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.\(^5\) 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 \( \gamma, \beta, \delta, \) and \( \alpha \) 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\(^2\) 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 \( \kappa \) 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 \( \eta \) (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 \( \beta, \gamma, \) and \( \delta \), 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 \( \kappa \) is small but never zero, attaining, for \( d = 3 \), a minimum value of about 0.08\( r^{-1} \) (\( r \) is the hard-core radius). In this

\(^{5}\) It is possible that the correct behavior of the YBG equation is given by \( \eta = 4 - d \), whereas for \( d > 4 \), \( \kappa = 0 \) is compatible with a positive pair correlation with \( \eta = 0 \). Further analysis 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 is not, as yet, capable of predicting either the numerical values of the exponents \( \beta, \gamma, \) and \( \delta \), 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) strongly support the following conclusions: (1) For \( d \leq 4 \), the YBG equation has solutions for which \( \kappa \) is small but never zero, attaining, for \( d = 3 \), a minimum value of about 0.08\( r^{-1} \) (\( r \) is the hard-core radius).
region the thermodynamic behavior is approxi-
matel)ly 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,\(^2\) the Ornstein-
Zernike form. In addition, the exponents $\gamma$, $\beta_s$, and $\delta$
have the classical mean-field values and the
compressibility $K_T$ is a homogeneous function of
the appropriate thermodynamic variables.

$$
\frac{d}{dr} \ln g(r) = \frac{u(r)}{r} + \frac{\lambda}{r} \int_{r-s}^{r+s} \frac{dG(s)}{ds} g(s) (s^{d-2t}) \cos \theta \sin^{d-\delta} \phi \delta [g(\theta) - 1] dt ds,
$$

(1)

where $g(r)$ is the pair correlation function, $u(r) = \varphi(r)/k_BT$ is the reduced intermolecular potential,
$\lambda = \rho(d - 1)!^2/\pi^{d+1/2}$, $\rho$ is the mole-
cular number density, and $\cos \theta = s^2 + t^2 - 2st \cos \phi$.\(^3\)
Our numerical method for solving (1) is, briefly,
to replace the upper limit of the $s$ integration
by a large but finite value (100$\sigma$), set $g(r) = 1$
for $r > 100\sigma$, discretize the continuous variables, and
compute the right-hand side of (1) by trap-
pezoidal-rule integration, with use of some initial choice
for $g(r)$. We then integrate (1) numerically from
$r$ to $100\sigma$ 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 suc-
cessive iterations empirically converge geometri-
cally, at least for well chosen initial $g(r)$, and
the iterative process is continued until certain
convergence criteria are satisfied. Our calcula-
tions have been done by using a hard-core, at-
tractive square-well intermolecular potential\(^1\)  of
hard-core radius unity and well radius 1.85. We
give our results in terms of a reduced in-
terface temperature $\theta = k_BT$, where $\epsilon$ is the well
depth, and the reduced density parameter $\lambda$. With
the above procedure we construct numerical solutions
for $g(r)$ for various points in the $(\theta, \lambda)$ plane, us-
ing the converged solutions at one point as the in-
put for the iterative process at a neighboring
point, in a search for values of $(\theta, \lambda)$ 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 $(\theta, \lambda)$ plane (the
stability line) such that as we approach any point
on that curve the inverse correlation range $\kappa$
tends to 0. We can determine $\kappa$ from the decay
of $g(r)$ at large $r$ but the analytic studies\(^2\) also
provide an expression for $\kappa$ which depends only
on values of $g(r)$ inside the potential range. The
$\kappa$ values determined in these two ways, from the
numerical solutions, agree to about 1% and this

Thus it appears that, as a theory of critical
phenomena, the YBG equation exhibits the cor-
rect 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 inter-
esting, approximate critical region which never-
thless ultimately fails to develop into a correct
description.

The YBG equation in spatial dimension $d$ can be
written as

comparison provides an internal check on the nu-
merical method.

The major difficulty in determining the stability
line is that the convergence rate of the iterative
process becomes very slow as $\kappa = 0$. A quantity
$X_n$ computed by a convergent first-order iterative
process will usually approach its limit $X$ geo-
metrically for large $n$, i.e., as $|X_n - X| = AC^n$
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 $\kappa$ near
zero, $C$ is very near 1 so that the process is slow-
ly 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 $\kappa$ 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-$\kappa$ regions of their $(\theta, \lambda)$ planes. Although
the $d = 3$ case will be described in some detail
elsewhere,\(^2\) it is useful here to contrast the $d = 3$ and the $d = 6$ results. We locate the line of stability
by fixing $\lambda$ and looking at the $\theta$ dependence
of $\kappa$. If we do this for the $d = 3$ case, say at $\lambda = 4.60$
which was previously\(^4\) thought to be the critical
isochore, we find that the $\kappa$ values determined in
the range $0.368 < \theta < 0.372$ appear to extrapolate
to zero at $\theta_0 \approx 0.374$; this led Green \textit{et al.}\(^4\) to
determine, for example, the exponent $\gamma$ by using
solutions in the above range of $\theta$. We have since
constructed five numerical solutions for larger
values of $\theta$, in the range $3.72 < \theta < 3.85$ and find
that the previous extrapolation of $\kappa = 0$ is not
followed but that $\kappa$ in fact passes through a minimum
of about 0.04 near $\theta = 0.375$. The convergence
rate is slow ($C \approx 0.997$) but very stable in this re-
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 $\theta$ varies from 0.04580 to 0.04585, $\kappa$ falls from 0.0943 to 0.0485 and extrapolates (by a method to be discussed) very accurately to zero at $\theta = 0.045868$. The convergence rates are very low ($C \approx 0.999$) but fairly stable and good quality solutions are found. Now, however, if we try to construct solutions for $\theta \geq \theta_c$, the values of $\kappa^2$, 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 $\lambda$ and fitting the $\kappa$ vs $\theta$ data by the usual algebraic form $\ln \kappa = \ln A + \nu \ln (\theta_c / \theta - 1)$, where $A$, $\theta_c$, and $\nu$ are fitting parameters. The quality of a typical fit can be seen from Table I. The best fit is for parameter values $\theta_c = 0.045868$, $\nu = 0.49985$, and $\ln A = 0.89448$. Any change in the last significant figure appreciably worsens the fit. In Table I, $\Delta$ is the fractional difference between the numerical values of $\kappa$ and the fitting curve. The fit is very good and shows no sign of worsening at values of $\theta$ nearest $\theta_c$. In Table II we show the results of a series of such fits at several $\lambda$ which we determine five points on the (low-$\lambda$ side) of the stability curve. Because of the large amount of computer time required we have less extensive data on the high-$\lambda$ side. The stability line is found by fitting this data by a quadratic curve $\theta_c(\lambda) = \theta_c + C(\lambda - \lambda_c)^2$. The best fit to the data of Table II is uniformly better than one part in $10^6$ and determines the critical values $\theta_c = 0.04586798$, $\lambda_c = 23.91$, and $C = 2.10474 \times 10^{-5}$. The curve is very flat near its minimum so that the data determine $\theta_c$ much more accurately than $\lambda_c$. 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 $\beta_\phi = 0.5$ for the exponent characterizing the stability line.

We have good quality solutions at 21 points in the $(\theta, \lambda)$ plane near the low-$\lambda$ 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 $\kappa^2$ 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 $\kappa$ 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 $\gamma$ and $\delta$ are to be found from the compressibility $K_T$. Here we are considerably helped by the prediction, from the analytic studies, that for $\kappa$ close to zero $K_T \propto \kappa^{-\gamma}$. 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 $K_T = [A(\theta_c - \theta) + B(\lambda_c - \lambda)]^{\gamma}$ 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 $K_T$ 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 ($\sim 1000$) 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>
<thead>
<tr>
<th>$\theta_0$</th>
<th>$\kappa_0$</th>
<th>$\Delta$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.04580</td>
<td>0.094297</td>
<td>$-4 \times 10^{-5}$</td>
</tr>
<tr>
<td>0.04582</td>
<td>0.079206</td>
<td>$7 \times 10^{-6}$</td>
</tr>
<tr>
<td>0.04583</td>
<td>0.070466</td>
<td>$3 \times 10^{-5}$</td>
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<tr>
<td>0.04584</td>
<td>0.060480</td>
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</tr>
<tr>
<td>0.04585</td>
<td>0.048494</td>
<td>$-6 \times 10^{-5}$</td>
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<table>
<thead>
<tr>
<th>$\lambda$</th>
<th>$\theta_0(\lambda)$</th>
<th>$\nu(\lambda)$</th>
</tr>
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<tbody>
<tr>
<td>22.40</td>
<td>0.045916</td>
<td>0.4942</td>
</tr>
<tr>
<td>22.60</td>
<td>0.045904</td>
<td>0.4946</td>
</tr>
<tr>
<td>22.80</td>
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<td>23.01</td>
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</tr>
<tr>
<td>23.24</td>
<td>0.045868</td>
<td>0.4999</td>
</tr>
</tbody>
</table>

TABLE II. Values of the stability temperature $\theta_0(\lambda)$ and exponent $\nu(\lambda)$ for various $\lambda$.
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 $\kappa$ rather than $K_T$.

We have compared several of our best numerical solutions for $\gamma(\nu)$, for $0.05 < \kappa < 0.08$ and $\nu > 20$, to the Ornstein-Zernike form and again found a satisfactory fit, indicating that the exponent $\eta$ 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 $\kappa$ 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 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 $\beta$ and $\gamma'$. If we assume, however, that the stability line and the coexistence curve have the same exponents, $\gamma' = \gamma = 0.5$, then the result $K_T = [A'(\bar{\beta} - \theta) + B'(\kappa_c - \lambda)]^{-1}$ 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)].

4S. Fishman, to be published.

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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