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Weak non-Gaussian approximation

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A superposition of Gaussian functionals is considered as a trial functional for the Bogoliubov inequality. The direct optimization of the Bogoliubov inequality generates a non-Gaussian approximation. This function may be strongly non-Gaussian but the kernel is the same as the usual one, up to a multiplicative constant.

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One of the limitations of the variational principle in field theory or statistical mechanics is that the only functionals $\omega[\phi]$ for which an average can be computed exactly is the Gaussian

$$\omega[\phi]=\exp\left[-\int dx\, dy\, \phi(x)K(x,y)\phi(y) + \int dx\, J(x)\phi(x)\right], \quad (1)$$

with K some positive definite operator [1]. This is something of a limitation and means that typically, a functional such as (1) is chosen as the trial state. A superposition of Gaussians can be considered as a straightforward non-Gaussian generalization. Some such special cases of weakly non-Gaussian functionals have been studied, and it may be shown that they correspond to exactly solvable models [2–5]. Such models have been chosen somewhat arbitrarily, in attempts to describe some of the fluctuations of the Landau-Ginzburg-Wilson Hamiltonian. Here we shall show that it is possible to refine such an approach, by optimizing the distribution over a large variational space. We define the superposition as

$$\int d^N\phi \exp[-F(\vec{\phi}\cdot\mathbf{K}\vec{\phi})+\vec{\mathrm{J}}\cdot\vec{\phi}] = \frac{(2\pi)^{N/2}}{\sqrt{\det\mathbf{K}}}\int_0^{+\infty} dt\, t^{N-1} \times\Omega_N(t\sqrt{\vec{\mathrm{J}}\cdot\mathbf{K}^{-1}\vec{\mathrm{J}}})\exp[-F(t^2)]\ , \quad (2)$$

where $\vec{\phi}$ is an N-dimensional vector, $\mathbf{K}$ is the $N\times N$-matrix,

$$\Omega_N(x)\equiv\frac{I_{(N-2)/2}(x)}{x^{(N-2)/2}}\ , \quad (3)$$

and I_N is the modified Bessel function of order N [6]. [Some integrals similar to (2) may be found in [7].]

The Eq. (2) is a discretized generalization of the well-known case, $F(t)=t$. We shall now attempt to determine the F by a variational procedure. Let us consider the Bogoliubov inequality

$$-\ln\int d^N\phi \exp(-H[\vec{\phi}])\le f=f_1+f_2+f_3\ , \quad (4)$$

$$f_1=-\ln\int d^N\phi\exp(-H_T[\vec{\phi}])\ , \quad (5)$$

$$f_2=\langle H\rangle_T\ ,\quad f_3=-\langle H_T\rangle_T\ , \quad (6)$$

where

$$\langle\cdots\rangle_T\equiv\frac{\int d^N\phi\cdots\exp(-H_T[\vec{\phi}])}{\int d^N\phi\exp(-H_T[\vec{\phi}])}\ . \quad (7)$$

Consider first the more straightforward case of a symmetric phase, so that the trial Hamiltonian may be written $H_T[\vec{\phi}]=F(\vec{\phi}\cdot\mathbf{K}\vec{\phi})$.

We then find, by variation,

$$F(t)=2^{(N-2)/2}\Gamma\left[\frac{N}{2}\right]H(\partial_{\vec{\mathrm{J}}}|_{J=0})\Omega_N(\sqrt{\vec{\mathrm{J}}\cdot\mathbf{K}^{-1}\vec{\mathrm{J}}})\ , \quad (8)$$

where we use the expression

$$\Omega_N(\sqrt{t})=\frac{1}{2^{(N-2)/2}}\sum_{k=0}^{\infty}\frac{t^k}{2^{2k}k!\Gamma\left[\frac{N}{2}+k\right]}\ . \quad (9)$$

As an example we may choose the Hamiltonian

$$H[\vec{\phi}]=\vec{\phi}\cdot\mathbf{B}\vec{\phi}+\lambda\sum_{j=1}^{N}\phi_j^4\ . \quad (10)$$

Then the optimal F yields

$$H_T[\vec{\phi}]=\frac{1}{N}\mathrm{Tr}\left[\frac{\mathbf{B}}{\mathbf{K}}\right]\vec{\phi}\cdot\mathbf{K}\vec{\phi} +\lambda\frac{3}{N(N+2)}\sum_{j=1}^{N}(\mathbf{K}^{-1})_{jj}^2(\vec{\phi}\cdot\mathbf{K}\vec{\phi})^2\ . \quad (11)$$

Equation (8) is encouragingly simple. Now we perform the minimization of Eq. (4) with respect to $\mathbf{K}$ and F simultaneously.

For a simple example we chose the Landau-Ginzburg model in three-dimensional Euclidean space,

$$H=\tfrac{1}{2}[\nabla\phi(\mathbf{x})]^2+\frac{a}{2}\phi^2(\mathbf{x})+\frac{b}{24}\phi^4(\mathbf{x})\ ,\quad b>0\ . \quad (12)$$

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The trial Hamiltonian

$$H_T[\phi]=F\left[\int d\mathbf{x}\,d\mathbf{y}[\phi(\mathbf{x})-\varphi]G^{-1}(\mathbf{x},\mathbf{y})[\phi(\mathbf{y})-\varphi]\right] \tag{13}$$

permits us to consider both symmetric and broken symmetry phases. It depends on φ, the kernel G^{-1}, and the function F. Note that φ is just the average value of the field: $\varphi=\langle\phi\rangle_T$.

Let us consider problem (12) on a lattice of $N=M^3$ sites with a mesh size Λ^{-1} and periodic boundary conditions. Recall that, on a Fourier lattice, $\langle\mathbf{k}_1|\Delta|\mathbf{k}_2\rangle=-4\Lambda^2\delta_{\mathbf{k}_1\mathbf{k}_2}\xi_{\mathbf{k}_1}$, $\xi_{\mathbf{k}}\equiv\sum_{j=1}^{3}\sin^2(\pi k_j/M)$, and $k_j=1,\ldots,M$ [8]. And we denote $g_{\mathbf{k}_1}\equiv\langle\mathbf{k}_1|G|\mathbf{k}_2\rangle$. Then

$$f_1=-\tfrac{1}{2}\sum_{\mathbf{k}}\ln g_{\mathbf{k}}+\ln\left[\frac{\Gamma(N/2)}{\Theta_{N/2}}\right]-\frac{N}{2}\ln\pi\ , \tag{14}$$

$$f_2=\frac{2\Lambda^5}{N^2}\frac{\Theta_{N/2+1}}{\Theta_{N/2}}\sum_{\mathbf{k}}\xi_{\mathbf{k}}g_{\mathbf{k}}+\frac{\Lambda^3}{N^2}\frac{\Theta_{N/2+1}}{\Theta_{N/2}}\left[\frac{a}{2}+\frac{b}{4}\varphi^2\right]\sum_{\mathbf{k}}g_{\mathbf{k}} +\frac{\Lambda^6}{8N^3(N+2)}\frac{\Theta_{N/2+2}}{\Theta_{N/2}}b\left[\sum_{\mathbf{k}}g_{\mathbf{k}}\right]^2+\frac{a}{2}\varphi^2+\frac{b}{24}\varphi^4\ , \tag{15}$$

$$f_3=-\frac{1}{\Theta_{N/2}}\int_0^{+\infty}d\tau\,\tau^{(N-2)/2}F(\tau)\exp[-F(\tau)]\ , \tag{16}$$

$$\Theta_n[F]\equiv\int_0^{+\infty}d\tau\,\tau^{n-1}\exp[-F(\tau)]\ . \tag{17}$$

Note that, if $F(\tau)=\tau$, the Θ_n becomes the gamma function $\Gamma(n)$.

Minimization of f with respect to $g_{\mathbf{k}}$, $\partial_{g_{\mathbf{k}}}f=0$, results in

$$g_{\mathbf{k}}=\frac{N^2}{4\Lambda^5}\frac{\Theta_{N/2}}{\Theta_{N/2+1}}\frac{1}{\xi_{\mathbf{k}}+\mu^2}\ , \tag{18}$$

where the parameter μ^2 is to be defined by minimization of f. Substitution of (18) into $f=f_1+f_2+f_3$ and minimization of f with respect to F, $\delta f/\delta F(\tau)=0$, yields

$$F(\tau)=q\tau+p\tau^2\ ,\quad p>0\ . \tag{19}$$

Notice that in the standard Gaussian case $p=0$.

Substitution of (19) into f and the minimization of f with respect to φ^2 yields

$$f(\mu,z)=\tfrac{1}{2}V_1+\frac{a}{8\Lambda^2}V-\frac{b}{24}\varphi^4-\frac{z^2}{4} +\frac{b}{128\Lambda^4}\frac{\Upsilon_{N+4}\Upsilon_N}{\Upsilon_{N+2}^2}V^2 -\frac{N}{2}z\frac{\Upsilon_{N+2}}{\Upsilon_N}-\frac{N(N+2)}{8}\frac{\Upsilon_{N+4}}{\Upsilon_N} +\frac{N}{2}\ln\frac{\Upsilon_{N+2}}{\Upsilon_N}-\ln\Upsilon_N+\frac{N}{2}\ln\left[\frac{2\Lambda^5}{\pi N}\right]\ , \tag{20}$$

where $\varphi^2=-6(a/b)-3V/(4\Lambda^2)$ if $6(a/b)+3/4\Lambda^2V<0$, and $\varphi=0$ otherwise. Here the following notations have been introduced:

$$z\equiv\frac{q}{\sqrt{2p}}\ , \tag{21}$$

$$V\equiv\sum_{\mathbf{k}}\frac{1}{\xi(\mathbf{k})+\mu^2}\ , \tag{22}$$

$$V_1\equiv\sum_{\mathbf{k}}\left[\frac{\xi(\mathbf{k})}{\xi(\mathbf{k})+\mu^2}+\ln[\xi(\mathbf{k})+\mu^2]\right]\ . \tag{23}$$

The symbol Υ_N stands for the parabolic cylinder function [9]

$$\Upsilon_N\equiv U\left[\frac{N-1}{2},z\right]\equiv D_{-(N-2)/2}(z)\ . \tag{24}$$

Thus, the minimization of $f(\mu,z)$ need be carried out only with respect to two parameters, μ and z. The standard Gaussian approximation implies $z=+\infty$ and

$$f(\mu,+\infty)=\tfrac{1}{2}V_1+\frac{a}{8\Lambda^2}V+\frac{b}{128\Lambda^4}V^2-\frac{b}{24}\varphi^4 +\frac{N}{2}\ln\left[\frac{2\Lambda^5}{\pi eN}\right]\ , \tag{25}$$

where φ^2 is defined above.

The more general result that we have presented, (20), can be computed numerically using Darwin's expansion of $U(\alpha,z)$ for α positive and $(4\alpha+z^2)$ large [9]. We applied this expansion including the polynomials $d_3,d_6,d_9,\ldots,$ up to d_{24} [9,10]. The standard Gaussian approximation (25) allows us to check the more general result with the same value of μ and for large z. Such numerical calculations show that for this model the corrections to the standard Gaussian approximation are very small, but are instructive in that they illustrate the interesting behavior of the "non-Gaussian" parameter z. We note that this parameter becomes negative in the symmetric phase. In Fig. 1 we have plotted z vs a for $\Lambda=1$, $N=1000$, and $b=6$ around the critical point $a\approx-85$. The correction to the free energy compared to the standard Gaussian approximation is small, of order 3×10^{-4}. The parameter z decreases gradually from ≈62 at $a\approx-100$ to ≈44 at the critical point, where it

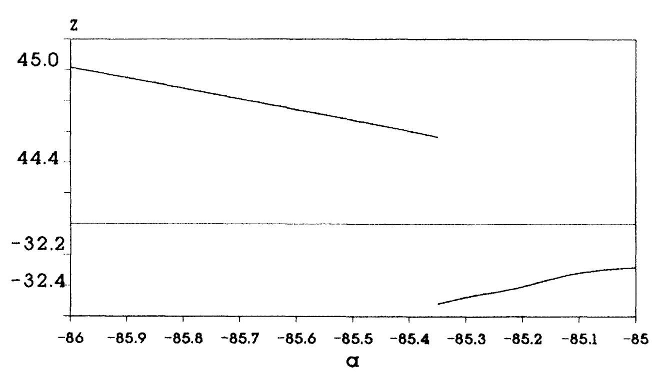

FIG. 1. Non-Gaussian parameter z is plotted against a. A region of z is cut to facilitate the picture.

changes sign and becomes negative: ≈ -32 in the symmetric phase.

In conclusion, we have considered the trial distribution (2) [or (13)] of a superposition of Gaussians, and found that optimization of the Bogoliubov inequality generates a weak non-Gaussian approximation with weight function in (8) and (19). This function can be strongly non-Gaussian [as for example, with $q<0$ in (19)] but in the sample calculation the kernel is not changed, up to a multiplicative constant [see (18)].

A similar analysis could improve the Gaussian effective potential approach in quantum field theory [11] and the corresponding calculations on a lattice [12]. It will be of some interest to consider more general superpositions of Gaussians with different kernels and a broader space of distributions. Perhaps, there lies the resolution to some problems that have plagued attempts to improve simple approximations in statistical mechanics and field theory of classical and quantum systems.

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