Improved Approximation for the Free Energy in Low Dimensions

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Abstract

We develop a recursive formula that gives a sequence of improved approximations for the partition function and free energy. In this paper we work with the generic non-linear $q^3 + q^4$ model in $d = 0$ dimensions. We compare the first, and simplest, approximation in the above sequence with the semi-classical approximation, as well as with the exact results calculated numerically.

It is well known that low dimensional models have played a crucial role in our understanding of the properties of various systems [1-4]. Apart from being relevant as models of particular materials that exhibit low dimensional behavior [5-7] they also offer a way to study and develop methods for calculating the thermodynamic properties.

In this paper we have studied a generic non-linear oscillator model with cubic and quartic couplings:

$$\mathcal{H}(q) = \frac{1}{2}\, q^2 + \frac{1}{3!}\, g_3\, q^3 + \frac{1}{4!}\, g_4\, q^4 \ . \tag{1}$$

In $d = 0$ the partition function of this system in an external field B is given by

$$Z(B) = \int dq\, e^{-\beta(\mathcal{H}(q) - B\, q)} \ . \tag{2}$$

Two other important objects are the free energy $F(B)$ defined through $Z(B) = e^{-\beta F(B)}$ and magnetization $M = \langle q \rangle = -\frac{\partial}{\partial B} F(B)$.

In the Gaussian approximation, we Taylor expand the Hamiltonian in the above integral around some reference point $q_{\rm ref}$, and keep terms that are at most quadratic in $q - q_{\rm ref}$. The integral in (2) is now a Gaussian and we find

$$F_{\rm Gauss}(B, q_{\rm ref}) = \mathcal{H}(q_{\rm ref}) - B\, q_{\rm ref} + \frac{1}{2\beta}\, \ln \beta \mathcal{H}''(q_{\rm ref}) - \frac{1}{2}\, \frac{(\mathcal{H}'(q_{\rm ref}) - B)^2}{\mathcal{H}''(q_{\rm ref})} \ . \tag{3}$$

For this approximation to make sense, the integral must get its dominant contribution from the vicinity of the reference point $q_{\rm ref}$. The standard semi-classical (SC) approximation corresponds to the choice $q_{\rm ref} = q_{\rm mf}\,(B)$, where $q_{\rm mf}$ is the solution of the mean field equation $\mathcal{H}' = B$ [8]. The mean field solution is the maximum of the integrand in (2).

On the other hand, we expand the integrand around the magnetization M. Although the mean field solution gives the maximum of the integrand, expansion around M gives a better approximation for the area under the curve. The Gaussian approximation around M is simply

$$F_{\rm Gauss}(B,M) = \mathcal{H}(M) - B\,M + \frac{1}{2\beta}\,\ln\beta\mathcal{H}''(M) - \frac{1}{2}\,\frac{(\mathcal{H}'(M)-B)^2}{\mathcal{H}''(M)}\ . \tag{4}$$

To be able to evaluate this *in closed form* we need to know $M(B)$, which is tantamount to knowing how to do the theory exactly, since M and its derivatives give all the thermodynamic response functions. The practical use of equation (4) comes about when one solves it iteratively. Using the definition of M in terms of F, as well as equation (3) we obtain the following iterative process

$$M_{n+1}(B) = -\,\frac{d}{dB}\,F_{\rm Gauss}(B, M_n(B))\ . \tag{5}$$

For the seed of this iteration we chose the mean field, i.e. $M_0 = q_{\rm mf}$. After one iteration we obtain the standard SC result $M_1 = M_{\rm sc}$. Continuing this process we obtain a sequence of approximations $M_0, M_1, M_2, \ldots$ or equivalently of approximations to the free energy $F_1, F_2, F_3, \ldots$ given by $F_{n+1}(B) = F_{\rm Gauss}(B, M_n(B))$.

To test this iteration scheme we first numerically calculated the exact magnetization $M_{\rm ex}$, and then compared it with our sequence of approximations M_n. The results of this analysis are shown in Figure 1. As we can see, successive iterates are better and better and converge (though slowly) to the best Gaussian approximation M_∞. We also see that M_∞ is still not equal to the exact result $M_{\rm ex}$, since we used the Gaussian approximation $F_{\rm Gauss}$ in defining our recursive relation. It is clear that this procedure offers a systematic improvement on the usual mean field and SC results.

It is interesting to look at the first new approximation in the above sequence $F_2(B) = F_{\rm Gauss}(B, M_1)$, where $M_1 = -\frac{d}{dB}F_1$. Even this simple approximation already gives a remarkable improvement on the SC result, while being only marginally harder to compute. We call it the improved Gaussian approximation (IGA). In what follows we compare IGA to SC and exact numerical results.

We first studied the case of the magnetization by evaluating IGA and SC for a range of couplings g_3 and g_4 such that the Hamiltonian (1) has a unique minimum ($g_4 > \frac{3}{8}\,g_3^2$). As a measure of the quality of an approximation let us consider the area of the region in the g_3–g_4 plane in which it differs from the exact result by less than 10%. Figure 2 shows these areas for $M_{\rm sc}$ and $M_{\rm iga}$. It is clear that IGA is superior. From these contour plots we also see that the same holds at 5% accuracy, etc.

To further test IGA we have calculated the quantity

$$\langle q^2\rangle = \frac{\int dq\, q^2\, e^{-\beta\mathcal{H}(q)}}{\int dq\, e^{-\beta\mathcal{H}(q)}}\ , \tag{6}$$

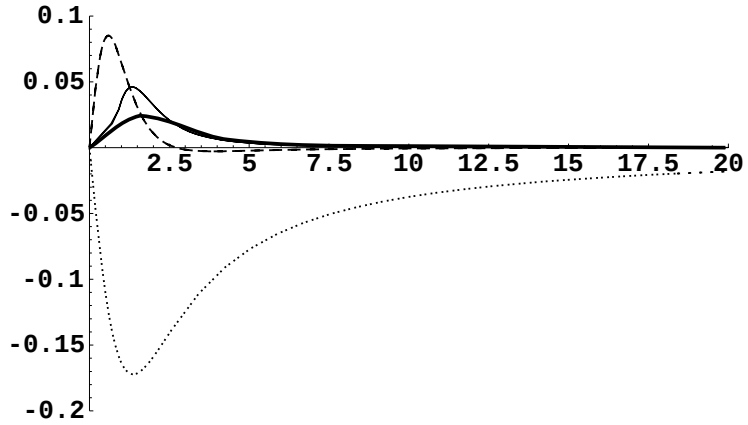

Figure 1: Plots of $M_{\rm ex} - M_0$ (dotted line), $M_{\rm ex} - M_1$ (dashed line), $M_{\rm ex} - M_2$ (thin line) and $M_{\rm ex} - M_\infty$ (thick line) as functions of B. The above plot is done for couplings $g_3 = 0$, $g_4 = 1$, and for $\beta = 1$.

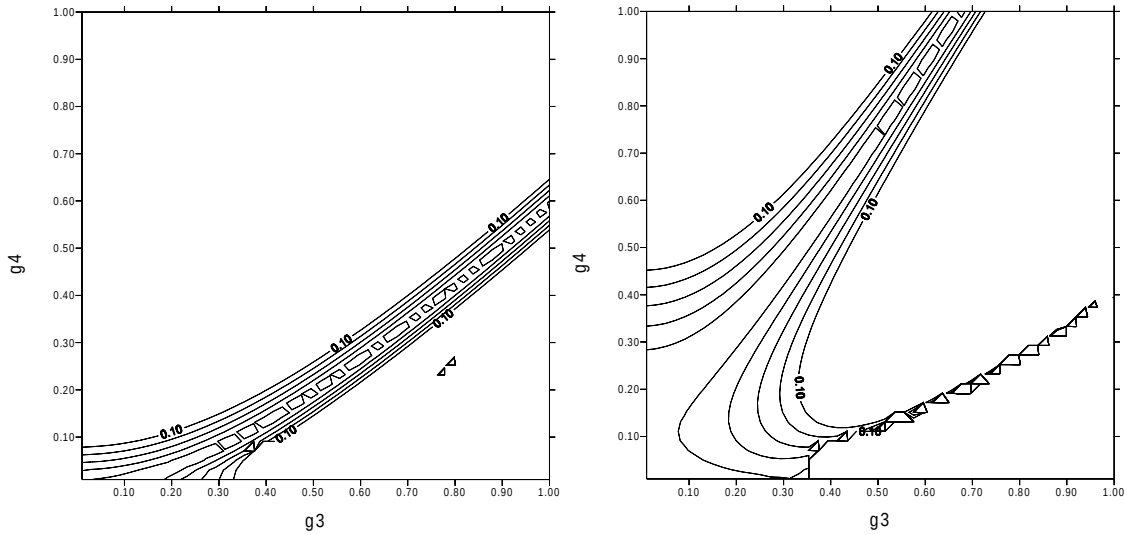

Figure 2: Contour plots of $|\frac{M_{\rm ex}-M_{\rm sc}}{M_{\rm ex}}| < 0.1$ (left) and $|\frac{M_{\rm ex}-M_{\rm iga}}{M_{\rm ex}}| < 0.1$ (right), for $\beta = 1$ and $B = 0$.

related to the zero field susceptibility. Again, IGA outperforms SC in a similar manner. The area in which IGA has better than 10% accuracy is in this case ≈ 2.5 times larger than the appropriate area for SC.

As a conclusion, we have shown in this paper that even the simplest improved Gaussian approximation (IGA) gives better agreement with the exact results than the semi-classical (SC) approximation. At the same time, its computational cost is only negligibly greater. We are currently working on extending the above results to interesting models in $d = 1$.

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