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# Nonperturbative renormalization-group calculations for continuum spin systems

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Wilson's exact smooth-cutoff renormalization-group (RG) equation for continuum spin Landau-Ginsburg models is shown to be equivalent to an easily constructed, infinite set of partial differential equations that provide a natural system of successive approximation for numerical calculation. It differs from other RG approaches in that an infinite number of couplings are included at each level of approximation. By way of illustration, preliminary results are presented for Ising-model critical exponents in three dimensions.

A continuing challenge for the improvement of renormalization-group (RG) calculations in both critical phenomena and quantum field theory is the proliferation of interactions that occur as the RG transformation is carried out.[1] So far, the successful application of the RG approach has generally depended on one being able to construct a transformation in which only a small number of couplings are needed to produce good results. This approach has been sufficient for isolating and describing the essential universal features of many systems. Yet, the need for greater accuracy and wider applicability requires an approach that will handle a far greater number of interactions without creating an impractical increase in computational complexity.[2]

This Rapid Communication presents a new method of RG calculation that makes some progress in this direction. Indeed, an infinite number of couplings are included from the very beginning. The method is based on a new approach to solving functional differential equations, presented here and applied to Wilson's exact RG equation for continuum spin Ising systems in $d$ dimensions.[3,4] It is quite simple and easily generalized to more complex sysems. It essentially involves constructing an infinite set of partial differential equations (PDE's) equivalent to the original functional differential equation. These PDE's then provide a natural system of successive approximation for numerical calculation. Though nonperturbative in character, it has a certain similarity to the effective-action expansion[5] in quantum field theory in that it involves an expansion of the effective RG Hamiltonian in an infinite series of local effective Hamiltonians arranged according to the powers of momenta which couple the Fourier-transformed spin variables. Thus, it may have application to the problem of spontaneous symmetry breaking in quantum field theory where perturbative approaches have run into difficulties.[6]

We start from Wilson's exact smooth-cutoff RG equation[3] for the effective Hamiltonian $\mathscr{H}[\sigma,t]$

$$\frac{\partial\mathscr{H}}{\partial t}=\int_{\mathbf{q}}\left(\frac{d}{2}\sigma_{\mathbf{q}}+\mathbf{q}\cdot\nabla_{\mathbf{q}}\sigma_{\mathbf{q}}\right)\frac{\delta\mathscr{H}}{\delta\sigma_{\mathbf{q}}}+\int_{\mathbf{q}}(1+\Delta+2q^2)\left(\sigma_{\mathbf{q}}\frac{\delta\mathscr{H}}{\delta\sigma_{\mathbf{q}}}+\frac{\delta^2\mathscr{H}}{\delta\sigma_{\mathbf{q}}\delta\sigma_{-\mathbf{q}}}+\frac{\delta\mathscr{H}}{\delta\sigma_{\mathbf{q}}}\frac{\delta\mathscr{H}}{\delta\sigma_{-\mathbf{q}}}+\delta(0)\right), \quad (1)$$

where $d$ is the dimensionality of the system, $\int_{\mathbf{q}}\equiv(2\pi)^{-d}\int d^d\mathbf{q}$, $\sigma_{\mathbf{q}}$ is the rescaled Fourier-transformed spin variable (a function of momentum $\mathbf{q}$), $\delta(0)$ represents the infinite volume of the system, and $\Delta$ is a free parameter which must be properly chosen ($\Delta=\Delta^*$) in order that the equation have a critical fixed point. This fixed-point value then determines the critical exponent $\eta$ according to $\eta=-2\Delta^*$. To proceed, we integrate the gradient term by parts and substitute $\mathscr{H}=\mathscr{H}'+\mathscr{H}^\infty$, $s_{\mathbf{q}}=\phi(q)\sigma_{\mathbf{q}}$, and $H[s_{\mathbf{q}},t]=\mathscr{H}'[\phi^{-1}(q)s_{\mathbf{q}},t]$, where $\mathscr{H}^\infty=-1/2\int_{\mathbf{q}}\sigma_{\mathbf{q}}\sigma_{-\mathbf{q}}$ is the $T=\infty$ fixed point of Eq. (1), and $\phi(q)$, with $\phi(0)=1$, is a momentum-dependent spin-rescaling function required in order to make the integrals $K_n$, defined below, finite. Our resulting equation for $H[s,t]$ is then

$$\frac{\partial H}{\partial t}=dH-\int_{\mathbf{q}}s_{\mathbf{q}}[B(q)+\mathbf{q}\cdot\nabla'_{\mathbf{q}}]\frac{\delta H}{\delta s_{\mathbf{q}}}+\int_{\mathbf{q}}C(q)\left(\frac{\delta^2H}{\delta s_{\mathbf{q}}\delta s_{-\mathbf{q}}}+\frac{\delta H}{\delta s_{\mathbf{q}}}\frac{\delta H}{\delta s_{-\mathbf{q}}}\right), \quad (2)$$

where

$$B(q)=d/2+1+\Delta+2q^2+\mathbf{q}\cdot\nabla_{\mathbf{q}}\ln[\phi(q)],$$

$$C(q)=(1+\Delta+2q^2)\phi^2(q),$$

and the prime on the gradient indicates that it is not to be applied to the momentum conserving $\delta$ functions in $H$.

Next, we expand $H[s,t]$ in powers of momenta:

$$H[s,t]=H_0[s,t]+H_2[s,t]+\sum_{i=1}^{3}H_{4i}[s,t]+\cdots, \quad (3a)$$

where

$$H_{pi}[s,t]=\sum_n a_{pin}(t)F_{pin}[s],$$

$$F_{pin}[s]=\int_{\mathbf{q}_1}\cdots\int_{\mathbf{q}_n}f_{pi}(\mathbf{q}_1,\ldots,\mathbf{q}_n)\delta(\mathbf{q}_1+\cdots+\mathbf{q}_n)\times s_{\mathbf{q}_1},\ldots,s_{\mathbf{q}_n},\quad F_{00}[s]=\delta(0), \quad (3b)$$

and the $f_{pi}(\mathbf{q}_1,\ldots,\mathbf{q}_n)$ are homogenous monomials in $\{\mathbf{q}_j\}$ of degree $p$, with the index $i$ present when needed to keep track of degeneracies. Because of the momentum conserving $\delta$ function we have, for spatially isotropic systems, only one linearly independent functional of degree 2: $f_2=\mathbf{q}_1\cdot\mathbf{q}_2$, and three of degree 4: $f_{41}=(\mathbf{q}_1\cdot\mathbf{q}_2)^2$, $f_{42}=(\mathbf{q}_1\cdot\mathbf{q}_2)(\mathbf{q}_1\cdot\mathbf{q}_3)$, $f_{43}=(\mathbf{q}_1\cdot\mathbf{q}_2)(\mathbf{q}_3\cdot\mathbf{q}_4)$, since all powers of $q_i^2$ can be re-expressed in terms of powers of $\mathbf{q}_i\cdot\mathbf{q}_j$, $i\neq j$.

Next we substitute the above expansion into Eq. (2) and,

 

by expanding $B(q)$ and $C(q)$ where appropriate, express the resulting series in terms of the functionals $F_{pin}[s]$, which we then regroup according to their contribution to $\partial H_{pi}[s,t]/\partial t$. Limiting ourselves here to the cases $p=0, 2$ we get

$$\frac{\partial}{\partial t}H_0[s,t] = d\sum_n a_{0n}F_{0n} - B_0\sum_n n a_{0n}F_{0n} + K_0\sum_n n(n-1)a_{0n}F_{0,n-2} - 2K_2\sum_n a_{2n}F_{0,n-2} + C_0\sum_{n,m} nm a_{0n}a_{0m}F_{0,n+m-2} + \cdots , \tag{4a}$$

$$\frac{\partial}{\partial t}H_2[s,t] = d\sum_n a_{2n}F_{2n} - 2\sum_n a_{2n}F_{2n} - B_0\sum_n n a_{2n}F_{2n} + B_2\sum_n n(n-1)a_{0n}F_{2n} + K_0\sum_n (n-2)(n-3)a_{2n}F_{2,n-2}$$
$$- C_2\sum_{n,m} n(n-1)m(m-1)a_{0n}a_{0m}F_{2,n+m-2} + 2C_0\sum_{n,m}[2n(n-1)+n(m-2)]a_{0n}a_{2m}F_{2,n+m-2} + \cdots , \tag{4b}$$

where the terms indicated by $\cdots$ are contributions from $H_{pin}[s,t]$ with $p \geq 4$, $B(q) = B_0 + B_2 q^2 + \cdots$, $C(q) = C_0 + C_2 q^2 + \cdots$, and $K_n = \int_q C(q) q^n$.

If we wished, we could now determine a set of ordinary differential equations (ODE's) for the $a_{pn}(t)$ by equating the coefficients of $F_{pn}[s]$ on both sides of Eq. (4). However, given the introductory remarks, one does not expect this approach to give any advantage over already existing techniques. Instead we define new functions $W_{pi}(x,t) \equiv \sum_n a_{pin}(t)x^n$ and construct PDE's for the $W_{pi}(x,t)$ that yield precisely the same ODE's for the $a_{pin}(t)$ as Eq. (4). These PDE's then provide an alternate representation of Wilson's exact RG equation which is not only a good starting point for numerical computation, but also has a number of other very attractive features which will be shown below.

Given the coefficient structure of Eq. (4) it is a simple matter to construct the desired PDE's, namely,

$$\frac{\partial W_0}{\partial t} = dW_0 - B_0 x\frac{\partial W_0}{\partial x} + K_0\frac{\partial^2 W_0}{\partial x^2} - 2K_2\frac{1}{x^2}W_2 + C_0\left(\frac{\partial W_0}{\partial x}\right)^2 \tag{5a}$$

$$\frac{\partial W_2}{\partial t} = (d-2)W_2 - B_0 x\frac{\partial W_2}{\partial x} + B_2 x^2\frac{\partial^2 W_0}{\partial x^2} + K_0 x^2\frac{\partial^2}{\partial x^2}\left(\frac{1}{x^2}W_2\right) - C_2 x^2\left(\frac{\partial^2 W_0}{\partial x^2}\right)^2 + 4C_0\left(\frac{\partial^2 W_0}{\partial x^2}\right)W_2 + 2C_0 x^2\frac{\partial W_0}{\partial x}\frac{\partial}{\partial x}\left(\frac{1}{x^2}W_2\right) . \tag{5b}$$

A still simpler form results if we substitute $\hat{W}_2(x,t) = W_2(x,t)/x^2$, but we will not reproduce it here.

One can easily extend this construction to include higher $p$ values. The $p=0$ equation has already been derived and studied (in somewhat different contexts) in an early paper by Nicoll, Chang, and Stanley,[7] and more recently by Tokar.[8] They demonstrated its equivalence to order $\epsilon$ with exact $\epsilon$-expansion results, and also[8] its suitability for approximate ($\eta = 0$) numerical calculations in three dimensions. However, neither investigation recognized the $p=0$ equation as the leading member of an exact hierarchy of equations which could be derived and studied to higher orders.

The hope is, of course, that such a hierarchy may provide a method of successive approximation to the exact solution, the higher $p$ values contributing only small corrections to the (presumed) dominant behavior of the small-$p$ terms. Because there is no small parameter available with which we can generate (as with the $\epsilon$ expansion) exact analytic solutions to higher and higher orders, we are instead forced into the rather *ad hoc* scheme of simple truncation of the hierarchy with the question of convergence to be answered empirically. In this respect the approach is similar to other nonperturbative approaches such as finite lattice[1] and scaling field methods.[9,10] Such approaches appear to share an advantage over exact analytic expansions in that one can try to optimize their results through an appropriate choice of what would be redundant parameters[4] in an exact approach. In fact, some such optimization appears to be necessary for such nonperturbative approaches to be useful in low orders of approximation.[1,10,11] In my own results, to be discussed below, I indeed find that the effect of the omitted higher powers of momenta can, to some extent, be controlled by the appropriate choice of the redundant rescaling function $\phi(q)$.

Before proceeding to numerical study of the equations it is first useful to study the physical significance of the function $W_0(x,t)$. This can be done by using Wilson's exact generating functional for spin correlation functions[3]

$$Z(j) = \int_{[\sigma]} \exp\left[\int_{\mathbf{q}} j(\mathbf{q})\sigma_{-\mathbf{q}} + \mathcal{H}[\sigma,0]\right] ,$$

where $\int_{[\sigma]}$ denotes functional integration. Following Wilson and Kogut[3] this can be written in terms of the Hamiltonian $H[s,t]$ as

$$Z(j) = \lim_{t\to\infty} \exp H[s_t',t] ,$$

where

$$s_t'(\mathbf{q}) = \phi(q)j(\mathbf{q}e^{-t})\exp[\beta_q(t) - dt/2]$$

and

$$\beta_q(t) = (1+\Delta)t + q^2(1-e^{-2t}) .$$

We may then calculate the free energy for the system in a spatially uniform (reduced) magnetic field $h = H/k_B T$ by expanding $H[s_t',t]$ in terms of Eqs. (3a) and (3b) and substituting

$$j(\mathbf{q}) = \int e^{i\mathbf{q}\cdot\mathbf{x}}h(\mathbf{x})d^d\mathbf{x} = (2\pi)^d h\delta(\mathbf{q}) .$$

Then all contributions from $H_{p\neq 0}[s_t',t]$ with $p\neq 0$ integrate to zero, resulting in the *exact* expression for the reduced free energy per unit volume:

$$f(K,h) = -1/\delta(0)\ln Z(h)$$
$$= -\lim_{t\to\infty} e^{-dt} W_0(he^{(1+\Delta+d/2)t},t) \ , \qquad (6)$$

where for completeness I have included $K = J/k_B T$, the reduced coupling, which is contained implicitly in $H[s,0]$.

Thus $W_0(x,t)$ is a useful function indeed! It is interesting that here it plays the role of the (magnetic) Gibbs free energy, while the analogous function for sharp-cutoff RG's is its Legendre transform, the Helmholtz free energy, or effective potential.[12] Thus, knowing the *zero-field* $W_0(x,t)$, one can calculate directly equations of state, crossover functions, etc., for the entire phase diagram.

At the $h=0$ critical point we have (for $\Delta=\Delta^*$)

$$\lim_{t\to\infty} W_{0,\text{crit}}(x,t) = W_0^*(x) \ ,$$

the critical fixed point. The corresponding free energy at $K=K_c$ for arbitrary $h$ is

$$f(K_c,h) = -\lim_{t\to\infty} e^{-dt} W_{0,\text{crit}}(he^{(1+\Delta^*+d/2)t},t) \ .$$

When there are no dangerous irrelevant variables[13] we can write, to leading order,

$$f(K_c,h) = -\lim_{t\to\infty} e^{-dt} W_0^*(he^{(1+\Delta^*+d/2)t}) \ .$$

For the limit to exist we must have $W_0^*(x)\propto x^{d/(1+\Delta^*+d/2)}$ as $x\to\infty$, and thus $f(K_c,h)\sim \text{const}\times h^{1+\delta}$, where $\delta=(d-2+\eta)/(d+2-\eta)$, the standard hyperscaling form for the free energy at $K_c$.[13]

If we now turn to the approximation Eqs. (5a) and (5b) it is easy to determine the asymptotic fixed-point solutions for large $x$, namely, $W_0^*(x)\propto x^u$, and $\hat{W}_2^*(x)\propto(A-2)x^{u-2}+\text{const}\times x^{2u-4}$, where $u=d/(1+\Delta+d/2)$, and $A$ is a redundant parameter contained in the rescaling function $\phi(q)=e^{-q^2}/(Aq^2+e^{-2q^2})$ chosen to allow comparison of our numerical results with those of the scaling-field method where the same function naturally appears.[9,10] We note the surprising result that the approximate equations yield the exact asymptotic behavior for $W_0^*(x)$,[14] i.e., that its behavior dominates that of the other $W_p^*(x)$ at large $x$. This is a natural result of the feedback structure of the hierarchy, and thus it gives us some encouragement that corrections from the higher-$p$ contributions might be small. These asymptotic results are also a useful guide in locating the numerical solutions to the fixed point equations, which we now discuss for the case $d=3$.

Rather than integrate the PDE's (5a) and (5b) from initial values $W_0(x,0)$ and $W_2(x,0)$ to locate the critical fixed point, it is simpler and more useful to solve the fixed point equations $\partial W_p(x,t)/\partial t=0$ directly. The problem then becomes one of ODE's. For fixed parameters $A$ and $\Delta$ we can determine the fixed point solution by locating initial values $W_0^*(0)$ and $\hat{W}_2^*(0)$ such that the integrated equations have the correct asymptotic behavior. For improper choices of the initial values, the integration instead results in singular behavior which is easily distinguished from the desired result. Once the fixed point is found, the equations linearized about this fixed point are then solved to determine the critical exponents.

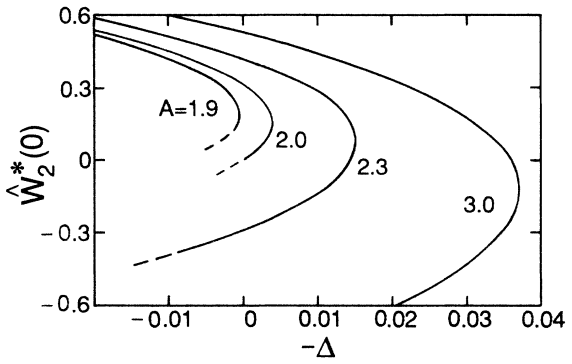


FIG. 1. The fixed point initial values $\hat{W}_2^*(0)$ vs $-\Delta$ for several values of $A$. The dashed lines indicate a region where the numerical routines have difficulty converging, though there is good evidence that the solutions continue to exist.

We find that as functions of $A$ and $\Delta$ the solutions of our equation have a structure similar to that of other nonperturbative linear RG approaches.[10,15] For fixed $A$, fixed-point solutions exist for a continuous range of $\Delta$ as shown in Fig. 1, where we have plotted the fixed-point initial value $\hat{W}_2^*(0)$ vs $-\Delta$ for several $A$ values. In contrast, the solution of the exact RG equations would exhibit a single vertical line (i.e., independent of $A$) at the physical value of $\Delta^*=-\eta/2$. The exact structure is due to the presence of a marginal redundant operator in the RG transformation which generates the line of physically equivalent fixed points parametrized by $\hat{W}_2^*(0)$.[9,15,16] Because the truncated form of the operator is no longer necessarily marginal or redundant, we get instead the results of Fig. 1. Typical of these results, however, is the existence of a marginal operator at that value of $\Delta$ where the slope of the curve becomes infinite, and we follow the standard practice[10,15] of choosing that value as the best approximation for the physical $\Delta^*$.

From Fig. 1 we see a strong nonuniversal dependence of $\Delta^*$ (and hence $\eta$) on $A$. This is also true for the thermal eigenvalue $y_1(\Delta^*(A))$ which determines the exponent $\nu=1/y_1$. In fact, over the range of $A$ studied so far, $2\leq A\leq 4$, the dependence is nearly linear and well approximated by $\eta=0.01+0.07(A-2)$, and $\nu=0.63-0.08(A-2)$. Thus we must choose a "best value" of $A$ for our approximation. In Fig. 2 we show $\hat{W}_2^*(K_0^{1/2}x)$ when $\Delta=\Delta^*(A)$ for several $A$ values. We see that $A$ indeed controls the

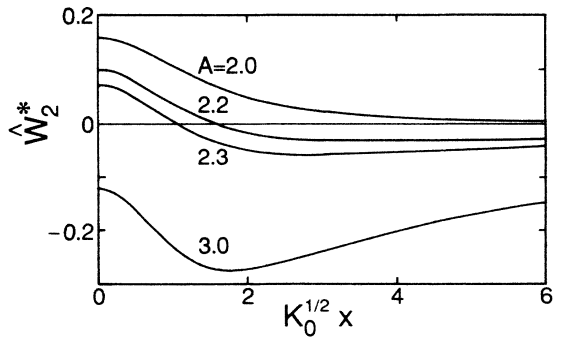


FIG. 2. The fixed point solution $\hat{W}_2^*(K_0^{1/2}x)$ at $\Delta=\Delta^*(A)$ for several values of $A$.

strength of the higher $p$ contributions to $H[s,t]$. If, without any more rigorous criterion, we choose $A$ to roughly minimize the "size" of $\hat{W}_2^*(K_0^{1/2}x)$, say $2.1 \leq A \leq 2.3$, we get $\eta = 0.024 \pm 0.007$ and $\nu = 0.617 \pm 0.008$. These values are a little lower than currently accepted estimates[17] from field theoretic, high-temperature, and scaling-field expansions, but given the simplicity of our calculation and the low order of approximation, they are quite acceptable.

To move toward greater accuracy the next step is obviously to extend the calculation to higher $p$ values and study the convergence properties of our simple truncation scheme. The ideal situation would be that for some appropriately chosen rescaling function $\phi(q)$ the higher $p$ terms become successively and rapidly less important. Then $\phi(q)$ could be used to optimize the solution, hopefully in a precise and unbiased fashion, to any order of truncation.

The essential point at this stage is the simplicity of extending this approach in many directions, e.g., higher $p$ values, $n$-component systems, equations of state and crossover scaling functions, and perhaps even gauge theories. Even in their present form Eqs. (5) and (7) should allow a fairly thorough numerical study of the wetting problem.[2] The ability to perform simple, nonperturbative RG calculations in an infinite-dimensional space of interactions gives this approach great flexibility and encourages its application to problems in many areas.

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