Interaction effects in the spectrum of the three-dimensional Ising model

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The two-point correlation functions of statistical models show, in general, both poles and cuts in momentum space. The former correspond to the spectrum of massive excitations of the model, while the latter originate from interaction effects, namely, the creation and annihilation of virtual pairs of excitations. We discuss the effect of such interactions on the long-distance behavior of correlation functions in configuration space, focusing on certain time-slice operators that are commonly used to extract the spectrum. For the three-dimensional Ising model in the scaling region of the broken-symmetry phase, a one-loop calculation shows that the interaction effects on time-slice correlations is non-negligible for distances up to a few times the correlation length and should therefore be taken into account when analyzing Monte Carlo data.
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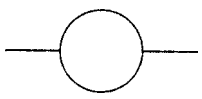
I. INTRODUCTION

When studying a statistical model, one is often interested in determining the spectrum of massive excitations, i.e., the eigenvalues of the transfer matrix. For many interesting models this cannot be done exactly and one has to rely on numerical methods, falling into two main classes: direct diagonalization of the transfer matrix and Monte Carlo simulations [for studies of the three-dimensional (3D) Ising model in these frameworks see, respectively, Refs. [1] and [2,3] and references therein]. The Monte Carlo method has been shown to provide greater accuracy in the evaluation of the eigenvalues; however, a careful analysis of the raw Monte Carlo data is required to extract the spectrum. The purpose of the present work is to study some physical effects that are relevant to this analysis.

The observables that are most suitable to investigate the spectrum of a model through a Monte Carlo simulation are the two-point correlation functions of operators: Their long-distance behavior is directly related to the spectrum. This is especially evident in momentum space, where each pole of the correlation function corresponds to a massive excitation and therefore to an eigenvalue of the transfer matrix.

In general, however, the momentum space correlators will have not only poles but also cuts, signaling the possibility of creating and annihilating virtual pairs of excitations. For example, if the effective Hamiltonian for the order parameter ϕ includes a ϕ^3 interaction, the Feynman diagram



will generate a cut in the $\langle\phi\phi\rangle$ correlator in momentum space.

Since, in general, Monte Carlo simulations give direct access to configuration-space correlation functions rather than their Fourier transforms, it is interesting to study the effect of such interactions on the long-distance behavior of configuration-space correlators. The purpose of this work is to compute this effect in the scaling region of the broken-symmetry phase of the 3D Ising model, where actual calculations can be performed in the framework of renormalized Euclidean quantum field theory.

A strong motivation for this analysis is provided by the continuous improvements in the accuracy of Monte Carlo simulations: Recent advances in both computer performances and simulation algorithms allow us to obtain numerical data of unprecedented precision. Their analysis requires more sophisticated theoretical tools as finer effects become observable. We will find that the effects that are the object of this study typically account for about 1% of the correlators in the region of physical interest: This is actually an order of magnitude larger than the statistical uncertainties typical of recent Monte Carlo studies of the 3D Ising model.

The paper is organized as follows. In Sec. II we introduce time-slice operators, which are particularly suitable for the Monte Carlo study of the spectrum of a statistical model. In Sec. III we compute the correlators of such operators in the Ising model using ϕ^4 field theory at one loop in three Euclidean dimensions. In particular, the interaction effects can be evaluated and expressed in terms of exponential integral functions. In Sec. IV we comment on the relevance of these effects to certain universal amplitude ratios, while Sec. V is devoted to the discussion of the results and their implications for the analysis of Monte Carlo data.

II. TIME-SLICE CORRELATORS

The spectrum of massive excitations of a statistical model can be obtained by studying the long-distance behavior of two-point correlation functions. Consider, for example, the Gaussian model, with the Hamiltonian

$$H=\int d^dx\left(\frac{1}{2}\,\partial_\mu\phi\partial_\mu\phi+\frac{m^2}{2}\,\phi^2\right). \tag{1}$$

The two-point correlation function is

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$$\langle \phi(x)\phi(y)\rangle = \int \frac{d^d p}{(2\pi)^d} \frac{e^{ip(x-y)}}{p^2+m^2} = \frac{1}{(2\pi)^{d/2}} \left(\frac{|x-y|}{m}\right)^{1-d/2} K_{1-d/2}(m|x-y|), \tag{2}$$

where $K_{1-d/2}$ is a modified Bessel function. Therefore, asymptotically for $|x-y|\to\infty$,

$$\langle \phi(x)\phi(y)\rangle \sim \text{const } m^{(d-3)/2}|x-y|^{-(d-1)/2} e^{-m|x-y|}. \tag{3}$$

We see that the long-distance behavior of correlators can be used to extract the value of the mass m, which in this case is obviously the only state in the spectrum.

The standard practice in Monte Carlo studies is to define time-slice operators

$$S(t) = \frac{1}{L^{d-1}} \int dx_1 \cdots dx_{d-1} \phi(x_1,\ldots,x_{d-1},t) \tag{4}$$

to obtain a purely exponential behavior of correlations. For example, in the Gaussian model it is easy to see that

$$\langle S(t)S(0)\rangle = \frac{1}{L^{d-1}} e^{-m|t|}. \tag{5}$$

When considering a nontrivial model, it is customary to generalize Eq. (5) to

$$\langle S(t)S(0)\rangle = \sum_k c_k e^{-m_k|t|}. \tag{6}$$

By fitting the values of the time-slice correlations with Eq. (6) one can extract the values of a certain number of low-lying states, depending on the precision of the available data.

Each exponential on the right-hand side of Eq. (6) corresponds to a pole in the Fourier transform of $\langle \phi(x)\phi(y)\rangle$. However, since a nontrivial model certainly involves interactions, Eq. (6) must be modified to take into account their contribution: in the next section we will compute the time-slice correlator $\langle S(0)S(t)\rangle$ for the 3D Ising model in the broken-symmetry phase, where a ϕ^3 interaction is present in the effective Hamiltonian so that cuts appear in the two-point function already at one loop. The calculation will teach us how to modify Eq. (6) to take into account the effect of the production and annihilation of virtual pairs of excitations.

III. THE CASE OF THE 3D ISING MODEL

It is a widely accepted conjecture that the 3D Ising model is in the same universality class as ϕ^4 field theory. This allows us to use renormalized 3D quantum field theory to study the Ising model in the scaling region, where lattice effects become negligible and universality holds. This program was initiated by Parisi [4] and has been vigorously pursued to study several aspects of the Ising model [5–7]. The agreement between field-theoretical calculations and Monte Carlo results is satisfactory.

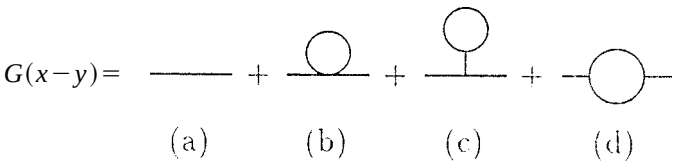
Therefore, from now on we will consider the 3D Euclidean field theory defined by the action (effective Hamiltonian, in the language of statistical mechanics)

$$S = \int d^3x \left[\frac{1}{2}\partial_\mu\phi\partial_\mu\phi + \frac{g}{24}(\phi^2-v^2)^2\right]. \tag{7}$$

We are interested in the two-point connected function

$$G(x-y) = \langle \phi(x)\phi(y)\rangle - \langle \phi(x)\rangle\langle \phi(y)\rangle. \tag{8}$$

The perturbative expansion must be performed around one of the stable classical solutions say, $\phi = v$. Defining a fluctuation field $\varphi = \phi - v$, a φ^3 term appears in the Lagrangian, with a coupling proportional to $\sqrt{g}$ (for details about the perturbative expansion in the broken-symmetry phase see, e.g., Ref. [6]). The correlation function (8) is then given at one loop by the sum of the Feynman diagrams



Using dimensional regularization we find

$$G_d(x-y) = \int \frac{d^d p}{(2\pi)^d} \tilde{G}_d(p) e^{ip(x-y)}, \tag{9}$$

with

$$\tilde{G}_d(p) = \frac{1}{p^2+m^2} + \frac{g}{m^2}\left(\frac{m^2}{4\pi}\right)^{d/2} \frac{\Gamma\left(1-\frac{d}{2}\right)}{(p^2+m^2)^2} + \frac{3m^2 g}{2} \frac{F_d(p)}{(p^2+m^2)^2} \tag{10}$$

and

$$F_d(p) = \frac{\Gamma(2-d/2)}{(4\pi)^{d/2}} \int_0^1 dx [m^2 + x(1-x)p^2]^{d/2-2}. \tag{11}$$

The first term on the right-hand side of Eq. (10) is the tree-level contribution with a pole in $p^2=-m^2$. The remaining diagrams are interaction effects: The second term, corresponding to diagrams (b)+(c), produces shift in the location of the pole, i.e., a quantum correction to the physical mass. The third term is the interesting one for our purpose: In addition to providing another quantum correction to the physical mass, it has a cut in $p^2=-4m^2$. Indeed, this term corresponds to diagram (d) in the expansion of $G(x-y)$, namely, to the production and annihilation of a virtual pair of particles.

The theory must be renormalized to be compared with experimental or Monte Carlo results. Notice that analytic continuation to $d=3$ gives a finite expression for $\widetilde{G}(p)$ without need for any subtraction. This is a peculiarity of dimensional regularization for odd d, which disappears when higher-loop effects are taken into account. It implies that the renormalized parameters in the minimal subtraction (MS) scheme coincide at one loop with the bare parameters.

However, the MS scheme is not particularly suited for direct comparison of field-theoretic calculations with experimental or Monte Carlo data. A more convenient scheme, where the renormalized parameters of the field theory have a direct lattice interpretation, was introduced in Ref. [8]. The renormalized parameters ϕ_R, m_R, g_R in this scheme were computed at three-loop order in [7], to which we refer the reader for the definitions and expressions of the renormalized parameters. In particular, the renormalized mass m_R^2 is defined as the momentum space correlation at $p=0$ and coincides with the inverse second-moment correlation length. Here we just need the expression of the connected two-point function of renormalized fields:

$$G_R(x-y)=\langle \phi_R(x)\phi_R(y)\rangle_c=\int \frac{d^3p}{(2\pi)^3}\,\widetilde{G}_R(p)e^{ip(x-y)} \tag{12}$$

with, denoting with $u_R=g_R/m_R$ the dimensionless renormalized coupling,

$$\widetilde{G}_R(p)=\left(1+\frac{u_R}{64\pi}\right)\left\{\frac{1}{p^2+m_R^2\left(1-\frac{3u_R}{64\pi}\right)}-\frac{m_R^2u_R}{4\pi}\frac{1}{(p^2+m_R^2)^2}+\frac{3m_R^3u_R}{8\pi}\frac{1}{(p^2+m_R^2)^2}\frac{1}{\sqrt{p^2}}\arctan\left(\frac{\sqrt{p^2}}{2m_R}\right)\right\}. \tag{13}$$

Defining the time-slice operators as

$$S(t)=\frac{1}{L^2}\int dx_1dx_2\phi_R(x_1,x_2,t), \tag{14}$$

we have

$$\langle S(t)S(0)\rangle_c=\frac{1}{L^2}\int\frac{dp}{2\pi}\,e^{ipt}\widetilde{G}_R(0,0,p). \tag{15}$$

After a simple calculation we obtain for $t>0$

$$\langle S(t)S(0)\rangle=\frac{1}{2m_RL^2}\,e^{-m_{\rm ph}t}\left[1+\frac{u_R}{128\pi}(24\ln 3-27)\right]+\frac{3u_R}{16\pi L^2m_R}\int_{2m_R}^{\infty}d\mu\,\frac{e^{-\mu t}}{\mu\left(1-\frac{\mu^2}{m_R^2}\right)^2}, \tag{16}$$

where $m_{\rm ph}$ is the physical mass, defined as the location of the zero of the inverse correlator in momentum space $G^{-1}(p)$,

$$m_{\rm ph}^2=m_R^2\left[1+\frac{u_R}{64\pi}(13-12\ln 3)\right]. \tag{17}$$

The integral appearing in Eq. (16) can be expressed in terms of exponential integral functions to give

$$\langle S(t)S(0)\rangle_c=\frac{1}{2m_RL^2}\,e^{-m_{\rm ph}t}\left[1+\frac{u_R}{128\pi}(24\ln 3-27)\right]+\frac{3u_R}{16\pi L^2m_R}\left[\frac{e^{-2m_{\rm ph}t}}{6}+\frac{m_{\rm ph}t+2}{4}\,e^{-m_{\rm ph}t}\times{\rm Ei}(-m_{\rm ph}t)+\frac{2-m_{\rm ph}t}{4}\,e^{m_{\rm ph}t}\,{\rm Ei}(-3m_{\rm ph}t)-{\rm Ei}(-2m_{\rm ph}t)\right]. \tag{18}$$

[The appearance of an exponential term e^{-2mt} in Eq. (18) could be misleading: Due to a cancellation between this term and the Ei functions the asymptotic behavior of the sum in square brackets is actually e^{-2mt}/t.] Equation (18) is our main result: It gives the contribution of interaction effects to the correlation function of time-slice operators as a modification of the simple exponential behavior (6).

IV. THE UNIVERSAL AMPLITUDE RATIO $\xi/\xi_{\rm 2nd}$

Universal amplitude ratios are certain dimensionless combinations of observables that are predicted to be universal at criticality (for a comprehensive review see Ref. [9]). Among these, of particular relevance to us is the ratio $\xi/\xi_{\rm 2nd}$ of the second-moment correlation length and the ''true'' correlation length (i.e., the inverse of the physical mass). This ratio defines two universal amplitude ratios F_+ (F_-) when the critical limit is taken from the symmetric (broken-symmetry) phase. It can be shown [3] that the presence of higher masses in the spectrum implies $F_\pm>1$. However, the corresponding analysis in ϕ^4 theory shows that the converse is not true: A value of F_- greater than one does not necessarily indicate the presence of higher mass states, but can simply be a signal of nontrivial interaction effects such as the ones studied in this work.

In fact, since the renormalized mass m_R is defined as $1/\xi_{\rm 2nd}$ (see [8]), from Eq. (17) we see that at one loop in ϕ^4 theory [10]

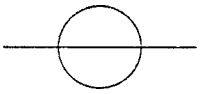
$$F_- = 1 - \frac{u_R^*}{128\pi}(13 - 12\ln 3) = 1.006\,68(3), \qquad (19)$$

in good agreement with the Monte Carlo result [3]

$$F_- = 1.009(5). \qquad (20)$$

Moreover, it is easy to see that the nontrivial contribution to F_- comes exclusively from diagram (d) in the expression of $G(x-y)$, namely, the diagram that produces the cut.

It would be interesting to study similar effects in the symmetric phase, however, we expect them to appear with the diagram



and therefore only at the two-loop level. This provides a qualitative explanation for the fact that in the symmetric phase the corresponding amplitude ratio F_+ is known to be much smaller than F_-: A strong coupling expansion gives [11]

$$F_+ = 1.000\,23(5), \qquad (21)$$

while Monte Carlo calculations give an upper bound [3]

$$F_+ < 1.0006. \qquad (22)$$

V. DISCUSSION

The relevance of the effect we have just computed can be best appreciated by considering the ratios

$$R(t) = -\ln \frac{\langle S(t+1)S(0)\rangle_c}{\langle S(t)S(0)\rangle_c}. \qquad (23)$$

For a purely exponential behavior, $R(t)$ is identically equal to $m_{\rm ph}$, while $R(t)$ as given by Eq. (18) is plotted in Fig. 1, where we have used the Monte Carlo estimate [3]

$$u_R^* = 14.3(1) \qquad (24)$$

for the value of the dimensionless renormalized coupling in the continuum limit and we have set $m_{\rm ph}=1$ (i.e., we are measuring distances in units of the correlation length). (The variation of u_R is anyway very slow in the whole scaling region, being governed by corrections to scaling.)

The figure shows that $R(t)$ is appreciably different from 1 for distances of the order of a few times the correlation length. For example, at $t=1$ the interaction effect is $\sim 0.8\%$ of R. State-of-the-art Monte Carlo simulations give statistical uncertainties about ten times smaller for the same quantity [3]. The magnitude of the effect becomes comparable to the statistical uncertainties at $t \sim 2.5$.

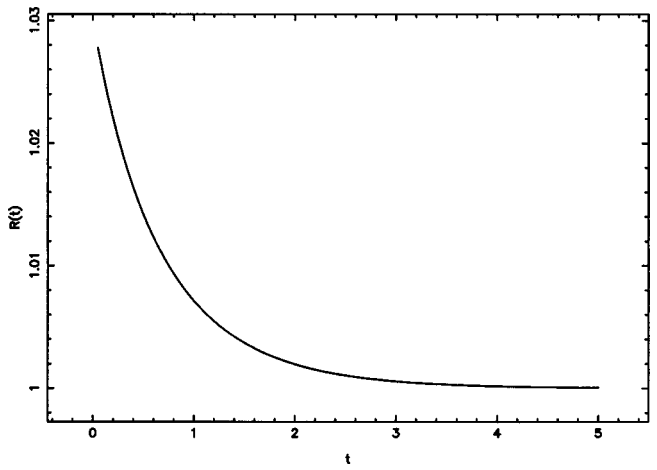


FIG. 1. Ratio $R(t)$ defined in Eq. (23) as predicted by Eq. (18) for $m_{\rm ph}=1$. A purely exponential behavior would give $R(t)=1$ identically.

The specific form of Eq. (18) suggests one more reason why the correction must be taken into account when analyzing numerical data. In fact, the behavior of the correlators when interaction contributions are included mimics very closely the contribution of a higher mass in the spectrum. Consider the ratio (23) when the contribution of two poles is included and the cut is neglected:

$$\widetilde{R}(t) = -\ln \frac{e^{-m(t+1)} + \alpha e^{-m'(t+1)}}{e^{-mt} + \alpha e^{-m't}} \qquad (25)$$

We have verified that by adjusting the parameters α and m'/m one can make $\widetilde{R}(t)$ look very similar to the cut contribution: Relative uncertainties in the data of less than one part in 10^4 would be needed to resolve the difference. The ''best-fit'' value is about $m'/m = 2.4$. Therefore, the effect of interaction can easily be mistaken for a higher mass state with $m' \sim 2.4m$. A more complete investigation of these issues, including a high-precision Monte Carlo analysis, is currently being pursued and will be presented elsewhere [12].

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