Improved calculation of the third virial coefficient of a free anyon gas

J. Law,* Avinash Khare,† R. K. Bhaduri, and Akira Suzuki‡
Department of Physics and Astronomy, McMaster University, Hamilton, Ontario, Canada L8S 4M1
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For three anyons confined in a harmonic oscillator, only the class of states that interpolates nonlinearly with the statistical parameter contributes to the third virial coefficient of a free anyon gas. Rather than evaluating the full three-body partition function as was done in an earlier publication [J. Law, A. Suzuki, and R. Bhaduri, Phys. Rev. A **46**, 4693 (1992)], here only the nonlinear contribution is calculated, thus avoiding delicate cancellations between the irrelevant linear part and the two-body partition function. Our numerical results are consistent with the simple analytical form suggested recently by Myrheim and Olaussen [Phys. Lett. B **299**, 267 (1993)].

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In this Brief Report we report an improved numerical calculation of the third virial coefficient of a free anyon gas using the method of the hyperspherical coordinates of an earlier publication [1]. Improved accuracy is obtained by exploiting the fact that only the nonlinearly interpolating states of the three-anyon system contribute to the third virial coefficient [2–4]. The virial expansion of the two-dimensional anyon gas may be written as

$$\frac{P\beta}{\rho} = 1 + A_2(\alpha)(\rho\lambda^2) + A_3(\alpha)(\rho\lambda^2)^2 + \cdots, \qquad (1)$$

where P, ρ, and β are the pressure, density, and the inverse temperature in units of the Boltzmann constant, and $\lambda = \hbar(2\pi\beta/m)^{1/2}$ is the thermal wavelength. The expansion parameter is the dimensionless quantity $(\rho\lambda^2)$, and A_2, A_3, are the second and third virial coefficients of the gas, as a function of the dimensionless statistical parameter α. Note that the coefficients A_2, A_3, etc. are temperature independent, since there is no length scale in the statistical interaction. To evaluate the virial coefficients it is convenient to confine the anyons in a two-dimensional harmonic oscillator of frequency ω, and take the limit of the appropriate combinations of the partition functions as $(\hbar\omega\beta) \to 0$. Denote the N-body partition function in the harmonic oscillator by Z_N. The center-of-mass part Z_1 may be separated out, and the relative part is given by $\tilde{Z}_N = Z_N/Z_1$. Then the second and the third virial coefficients are given by $(x = \hbar\omega\beta)$

$$\begin{aligned} A_2(\alpha) &= \lim_{x\to 0} A_2(\alpha, x) \\ &= \lim_{x\to 0} x^{-2}[1 - 2\tilde{Z}_2/Z_1], \qquad (2) \\ A_3(\alpha) &= \lim_{x\to 0} A_3(\alpha, x) \\ &= \lim_{x\to 0} 2x^{-4}[1 + 8(\tilde{Z}_2/Z_1)^2 - 5(\tilde{Z}_2/Z_1) \\ &\quad -3(\tilde{Z}_3/Z_1^2)]. \qquad (3) \end{aligned}$$

The calculations are performed in the fermionic basis, i.e., for $\alpha = 0$, the particles are noninteracting fermions while for $\alpha = 1$ they behave like noninteracting bosons. In Eqs. (2) and (3), Z_1 and $\tilde{Z}_2$ are analytically known $[t = \exp(-x)]$:

$$Z_1 = t/(1-t)^2, \qquad \tilde{Z}_2 = t^2(t^\alpha + t^{-\alpha})/(1-t^2)^2, \quad (4)$$

while $\tilde{Z}_3$ in Ref. [1] was calculated from the numerically obtained spectrum of the three-anyon system. Three particles in two dimensions, after elimination of the center of mass, have four independent degrees of freedom. The problem may be regarded as that of one body in four dimensions. Moreover, it is convenient to use the hyperspherical coordinates [5] of a four-dimensional sphere with radius R and three independent angles θ, ϕ, and ψ. This is because in these coordinates, the fermionic (or bosonic) basis of states may be constructed by specifying their quantum numbers using a simple set of rules [6]. The three-anyon Hamiltonian may be separated in a radial and an angular part, and the eigenvalue spectrum obtained by diagonalizing the angular part [1,7] of the Hamiltonian in the basis of the hyperspherical harmonics $Y_{N,\nu,\lambda}(\theta,\phi,\psi)$. In addition, there is another quantum number n' associated with the radial excitations. The eigenstates of the harmonic oscillator are completely specified by the set of quantum numbers (N,ν,λ,n') with eigenenergies given by $E_{N,n'} = (N+2n'+2)\hbar\omega$. The form of the Hamiltonian and other mathematical details will not be repeated here, since these are given in Ref. [1].

The calculation of A_3 in Ref. [1] involved a delicate cancellation of terms in the square brackets on the right-hand side of Eq. (3). Since A_3 is known to be finite [7–9], there should be no terms of order x and x^3 within the brackets, and all terms of order x^2 should cancel exactly as $x^2 \to 0$, if the numerical calculations were exact. In practice, due to the truncation of the basis and numerical inaccuracies, these are not satisfied. The numerical calculations in Ref. [1] were reliable for $x^2 \geq 0.8$, and careful interpolation was necessary to reach the limit of $x^2 = 0$. Part of the error resulting from this incomplete cancellation takes place between the terms involving $\tilde{Z}_2$ and only that portion of $\tilde{Z}_3$ which originates from the linearly interpolating eigenvalues of the three-body problem. The

*Physics Department, University of Guelph, Guelph, Ontario, N1G 2W1, Canada.
†Institute of Physics, Sachivalaya Marg, Bhubaneswar-751 005, India.
‡Physics Department, Science University of Tokyo, Tokyo 162, Japan.

analytical expression of this part of $\tilde{Z}_3$ is known [7,10]. We may decompose $\tilde{Z}_3$ into two parts:

$$\tilde{Z}_3 = \tilde{Z}_3^{\mathrm{L}} + \tilde{Z}_3^{\mathrm{NL}}, \tag{5}$$

where

$$\tilde{Z}_3^{\mathrm{L}} = \frac{t^5(t^{3\alpha} + t^{-3\alpha})}{(t-1)^4(t+1)^2(1+t+t^2)^2} \tag{6}$$

is the portion from the linearly interpolating states, and $\tilde{Z}_3^{\mathrm{NL}}$ is the nonlinear part. Although $\tilde{Z}_3^{\mathrm{NL}}$ diverges as x^{-4} for $x \to 0$, the quantity

$$\Delta\tilde{Z}_3^{\mathrm{NL}}(\alpha) = [\tilde{Z}_3^{\mathrm{NL}}(\alpha) - \tilde{Z}_3^{\mathrm{NL}}(0)] \tag{7}$$

is finite. Using Eqs. (3)–(6), it is straightforward to show that

$$\Delta A_3(\alpha) = A_3(\alpha) - A_3(0) = -6 \lim_{x\to 0} \Delta\tilde{Z}_3^{\mathrm{NL}}(\alpha). \tag{8}$$

It follows from the above equation that it is only necessary to compute $\Delta\tilde{Z}_3^{\mathrm{NL}}(\alpha)$ numerically. This necessitates identifying and excluding the linearly interpolating states (after diagonalizing the three-body Hamiltonian) from the calculation of the partition function. These linearly interpolating states change by three units of $\hbar\omega$ as the statistical parameter α varies from 0 to 1, and may be identified by the set of rules given in the Appendix.

The diagonalization of the angular part of the Hamiltonian (as specified in Ref. [1]) was performed with a basis truncated at

$$N_{\max} = \begin{cases} 130 & \text{for } 0 \le |\lambda| \le 20 \\ 100 & \text{for } 21 \le |\lambda| \le 72. \end{cases} \tag{9}$$

The quantum number λ determines the angular momentum of the three-body system. Note that this basis for diagonalization is considerably bigger than that used in Ref. [1]. After the diagonalization, only the nonlinearly interpolating states were used to calculate $\Delta\tilde{Z}_3^{\mathrm{NL}}(\alpha)$ as a function of x^2 for various values of α. The nodeless ($n' = 0$) states were included in the evaluation of $\sum_i \exp(\beta E_i)$, and the infinite tower of nodal excitations was taken into account by the multiplicative overall factor of $[1 - \exp(-2x)]^{-1}$. The numerical results changed insignificantly even if the sum over all the eigenstates, including the tower of nodal excitations, was cut off at $90\hbar\omega$. The quantity $[-6\Delta\tilde{Z}_3^{\mathrm{NL}}(\alpha)]$ is computed as a function of x^2 for $\alpha = 0.05$ to 0.5 in steps of 0.05. In principle, its value at $x^2 = 0$ should yield $\Delta A_3(\alpha)$. In practice, there is still a divergence due to numerical inaccuracies, since the cancellation of singularities between $\tilde{Z}_3^{\mathrm{NL}}(\alpha)$ and $\tilde{Z}_3^{\mathrm{NL}}(0)$ is not perfect as $x^2 \to 0$, since $\tilde{Z}_3^{\mathrm{NL}}(\alpha)$ is calculated less accurately than $\tilde{Z}_3^{\mathrm{NL}}(0)$. The spurious singularities in $\Delta\tilde{Z}_3^{\mathrm{NL}}(\alpha)$ have to be isolated to extract $\Delta A_3(\alpha)$. To this end, we define $\Delta A_3(\alpha, x^2) = -6\Delta\tilde{Z}_3^{\mathrm{NL}}(\alpha)$ for any x, and fit [11] this function by the following form containing six α-dependent parameters in the range $0.05 \le x^2 \le 3.4$:

$$\Delta A_3(\alpha, x^2) = \frac{a}{x^{2n}} + c\,\exp[b_2x^2 + b_4x^4 + b_6x^6 + b_8x^8]. \tag{10}$$

The computed $\Delta\tilde{Z}_3^{\mathrm{NL}}(\alpha)$ is sensitive to the basis size only for $x^2 \le 0.2$.

In the above fit, the coefficient $c = \Delta A_3(\alpha)$, and is found to be numerically stable even when higher order terms $b_{10}x^{10} + b_{12}x^{12} + b_{14}x^{14}$ are added in the exponent of Eq. (10). The parameter n in Eq. (10) is close to 2 up to $\alpha = 0.20$, but decreased monotonically for larger α, with $n = 1.56$ for $\alpha = 0.50$. The convergence of the extracted $\Delta A_3(\alpha)$ value is also tested by performing the same calculation of $\Delta\tilde{Z}_3^{\mathrm{NL}}(\alpha)$, but including only eigenvalues up to $N_{\max} = 60$. The $\Delta A_3(\alpha)$ values so obtained are displayed in Table I for various values of α in the range 0.05–0.40. For $\alpha > 0.40$, the extracted $\Delta A_3(\alpha)$ is not too stable, and is too inaccurate to be listed. This is because the eigenvalues of the Hamiltonian matrix for the larger α values tend to be more and more inaccurate.

Numerically, of course, only A_3 values up to $\alpha = 0.5$ would suffice, because of the relation $A_3(\alpha) = A_3(1-\alpha)$ derived by Sen [10] . Recently, Myrheim and Olaussen [8] have calculated $A_3(\alpha)$ numerically using a path integral representation of the three-body partition function. Their method of calculation is completely different, and uses the winding number formalism rather than the statistical interaction. From their extensive numerical work, they suggest [8,12] that perhaps $\Delta A_3(\alpha)$ obeys the remarkably simple relation

$$\Delta A_3(\alpha) = \frac{\sin^2(\pi\alpha)}{12\pi^2}. \tag{11}$$

For small α, this is in agreement with the perturbative analytical result of $\alpha^2/12$ of de Veigy and Ouvry [9]. In Fig. 1, the computed values $\Delta A_3(\alpha)$ of the present calculation are compared with the simple form given by Eq. (11). Our calculated $\Delta A_3(\alpha)$ values confirm Eq. (11) with good accuracy up to $\alpha = 0.25$, beyond which our numerical method starts to lose accuracy. This independent check of the Myrheim-Olaussen calculation is the main content of this paper. Figure 1 also shows that the inaccuracies for larger α build up rapidly in the method of Ref. [1], where the nonlinear part $\tilde{Z}_3^{\mathrm{NL}}$ was not isolated.

TABLE I. The calculated quantity $\Delta A_3(\alpha) = [A_3(\alpha) - A_3(0)]$ is tabulated as a function of α. The first row of $\Delta A_3(\alpha)$ is obtained by including all the eigenenergies in the space defined by Eq. (9). The six-parameter fit, as given by Eq. (10), is used. The second row is computed by including only eigenvalues up to $E_{\mathrm{cut}} = 60\hbar\omega$.

α	0.05	0.10	0.15	0.20	0.25	0.30	0.35	0.40
$10^4\Delta A_3(\alpha)$	2.08	8.22	17.3	29.0	41.8	53.8	62.7	65.7
$10^4\Delta A_3(\alpha)$	2.13	8.34	17.6	29.4	42.4	54.7	63.9	67.4

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APPENDIX

The exact solutions for the linear states with slopes of $\pm 3\hbar\omega$ have been written down by Wu [13] in Jacobi coordinates. Using the details given in Ref. [6], we can easily write down these solutions in hyperspherical coordinates and identify the quantum numbers N, ν, λ, n' and the degeneracy of these states. We find that for $N = (6p-3)$, $(6p-1)$, or $(6p+1)$ (with $p = 1, 2, 3, ...$), there are $2p^2$ degenerate states with $n' = 0$ (and hence total energy $E = N + 2$), while for $N = 6p$, $(6p+2)$, or $(6p+4)$ (with $p = 1, 2, 3, ...$) there are $2p(p+1)$ degenerate states with $n' = 0$. For example, for $N = (6p-3)$, one finds that the states with $\lambda = \pm(6p-3)$ are both p-fold degenerate with the corresponding ν quantum number being $\nu = (6p-3), (6p-9), ..., 3$ (note that $\nu, N > 0$; $\nu, |\lambda| \leq N$; $\nu, N, |\lambda|$ have the same parity, and ν is always a multiple of 3). For the same N, the four states with $\lambda = \pm(6p-5), \pm(6p-7)$ are all $(p-1)$-fold degenerate $[\nu = (6p-3), (6p-9), ..., 9]$. The next four states with $\lambda = \pm(6p-9), \pm(6p-11)$ are all $(p-2)$-fold degenerate $[\nu = (6p-3), (6p-9), ..., 15]$, and so on. Finally the four states with $\lambda = \pm(2p+7), \pm(2p+5)$ are all nondegenerate. Exactly the same rules also apply when $N = (6p-1)$ or $(6p+1)$. On the other hand, when N is even, for $N = 6p$, we find that the four states with $\lambda = \pm 6p, \pm(6p-2)$, are all p-fold degenerate with $\nu = 6p, (6p-6), ..., 3$. The next four states with $\lambda = \pm(6p-4), \pm(6p-6)$ are all $(p-1)$-fold degenerate and so on. Finally the four states with $\lambda = \pm(2p+2), \pm(2p+4)$ are all nondegenerate. Similar rules also apply when $N = (6p+2)$ or $(6p+4)$. In this way we are able to identify all the linear states in the spectra and exclude them from the evaluation of the partition function.

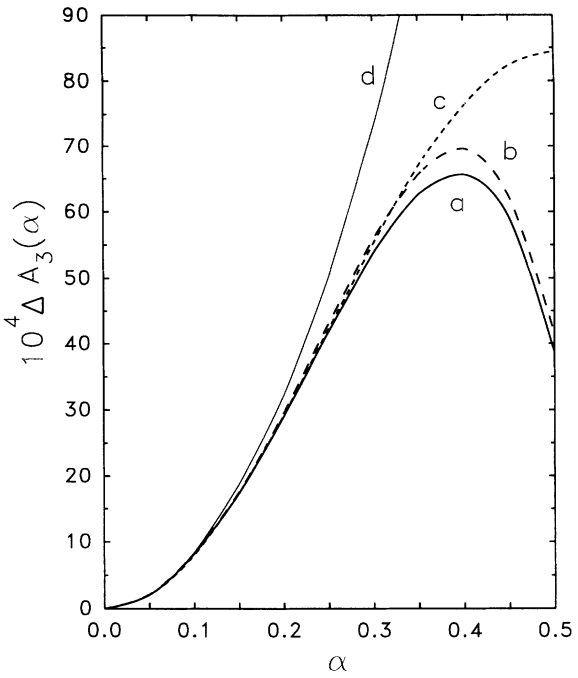

FIG. 1. Plot of $\Delta A_3(\alpha)$ as a function of the statistical parameter α in the fermionic basis. Curve *a*, present calculation (top row of Table I), with the six-parameter fit of Eq. (10). Curve *b*, the variations in the extracted $\Delta A_3(\alpha)$, with a nine-parameter fit to $\Delta A_3(\alpha, x^2)$. This is done by including the terms $b_{10}x^{10} + b_{12}x^{12} + b_{14}x^{14}$ in the exponent of Eq. (10). Curve *c*, the plot of Eq. (11), [the Myrheim-Olaussen conjecture for $\Delta A_3(\alpha)$]. Curve *d*, the $\Delta A_3(\alpha)$ values calculated by the method given in Ref. [1], but in the enlarged basis, Eq. (9).

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