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PATH INTEGRAL TREATMENT OF INTERACTING BOSONS OR FERMIONS

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A generalization of symmetrized density matrices in combination with the technique of generating functions allows one to calculate the partition function and the static correlation functions of identical particles in a parabolic confining well with harmonic two-body interactions.

1. INTRODUCTION

In the present paper we summarize the essential ingredients, which enabled us to derive the path-integral for a system of harmonically interacting spin-polarized identical particles in a parabolic confining potential, including both the statistics (Bose–Einstein or Fermi–Dirac) and the harmonic interaction between the particles. More details can be found in a series of papers [2]. This quadratic model, giving rise to repetitive Gaussian integrals, allows one to derive an analytical expression for the generating function of the partition function. The calculation of this generating function circumvents the constraints on the summation over the cycles of the permutation group. Moreover, it allows one to calculate the canonical partition function recursively for the system with harmonic two-body interactions.

2. PROPAGATOR OF THE MODEL SYSTEM

In atomic units ($\hbar = m = 1$), the potential energy of the quadratic model system under consideration is given by

$$V = \frac{\Omega^2}{2} \sum_{j=1}^{N} \mathbf{r}_j^2 \mp \frac{\omega^2}{4} \sum_{j,l=1}^{N} \left(\mathbf{r}_j - \mathbf{r}_l\right)^2,\tag{1}$$

where Ω is the frequency of the confinement potential, and ω is the frequency of the harmonic interparticle interaction, which might be either attractive or repul-

sive. The classical equations of motion of this system lead to

$$\ddot{\mathbf{r}}_{j} = -w^{2}\mathbf{r}_{j} \mp \omega^{2} \sum_{l=1}^{N} \mathbf{r}_{l} \text{ with } w = \sqrt{\Omega^{2} \mp N\omega^{2}}, \qquad (2)$$

from which it readily follows that the centre-of-mass coordinate $\mathbf{R} = \frac{1}{N} \sum_{j=1}^{N} \mathbf{r}_{j}$ obeys the equation of motion $\ddot{\mathbf{R}} = -\Omega^2 \mathbf{R}$. The equations of motion for the relative coordinates $\mathbf{u}_j = \mathbf{r}_j - \mathbf{R}$ become $\ddot{\mathbf{u}}_j = -w^2 \mathbf{u}_j$. It is straightforward to rewrite the potential energy as $V = \frac{1}{2}N\Omega^2 \mathbf{R}^2 + \frac{1}{2}w^2 \sum_{j=1}^{N} \mathbf{u}_j^2$. However, it should be noted that this transformation does not diagonalize the Hamiltonian, because of the subsidiary condition $\sum_{j=1}^{N} \mathbf{u}_j = 0$ which mixes up the relative coordinates. This condition does not hinder the path-integral approach, because it is easily incorporated in the derivation of the classical path, and hence of the classical action. The derivation of the resulting path integral over the deviations from the classical trajectory is a standard path-integral technique for quadratic systems. In the Euclidean time variable, the resulting path integral K_D for the system of distinguishable particles becomes

$$K_D\left(\mathbf{\bar{r}}^{\prime\prime},\beta|\mathbf{\bar{r}}^{\prime},0\right) = \frac{\mathcal{K}\left(\mathbf{R}^{\prime\prime},\beta|\mathbf{R}^{\prime},0\right)_{\Omega}}{\mathcal{K}\left(\mathbf{R}^{\prime\prime},\beta|\mathbf{R}^{\prime},0\right)_{w}} \prod_{j=1}^{N} K\left(\mathbf{r}_{j}^{\prime\prime},\beta|\mathbf{r}_{j}^{\prime},0\right)_{w},\tag{3}$$

where $K(\mathbf{r}_{\beta},\beta|\mathbf{r}_{0},0)_{w}$ is the standard path integral for a 3D harmonic oscillator with frequency w $K(\mathbf{n}, \beta | \mathbf{n}, 0)$

$$K \left(\mathbf{r}_{\beta}, \beta | \mathbf{r}_{0}, 0 \right)_{w} =$$

$$= \sqrt{\frac{w}{2\pi \sinh w\beta}} \exp \left(-\frac{w}{2} \frac{\left(\mathbf{r}_{\beta}^{2} + \mathbf{r}_{0}^{2} \right) \cosh w\beta - 2\mathbf{r}_{\beta} \cdot \mathbf{r}_{0}}{\sinh w\beta} \right). \tag{4}$$

Similarly, $\mathcal{K}(\mathbf{R}_{\beta},\beta|\mathbf{R}_{0},0)_{w}$ is the path integral for the centre-of-mass, which has mass N (in units of the particle mass)

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$$\mathcal{K} \left(\mathbf{R}_{\beta}, \beta | \mathbf{R}_{0}, 0 \right)_{w} =$$

$$= \sqrt{\frac{w}{2\pi \sinh w\beta}} \exp \left(-\frac{Nw}{2} \frac{\left(\mathbf{R}_{\beta}^{2} + \mathbf{R}_{0}^{2} \right) \cosh w\beta - 2\mathbf{R}_{\beta} \cdot \mathbf{R}_{0}}{\sinh w\beta} \right). \quad (5)$$

The path integral K_I for *identical* particles is obtained by imposing the proper symmetry ($\xi = +1$ for bosons) or antisymmetry ($\xi = -1$ for fermions), i.e.,

$$K_{I}\left(\mathbf{\bar{r}}^{\prime\prime},\beta|\mathbf{\bar{r}}^{\prime},0\right) = \frac{1}{N!} \sum_{p} \xi^{p} K_{D}\left(P\mathbf{\bar{r}}^{\prime\prime},\beta|\mathbf{\bar{r}}^{\prime},0\right),\tag{6}$$

where \sum_{p} denotes the sum over all possible permutations, and $\bar{\mathbf{r}}$ is the generalized coordinate $\bar{\mathbf{r}}^{T} = (\mathbf{r}_{1}, \cdots, \mathbf{r}_{N})$. The centre of mass is clearly not affected by the permutations, which therefore only have to be studied in the product $\prod_{i=1}^{N} K(\mathbf{r}'_{i}, \beta | \mathbf{r}'_{i}, 0)_{w}$.

 $\prod_{j=1}^{N} K\left(\mathbf{r}'_{j}, \beta | \mathbf{r}'_{j}, 0\right)_{w}.$ This method is also applicable in the presence of a magnetic field [1], although the anisotropy induced by the magnetic field considerably complicates the algebra.

3. THERMODYNAMICS

The partition function Z_I for the system of identical particles is obtained by integrating the path integral over the configuration space:

$$Z_{I} = \int d\mathbf{\bar{r}} K_{I}(\mathbf{\bar{r}},\beta|\mathbf{\bar{r}},0) = \frac{1}{N!} \int d\mathbf{\bar{r}} \sum_{p} \xi^{p} K_{D}(P\mathbf{\bar{r}},\beta|\mathbf{\bar{r}},0).$$
(7)

The explicit evaluation [2] involves the following major steps.

3.1. The Centre of Mass. The centre-of-mass coordinate $\mathbf{R} = \frac{1}{N} \sum_{j=1}^{N} \mathbf{r}_{j}$ does not only depend on the coordinates of all the particles, but it also has its own propagator. Therefore substituting \mathbf{R} by its expression in terms of the particle positions and then performing the integration seems not to be the most adequate way to deal with the integration over the configuration space. Instead, the following identity is used for the formal treatment of \mathbf{R} as an independent coordinate, at the expense of additional integrations:

$$\int d\mathbf{\bar{r}} f\left(\mathbf{\bar{r}}, \frac{1}{N} \sum_{j=1}^{N} \mathbf{r}_{j}\right) = \int d\mathbf{R} \int d\mathbf{\bar{r}} f\left(\mathbf{\bar{r}}, \mathbf{R}\right) \delta\left(\mathbf{R} - \frac{1}{N} \sum_{j=1}^{N} \mathbf{r}_{j}\right).$$
(8)

Fourier transformation of the δ function then leads to

$$\int d\mathbf{\bar{r}} f\left(\mathbf{\bar{r}}, \frac{1}{N} \sum_{j=1}^{N} \mathbf{r}_{j}\right) = \int d\mathbf{R} \int \frac{d\mathbf{k}}{\left(2\pi\right)^{3}} e^{i\mathbf{k}\cdot\mathbf{R}} \int d\mathbf{\bar{r}} f\left(\mathbf{\bar{r}}, \mathbf{R}\right) e^{-i\mathbf{\bar{k}}\cdot\mathbf{\bar{r}}}, \quad (9)$$

where $\bar{\mathbf{k}}^T = \frac{k}{N} ((1,1,1), \cdots, (1,1,1))$ is a 3*N*-dimensional row vector. Applying this transformation to the partition function Z_I and rearranging the factors one obtains

$$Z_{I} = \int d\mathbf{R} \int \frac{d\mathbf{k}}{(2\pi)^{3}} e^{i\mathbf{k}\cdot\mathbf{R}} \frac{\mathcal{K}(\mathbf{R},\beta|\mathbf{R},0)_{\Omega}}{\mathcal{K}(\mathbf{R},\beta|\mathbf{R},0)_{w}} \times \int d\mathbf{\bar{r}} \frac{1}{N!} \sum_{p} \xi^{p} \prod_{j=1}^{N} K\left((P\mathbf{\bar{r}})_{j},\beta|\mathbf{r}_{j},0\right)_{w} e^{-\frac{i}{N}\mathbf{k}\cdot\mathbf{r}_{j}}.$$
 (10)

This transformation makes **R** independent of the particle positions relative to the centre of mass. The real dependence on the relative positions is reintroduced by the Fourier transform. It should be noted that the explicit dependence of the propagator on **R**, and the presence of the factor $e^{-\frac{i}{N}\mathbf{k}\cdot\mathbf{r}_j}$, are consequences of the two-body interactions.

3.2. Cyclic Decomposition. The remaining sum over the permutations is converted into a sum over their cyclic decompositions [3]. A permutation can be broken up into cycles. Suppose that a particular permutation contains M_{ℓ} cycles of length ℓ . The positive integers M_{ℓ} and ℓ then have to satisfy the constraint

$$\sum_{\ell} \ell M_{\ell} = N. \tag{11}$$

Furthermore, the number $M(M_1, \dots M_N)$ of cyclic decompositions with M_1 cycles of length $1, \dots, M_\ell$ cycles of length ℓ, \dots is known to be

$$M(M_1, \cdots M_N) = \frac{N!}{\prod_{\ell} M_{\ell}! \ell^{M_{\ell}}}.$$
(12)

A cycle of length ℓ will be obtained from $(\ell - 1)$ permutations. Therefore the sign factor ξ^p can be decomposed as

$$\xi^p = \prod_{\ell} \xi^{(\ell-1)M_{\ell}}.$$
(13)

Combining these result originating from the permutation symmetry one obtains

$$Z_{I} = \int d\mathbf{R} \int \frac{d\mathbf{k}}{(2\pi)^{3}} e^{i\mathbf{k}\cdot\mathbf{R}} \frac{K\left(\sqrt{N}\mathbf{R},\beta|\sqrt{N}\mathbf{R},0\right)_{\Omega}}{K\left(\sqrt{N}\mathbf{R},\beta|\sqrt{N}\mathbf{R},0\right)_{w}} \times \sum_{M_{1}\cdots M_{N}} \prod_{\ell} \frac{\xi^{(\ell-1)M_{\ell}}}{M_{\ell}!\ell^{M_{\ell}}} \left(\mathcal{K}_{\ell}\left(\mathbf{k}\right)\right)^{M_{\ell}},$$
(14)

$$\mathcal{K}_{\ell}(\mathbf{k}) = \int d\mathbf{r}_{\ell+1} \int d\mathbf{r}_{\ell} \cdots \int d\mathbf{r}_{1} \delta\left(\mathbf{r}_{\ell+1} - \mathbf{r}_{1}\right) \prod_{j=1}^{N} K\left(\mathbf{r}_{j+1}, \beta | \mathbf{r}_{j}, 0\right)_{w} e^{-i\mathbf{k} \cdot \mathbf{r}_{j}/N}.$$

The main ingredient in this calculation then become path-integrals $\mathcal{K}_{\ell}(\mathbf{k})$ over all cycles with length ℓ , which can be evaluated in closed form, using the path integral of the driven harmonic oscillator:

$$\mathcal{K}_{\ell}\left(\mathbf{k}\right) = \left(\frac{1}{2\sinh\frac{1}{2}\ell\beta w}\right)^{3} \exp\left(-\frac{\ell}{4N^{2}}\frac{k^{2}}{w}\frac{1+e^{-\beta w}}{1-e^{-\beta w}}\right).$$
(15)

As a result, the partition function can be written as a product

$$Z_{I} = \left(\frac{\sinh\frac{1}{2}\beta w}{\sinh\frac{1}{2}\beta\Omega}\right)^{3} \mathbb{Z}_{I}(N);$$
(16)

$$\mathbb{Z}_{I}(N) \equiv \sum_{M_{1}\cdots M_{N}} \prod_{\ell=1}^{N} \frac{\xi^{(\ell-1)M_{\ell}}}{M_{\ell}!\ell^{M_{\ell}}} \left(\frac{e^{-\frac{1}{2}\ell\beta w}}{1-e^{-\ell\beta w}}\right)^{3M_{\ell}},$$
(17)

where $\mathbb{Z}_{I}(N)$ is the contribution from the internal degrees of freedom, which in Z_{I} is multiplied by a centre-of-mass correction. The constraint $\sum_{\ell} \ell M_{\ell} = N$ on the cycles substantially complicates the direct summation of $\mathbb{Z}_{I}(N)$.

3.3. Generating Function. The introduction of the generating function

$$\Xi_{I}(u) = \sum_{N=0}^{\infty} \mathbb{Z}_{I}(N) u^{N}, \qquad (18)$$

lifts the restrictions on the cycles. The summations can then be performed analytically. The result is

$$\Xi_{I}(u) = \exp\left(\sum_{\ell=1}^{\infty} \frac{\xi^{\ell-1}}{\ell} \frac{e^{-\frac{3}{2}\ell\beta w} u^{\ell}}{(1 - e^{-\ell\beta w})^{3}}\right).$$
 (19)

By expanding $(1 - e^{-\ell\beta w})^{-3}$ as a power series $e^{-\ell\beta w}$ and then performing the summation over the cycle lenghts ℓ , this generating function can be written in the form

$$\Xi_{I}(u) = \prod_{\nu=0}^{\infty} \left(1 - \xi u e^{-\beta \epsilon_{\nu}}\right)^{-\xi \frac{(\nu+1)(\nu+2)}{2}},$$
(20)

where $\epsilon_{\nu} = w\left(\frac{3}{2} + \nu\right)$ are the harmonic oscillator energy levels of the internal degrees of freedom.

It should be stressed that $\Xi_I(u)$ is <u>not</u> the grand canonical partition function of the model system, but a generating function introduced for finding the partition function $\mathbb{Z}_I(N)$. This can be realized in two natural ways:

(1) by a Taylor series expansion in powers of u;

(2) by contour integration.

The first method gives a recurrence relation for $\mathbb{Z}_{I}(N)$, whereas the second method results in an integral which is numerically tractable.

3.3.1. Recurrence Relations for the Partition Function. Starting from the defining equation of the generating function $\Xi_I(u)$, a recursion relation can be obtained for the partition function $\mathbb{Z}_I(N)$. Introducing:

$$b = e^{-\beta w} \tag{21}$$

for brevity in the notations, we observe that

$$\frac{d}{du}\Xi_I(u) = \Xi_I(u) \sum_{\nu=0}^{\infty} \frac{1}{2} (\nu+1) (\nu+2) \frac{b^{\frac{3}{2}+\nu}}{1-\xi u b^{\frac{3}{2}+\nu}}.$$

Considering next $\mathbb{Z}_{I}(N) = \frac{1}{N!} \frac{d^{N-1}}{du^{N-1}} \frac{d}{du} \Xi(u) \big|_{u=0}$, the product rule and an elementary binomial expansion can be used to find

$$\mathbb{Z}_{I}(N) = \frac{1}{N} \sum_{m=0}^{N-1} \xi^{N-m-1} \left(\frac{b^{\frac{1}{2}(N-m)}}{1-b^{N-m}} \right)^{3} \mathbb{Z}_{I}(m) \,. \tag{22}$$



Fig. 1. Boson specific heat C_B/Nk per particle in units of the Boltzmann constant k for N = 10, 100, 1000 as a function of T/T_c , where T_c is the condensation temperature in the limit $N \rightarrow \infty$

Of course, the corresponding recursion relations for the free energy $F = -\frac{1}{\beta} \ln Z$, the internal energy $U = d(\beta F)/d\beta$ and the specific heat C = dU/dT can readily be derived. The resulting specific heat contribution from the internal degrees of freedom clearly illustrates the effect of condensation for a finite number of particles, as can be seen from the plot in the Figure for 10, 100 and 1000 bosons, with the temperature expressed in units of $T_c = w/k (\zeta(3)/N)^{1/3}$ which is the condensation temperature in the limit $N \to \infty$. For fermions the recurrence relation, although correct, is not appropriate for numerical evaluation, because of the alternating signs in the subsequent contributions, with terms of the same order of magnitude. But the contour integration method, discussed below, overcomes this difficulty.

The corresponding one-dimensional version of the recurrence relation (indicated with the subscript i to distinguish it from the 3D case with capital subscript) becomes

$$\mathbb{Z}_{i}(N) = \frac{1}{N} \sum_{m=0}^{N-1} \xi^{N-m-1} \frac{b^{\frac{1}{2}(N-m)}}{1-b^{N-m}} \mathbb{Z}_{i}(m)$$

leading to the following partition functions in closed form for one-dimensional bosons and one-dimensional fermions

$$\mathbb{Z}_b = \frac{b^{\frac{1}{2}N}}{\prod_{j=1}^N (1-b^j)}; \quad \mathbb{Z}_f = \frac{b^{\frac{1}{2}N^2}}{\prod_{j=1}^N (1-b^j)};$$

It is easy to check that these partition functions are the solution of the recurrence relation for $\mathbb{Z}_i(N)$ with $\xi = 1$ for bosons and $\xi = -1$ for fermions. However, in the two-dimensional and the three-dimensional case we did not find a systematic method to obtain analytical solutions for this type of recurrence relations.

3.3.2. Contour Integration and Steepest Descent. For fermions the numerical evaluation of the thermodynamical quantities from the recurrence relations for the partition function is found to be inaccurate. For a very large number of bosons $(N \gtrsim 10000)$ it becomes very time consuming. For these cases an alternative derivation using

$$\mathbb{Z}_{I}\left(N\right) = \frac{1}{2\pi i} \oint_{c} \frac{\Xi_{I}\left(z\right)}{z^{N+1}} dz = \frac{1}{2\pi} \int_{0}^{2\pi} \frac{\Xi_{I}\left(ue^{i\theta}\right)}{u^{N}} e^{-iN\theta} d\theta,$$

becomes very useful and numerically accurate if the radius u of the contour integral is determined from the steepest descent approximation, i.e., determine u from the following transcendental equation

$$N = u \frac{d \ln \Xi_I(u)}{du} \to N = \sum_{\nu=0}^{\infty} \frac{1}{2} \left(\nu+1\right) \left(\nu+2\right) \frac{u}{u-\xi e^{\beta \epsilon_\nu}}$$

which is precisely the expression for the expected number of particles N in the «grand canonical ensemble» if u is interpreted as $u = e^{\beta\mu}$. A more detailed discussion about the relation between the grand canonical ensemble and the statistics of a finite number of particles can be found in [4]. Using this optimized expression for u, the integral for $\mathbb{Z}_I(N)$ can be written as

$$\mathbb{Z}_{I}(N) = \frac{\Xi_{I}(u)}{u^{N}} \int_{0}^{\pi} \Psi(\theta) \, d\theta,$$
(23)

with

$$\Psi\left(\theta\right) = \frac{1}{\pi} \frac{\Xi_{I}\left(ue^{i\theta}\right)}{\Xi_{I}\left(u\right)} e^{-iN\theta} = \frac{1}{\pi} e^{-\sum_{\ell=1}^{\infty} (1-\cos\ell\theta)C_{\ell}} \cos\left(\theta N - \sum_{\ell=1}^{\infty} C_{\ell}\sin\ell\theta\right),\tag{24}$$

where

$$C_{\ell} = \frac{\xi^{\ell-1}}{\ell} \frac{\left(b^{\frac{3}{2}}u\right)^{\ell}}{\left(1 - b^{\ell}\right)^{3}}.$$
(25)

For the free energy one readily obtains

$$\mathbb{F}_{F}(N) = \mathbb{F}_{F}^{(0)}(N) - \frac{1}{\beta} \ln\left(\int_{0}^{\pi} \Psi(\theta) \, d\theta\right) \text{ with } \mathbb{F}_{F}^{(0)}(N) = -\frac{1}{\beta} \ln\frac{\Xi_{F}(u)}{u^{N}},$$
(26)

where $\mathbb{F}_{F}^{(0)}(N)$ is the zero-order steepest descent result, which would be obtained from the «grand-canonical» treatment.

For bosons it turns out that the integral correction from $\int_0^{\pi} \Psi(\theta) d\theta$ to the free energy, which accounts for the finite number of particles, becomes negligible as compared to the «grand canonical contribution» $\mathbb{F}_F^{(0)}(N)$ if $N \gtrsim 100$.

For fermions, the integrandum $\Psi(\theta)$ is well-behaved, and very suitable for numerical integration. More details can be found in Ref. 1.

4. STATIC CORRELATIONS

The static correlation functions, in particular the density and the pair correlation function

$$n(\mathbf{r}) = \frac{1}{N} \left\langle \sum_{l=1}^{N} \delta(\mathbf{r} - \mathbf{r}_{l}) \right\rangle$$

$$= \frac{1}{N} \int \frac{d^{3}q}{(2\pi)^{3}} e^{i\mathbf{q}\cdot\mathbf{r}} \left\langle \sum_{l=1}^{N} e^{-i\mathbf{q}\cdot\mathbf{r}_{l}} \right\rangle$$

$$g(\mathbf{r}) = \frac{1}{N(N-1)} \left\langle \sum_{l=1,l'\neq l}^{N} \delta(\mathbf{r} - \mathbf{r}_{l} + \mathbf{r}_{l'}) \right\rangle$$

$$= \frac{1}{N(N-1)} \int \frac{d^{3}q}{(2\pi)^{3}} e^{i\mathbf{q}\cdot\mathbf{r}} \left\langle \sum_{l=1,l'\neq l}^{N} e^{-i\mathbf{q}\cdot(\mathbf{r}_{l} - \mathbf{r}_{l'})} \right\rangle$$

could be derived (see [2]) using the same techniques, i.e.,

- 1. transformation of the centre of mass into an independent variable,
- 2. cyclic decomposition of the permutations,
- 3. calculation of the generating function,
- 4. inversion of the generating function series.

For example, for the spatial Fourier transform $n_{\mathbf{q}}$ of the density we found

$$n_{\mathbf{q}} = \exp\left[-\frac{\hbar q^2}{4mN} \left(\frac{\coth\frac{1}{2}\beta\hbar\Omega}{\Omega} - \frac{\coth\frac{1}{2}\beta\hbar w}{w}\right)\right] \tilde{n}_{\mathbf{q}},\tag{27}$$

where the exponent in front of \tilde{n}_{q} accounts for the centre-of-mass correction, whereas \tilde{n}_{q} is the contribution from the internal degrees of freedom. Its explicit expression is

$$\tilde{n}_{\mathbf{q}} = \frac{1}{N} \sum_{\ell=1}^{N} \frac{\xi^{\ell-1} \exp\left(-\frac{\hbar q^2}{4mw} \coth\frac{1}{2}\ell\beta\hbar w\right)}{\left(2\sinh\frac{1}{2}\ell\beta\hbar w\right)^3} \frac{\mathbb{Z}_I \left(N-\ell\right)}{\mathbb{Z}_I \left(N\right)}.$$
(28)

For the spatial Fourier transform g_q of the pair correlation function we found that

$$g_{\mathbf{q}} = \frac{1}{N} \sum_{\ell=2}^{N} \frac{\mathbb{Z}_{I} \left(N-\ell\right)}{\mathbb{Z}_{I} \left(N\right)} \frac{\xi^{\ell-1} b^{\frac{3}{2}\ell}}{\left(1-b^{\ell}\right)^{3}} \sum_{j=1}^{\ell-1} \left(\begin{array}{c} \exp\left(-\frac{\hbar q^{2}}{2mw} \frac{1}{Q_{\ell,j}(b)}\right) \\ +\xi \left(Q_{\ell,j}\left(b\right)\right)^{3} \exp\left(-\frac{\hbar q^{2}}{2mw} Q_{\ell,j}\left(b\right)\right) \end{array} \right),$$
(29)

where

$$Q_{\ell,j} = \frac{1 - b^{\ell}}{(1 - b^j) \left(1 - b^{\ell-j}\right)}.$$
(30)

The centre of mass does not contribute directly to the pair correlation function.

These results were obtained by a Taylor series expanding the generating functions for the density and the pair correlation function, and are appropriate for a limited number of bosons.

Similarly as for the partition function, for fermions or for a very large number of bosons the inversion of the generating function by contour integration is again to be preferred for numerical purposes.

5. CONCLUSIONS

In the present paper, we sketched the methodology which we introduced to calculate the partition function and the static correlation functions of a system of harmonically interacting identical particles (bosons or fermions) with the techniques of path integration. The main point in the derivation is the conversion of the sum over all permutations into a sum over their cyclic decompositions, which in turn can be evaluated using a generating function technique. Detailed explicit results can be found in some of our papers [1,2]. Among the main results, we mention that this model in itself already shows the onset of Bose–Einstein

condensation in the specific heat for a number of bosons of order 10. For 1000 or 10000 bosons, the peak in the specific heat becomes very pronounced. Since also the static correlation functions could be obtained explicitly, the model is a powerful candidate to serve as the trial system for applying the Jensen–Feynman inequality for more realistic systems of identical particles.

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