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Critical Behavior of the Yvon-Born-Green Equation: Effects of Dimensionality

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Analytic studies of the Yvon-Born-Green equation have suggested that it may show no true critical region for spatial dimension $d \leq 4$ but that for $d > 4$ there is a critical point of the mean-field type. Presented here are the results of numerical solution of the equation which strongly support these suggestions. Thus the Yvon-Born-Green equation exhibits the correct borderline dimensionality of four and the expected mean-field behavior for $d \geq 4$, but for $d < 4$ has only a region of long, but finite, ranged correlations.

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The critical behavior of the Yvon-Born-Green (YBG) integral equation, in the theory of fluids, has been the subject of a number of recent investigations.[1-5] Interest was attracted to this problem by numerical studies[1] of the spatial dimension $d = 3$, square-well, YBG equation which appeared to have a region of long-ranged solutions characterized by values of the critical exponents γ, β, δ, and α very close to those believed to be correct. This suggests that the YBG equation might provide an asymptotically correct description of the critical region of fluids. This perspective was changed by the publication of analytic studies[2,3] in which the full YBG integral equation was reduced, in the region of long-ranged solutions, to a nonlinear differential equation by use of a moment expansion. In particular, it was shown[2] that, for $d \leq 4$, if the inverse correlation length κ were to become zero then the pair correlation must necessarily be negative (in disagreement with the numerical studies[1]) at intermediate and long range, with the critical exponent η (incorrectly) given by $\eta = 4 - d$, whereas for $d > 4$, $\kappa = 0$ is compatible with a positive pair correlation with $\eta = 0$. Further analysis[3] has led to the prediction that the correlations have the Ornstein-Zernike form in the critical region for $d > 4$ but that for $d \leq 4$, the isothermal compressibility K_T must remain bounded unless the correlations become negative. The analytic work[2-4] is not, as yet, capable of predicting either the numerical values of the exponents β, γ, and δ, or their dependence on spatial dimension d. Hence a full understanding of the critical behavior of the YBG equation, and its dependence on spatial dimensionality, must rely on a combination of analytic results and careful numerical solutions. We believe that the analytic studies and the improved and more extensive numerical results we present here (and elsewhere[5]) strongly support the following conclusions: (1) For $d \leq 4$, the YBG equation has solutions for which κ is small but never zero, attaining, for $d = 3$, a minimum value of about $0.08\sigma^{-1}$ (σ is the hard-core radius). In this

region the thermodynamic behavior is approximately characterized by algebraic singularities with realistic exponent values; however, no true critical point ($\kappa = 0$) is present. (2) For $d > 4$ a true critical point occurs, and in its vicinity the correlations have, as predicted,[3] the Ornstein-Zernike form. In addition, the exponents γ, β_s, and δ have the classical mean-field values and the compressibility K_T is a homogeneous function of the appropriate thermodynamic variables.

Thus it appears that, as a theory of critical phenomena, the YBG equation exhibits the correct upper borderline dimensionality[2] of $d = 4$ and largely the correct mean-field-like behavior for $d > 4$, but that for $d < 4$ it shows a, perhaps interesting, approximate critical region which nevertheless ultimately fails to develop into a correct description.

The YBG equation in spatial dimension d can be written as

$$\frac{d}{dr}\ln g(r) = \frac{du(r)}{dr} + \frac{\lambda}{r}\int_0^\infty \int_{|r-s|}^{r+s} \frac{du(s)}{ds} g(s)(s^{d-2}t)\cos\theta \sin^{d-3}\theta\,[g(t)-1]\,dt\,ds, \tag{1}$$

where $g(r)$ is the pair correlation function, $u(r) = \varphi(r)/k_B T$ is the reduced intermolecular potential, $\lambda = \rho(d-1)\pi^{(d-1)/2}/\Gamma(d+1/2)$, ρ is the molecular number density,[4] and $\cos\theta = (r^2+s^2-t^2)/2rs$. Our numerical method for solving (1) is, briefly, to replace the upper limit of the s integration by a large but finite value (100σ), set $g(r) = 1$ for $r > 100\sigma$, discretize the continuous variables, and compute the right-hand side of (1) by trapezoidal-rule integration, with use of some initial choice for $g(r)$. We then integrate (1) numerically from r to 100σ and exponentiate to obtain from the left-hand side of (1) the iterated values of $g(r)$, which are used as input for the next iteration. The successive iterations empirically converge geometrically, at least for well chosen initial $g(r)$, and the iterative process is continued until certain convergence criteria are satisfied. Our calculations have been done by using a hard-core, attractive square-well intermolecular potential[1] of hard-core radius unity and well radius 1.85. We give our results in terms of a reduced inverse temperature $\theta = \epsilon/k_B T$, where ϵ is the well depth, and the reduced density parameter λ. With the above procedure we construct numerical solutions for $g(r)$ for various points in the (θ,λ) plane, using the converged solutions at one point as the input for the iterative process at a neighboring point, in a search for values of (θ,λ) for which $g(r)$ becomes long ranged and the compressibility K_T [i.e., the integral of $g(r)$] becomes large. Now if the YBG equation exhibits critical behavior we expect[1,2] to find a curve in the (θ,λ) plane (the stability line) such that as we approach any point on that curve the inverse correlation range κ tends to 0. We can determine κ from the decay of $g(r)$ at large r but the analytic studies[2] also provide an expression for κ which depends only on values of $g(r)$ inside the potential range. The κ values determined in these two ways, from the numerical solutions, agree to about 1% and this comparison provides an internal check on the numerical method.

The major difficulty in determining the stability line is that the convergence rate of the interative process becomes very slow as $\kappa \to 0$. A quantity X_n computed by a convergent first-order iterative process will usually approach its limit $\bar{X}$ geometrically for large n, i.e., as $|X_n - \bar{X}| = AC^n$ where $0 < C < 1$. If C is close to 1 the process converges very slowly. Our iterative procedures follow, quite accurately for large n, the above geometric pattern but for solutions with κ near zero, C is very near 1 so that the process is slowly convergent. It appears empirically, and there is some theoretical reason to believe, that $C = 1$ at, or very close to, the stability line. Because of this solutions with κ very small are very time consuming to construct and the stability line must be found by careful extrapolation to $\kappa = 0$.

We have now a large set of solutions for $d = 3$ and $d = 6$, and some solutions for $d = 5$, in the small-κ regions of their (θ,λ) planes. Although the $d = 3$ case will be described in some detail elsewhere,[5] it is useful here to contrast the $d = 3$ and the $d = 6$ results. We locate the line of stability by fixing λ and looking at the θ dependence of κ. If we do this for the $d = 3$ case, say at $\lambda = 4.60$ which was previously[1] thought to be the critical isochore, we find that the κ values determined in the range $0.368 \leq \theta \leq 0.372$ *appear* to extrapolate to zero at $\theta_c \simeq 0.374$; this led Green *et al.*[1] to determine, for example, the exponent γ by using solutions in the above range of θ. We have since constructed five numerical solutions for larger values of θ, in the range $3.72 < \theta \leq 3.85$ and find that the previous extrapolation of $\kappa \to 0$ is *not* followed but that κ in fact passes through a minimum of about 0.08 near $\theta \simeq 0.375$. The convergence rate is slow ($C \simeq 0.997$) but very stable in this region and good quality solutions can be found at the

expense of considerable computer time. For the $d=6$ case, say at $\lambda=23.94$, as θ varies from 0.045 80 to 0.045 85, κ falls from 0.0943 to 0.0485 and extrapolates (by a method to be discussed) very accurately to zero at $\theta=0.045\,868$. The convergence rates are *very* low ($C\simeq 0.999$) but fairly stable and good quality solutions are found. Now, however, if we try to construct solutions for $\theta \gtrsim \theta_c$, the values of κ^2, determined by the first hundred or so iterations, become negative and the iterative process also begins to diverge ($C>1$) rapidly; i.e., we are unable to find solutions inside the line of stability. We believe that this and the following numerical results are strong evidence that the YBG equation has for $d=6$ (and $d=5$) a true stability line along which $\kappa=0$.

For the $d=6$ case we determine the line of stability by fixing λ and fitting the κ vs θ data by the usual algebraic form $\ln\kappa=\ln A+\nu\ln(\theta_s/\theta-1)$, where A, θ_s, and ν are fitting parameters. The quality of a typical fit can be seen from Table I. The best fit is for parameter values $\theta_s=0.045\,868$, $\nu=0.499\,93$, and $\ln A=0.894\,48$. Any change in the last significant figure appreciably worsens the fit. In Table I, Δ is the fractional difference between the numerical values of κ and the fitting curve. The fit is *very* good and shows no sign of worsening at values of θ nearest θ_s. In Table II we show the results of a series of such fits at several λ which determines five points on the (low-λ side) of the stability curve. Because of the large amount of computer time required we have less extensive data on the high-λ side. The stability line is found by fitting this data by a quadratic curve $\theta_s(\lambda)=\theta_c+C(\lambda-\lambda_c)^2$. The best fit to the data of Table II is uniformly better than one part in 10^6 and determines the critical values $\theta_c=0.045\,867\,98$, $\lambda_c=23.91$, and $C=2.104\,74\times10^{-5}$. The curve is very flat near its minimum so that the data determine θ_c much more accurately than λ_c. In fact we can assume that the last point in Table II is the critical point and still obtain a satisfactory quadratic fit. These results, of course, imply the mean-field value of $\beta_s=0.5$ for the exponent characterizing the stability line.

We have good quality solutions at 21 points in the (θ,λ) plane near the low-λ side of the stability line. To see if the data describe mean-field like behavior we have fitted all the data by the form $\kappa^2=D[(\theta_c-\theta)+C(\lambda-\lambda_c)^2]$, where D is the only remaining unknown parameter. For $D=131$ all of our values of κ^2 are uniformly fitted to better than 1%. It is difficult to make a firm estimate of the absolute accuracy to which our numerical solutions determine κ but various tests and internal consistency checks suggest an accuracy of around 1%, and so we regard the above agreement with mean-field behavior to be as good as, or perhaps slightly better than, can be expected. In fact we do not fully understand the considerably higher accuracy of the stability-line fits.

The critical exponents γ and δ are to be found from the compressibility K_T. Here we are considerably helped by the prediction,[3] from the analytic studies, that for κ close to zero $K_T\propto\kappa^{-2}$. We have checked this relation along two isochores and find that it holds to much better than 1%. We thus assume that it is true near the stability line and this implies the mean-field form $K_T=[A'(\theta_c-\theta)+B'(\lambda_c-\lambda)^2]^{-1}$ for the compressibility, and that the exponents have the classical values $\gamma=1$ and $\delta=3$. The relationship $K_T\propto\kappa^{-2}$ is of considerable practical importance to us because κ is computed from short-range values of $g(r)$ whereas K_T is found by integrating $g(r)$ and strongly depends on accurate values of $g(r)$ at large r. It is an empirical characteristic of our iterative method that after a large number of iterations (~ 1000) the convergence rate is the same, and slow, for all r but that for the first few hundred iterations, the convergence rate for $g(r)$ at small r is much higher than its asymptotic value. Thus the short-range values of $g(r)$ are known to good relative accuracy after a few hundred iterations while it

TABLE I. Data for determination of the stability temperature θ_s at $\lambda=23.94$.

θ	κ	Δ
0.045 80	0.094 297	-4×10^{-5}
0.045 82	0.079 206	7×10^{-6}
0.045 83	0.070 466	3×10^{-5}
0.045 84	0.060 480	7×10^{-5}
0.045 85	0.048 494	-6×10^{-5}

TABLE II. Values of the stability temperature $\theta_s(\lambda)$ and exponent $\nu(\lambda)$ for various λ.

λ	$\theta_s(\lambda)$	$\nu(\lambda)$
22.40	0.045 916	0.4942
22.60	0.045 904	0.4946
22.80	0.045 894	0.4993
23.01	0.045 885	0.4967
23.94	0.045 868	0.4999

requires perhaps 2000 iterations to construct K_T to the same accuracy. Thus once we are convinced that $K_T \propto \kappa^{-2}$ we save large amounts of computer time by working with κ rather than K_T.

We have compared several of our best numerical solutions for $g(r)$, for $0.05 < \kappa < 0.08$ and $r \geq 20$, to the Ornstein-Zernike form and again found a satisfactory fit, indicating that the exponent η is equal to 0, as predicted by the analytic studies. Finally we have done enough work on the $d = 5$ case to locate the critical point and check that κ along the critical isochore is characterized by an exponent $\nu = 0.5045$ which we regard as agreement with the $d = 6$ case.

We feel that the combination of the analytic studies[2,3] and these numerical results make a convincing case that the YBG equation shows no true critical region for $d \leq 4$ and that its critical behavior is largely mean-field-like for $d > 4$. There is no way within the YBG framework to directly determine the phase coexistence boundary, which presumably lies outside the line of stability. Hence we cannot determine the traditional exponents β and γ'. If we *assume*, however, that the stability line and the coexistence curve have the same exponents, $\beta = \beta_s = 0.5$, then the result $K_T = [A'(\theta_c - \theta) + B'(\lambda_c - \lambda)^2]^{-1}$ implies that $\gamma' = \gamma = 1$. We emphasize that the above form for K_T is valid into the stability line, not just to the coexistence curve. Whether or not the solutions of the YBG equation in the region between the coexistence curve and the stability line have any "physical" interpretation as metastable states is not clear to us.

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Note added.—We have recently obtained numerical solutions along two isochores on the high-density side of the stability line. These data are well described by the same expressions used in this paper and so the critical behavior is symmetric between the high- and low-density sides of the critical point, as is expected. This is of some interest in view of the recently discovered strong asymmetry of the coexistence curve of the Percus-Yevick equation [see S. Fishman and M. E. Fisher, Physica (Utrecht) 108A, 1 (1981)].

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Unification and Family Structure as Consequences of Universality

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Implementation of universality "reduces" the most general simple gauge group that treats all fermions of one color irreducibly to the gauge group $G = U(1) \otimes SU(2) \otimes SU(2)'$. For the natural choice of Higgs representation, the G gauge theory is the same, at low energy, as the standard $U(1) \otimes SU(2)$ theory. The fundamental representation of the unifying group breaks up into identical families of SU(2) doublets.

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In spite of the overwhelming experimental success[1] of the standard $U(1) \otimes SU(2)$ model of weak (including electromagnetic; the term "weak" is used in this sense throughout this Letter) interactions, theoretical questions remain, notably an understanding of families or generations of fermions. Current grand unified models[2] do not address this problem: They deal with a fixed small number of families [1 in the case of SU(5) and SO(10)] at a time. In this note, I indicate the basic features of an approach[3] to the description of families based on a proper incorporation of the