = 2$  or can be proved directly from the Fourier expansion (42) of the field.

We are now in a position to solve the functional integral (47) at finite volume. First, the functional integration variables are separated from those that are not integrated,

<sup>3</sup> Henceforth, the capital letter  $\Psi$  will denote field operators, while for field functions we will use the small letter  $\psi$ .

i.e. the field values outside  $V$  ( $\bar{V}$  denotes the complement of  $V$ ):

$$\begin{aligned}
& |\langle \psi | 0 \rangle|^2 \\
&= |\mathcal{N}|^2 \exp \left[ -\frac{1}{2} \int d^3x_1 \int d^3x_2 \psi(\mathbf{x}_1) K(\mathbf{x}_1 - \mathbf{x}_2) \psi(\mathbf{x}_2) \right] \\
&= |\mathcal{N}|^2 \exp \left[ -\frac{1}{2} \int_V d^3x_1 \int_V d^3x_2 \psi(\mathbf{x}_1) K(\mathbf{x}_1 - \mathbf{x}_2) \psi(\mathbf{x}_2) \right] \\
&\quad \times \exp \left[ -\frac{1}{2} \int_{\bar{V}} d^3x_1 \int_{\bar{V}} d^3x_2 \psi(\mathbf{x}_1) K(\mathbf{x}_1 - \mathbf{x}_2) \psi(\mathbf{x}_2) \right] \\
&\quad \times \exp \left[ -\int_V d^3x_1 \int_{\bar{V}} d^3x_2 \psi(\mathbf{x}_1) K(\mathbf{x}_1 - \mathbf{x}_2) \psi(\mathbf{x}_2) \right], \tag{56}
\end{aligned}$$

where we have taken advantage of the symmetry of the kernel  $K$ . Equation (56) is a gaussian functional, with a general quadratic form in the field values in the region  $V$ ; it can be integrated in (47) according to standard rules [14], yielding

$$\begin{aligned}
& \int_V \mathcal{D}\psi |\langle 0 | \psi \rangle|^2 \psi(\mathbf{x}') \psi(\mathbf{x}) \\
&= K_V^{-1}(\mathbf{x}', \mathbf{x}) |\mathcal{N}|^2 \det \left[ \frac{K_V}{2\pi} \right]^{-1/2} \\
&\quad \times \exp \left[ \frac{1}{2} \int_V d^3x_1 d^3x'_1 \int_V d^3x_2 d^3x'_2 K_V^{-1}(\mathbf{x}_1, \mathbf{x}'_1) \right. \\
&\quad \times K(\mathbf{x}_1 - \mathbf{x}_2) K(\mathbf{x}'_1 - \mathbf{x}'_2) \psi(\mathbf{x}'_2) \psi(\mathbf{x}_2) \\
&\quad \left. - \frac{1}{2} \int_{\bar{V}} d^3x_1 \int_{\bar{V}} d^3x_2 \psi(\mathbf{x}_1) K(\mathbf{x}_1 - \mathbf{x}_2) \psi(\mathbf{x}_2) \right] \\
&= K_V^{-1}(\mathbf{x}', \mathbf{x}) \int_V \mathcal{D}\psi |\langle 0 | \psi \rangle|^2 = K_V^{-1}(\mathbf{x}', \mathbf{x}) \langle 0 | \mathbf{P}_V | 0 \rangle. \tag{57}
\end{aligned}$$

The function  $K_V^{-1}$  is the inverse of  $K$  over the region  $V$ , namely the inverse of

$$K(\mathbf{x}' - \mathbf{x}) \Theta_V(\mathbf{x}') \Theta_V(\mathbf{x}) \equiv K_V(\mathbf{x}' - \mathbf{x}), \tag{58}$$

the function  $\Theta_V(\mathbf{x})$  being the Heaviside function:

$$\Theta_V(\mathbf{x}) = \begin{cases} 1 & \text{if } \mathbf{x} \in V, \\ 0 & \text{otherwise.} \end{cases} \tag{59}$$

The inverse kernel  $K_V^{-1}$  fulfills, by definition, the integral equation,

$$\int_V d^3x' K_V(\mathbf{y} - \mathbf{x}') K_V^{-1}(\mathbf{x}', \mathbf{x}) = \delta^3(\mathbf{x} - \mathbf{y}) \quad \forall \mathbf{x}, \mathbf{y} \in V. \tag{60}$$

Note that, because of the finite region of integration, the inverse kernel may now depend on both space variables instead of just their difference. Also note that  $K_V^{-1}$  is real and symmetric,  $K_V$  being real and symmetric. Therefore, the result of the functional integration yields the simple formula

$$\langle 0 | \Psi(\mathbf{x}') \mathbf{P}_V \Psi(\mathbf{x}) | 0 \rangle = K_V^{-1}(\mathbf{x}', \mathbf{x}) \langle 0 | \mathbf{P}_V | 0 \rangle, \tag{61}$$

where the factor  $\langle 0 | \mathbf{P}_V | 0 \rangle$  is a positive constant, which we will leave unexpanded.

Taking it altogether, the presence of the projector  $\mathbf{P}_V$  in (61) modifies the two-point correlation function by introducing a constant factor  $\langle 0 | \mathbf{P}_V | 0 \rangle$  and replacing the inverse kernel,  $K^{-1}$ , with a different one,  $K_V^{-1}$ . It can easily be proved, by using the general formulae of gaussian integrals, that this holds true in the more general case of the many-point correlation function. In fact, (53) holds for general quadratic forms in the field  $\psi$ , and so (61) can be generalized to

$$\begin{aligned}
& \langle 0 | \prod_{n=1}^N \Psi(\mathbf{x}_n) \mathbf{P}_V \prod_{n=N+1}^{2N} \Psi(\mathbf{x}_n) | 0 \rangle \\
&= \langle 0 | \mathbf{P}_V | 0 \rangle \sum_{\substack{\text{pairings} \\ \text{of } \mathbf{x}_1, \dots, \mathbf{x}_{2N}}} \prod_{\text{pairs}} K_V^{-1}(\text{paired var.}). \tag{62}
\end{aligned}$$

The remaining task is to calculate the inverse kernel  $K_V^{-1}$  by means of (60). In fact, we will look for a solution of the more general equation,

$$\int_V d^3x' K(\mathbf{y} - \mathbf{x}') K_V^{-1}(\mathbf{x}', \mathbf{x}) = \delta^3(\mathbf{x} - \mathbf{y}) \quad \forall \mathbf{x} \in V, \mathbf{y}, \tag{63}$$

with unbounded  $\mathbf{y}$ . It is clear that a solution  $K_V^{-1}$  of equation (63) is also a solution of (60), because  $K_V$  equals  $K$  when  $\mathbf{y} \in V$ . Setting  $\mathbf{y}$  unbounded allows us to find an implicit form for  $K_V^{-1}$ . In fact, (63) implies

$$\frac{1}{(2\pi)^3} \int_V d^3x' e^{i\mathbf{p} \cdot \mathbf{x}'} 2\varepsilon K_V^{-1}(\mathbf{x}', \mathbf{x}) = \frac{e^{i\mathbf{p} \cdot \mathbf{x}}}{(2\pi)^3}, \tag{64}$$

which is obtained by multiplying both sides of (63) by  $e^{i\mathbf{p} \cdot \mathbf{y}} / (2\pi)^3$  and integrating over the *whole space* in  $d^3y$ .

We are now in a position to accomplish our task of calculating  $\langle p | \mathbf{P}_V | p \rangle$ . By plugging (61) into (46), we get

$$\begin{aligned}
\langle 0 | a(p) \mathbf{P}_V a^\dagger(p) | 0 \rangle &= \frac{1}{(2\pi)^3} \int d^3x \int d^3x' e^{i\mathbf{p} \cdot (\mathbf{x} - \mathbf{x}')} \\
&\quad \times 2\varepsilon K_V^{-1}(\mathbf{x}', \mathbf{x}) \langle 0 | \mathbf{P}_V | 0 \rangle. \tag{65}
\end{aligned}$$

The integration domain in (65) can be split into the region  $V$  and the complementary  $\bar{V}$  for both variables. The inverse kernel  $K_V^{-1}$  is not defined outside  $V$  and can thus be set to an arbitrary value, e.g. zero. Otherwise, even if one chose a non-vanishing continuation of  $K_V^{-1}$ , an integration outside the domain  $V$  would involve the degrees of freedom of the field outside  $V$ , and, according to the general discussion at the end of Sect. 4, the contributing term should be dropped. Therefore, retaining only the physically meaningful term, (65) turns into

$$\begin{aligned}
\langle 0 | a(p) \mathbf{P}_V a^\dagger(p) | 0 \rangle &= \frac{1}{(2\pi)^3} \int_V d^3x \int_V d^3x' e^{i\mathbf{p} \cdot (\mathbf{x} - \mathbf{x}')} \\
&\quad \times 2\varepsilon K_V^{-1}(\mathbf{x}', \mathbf{x}) \langle 0 | \mathbf{P}_V | 0 \rangle. \tag{66}
\end{aligned}$$

In the above equation one can easily recognize the complex conjugate of the left hand side of (64). Hence, replacing



it with the complex conjugate of the right hand side, one gets

$$\begin{aligned} \langle 0| a(p) \mathbf{P}_V a^\dagger(p) |0\rangle &= \frac{1}{(2\pi)^3} \int_V d^3\mathbf{x} \langle 0| \mathbf{P}_V |0\rangle \\ &= \frac{V}{(2\pi)^3} \langle 0| \mathbf{P}_V |0\rangle, \end{aligned} \quad (67)$$

which is the same as the result of NRQM in (33) in the simple case  $N = 1$  times a factor  $\langle 0| \mathbf{P}_V |0\rangle$ . This factor still contains dependence on the field degrees of freedom outside  $V$ , according to the projector expression in (41), which should disappear at some point. However, we will see that this factor appears at any multiplicity and therefore becomes irrelevant for the calculations of the statistical averages.

## 5.2 Charged scalar field

The calculation done for a neutral scalar field can easily be extended to a charged scalar field. The 2-component charged scalar field in Schrödinger representation reads

$$\begin{aligned} \Psi(\mathbf{x}) &= \frac{1}{(2\pi)^{\frac{3}{2}}} \int \frac{d^3\mathbf{p}}{\sqrt{2\varepsilon}} (a(p) e^{i\mathbf{p}\cdot\mathbf{x}} + b^\dagger(p) e^{-i\mathbf{p}\cdot\mathbf{x}}) \quad (68) \\ \Psi^\dagger(\mathbf{x}) &= \frac{1}{(2\pi)^{\frac{3}{2}}} \int \frac{d^3\mathbf{p}}{\sqrt{2\varepsilon}} (b(p) e^{i\mathbf{p}\cdot\mathbf{x}} + a^\dagger(p) e^{-i\mathbf{p}\cdot\mathbf{x}}), \end{aligned}$$

where  $a$ ,  $a^\dagger$  and  $b$ ,  $b^\dagger$  are annihilation and creation operators of particles and antiparticles, respectively. They satisfy the commutation relations

$$\begin{aligned} [a(p), a^\dagger(p')] &= [b(p), b^\dagger(p')] = \delta^3(\mathbf{p} - \mathbf{p}') \quad (69) \\ [a(p), b(p')] &= [a^\dagger(p), b^\dagger(p')] = 0. \end{aligned}$$

Likewise, the fields obey the commutation relations

$$[\Psi(\mathbf{x}), \Psi^\dagger(\mathbf{y})] = 0, \quad (70)$$

and it is then possible to construct field states  $|\psi, \psi^\dagger\rangle$ . The projector  $\mathbf{P}_V$  can be written as

$$\mathbf{P}_V \equiv \int_V \mathcal{D}(\psi^\dagger, \psi) |\psi, \psi^\dagger\rangle \langle \psi, \psi^\dagger|, \quad (71)$$

with suitable state normalization and arbitrary field functions  $\psi(\mathbf{x})$  outside the region  $V$ .<sup>4</sup> Similar to (45), one can write

$$\begin{aligned} \langle 0| a(p) &= \langle 0| \frac{1}{(2\pi)^{\frac{3}{2}}} \int d^3\mathbf{x} e^{-i\mathbf{p}\cdot\mathbf{x}} \sqrt{2\varepsilon} \Psi(\mathbf{x}) \quad (72) \\ a^\dagger(p) |0\rangle &= \frac{1}{(2\pi)^{\frac{3}{2}}} \int d^3\mathbf{x} e^{i\mathbf{p}\cdot\mathbf{x}} \sqrt{2\varepsilon} \Psi^\dagger(\mathbf{x}) |0\rangle \\ \langle 0| b(p) &= \langle 0| \frac{1}{(2\pi)^{\frac{3}{2}}} \int d^3\mathbf{x} e^{-i\mathbf{p}\cdot\mathbf{x}} \sqrt{2\varepsilon} \Psi^\dagger(\mathbf{x}) \end{aligned}$$

<sup>4</sup> The functional measure in (71) reads  $\prod_{\mathbf{x}} d\psi(\mathbf{x}) d\psi^*(\mathbf{x})/i\pi$ . Anyhow, its explicit form is not important for our purposes.

$$b^\dagger(p) |0\rangle = \frac{1}{(2\pi)^{\frac{3}{2}}} \int d^3\mathbf{x} e^{i\mathbf{p}\cdot\mathbf{x}} \sqrt{2\varepsilon} \Psi(\mathbf{x}) |0\rangle.$$

The chain of arguments of the previous subsection can be repeated, and the functional integral

$$\begin{aligned} \langle 0| \prod_{n=1}^N \Psi(\mathbf{x}_n) \mathbf{P}_V \prod_{n=1}^N \Psi^\dagger(\mathbf{x}'_n) |0\rangle \\ = \int_V \mathcal{D}(\psi^\dagger, \psi) |\langle 0| \psi, \psi^\dagger\rangle|^2 \prod_{n=1}^N \psi(\mathbf{x}_n) \psi^\dagger(\mathbf{x}'_n) \end{aligned} \quad (73)$$

is found to be a multiple Gaussian integral. Letting  $\rho$  be a permutation of the integers  $1, \dots, N$ , the integration on the right hand side of (73) yields

$$\begin{aligned} \langle 0| \prod_{n=1}^N \Psi(\mathbf{x}_n) \mathbf{P}_V \prod_{n=1}^N \Psi^\dagger(\mathbf{x}'_n) |0\rangle \\ = \langle 0| \mathbf{P}_V |0\rangle \sum_{\rho \in S_N} \prod_{n=1}^N K_V^{-1}(\mathbf{x}_n, \mathbf{x}'_{\rho(n)}), \end{aligned} \quad (74)$$

which differs from the corresponding expression for the real scalar field, because now the field is complex, and  $\psi$  can only be coupled to  $\psi^\dagger$  [15]:

$$\begin{aligned} \int \mathcal{D}(\psi^\dagger, \psi) \prod_{n=1}^N (\psi(\boldsymbol{\xi}_n) \psi^\dagger(\boldsymbol{\xi}'_n)) \\ \times \exp \left[ - \int d^3\mathbf{x}_1 \int d^3\mathbf{x}_2 \psi^\dagger(\mathbf{x}_1) K(\mathbf{x}_1 - \mathbf{x}_2) \psi(\mathbf{x}_2) \right] \\ = I_0 \sum_{\rho \in S_N} \prod_{n=1}^N K^{-1}(\boldsymbol{\xi}_n - \boldsymbol{\xi}'_{\rho(n)}). \end{aligned} \quad (75)$$

However, the functional integral involving only the two fields  $\psi$  and  $\psi^\dagger$  yields the same result as for neutral particles. Thus, the kernel  $K$  is still the same and so is the integral equation (64) defining  $K_V^{-1}$ . The expectation value of  $\mathbf{P}_V$  in a state with only one particle (or antiparticle) will also be the same as in (67); that is,

$$\begin{aligned} \langle 0| a(p) \mathbf{P}_V a^\dagger(p) |0\rangle &= \langle 0| b(p) \mathbf{P}_V b^\dagger(p) |0\rangle \\ &= \frac{V}{(2\pi)^3} \langle 0| \mathbf{P}_V |0\rangle. \end{aligned} \quad (76)$$

## 6 Multiparticle channels

We have seen in the previous section that the expectation value  $\langle p| \mathbf{P}_V |p\rangle$  for a single spinless particle is the same as obtained in a NRQM approach [5] times an overall immaterial factor  $\langle 0| \mathbf{P}_V |0\rangle$ . In this section, we will tackle the calculation of the general multiparticle state. We will see that, by using the projector definitions in (41) and (71) and subtracting the spurious contributions stemming from external field degrees of freedom, the final result is still

the same as in the NRQM calculation times the factor  $\langle 0 | \mathbf{P}_V | 0 \rangle$ .

We will first address the case of  $N$  charged particles.

### 6.1 Identical charged particles

We will consider a state with  $N$  identical charged particles; for  $N$  antiparticles the result is trivially the same.

We want to calculate

$$\langle N, \{p\} | \mathbf{P}_V | N, \{p\} \rangle = \langle 0 | \prod_n^N a(p_n) \mathbf{P}_V \prod_n^N a^\dagger(p_n) | 0 \rangle. \quad (77)$$

Since

$$[a^\dagger, \Psi^\dagger] = [a, \Psi] = [b, \Psi^\dagger] = [b^\dagger, \Psi] = 0, \quad (78)$$

one can replace creation and annihilation operators with their expressions in (72) disregarding the position of the operators with respect to the vacuum state. Expressed in a formula we have

$$\begin{aligned} & \langle N, \{p\} | \mathbf{P}_V | N, \{p\} \rangle \\ &= \prod_{n=1}^N \left[ \frac{1}{(2\pi)^3} \int d^3x_n \int d^3x'_n e^{-i\mathbf{p}_n \cdot (\mathbf{x}_n - \mathbf{x}'_n)} 2\varepsilon_n \right] \\ & \times \langle 0 | \prod_{n=1}^N \Psi(\mathbf{x}_n) \mathbf{P}_V \prod_{n=1}^N \Psi^\dagger(\mathbf{x}'_n) | 0 \rangle \\ &= \prod_{n=1}^N \left[ \frac{1}{(2\pi)^3} \int d^3x_n \int d^3x'_n e^{-i\mathbf{p}_n \cdot (\mathbf{x}_n - \mathbf{x}'_n)} 2\varepsilon_n \right] \\ & \times \sum_{\rho \in S_N} \prod_{n=1}^N K_V^{-1}(\mathbf{x}_n, \mathbf{x}'_{\rho(n)}) \langle 0 | \mathbf{P}_V | 0 \rangle, \end{aligned} \quad (79)$$

where  $S_N$  is the permutation group of rank  $N$ . Now, like for the single-particle case, we restrict the integration domain to  $V$  in (79) in order to get rid of external degrees of freedom and, by repeatedly using (64), we are left with

$$\begin{aligned} & \frac{\langle N, \{p\} | \mathbf{P}_V | N, \{p\} \rangle}{\langle 0 | \mathbf{P}_V | 0 \rangle} \\ &= \sum_{\rho \in S_N} \prod_{n=1}^N \left[ \frac{1}{(2\pi)^3} \int_V d^3x'_n e^{-i\mathbf{p}_n \cdot (\mathbf{x}'_{\rho(n)} - \mathbf{x}'_n)} \right] \\ &= \sum_{\rho \in S_N} \prod_{n=1}^N \left[ \frac{1}{(2\pi)^3} \int_V d^3x'_n e^{-i(\mathbf{p}_{\rho^{-1}(n)} - \mathbf{p}_n) \cdot \mathbf{x}'_n} \right]. \end{aligned} \quad (80)$$

Hence, using the definition (25), we have

$$\langle N, \{p\} | \mathbf{P}_V | N, \{p\} \rangle = \sum_{\rho \in S_N} \prod_{n=1}^N F_V(\mathbf{p}_{\rho(n)} - \mathbf{p}_n) \langle 0 | \mathbf{P}_V | 0 \rangle, \quad (81)$$

which is exactly the expression (33) obtained in NRQM for  $N$  identical bosons times the factor  $\langle 0 | \mathbf{P}_V | 0 \rangle$ .

### 6.2 Identical neutral particles

The case of  $N$  identical neutral particles is more complicated, because of the possibility of particle pair creation. This is reflected in the formalism in the occurrence of many additional terms in working out (77). We start with the calculation for a state with two neutral particles of four-momenta  $p_1$  and  $p_2$ , respectively, generalizing to  $N$  particles thereafter. In terms of creation and annihilation operators we have

$$\langle p_1, p_2 | \mathbf{P}_V | p_1, p_2 \rangle = \langle 0 | a(p_1) a(p_2) \mathbf{P}_V a^\dagger(p_2) a^\dagger(p_1) | 0 \rangle, \quad (82)$$

which we can rewrite using (45) for  $a(p_1)$  and  $a^\dagger(p_1)$  as

$$\begin{aligned} & \langle p_1, p_2 | \mathbf{P}_V | p_1, p_2 \rangle \\ &= \frac{1}{(2\pi)^3} \int d^3x_1 \int d^3x'_1 e^{-i\mathbf{p}_1 \cdot (\mathbf{x}_1 - \mathbf{x}'_1)} \\ & \times 2\varepsilon_1 \langle 0 | \Psi(\mathbf{x}_1) a(p_2) \mathbf{P}_V a^\dagger(p_2) \Psi(\mathbf{x}'_1) | 0 \rangle. \end{aligned} \quad (83)$$

In order to use the expression (45) for the annihilation and creation operators  $a(p_2)$  and  $a^\dagger(p_2)$ , we have to get them acting on the vacuum state; hence they should be moved from their position in (84) outwards. This can be done by taking advantage of the following commutation rules:

$$\begin{aligned} [\Psi(\mathbf{x}), a(p)] &= -\frac{e^{-i\mathbf{p} \cdot \mathbf{x}}}{(2\pi)^{\frac{3}{2}} \sqrt{2\varepsilon}} \\ [a(p)^\dagger, \Psi(\mathbf{x})] &= -\frac{e^{i\mathbf{p} \cdot \mathbf{x}}}{(2\pi)^{\frac{3}{2}} \sqrt{2\varepsilon}}. \end{aligned} \quad (84)$$

Using (85) and then plugging (45) in (84) we get

$$\begin{aligned} & \langle p_1, p_2 | \mathbf{P}_V | p_1, p_2 \rangle \\ &= \frac{\varepsilon_1}{\varepsilon_2 (2\pi)^6} \int d^3x_1 \int d^3x'_1 e^{-i\mathbf{p}_1 \cdot (\mathbf{x}_1 - \mathbf{x}'_1)} e^{-i\mathbf{p}_2 \cdot (\mathbf{x}_1 - \mathbf{x}'_1)} \\ & \times \langle 0 | \mathbf{P}_V | 0 \rangle \\ & - \frac{2\varepsilon_1}{(2\pi)^6} \int d^3x_1 \int d^3x'_1 \int d^3x_2 e^{-i\mathbf{p}_1 \cdot (\mathbf{x}_1 - \mathbf{x}'_1)} \\ & \times e^{-i\mathbf{p}_2 \cdot (\mathbf{x}_2 - \mathbf{x}'_1)} \langle 0 | \Psi(\mathbf{x}_2) \mathbf{P}_V \Psi(\mathbf{x}_1) | 0 \rangle \\ & - \frac{2\varepsilon_1}{(2\pi)^6} \int d^3x_1 \int d^3x'_1 \int d^3x_2 e^{-i\mathbf{p}_1 \cdot (\mathbf{x}_1 - \mathbf{x}'_1)} \\ & \times e^{-i\mathbf{p}_2 \cdot (\mathbf{x}_1 - \mathbf{x}'_2)} \langle 0 | \Psi(\mathbf{x}'_1) \mathbf{P}_V \Psi(\mathbf{x}'_2) | 0 \rangle \\ & + \frac{4\varepsilon_1 \varepsilon_2}{(2\pi)^6} \int d^3x_1 \int d^3x'_1 \int d^3x_2 \int d^3x'_2 e^{-i\mathbf{p}_1 \cdot (\mathbf{x}_1 - \mathbf{x}'_1)} \\ & \times e^{-i\mathbf{p}_2 \cdot (\mathbf{x}_2 - \mathbf{x}'_2)} \langle 0 | \Psi(\mathbf{x}_2) \Psi(\mathbf{x}_1) \mathbf{P}_V \Psi(\mathbf{x}'_1) \Psi(\mathbf{x}'_2) | 0 \rangle, \end{aligned} \quad (85)$$

where advantage has been taken of the fact that  $[\mathbf{P}_V, \Psi(\mathbf{x})] = 0$ . Equation (86) has four different terms, among which only the last one was present in the case of two charged particles in Sect. 6.1. Instead, the first three terms arise from contractions of the annihilation and creation operators with field operators on the same side with respect to

$\mathbf{P}_V$ . By using (62) and replacing all unbounded integrations with integrations over  $V$  to eliminate spurious degrees of freedom of the field, (86) yields

$$\begin{aligned}
& \frac{\langle p_1, p_2 | \mathbf{P}_V | p_1, p_2 \rangle}{\langle 0 | \mathbf{P}_V | 0 \rangle} \\
&= \frac{\varepsilon_1}{\varepsilon_2 (2\pi)^6} \int_V d^3 x_1 \int_V d^3 x'_1 e^{-i\mathbf{p}_1 \cdot (\mathbf{x}_1 - \mathbf{x}'_1)} e^{-i\mathbf{p}_2 \cdot (\mathbf{x}_1 - \mathbf{x}'_1)} \\
&\quad - \frac{2\varepsilon_1}{(2\pi)^6} \int_V d^3 x_1 \int_V d^3 x_2 \int_V d^3 x'_1 e^{-i\mathbf{p}_1 \cdot (\mathbf{x}_1 - \mathbf{x}'_1)} \\
&\quad \times e^{-i\mathbf{p}_2 \cdot (\mathbf{x}_2 - \mathbf{x}'_1)} K_V^{-1}(\mathbf{x}_2, \mathbf{x}_1) \\
&\quad - \frac{2\varepsilon_1}{(2\pi)^6} \int_V d^3 x_1 \int_V d^3 x'_1 \int_V d^3 x'_2 e^{-i\mathbf{p}_1 \cdot (\mathbf{x}_1 - \mathbf{x}'_1)} \\
&\quad \times e^{-i\mathbf{p}_2 \cdot (\mathbf{x}_1 - \mathbf{x}'_2)} K_V^{-1}(\mathbf{x}'_1, \mathbf{x}'_2) \\
&\quad + \frac{4\varepsilon_1 \varepsilon_2}{(2\pi)^6} \int_V d^3 x_1 \int_V d^3 x'_1 \int_V d^3 x_2 \\
&\quad \times \int_V d^3 x'_2 e^{-i\mathbf{p}_1 \cdot (\mathbf{x}_1 - \mathbf{x}'_1)} e^{-i\mathbf{p}_2 \cdot (\mathbf{x}_2 - \mathbf{x}'_2)} \\
&\quad \times [K_V^{-1}(\mathbf{x}_1, \mathbf{x}'_1) K_V^{-1}(\mathbf{x}_2, \mathbf{x}'_2) + K_V^{-1}(\mathbf{x}_1, \mathbf{x}'_2) K_V^{-1}(\mathbf{x}_2, \mathbf{x}'_1) \\
&\quad \quad + K_V^{-1}(\mathbf{x}_1, \mathbf{x}_2) K_V^{-1}(\mathbf{x}'_2, \mathbf{x}'_1)] . \quad (87)
\end{aligned}$$

We can now use (64) to integrate out the inverse kernel in (87). For the second term on the right hand side, we choose to integrate  $\exp(-i\mathbf{p}_2 \cdot \mathbf{x}_2) K_V^{-1}(\mathbf{x}_2, \mathbf{x}_1)$  in  $x_2$  and for the third term  $\exp(i\mathbf{p}_1 \cdot \mathbf{x}'_1) K_V^{-1}(\mathbf{x}'_1, \mathbf{x}'_2)$  in  $x'_1$ . At the same time, we perform the integration of the last term in an arbitrary couple of variables with indices 1 and 2, obtaining

$$\begin{aligned}
& \frac{\langle p_1, p_2 | \mathbf{P}_V | p_1, p_2 \rangle}{\langle 0 | \mathbf{P}_V | 0 \rangle} \\
&= \frac{1}{(2\pi)^6} \int_V d^3 x_1 \int_V d^3 x'_1 e^{-i\mathbf{p}_1 \cdot (\mathbf{x}_1 - \mathbf{x}'_1)} e^{-i\mathbf{p}_2 \cdot (\mathbf{x}_1 - \mathbf{x}'_1)} \frac{\varepsilon_1}{\varepsilon_2} \\
&\quad - \frac{1}{(2\pi)^6} \int_V d^3 x_1 \int_V d^3 x'_1 e^{-i\mathbf{p}_1 \cdot (\mathbf{x}_1 - \mathbf{x}'_1)} 2\varepsilon_1 \frac{e^{-i\mathbf{p}_2 \cdot (\mathbf{x}_1 - \mathbf{x}'_1)}}{2\varepsilon_2} \\
&\quad - \frac{1}{(2\pi)^6} \int_V d^3 x_1 \int_V d^3 x'_2 e^{-i\mathbf{p}_1 \cdot (\mathbf{x}_1 - \mathbf{x}'_2)} e^{-i\mathbf{p}_2 \cdot (\mathbf{x}_1 - \mathbf{x}'_2)} \\
&\quad + \frac{V^2}{(2\pi)^6} + \frac{1}{(2\pi)^6} \int_V d^3 x_1 \int_V d^3 x_2 e^{-i(\mathbf{p}_1 - \mathbf{p}_2) \cdot (\mathbf{x}_1 - \mathbf{x}_2)} \\
&\quad + \frac{1}{(2\pi)^6} \int_V d^3 x_1 \int_V d^3 x'_2 e^{-i\mathbf{p}_1 \cdot (\mathbf{x}_1 - \mathbf{x}'_2)} e^{-i\mathbf{p}_2 \cdot (\mathbf{x}_1 - \mathbf{x}'_2)} . \quad (88)
\end{aligned}$$

Four terms in the above sum cancel, and we are left with

$$\begin{aligned}
\frac{\langle p_1, p_2 | \mathbf{P}_V | p_1, p_2 \rangle}{\langle 0 | \mathbf{P}_V | 0 \rangle} &= \frac{V^2}{(2\pi)^6} + |F_V(\mathbf{p}_1 - \mathbf{p}_2)|^2 \\
&= \sum_{\rho \in S_2} \prod_{n=1}^2 F_V(\mathbf{p}_{\rho(n)} - \mathbf{p}_n) . \quad (89)
\end{aligned}$$

This is the same result as one would obtain for two identical bosons in a NRQM framework [5]. The second term on the right hand side accounts for the well known phenomenon of Bose–Einstein correlation in the emission of identical boson pairs.

Looking back at the whole derivation, we find that the terms arising from pairings of field variables on the same side with respect to  $\mathbf{P}_V$  have cancelled with the terms stemming from commutation of annihilation and creation operators with field operators; the only surviving terms are  $N!$  pairings of field variables on different sides of  $\mathbf{P}_V$ , just like in the case of charged particles. This cancellation property holds, and so the formula (82) applies to the case of  $N$  neutral particles as well. A proof based on the form of the thermodynamic limit  $V \rightarrow \infty$  is given in Appendix B.

### 6.3 Particle–antiparticle case

For a state with one particle and one antiparticle, the expectation value of  $\mathbf{P}_V$  reads

$$\langle 0 | a(p_1) b(p_2) \mathbf{P}_V b^\dagger(p_2) a^\dagger(p_1) | 0 \rangle \quad (90)$$

implying, in view of (72),

$$\begin{aligned}
& \langle 0 | a(p_1) b(p_2) \mathbf{P}_V b^\dagger(p_2) a^\dagger(p_1) | 0 \rangle \\
&= \frac{1}{(2\pi)^3} \int d^3 x_1 \int d^3 x'_1 e^{-i\mathbf{p}_1 \cdot (\mathbf{x}_1 - \mathbf{x}'_1)} \\
&\quad \times 2\varepsilon_1 \langle 0 | \Psi(\mathbf{x}_1) b(p_2) \mathbf{P}_V b^\dagger(p_2) \Psi^\dagger(\mathbf{x}'_1) | 0 \rangle . \quad (91)
\end{aligned}$$

Like for neutral particles, the  $b$  and  $b^\dagger$  operators are moved outwards to get them acting on the vacuum state by using the commutators:

$$\begin{aligned}
[\Psi(\mathbf{x}), b(p)] &= \frac{e^{-i\mathbf{p} \cdot \mathbf{x}}}{(2\pi)^{\frac{3}{2}} \sqrt{2\varepsilon}} \\
[b(p)^\dagger, \Psi^\dagger(\mathbf{x})] &= \frac{e^{i\mathbf{p} \cdot \mathbf{x}}}{(2\pi)^{\frac{3}{2}} \sqrt{2\varepsilon}} . \quad (92)
\end{aligned}$$

By using (72) and, like in the previous subsection, restricting the integration to the region  $V$  to eliminate external degrees of freedom, we obtain

$$\begin{aligned}
& \langle 0 | a(p_1) b(p_2) \mathbf{P}_V b^\dagger(p_2) a^\dagger(p_1) | 0 \rangle \\
&= \frac{\varepsilon_1}{\varepsilon_2 (2\pi)^6} \int_V d^3 x_1 \int_V d^3 x'_1 e^{-i\mathbf{p}_1 \cdot (\mathbf{x}_1 - \mathbf{x}'_1)} e^{-i\mathbf{p}_2 \cdot (\mathbf{x}_1 - \mathbf{x}'_1)} \\
&\quad \times \langle 0 | \mathbf{P}_V | 0 \rangle \\
&\quad - \frac{2\varepsilon_1}{(2\pi)^6} \int_V d^3 x_1 \int_V d^3 x'_1 \int_V d^3 x_2 e^{-i\mathbf{p}_1 \cdot (\mathbf{x}_1 - \mathbf{x}'_1)} \\
&\quad \times e^{-i\mathbf{p}_2 \cdot (\mathbf{x}_2 - \mathbf{x}'_1)} \langle 0 | \Psi^\dagger(\mathbf{x}_2) \mathbf{P}_V \Psi(\mathbf{x}_1) | 0 \rangle \\
&\quad - \frac{2\varepsilon_1}{(2\pi)^6} \int_V d^3 x_1 \int_V d^3 x'_1 \int_V d^3 x'_2 e^{-i\mathbf{p}_1 \cdot (\mathbf{x}_1 - \mathbf{x}'_1)} \\
&\quad \times e^{-i\mathbf{p}_2 \cdot (\mathbf{x}_1 - \mathbf{x}'_2)} \langle 0 | \Psi^\dagger(\mathbf{x}'_1) \mathbf{P}_V \Psi(\mathbf{x}'_2) | 0 \rangle \\
&\quad + \frac{4\varepsilon_1 \varepsilon_2}{(2\pi)^6} \int_V d^3 x_1 \int_V d^3 x'_1 \int_V d^3 x_2 \\
&\quad \times \int_V d^3 x'_2 e^{-i\mathbf{p}_1 \cdot (\mathbf{x}_1 - \mathbf{x}'_1)} e^{-i\mathbf{p}_2 \cdot (\mathbf{x}_2 - \mathbf{x}'_2)} \\
&\quad \times \langle 0 | \Psi^\dagger(\mathbf{x}_2) \Psi(\mathbf{x}_1) \mathbf{P}_V \Psi^\dagger(\mathbf{x}'_1) \Psi(\mathbf{x}'_2) | 0 \rangle , \quad (93)
\end{aligned}$$

whose result is (87) except the last term but one, because now

$$\frac{\langle 0 | \Psi^\dagger(\mathbf{x}_2) \Psi(\mathbf{x}_1) \mathbf{P}_V \Psi^\dagger(\mathbf{x}'_1) \Psi(\mathbf{x}'_2) | 0 \rangle}{\langle 0 | \mathbf{P}_V | 0 \rangle} \quad (94)$$

$$= K_V^{-1}(\mathbf{x}_1, \mathbf{x}'_1) K_V^{-1}(\mathbf{x}_2, \mathbf{x}'_2) + K_V^{-1}(\mathbf{x}_1, \mathbf{x}_2) K_V^{-1}(\mathbf{x}'_2, \mathbf{x}'_1),$$

which is a consequence of the general expression (74). Again, four out of five terms cancel in (93), and we get

$$\frac{\langle 0 | a(p_1) b(p_2) \mathbf{P}_V b^\dagger(p_2) a^\dagger(p_1) | 0 \rangle}{\langle 0 | \mathbf{P}_V | 0 \rangle} = \frac{V^2}{(2\pi)^6}, \quad (95)$$

where the missing term with respect to the neutral particle case (89) is the one involving permutations; this is a natural result, because particles and antiparticles are, of course, not identical. Hence, the expectation value of  $\mathbf{P}_V$  on a particle–antiparticle pair shows a remarkable factorization property; that is,

$$\langle 0 | a(p_1) b(p_2) \mathbf{P}_V b^\dagger(p_2) a^\dagger(p_1) | 0 \rangle$$

$$= \langle 0 | a(p_1) \mathbf{P}_V a^\dagger(p_1) | 0 \rangle \langle 0 | b(p_2) \mathbf{P}_V b^\dagger(p_2) | 0 \rangle, \quad (96)$$

where the = sign holds provided that the integrations are restricted to the region  $V$ .

Extrapolating to the most general case of  $N_+$  particles and  $N_-$  antiparticles, it can be argued, by using the limit  $V \rightarrow \infty$ , that the factorization of the microcanonical state weight holds (see Appendix B) at any multiplicity, i.e. particles and antiparticles behave like two different species:

$$\langle \{N_+\}, \{p_+\}, \{N_-\}, \{p_-\} | \mathbf{P}_V | \{N_+\}, \{p_+\}, \{N_-\}, \{p_-\} \rangle$$

$$= \sum_{\rho_+ \in S_{N_+}} \prod_{n_+=1}^{N_+} F_V(\mathbf{p}_{\rho_+(n_+)} - \mathbf{p}_{n_+})$$

$$\times \sum_{\rho_- \in S_{N_-}} \prod_{n_-=1}^{N_-} F_V(\mathbf{p}_{\rho_-(n_-)} - \mathbf{p}_{n_-}) \langle 0 | \mathbf{P}_V | 0 \rangle. \quad (97)$$

## 7 Summary and discussion

On the basis of (19), (21), (16) and (82), which apply to charged as well as neutral particles, and taking into account that the states  $|N, \{p\}\rangle$  have been chosen to be eigenvectors of four-momentum, we can finally write down the full expression of the microcanonical partition function of a relativistic quantum gas of neutral spinless bosons:

$$\Omega = \langle 0 | \mathbf{P}_V | 0 \rangle \sum_{N=0}^{\infty} \frac{1}{N!} \left[ \prod_{n=1}^N \int d^3 p_n \right] \delta^4 \left( P - \sum_{n=1}^N p_n \right)$$

$$\times \sum_{\rho \in S_N} \prod_{n=1}^N \int_V d^3 x \exp[i\mathbf{x} \cdot (\mathbf{p}_{\rho(n)} - \mathbf{p}_n)], \quad (98)$$

with  $P = (M, \mathbf{0})$  and the factor  $1/N!$  has been introduced in order to avoid multiple counting when integrating over

particle momenta. Similarly, on the basis of (20), (22) and (97), the microcanonical partition function of a relativistic quantum gas of charged spinless bosons can be written as

$$\Omega = \langle 0 | \mathbf{P}_V | 0 \rangle \sum_{N_+, N_- = 0}^{\infty} \frac{1}{N_+! N_-!} \left[ \prod_{n=1}^{N_+ + N_-} \int d^3 p_n \right]$$

$$\times \delta^4 \left( P - \sum_{n=1}^{N_+ + N_-} p_n \right)$$

$$\times \sum_{\rho_+ \in S_{N_+}} \prod_{n_+=1}^{N_+} \int_V d^3 x \exp[i\mathbf{x} \cdot (\mathbf{p}_{\rho_+(n_+)} - \mathbf{p}_{n_+})]$$

$$\times \sum_{\rho_- \in S_{N_-}} \prod_{n_-=1}^{N_-} \int_V d^3 x \exp[i\mathbf{x} \cdot (\mathbf{p}_{\rho_-(n_-)} - \mathbf{p}_{n_-})]. \quad (99)$$

The generalization to a multi-species gas of spinless bosons is then easily achieved:

$$\Omega = \langle 0 | \mathbf{P}_V | 0 \rangle \sum_{\{N_j\}} \left[ \prod_{j=1}^K \frac{1}{N_j!} \prod_{n_j=1}^{N_j} \int d^3 p_{n_j} \right]$$

$$\times \delta^4 \left( P - \sum_{n=1}^N p_n \right)$$

$$\times \prod_{j=1}^k \sum_{\rho_j \in S_{N_j}} \prod_{n_j=1}^{N_j} \int_V d^3 x \exp[i\mathbf{x} \cdot (\mathbf{p}_{\rho_j(n_j)} - \mathbf{p}_{n_j})], \quad (100)$$

where  $N = \sum_j N_j$ . The formulae (98), (99) and (100) are our final results. The finite volume Fourier integrals in the above expressions nicely account for the quantum statistics correlations known as Bose–Einstein and Fermi–Dirac correlations. We stress once more that for a charged quantum gas, particles and antiparticles can be handled as belonging to distinct species, and they correspond to different labels  $j$  in the multi-species generalization of (100).

The expression of the MPF (98) is the same as obtained in a NRQM calculation in [5], quoted in this work in (24), times an overall factor  $\langle 0 | \mathbf{P}_V | 0 \rangle$ , which is immaterial for the calculation of statistical averages in the microcanonical ensemble. More specifically, the expectation value of  $\mathbf{P}_V$  on a free multi-particle state (see (82) and (97)) is the same as in the NRQM calculation (33) times  $\langle 0 | \mathbf{P}_V | 0 \rangle$ . This result has been achieved enforcing a subtraction prescription, namely that all terms depending on the degrees of freedom outside the system region  $V$  must be subtracted “by hand” in all terms at fixed multiplicities. The factor  $\langle 0 | \mathbf{P}_V | 0 \rangle$  is still dependent on those spurious degrees of freedom, according to the  $\mathbf{P}_V$  definition in (41), but this does not affect any statistical average, because it always cancels. In the thermodynamic limit, this factor tends to 1 as  $\mathbf{P}_V \rightarrow \mathbf{I}$  and the large-volume limit result known in the literature [4] (i.e. (27)) is recovered.

This result looks surprising in a sense, because one would have expected a priori that quantum relativistic effects would affect the statistical averages bringing in a dependence on the ratio between the Compton wavelength and the linear size of the region, getting negligible at small values, i.e. when  $V \rightarrow \infty$ . This is because the condition (32), from which the MPF expressions (23) and (24) ensue, no longer holds in quantum field theory at finite volume and only applies to good approximation at very large volumes, as discussed in Sect. 4. However, in the calculation of statistical averages, only the projector  $\mathbf{P}_V$  enters, and this implies the summation over all states at different integrated occupation numbers  $|\tilde{N}\rangle_V$ , according to (31). So, even though the coefficients in the expansion (34) are different from zero and do depend on the volume, it turns out that, summing all of them at fixed  $N$ , one gets the same result as in the NRQM approximation (32). Expressed in a formula, by using (31), we have

$$\begin{aligned} & \langle N, \{p\} | \mathbf{P}_V | N \{p\} \rangle \\ &= \sum_{\tilde{N}, \{k_V\}} \left| \langle N, \{p\} | \tilde{N}, \{k_V\} \rangle \right|^2 \\ &= \sum_{\tilde{N}, \{k_V\}} \left| \langle 0 | \tilde{N}, \{k_V\} \rangle \right|^2 \sum_{\{k_V\}} |\langle N, \{p\} | N, \{k_V\} \rangle|_{\text{NR}}^2, \end{aligned} \quad (101)$$

where the index NR means that one should make a non-relativistic quantum mechanical calculation.

This calculation can be extended to the most general case of the microcanonical ensemble of an ideal relativistic quantum gas by fixing the maximal set of observables of the Poincaré algebra, i.e. spin, third component of the spin and parity, besides the energy-momentum four-vector. This will be the subject of a forthcoming publication.

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## Appendix A: Bogoliubov relations for a real scalar field

The Bogoliubov relations for a real scalar field can be derived by first expressing the localized annihilation operator as a function of the field  $\Psi$  and its conjugated moment  $\dot{\Psi}$ . For the localized problem we have

$$\Psi(x) = \sum_{\mathbf{k}} \frac{1}{\sqrt{2\varepsilon_{\mathbf{k}}}} a_{\mathbf{k}} u_{\mathbf{k}}(\mathbf{x}) e^{-i\varepsilon_{\mathbf{k}}t} + \text{c.c.}, \quad (A.1)$$

where  $\mathbf{k}$  is a vector of three numbers labeling the modes in the region  $V$ ,  $\varepsilon_{\mathbf{k}}$  is the associated energy and  $u_{\mathbf{k}}$  is a complete set of orthogonal wavefunctions over the region  $V$ :

$$\begin{aligned} & \sum_{\mathbf{k}} u_{\mathbf{k}}^*(\mathbf{x}) u_{\mathbf{k}}(\mathbf{x}') = \delta^3(\mathbf{x} - \mathbf{x}') \\ & \int_V d^3x u_{\mathbf{k}}^*(\mathbf{x}) u_{\mathbf{k}'}(\mathbf{x}) = \delta_{\mathbf{k}, \mathbf{k}'} \end{aligned} \quad (A.2)$$

and vanishing outside  $V$ . Inverting (A.1), we have

$$a_{\mathbf{k}} = \frac{i}{\sqrt{2\varepsilon_{\mathbf{k}}}} \int_V d^3x u_{\mathbf{k}}^*(\mathbf{x}) e^{i\varepsilon_{\mathbf{k}}t} \overleftrightarrow{\partial}_t \Psi(x), \quad (A.3)$$

which are valid at any time. We now enforce the mapping (35) and replace the localized field operators at  $t = 0$ , i.e. in the Schrödinger representation, with those in the full Hilbert space. In other words, we replace in (A.3)

$$\begin{aligned} \Psi(\mathbf{x}) &\rightarrow \frac{1}{(2\pi)^{3/2}} \int d^3p \frac{1}{\sqrt{2\varepsilon_{\mathbf{p}}}} e^{i\mathbf{p}\cdot\mathbf{x}} a_{\mathbf{p}} + \text{c.c.} \\ \dot{\Psi}(\mathbf{x}) &\rightarrow \frac{1}{(2\pi)^{3/2}} \int d^3p \frac{-i\sqrt{\varepsilon_{\mathbf{p}}}}{\sqrt{2}} e^{i\mathbf{p}\cdot\mathbf{x}} a_{\mathbf{p}} + \text{c.c.}, \end{aligned} \quad (A.4)$$

where  $\varepsilon_{\mathbf{p}} = \sqrt{p^2 + m^2}$ , obtaining

$$a_{\mathbf{k}} = \int d^3p F(\mathbf{k}, \mathbf{p}) \frac{\varepsilon_{\mathbf{k}} + \varepsilon_{\mathbf{p}}}{2\sqrt{\varepsilon_{\mathbf{k}}\varepsilon_{\mathbf{p}}}} a_{\mathbf{p}} + F(\mathbf{k}, -\mathbf{p}) \frac{\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{p}}}{2\sqrt{\varepsilon_{\mathbf{k}}\varepsilon_{\mathbf{p}}}} a_{\mathbf{p}}^\dagger, \quad (A.5)$$

where

$$F(\mathbf{k}, \mathbf{p}) = \frac{1}{(2\pi)^{3/2}} \int_V d^3x u_{\mathbf{k}}^*(\mathbf{x}) e^{i\mathbf{p}\cdot\mathbf{x}}; \quad (A.6)$$

that is, the Bogoliubov relations (36). We observe that the localized annihilation operator is a non-trivial combination of annihilation and creation operators in the whole space. However, the term in (A.5) depending on the creation operator  $a_{\mathbf{p}}^\dagger$  vanishes in the thermodynamic limit, as expected. This is most easily shown for a rectangular region, where one has  $u_{\mathbf{k}}(\mathbf{x}) = \exp[i\mathbf{k}\cdot\mathbf{x}]/\sqrt{V}$ ;  $\mathbf{k}$  is given by (9) and  $\varepsilon_{\mathbf{k}} = \sqrt{\mathbf{k}^2 + m^2}$ . Hence we have

$$\lim_{V \rightarrow \infty} F(\mathbf{k}, -\mathbf{p}) \propto \lim_{V \rightarrow \infty} \int_V d^3x e^{-i(\mathbf{p}+\mathbf{k})\cdot\mathbf{x}} \propto \delta^3(\mathbf{p} + \mathbf{k}), \quad (A.7)$$

and consequently  $\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{p}} \rightarrow 0$ , which makes the second term in (A.5) vanishing.

We can use (A.5) to work out linear relations between Fock space states of the localized problem and asymptotic Fock space states. These can be obtained enforcing the destruction of the localized vacuum state:

$$a_{\mathbf{k}} |0\rangle_V = 0$$

and writing

$$\begin{aligned} |0\rangle_V &= \alpha_0 |0\rangle + \int d^3p \alpha_1(\mathbf{p}) |\mathbf{p}\rangle \\ &+ \int d^3p_1 d^3p_2 \alpha_2(\mathbf{p}_1, \mathbf{p}_2) |\mathbf{p}_1, \mathbf{p}_2\rangle + \dots \end{aligned} \quad (A.8)$$

Working out such relations is beyond the scope of this paper.

## Appendix B: Multiparticle state with $N$ particles

In order to prove (82) for neutral particles, the first step is to realize that a general expansion of

$$\langle 0 | a_1 \dots a_N \mathbf{P}_V a_N^\dagger \dots a_1^\dagger | 0 \rangle \quad (\text{B.1})$$

( $a_i$  is a shorthand for  $a(p_i)$ ) must yield, on the basis of what shown for the case of two particles, a sum of terms like these:

$$\int_V d^3x_1 \dots \int_V d^3x_N \times \prod_{n,m=1}^N e^{\pm i \mathbf{p}_n \cdot \mathbf{x}_m} f(\varepsilon_1, \dots, \varepsilon_N) \langle 0 | \mathbf{P}_V | 0 \rangle, \quad (\text{B.2})$$

where  $f$  is a generic function involving a sum of ratios or product of any number of particle energies and  $\pm$  stands for either a + or a - sign. That (B.2) ought to be the final expression can be envisaged on the basis of a repeated application of (45), (85), (62) and (64) in turn. Equation (B.2) can also be written as

$$\int_V d^3x_1 \dots \int_V d^3x_N e^{i \sum'_n \mathbf{p}_n \cdot \mathbf{x}_1} \dots e^{i \sum'_n \mathbf{p}_n \cdot \mathbf{x}_n} \times f(\varepsilon_1, \dots, \varepsilon_N) \langle 0 | \mathbf{P}_V | 0 \rangle, \quad (\text{B.3})$$

where  $\sum'$  stands for an algebraic sum with terms having either sign.

If we now take the thermodynamic limit  $V \rightarrow \infty$  of (B.1), one has  $\mathbf{P}_V \rightarrow \mathbf{I}$ ; therefore,

$$\begin{aligned} & \lim_{V \rightarrow \infty} \langle 0 | a_1 \dots a_N \mathbf{P}_V a_N^\dagger \dots a_1^\dagger | 0 \rangle \\ &= \langle 0 | a_1 \dots a_N a_N^\dagger \dots a_1^\dagger | 0 \rangle \\ &= \sum_{\rho \in S_N} \prod_{n=1}^N \delta^3(\mathbf{p}_n - \mathbf{p}_{\rho(n)}). \end{aligned} \quad (\text{B.4})$$

This tells us that the functions  $f$  in each term (B.2) must reduce to a trivial factor 1, because they would otherwise survive in the thermodynamic limit, being a factor depending only on the  $p_n$ . Moreover, since the thermodynamic limit involves only Dirac  $\delta$ s with differences of two momenta as argument, there can be only a difference of two momenta as an argument of the exponential functions in (B.3). Finally, by comparing (B.3) with (B.4), we conclude that the only possible expression at finite  $V$  is

$$\begin{aligned} & \langle 0 | a_1 \dots a_N \mathbf{P}_V a_N^\dagger \dots a_1^\dagger | 0 \rangle \\ &= \langle 0 | \mathbf{P}_V | 0 \rangle \sum_{\rho \in S_N} \prod_{n=1}^N \frac{1}{(2\pi)^3} \int_V d^3x_n e^{-i(\mathbf{p}_n - \mathbf{p}_{\rho(n)}) \cdot \mathbf{x}_n}, \end{aligned} \quad (\text{B.5})$$

which is precisely (82).

For a state with  $N_+$  particles and  $N_-$  antiparticles, the validity of (97) can be argued for with a similar argument, i.e. by constraining the form of general terms like (B.2) taking advantage of the limit  $V \rightarrow \infty$ . In the case of particles and antiparticles, the thermodynamic limit tells us that

$$\begin{aligned} & \lim_{V \rightarrow \infty} \langle 0 | a_1 \dots a_{N_+} b_1 \dots b_{N_-} \mathbf{P}_V a_{N_+}^\dagger \dots a_1^\dagger b_{N_-}^\dagger \dots b_1^\dagger | 0 \rangle \\ &= \langle 0 | a_1 \dots a_{N_+} b_1 \dots b_{N_-} a_{N_+}^\dagger \dots a_1^\dagger b_{N_-}^\dagger \dots b_1^\dagger | 0 \rangle \\ &= \sum_{\rho_+ \in S_{N_+}} \prod_{n_+=1}^{N_+} \delta^3(\mathbf{p}_{n_+} - \mathbf{p}_{\rho_+(n_+)}) \\ & \times \sum_{\rho_- \in S_{N_-}} \prod_{n_-=1}^{N_-} \delta^3(\mathbf{p}_{n_-} - \mathbf{p}_{\rho_-(n_-)}), \end{aligned} \quad (\text{B.6})$$

and this determines the form of the expression

$$\langle 0 | a_1 \dots a_{N_+} b_1 \dots b_{N_-} \mathbf{P}_V a_{N_+}^\dagger \dots a_1^\dagger b_{N_-}^\dagger \dots b_1^\dagger | 0 \rangle$$

at finite  $V$  to be (97). The absence of integrals mixing particle with antiparticle momenta such as

$$\int d^3x_i e^{i(\mathbf{p}_{n_+} - \mathbf{p}_{n_-}) \cdot \mathbf{x}_i}$$

is owing to the absence of such differences as arguments of the  $\delta$ s in (B.6).

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