Recent investigations show that the statistical mechanics of a finite number of particles in ideal harmonic systems predicts different results for the same physical properties, depending on the ensemble under consideration. Path integral methods for a finite number of bosons with equidistant energy levels give the same answers for the mean energy, the specific heat and the condensation temperature etc., irrespective whether their calculation results from the density of states, from the partition function or from the generating function.

We show that this contradiction is due either to the use of approximate relations between quantum statistical expressions, or to a misinterpretation of the generating function.

Since Bose–condensed vapors became available to experimentation [1–4], considerable theoretical interest has been raised in the statistical mechanics of an idealization of the vapor, i.e. a system with equally spaced energy levels for a finite number of particles. Conventional statistical mechanics for a system in equilibrium at a given temperature (expressed by \( \beta = 1/kT \)) states that the probability of the system having energy \( E_n \) is proportional to \( \exp(-\beta E_n) \).

The calculation of the energies \( E_n \) is a quantum mechanical problem. Equally spaced energy levels are justified by the parabolic confinement potential. The quantum statistical theory takes into account the discreteness of the levels and the limited number of particles and contrasts therefore with earlier studies of Bose–Einstein condensation, because the thermodynamic limit and the quasi–continuity of the levels cannot be used as a justification [5]. In the path integral approach to quantum statistical theory [6,7], the calculation of the levels as well as the density of states or the partition function form an intrinsic part of the same study and are obtained simultaneously, in contradistinction with the approach where a quantum problem gives the energy levels and where subsequently statistical theory is used to study the cooperative behavior.

For identical particles the conditional probability to find a system containing \( N \) particles in the neighborhood of the configuration \( r \) can be calculated by the path integral method [8,9]. We have calculated the partition function \( Z(\beta, N) \) and some static response functions of a Gaussian model for bosons as well as for fermions using this approach. The related thermodynamical quantities have been obtained from the free energy that was calculated using the probability generating function \( \Xi(\beta, \gamma) \). The partition function \( Z(\beta, N) \) relates to the density of states \( \Omega(E, N) \) as follows:

\[
Z(\beta, N) = \int e^{-\beta E} \Omega(E, N) dE,
\]

while the generating function is defined by:

\[
\Xi(\beta, \gamma) = \sum_N \gamma^N Z(\beta, N).
\]

It should be remarked that the real variables \( \gamma \) and \( \beta \) used to interrelate the three quantities \( \Omega(E, N) \), \( Z(\beta, N) \) and \( \Xi(\beta, \gamma) \) are independent variables [10]. The inversion formula to obtain \( \Omega(E, N) \) from \( Z(\beta, N) \) is the inverse Laplace transform

\[
\Omega(E, N) = \frac{1}{2\pi i} \int_{\beta-i\infty}^{\beta+i\infty} e^{\tau E} Z(\tau, N) d\tau,
\]
where $\beta$ is larger than the real part of all poles of $Z(\tau, N)$ in the complex $\tau$ plane. For the inversion of $\Xi(\beta, \gamma)$ the residue theorem can be used:

$$Z(\beta, N) = \frac{1}{2\pi i} \oint \frac{\Xi(\beta, z)}{z^{N+1}} dz.$$  \hspace{1cm} (4)

It is generally accepted that the probabilities associated with events by statistical mechanics, are consistent with those of quantum statistical theory \cite{11}. Referring to the normalization factor $Q = \sum_n \exp (-\beta E_n)$ of the probability in statistical mechanics as the canonical partition function, it is implicitly assumed that $Q$ and $Z$ are the same for the same system, and lead consequently to the same predictions. Therefore it should not matter which one of the three quantities $\Omega$, $Z$ or $\Xi$ is calculated because of their exact interrelationship. Quantum statistical theory would be in conflict with statistical mechanics if in statistical mechanics the quantities corresponding with $\Omega$, $Z$ and $\Xi$ (usually indicated by their ensemble: microcanonical, canonical or grand canonical), would lead to different predictions, what they do according to \cite{12}. Recently this puzzle even gave rise to the introduction of a new fourth ensemble, coined the “Maxwell Demon” ensemble \cite{13,14}, with the aim to take the ensemble conditions for condensation better into account. The quantum statistical analogue of this “Maxwell Demon” ensemble is obtained by performing the inversions starting from $\Xi$ in the appropriate order

$$\Upsilon(E, \gamma) = \frac{1}{2\pi i} \int_{\beta-i\infty}^{\beta+i\infty} e^{\tau E} \Xi(\tau, \gamma) d\tau \sum_N \Omega(E, N) \gamma^N,$$  \hspace{1cm} (5)

expressing also this quantity in a unique way in terms of the density of states.

The main question that will be addressed in the present letter is: what is the origin of the apparent discrepancies between predictions based on statistical mechanics? We will discuss here two possibilities. The first one is based on probability considerations. The second one elaborates upon an old warning of Zip, Uhlenbeck and Kac \cite{11} against grand canonical partition functions calculated from $\Xi$ in the appropriate order $\Xi_B(\gamma, \beta) = Tr [\exp (-\beta (H - \mu N))]$.\footnote{Referring to the normalization factor $Q = \sum_n \exp (-\beta E_n)$ of the probability in statistical mechanics as the canonical partition function, it is implicitly assumed that $Q$ and $Z$ are the same for the same system, and lead consequently to the same predictions. Therefore it should not matter which one of the three quantities $\Omega$, $Z$ or $\Xi$ is calculated because of their exact interrelationship. Quantum statistical theory would be in conflict with statistical mechanics if in statistical mechanics the quantities corresponding with $\Omega$, $Z$ and $\Xi$ (usually indicated by their ensemble: microcanonical, canonical or grand canonical), would lead to different predictions, what they do according to \cite{12}. Recently this puzzle even gave rise to the introduction of a new fourth ensemble, coined the “Maxwell Demon” ensemble \cite{13,14}, with the aim to take the ensemble conditions for condensation better into account. The quantum statistical analogue of this “Maxwell Demon” ensemble is obtained by performing the inversions starting from $\Xi$ in the appropriate order}

The same function can be obtained directly using combinatorial analysis within the assumptions of statistical mechanics. \cite{13,20}. In our case $\Xi_B(\gamma, \beta)$ is only formally the grand canonical partition function of a set of identical particles in a parabolic well. To become really a grand canonical partition function the substitution $\gamma \rightarrow \exp (\mu \beta)$ has to be made and a calculation procedure for $\mu$ has to be given. If $N$ is sufficiently large, stationary phase or steepest
descent methods can be used to approximate the inversion formulas \([10]\) and give a meaning to the chemical potential \(\mu\).

As an illustration, let us consider the partition function \(Z_B(\beta, N)\) based on the contour integral \([3]\) for the specific example of harmonically interacting bosons in an harmonic confinement potential, i.e. the actual calculations are performed using the explicit form \([4]\). The generating function \(\Xi_B(z, \beta)\) makes the direct numerical evaluation of \([1]\) unfeasible. The interested reader is referred to \([8,9]\) for a discussion. However, considering a circular contour around the origin with radius \(u\), the substitution \(z = ue^{i\theta}\) transforms the contour integral into

\[
Z_B(\beta, N) = \frac{1}{2\pi} \int_0^{2\pi} \Xi \left(ue^{i\theta}, \beta\right) e^{-in\theta} d\theta = \frac{1}{2\pi} \int_0^{2\pi} e^{[\ln \Xi(ue^{i\theta}, \beta) - N\ln u]} e^{-in\theta} d\theta. \tag{9}
\]

The extrema of \([\ln \Xi(ue^{i\theta}, \beta) - N\ln u]\) on the real axis satisfies the condition

\[
N = u \frac{d}{du} \ln \Xi(u, \beta), \tag{10}
\]

which is precisely the expression for the expected number of particles \(N\) in the “grand canonical ensemble” if \(u\) is interpreted as \(u = e^{\beta\mu}\). Factorizing out this steepest descent contribution and extracting the real part, one obtains with little effort

\[
Z_B(\beta, N) = Z_B^{(0)}(\beta, N) \int_0^\pi \Psi(\theta) d\theta, \tag{11}
\]

\[
Z_B^{(0)}(\beta, N) = \frac{\Xi_B(u, \beta)}{uN}, \tag{12}
\]

\[
\Psi(\theta) = \frac{1}{\pi} \frac{\Xi_B(ue^{i\theta}, \beta)}{\Xi_B(u, \beta)} e^{-in\theta}. \tag{13}
\]

The corresponding free energy thus becomes the sum of two contributions

\[
F_B(\beta, N) = F_B^{(0)}(\beta, N) - \frac{1}{\beta} \ln \left(\int_0^\pi \Psi(\theta) d\theta\right), \tag{14}
\]

\[
F_B^{(0)}(\beta, N) = -\frac{1}{\beta} \ln \frac{\Xi_B(u, \beta)}{uN}. \tag{15}
\]

\(F_B^{(0)}(\beta, N)\) is the result which one would obtain in the “grand canonical treatment”. The remainder \(\frac{1}{\beta} \ln \left(\int_0^\pi \Psi(\theta) d\theta\right)\) can be obtained by integration and this correction is crucial for a finite number of particles. The integrand \(\Psi(\theta)\) is shown in Fig. 1 for \(N = 10\) as a function of \(\theta\) for various temperatures \(T\), expressed in units of the condensation temperature \(T_c = (N/\zeta(3))^{1/3} \hbar w/k\). Below the condensation temperature the oscillations in \(\Psi(\theta)\) are distributed more or less uniformly (for bosons) over the integration interval \([0, \pi]\) and above the condensation temperature they are strongly damped. The difference between \(F_B(\beta, N)\) and the zero-order approximation \(F_B^{(0)}(\beta, N)\) decreases with an increasing number of particles. The results for the free energy are shown in Fig. 2–4 for \(N = 1, 10\) and 100, where \(f(\beta, N) \equiv F_B(\beta, N)/N\hbar w\) is plotted versus \(T/T_c\). For comparison, the zero-order approximation \(F_B^{(0)}(\beta, N)/N\hbar w\) is also plotted. The numerical results for \(F_B(\beta, N)\) are to within 6 digits in agreement with those obtained earlier \([3]\) from a recurrence relation for the partition function.

If the partition function obtained using our path integral method relates to the conditional probability function for the energy density given the number of particles, we may summarize that the predictions based on the canonical partition function in statistical mechanics are not in conflict with quantum statistical theory, provided the density of states (microcanonical) is correctly derived by the inversion formulas. This concludes our discussion based on the conditional probability interpretation of the density of states.

2. The joint probability density approach

It is a common error to interpret a conditional probability as a joint probability function. In order to analyse the consequences of this possibility, let us assume that the function \(\Xi_B(\gamma, \beta)\) is the generator of such a joint probability function for the energy \(E\) and the number particles \(N\), i.e. we give ourselves a marginal distribution for the number of particles consistent with that generating function. The theory of continuous-time Markov processes for a queue with
states containing a different number of bosons, what is not the case in the quantum statistical theory leading to (7).

We will discuss the particle fluctuations of the “grand canonical ensemble” in this interpretation and elucidate the remark of ref. [11] earlier cited on that ensemble. In order to do so it is instructive to introduce an alternative to invert a power series. This inversion will allow to make a connection between the generating function in this interpretation and coherent states. Using

$$\frac{1}{N!} \int e^{-|z|^2} z^N \bar{z}^L d^2 z = \delta_{N,L},$$

where $\bar{z}$ denotes the complex conjugate of $z$, one obtains the following expression for the partition function $Z(\beta, N)$ from $\Xi(z, \beta)$:

$$Z(\beta, N) = \frac{1}{N!} \int e^{-|z|^2} z^N \Xi(z, \beta) d^2 z.$$

Filling out the power series (2) and summing over $N$ one finds:

$$\sum_{N=0}^{\infty} Z(\beta, N) = \frac{1}{\pi} \int \sum_{N=0}^{\infty} \sum_{L=0}^{\infty} \frac{z^N e^{-\frac{1}{2}|z|^2}}{\sqrt{N!}} Z(\beta, L) \frac{z^L e^{-\frac{1}{2}|z|^2}}{\sqrt{L!}} d^2 z,$$

where use has been made of the orthogonality relation (18) to replace a denominator $N!$ by $\sqrt{N!L!}$.

Introducing formally a Hamiltonian $\mathcal{H}$ that allows for transitions between systems with different numbers of particles, the following form

$$\sum_{N=0}^{\infty} Z(\beta, N) = \frac{1}{\pi} \int \langle z | e^{-\beta \mathcal{H}} | z \rangle d^2 z$$

helps to recognize the coherent state representation for the normalization of the probability for the event that “the system contains $N$ particles given the inverse temperature $\beta$”. The state $|z\rangle$ can be considered as a coherent matter state built up from Bose systems containing a different number of particles:

$$|z\rangle = \sum_{N} \frac{z^N}{\sqrt{N!}} e^{-\frac{1}{2}|z|^2} |N\rangle.$$

The derivation of the actual form of the Hamiltonian $\mathcal{H}$ needed to study other than equilibrium properties is beyond the scope of this letter. In order that the equilibrium properties predicted by $\mathcal{H}$ coincide with those derived from the generating function, $\mathcal{H}$ should satisfy the condition $\sum_{L} \langle N | \mathcal{H} | L \rangle \sqrt{\frac{N!}{N!}} = 0$, which expresses the conservation of probability [22,23], for a generator of a stochastic process. When the equilibrium properties of a model with fluctuations in the number of particles are considered, information on this model can be extracted from the generating function $\Xi(z, \beta)$ by making the following identification

$$\langle z | e^{-\beta \mathcal{H}} | z \rangle = e^{-\bar{z}(z-1)} \Xi(z, \beta).$$

The analogy with the queue suggests that if the generating function derives from a density of states that is interpreted as a joint probability density, it leads to a marginal distribution of the fluctuating number of particles. Also the assumed stochastic behavior requires a specific form for the transitions between a well with $N$ bosons and one with $N \pm 1$ bosons. These “a priori” properties of that model are certainly not satisfied in the experimental set-up [1, 2, 24] where the number of particles are monitored. Therefore, interpreting $\Xi(z, \beta)$ given by (17) as the generator of a joint probability density does in our opinion not allow to draw conclusions on the Bose condensed systems, discussed in the introduction. Changing the order of inversion to obtain the “Maxwell demon” distribution without changing the interpretation will not alter our objections. This means that the study of a Bose condensed system with respect to a fluctuating number of particles requires a quantum statistical theory incorporating explicitly the transitions between states containing a different number of bosons, what is not the case in the quantum statistical theory leading to (17).
3. Conclusion

In general we conclude that for a given number of particles the concepts put forward in [6] and worked out partially in [8] and [9] for systems of identical particles with equally spaced energy levels, allow to trace back differences linked with the statistical ensembles to different approximations in the inversion of the generating function. These differences have been quantified for the free energy and are identified with oscillatory behavior in our integrand \( \Psi (\theta) \). At least for indistinguishable (identical) particles, these oscillations become negligible in the large \( N \) limit. It should be stressed that the large \( N \) behavior is a direct consequence of the projection on the symmetric (antisymmetric) representation of the permutation group ensuring indistinguishability of the identical particles. Without the projection on the symmetric irreducible representation, this large \( N \) behavior for the oscillations is absent. In that case the relative error made by replacing the integral by its steepest descent approximation does not become negligible. This observation raises a new challenging question in the statistical description of identical particles: is the projection on the symmetric (antisymmetric) representation necessary in all circumstances?

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Figure captions

Fig. 1: Integrand $\Psi (\theta)$ [see (13)] for the remainder term of the partition function, calculated for 10 bosons at various temperatures.

Fig. 2: Scaled free energy $f(\beta, N) \equiv F_B(\beta, N)/N\hbar w$ as a function of $T/T_c$ for $N = 1$. For comparison, the zero-order steepest descent approximation $F_B^{(0)}(\beta, N)/N\hbar w$ is also plotted (dashed line).

Fig. 3: Same as Fig. 2, for $N = 10$ bosons.

Fig. 4: Same as Fig. 3, for $N = 100$ bosons.
Fig. 1 Lemmens et al.
Fig. 2 Lemmens et al.
Fig. 3 Lemmens et al.

- **Exact**
- **Zero order steepest descent**
ExactZero order steepest descent

Fig. 4 Lemmens et al.