Partition function of the rigid rotator at high temperatures using the Hubbard-Statanovich transformation

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It is shown that using the Hubbard-Statanovich transformation one can derive the asymptotic series and the remainder term for the partition function of the rigid rotator at high temperatures in a fairly simple way.

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Even though the rigid-rotator partition function is fairly simple in appearance, it poses quite a bit of problem when one needs its asymptotic form at high temperatures. The complication arises mainly because the summation index enters as a square in the exponent. In the many-body physics problems the Hubbard-Statanovich (HS) transformation [1] has been found to be very useful in linearizing the power in the exponent. In the present problem it turns out that a straightforward application of the transformation leads to nonconvergence of the summation. We would like to show in the present Brief Report that a convergence factor together with HS transformation makes it possible to find the asymptotic form as well as the remainder term of the partition function of the rigid rotator in an extremely simple way. The present method is not only simpler than the earlier methods given by Mulholland and Joyce [2] but can also be used when correction terms are to be added to the rotational energy.

Let the partition function of the rigid rotator be denoted by $Z(\sigma)$. It is given by [2]

$$Z(\sigma)=\sum_{n=0}^{\infty}(2n+1)\exp[-n(n+1)\sigma]\ , \tag{1}$$

where σ is a dimensionless quantity and inversely proportional to the temperature.

To develop the asymptotic series for $Z(\sigma)$ at high temperatures we write [2]

$$Z(\sigma)=2[\exp(\tfrac{1}{4}\sigma)]f(\sigma)\ , \tag{2}$$

where $f(\sigma)$ is given by

$$f(\sigma)=\sum_{n=0}^{\infty}(n+\tfrac{1}{2})\exp[-(n+\tfrac{1}{2})^2\sigma]\ . \tag{3}$$

For the present problem, the HS transformation is given by

$$\exp(-b^2)=\pi^{-1/2}\int_{-\infty}^{\infty}dx\,\exp(-x^2+2ibx)\ .$$

Using this transformation in expression (3) we can write $f(\sigma)$ as

$$f(\sigma)=\frac{1}{\sqrt{\pi}}\int_{-\infty}^{\infty}dx[\exp(-x^2)]\times\sum_{n=0}^{\infty}(n+\tfrac{1}{2})\exp[2ix\sqrt{\sigma}(n+\tfrac{1}{2})]\ . \tag{4}$$

The usefulness of the HS transformation lies in the fact that it can be used twice if one has also anharmonic terms of the form $(n+\frac{1}{2})^4$ in expression (3).

We now introduce a convergence factor

$$\exp[-(n+\tfrac{1}{2})\gamma]\ , \tag{5}$$

γ being a real parameter which goes to zero in the end. The convergence factor given by (5) is also useful to take care of the factor $(n+\frac{1}{2})$ in expression (4) by writing the derivative of it with respect to γ.

Using expressions (4) and (5) and carrying out summation over n, we get

$$f(\sigma)=\frac{1}{2\sqrt{\pi}}\left[-\frac{\partial}{\partial\gamma}\right]\int_{-\infty}^{\infty}dx[\exp(-x^2)]\times\operatorname{csch}[\tfrac{1}{2}(\gamma-2i\sqrt{\sigma}x)]\qquad \gamma\to 0\ . \tag{6}$$

This is the exact integral representation of the rigid-rotator partition function. In order to find the asymptotic series and the remainder, we write the following expansion [3] of the function csch$t$,

$$\operatorname{csch}t=\frac{1}{t}-\sqrt{\pi}\sum_{m=1}^{N}\frac{(1-2^{1-2m})}{\Gamma(m+\frac{1}{2})m!}B_{2m}t^{2m-1}+2(-1)^N t^{2N+1}\sum_{k=1}^{\infty}\frac{(-1)^k}{(\pi^2k^2)^{N+1}}\times\left[1+\frac{t^2}{4\pi^2k^2}\right]^{-1}\ , \tag{7}$$

where B_{2m} are Bernoulli numbers, and the last term which gives the remainder has been written using the Fourier expansion of Bernoulli polynomials [3].

Consider first the terms $m=1$–N. Writing

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$t=\frac{1}{2}(\gamma-2i\sqrt{\sigma}x)$ and realizing that only the terms linear in γ survive, we get, after integrating over x, the series

$$\frac{1}{2}\sum_{m=1}^{N}\frac{(-1)^m(2^{1-2m}-1)B_{2m}}{m!}\sigma^{m-1} . \tag{8}$$

This is in agreement with the asymptotic series as given by Eqs. (1) and (3) of Mulholland [2] as well as the one given by Joyce [2] in his Eqs. (2.23) and (2.24).

To calculate the value of the term corresponding to $1/t$ in expansion (6), we use the integral representation of the function $w(z)$ given by [3]

$$w(z)=\frac{i}{\pi}\int_{-\infty}^{\infty}\frac{\exp(-t^2)dt}{z-t}, \quad \text{Im}z>0 . \tag{9}$$

This gives the first term of the asymptotic series as

$$\frac{1}{2\sigma} , \tag{10}$$

again in agreement with [2].

The remainder R_{N+1} after $(N+1)$ terms is given by the integral of the last term in expression (7), by setting

$$t=\tfrac{1}{2}(\gamma-2i\sqrt{\sigma}x) .$$

The numerator t^{2N+1} is expanded and even powers of x are taken care of by introducing a parameter λ in $\exp(-x^2)$ and taking derivatives with respect to λ and setting it to unity in the end. Only the terms linear in γ will contribute as $\gamma\to 0$. The integrals are of the form (9) and can be written down in terms of $w(z)$, which is given in terms of the confluent hypergeometric function ${}_1F_1(a;b;z)$ as [3]

$$w(z)=\exp(-z^2)+\frac{2i}{\sqrt{\pi}}z\,{}_1F_1(1,\tfrac{3}{2},-z^2) . \tag{11}$$

After some simplification, one finds that the remainder R_{N+1} is given by

$$R_{N+1}=\sigma^{N-1}\frac{\Gamma(N+\frac{1}{2})}{\sqrt{\pi}} \times\sum_{k=1}^{\infty}\frac{(-1)^k}{(\pi^2k^2)^N}\,{}_1F_1\left[1;-N+\tfrac{1}{2};-\frac{\pi^2k^2}{\sigma}\right] , \tag{12}$$

same as recently given by Joyce [2].

Using (2), (3), (6)–(8), (10), and (12), we find that $Z(\sigma)$ at high temperatures is given by

$$Z(\sigma)=2\exp(\tfrac{1}{4}\sigma)\left[\frac{1}{2\sigma}+\frac{1}{2}\sum_{m=1}^{N}\frac{(-1)^m(2^{1-2m}-1)B_{2m}}{m!}\sigma^{m-1} +\sigma^{N-1}\frac{\Gamma(N+\frac{1}{2})}{\sqrt{\pi}}\sum_{k=1}^{\infty}\frac{(-1)^k}{(\pi^2k^2)^N}\,{}_1F_1\left[1;-N+\tfrac{1}{2};-\frac{\pi^2k^2}{\sigma}\right]\right] . \tag{13}$$

Thus we have shown that the HS transformation together with a convergence factor gives the asymptotic series as well as remainder for the rigid-rotator partition function in a fairly simply way. The present formulation shows how to use the powerful HS transformation in many-body physics where problems of convergence may arise. As was mentioned above, the added advantage of the present derivation is that it can also be used if the correction terms are to be added to the rotational energy. This advantage is not there in the earlier derivations [2].

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