Erratum: "Path-integral calculation of the third virial coefficient of quantum gases at low temperatures" [J. Chem. Phys. 134, 134106 (2011)]

Giovanni Garberoglio[1,2,a)] and Allan H. Harvey[3,b)]
[1)]*European Centre for Theoretical Studies in Nuclear Physics and Related Areas (FBK-ECT*)
Trento I-38123, Italy*
[2)]*Trento Institute for Fundamental Physics and Applications (TIFPA-INFN)
Trento I-38123, Italy*
[3)]*Applied Chemicals and Materials Division, National Institute of Standards and Technology, Boulder, CO 80305*

(Dated: 8 April 2020)

In our original paper[1], the effect of nuclear spin states was not properly taken into account in the derivation of the formulae for the second and third virial coefficient. Equation (7) should read

$$B_{\rm xc}(T) = -\frac{(-1)^{2I}\Lambda^6}{(2I+1)2V}\int \mathrm{d}\boldsymbol{r}_1 \mathrm{d}\boldsymbol{r}_2 \langle \boldsymbol{r}_1\boldsymbol{r}_2|\exp\left[-\beta(\hat{K}_2+\hat{U}_2(|\boldsymbol{r}_2-\boldsymbol{r}_1|))\right]|\boldsymbol{r}_2\boldsymbol{r}_1\rangle, \quad (1)$$

where I is the nuclear spin of the atom under consideration in units of $\hbar$, that is $I = 0$ for ^{4}He and $I = 1/2$ for ^{3}He. Analogously, Equation (22) for the third virial coefficient $C(T)$ should read

$$C(T) = C_{\rm Boltzmann}(T) + (-1)^{2I}\frac{C_{\rm odd}(T)}{2I+1} + \frac{C_{\rm even}(T)}{(2I+1)^2} + C_{\rm B}(T). \quad (2)$$

Equation (23) in the original manuscript is correct, provided that $B_{\rm xc}(T)$ is taken from Eq. (1) above.

The results reported in Table I of the original manuscript regarding the third virial coefficient for ^{4}He are not affected since in this case $I = 0$, but the values of $C(T)$ for ^{3}He in Table II below about 4.5 K are significantly modified as a result of the changes in Eq. (2). We report the correct values in a revised Table II below. Additionally, Figs. 2 and 3 in the original paper should be replaced with those given here.

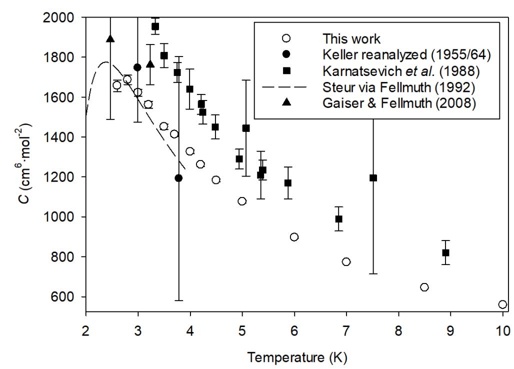

FIG. 3. The third virial coefficient of ^{3}He.

These corrected results for ^{3}He do not alter the Conclusions in the original paper, although they somewhat improve our agreement (as shown in Fig. 3) with the available experimental data below 5 K.

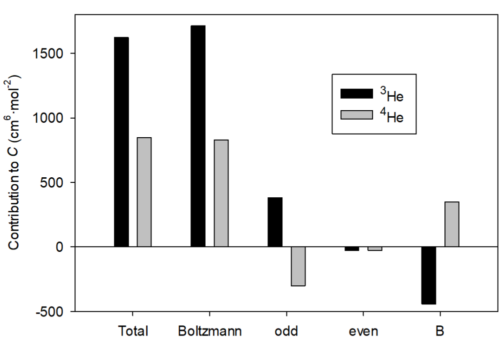

FIG. 2. The magnitude and sign of the various contributions to $C(T)$ at $T = 3$ K.

[1]G. Garberoglio and A. H. Harvey, "Path-integral calculation of the third virial coefficient of quantum gases at low temperatures," J. Chem. Phys. **134**, 134106 (2011).
[2]G. Garberoglio, M. R. Moldover, and A. H. Harvey, "Improved first-principles calculation of the third virial coefficient of Helium," J. Res. Natl. Inst. Stand. Technol. **116**, 729–742 (2011).

[a)]Electronic mail: garberoglio@ectstar.eu
[b)]Electronic mail: allan.harvey@nist.gov

Temperature (K)	C ($\mathrm{cm^6\ mol^{-2}}$)		$C_{\mathrm{Boltzmann}}$ ($\mathrm{cm^6\ mol^{-2}}$)		C_{odd} ($\mathrm{cm^6\ mol^{-2}}$)		C_{even} ($\mathrm{cm^6\ mol^{-2}}$)		C_{B} ($\mathrm{cm^6\ mol^{-2}}$)	
2.6	1657	±29	1857	±28	−1803	±4	−274.8	±0.8	−1033	±5
2.8	1686	±23	1817	±23	−1164	±3	−167.9	±0.6	−671	±4
3	1622	±17	1712	±17	−760.2	±2.2	−105.7	±0.4	−443.3	±2.2
3.2	1561	±17	1621	±17	−503.5	±1.7	−66.8	±0.3	−295	±1.6
3.5	1451	±13	1487	±13	−277.2	±1.2	−34.89	±0.15	−165.8	±1.1
3.7	1412	±11	1439	±11	−189.2	±0.8	−23.12	±0.11	−115.5	±1
4	1326	±9	1342	±9	−107	±0.5	−12.69	±0.07	−66.5	±0.7
4.2	1261	±9	1273	±9	−73.9	±0.5	−8.65	±0.05	−46.8	±0.2
4.5	1183	±7	1190	±7	−43.7	±0.3	−4.86	±0.03	−27.9	±0.2
5	1075	±6	1079	±6	−18.41	±0.16	−1.963	±0.016	−12.31	±0.13
6	896	±4	897	±4	−3.56	±0.06	−0.353	±0.005	−2.52	±0.04
7	773	±3	773	±3	−0.78	±0.02	−0.0784	±0.002	−0.6	±0.01
8.5	645	±2	645	±2	−0.059	±0.006	−0.0087	±0.0003	−0.072	±0.003
10	558.3	±1.6	558.3	±1.6						
12	475.5	±1.1	475.5	±1.1						
13.8033	426.2	±0.8	426.2	±0.8						
15	402	±0.7	402	±0.7						
17	369.6	±0.5	369.6	±0.5						
18.689	347.8	±0.4	347.8	±0.4						
20	333.4	±0.4	333.4	±0.4						
24.5561	297.8	±0.3	297.8	±0.3						

TABLE II. Values of the third virial coefficient of ^{3}He and its components at selected temperatures. Note that the various contributions should be summed with the weights appearing in Eq. (2) with $I = 1/2$. The ± values reflect only the standard uncertainty of the Monte Carlo integration; see Ref. 2 for complete uncertainty analysis.