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# Surface effects on the susceptibility of confined systems near the critical point

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On the basis of the $\varphi^4$ model we describe the effect of non-periodic boundary conditions (b.c.) on the susceptibility or compressibility of three-dimensional (3D) confined systems for $T \geq T_c$ by taking into account a surface coupling. The result is compared with new Monte Carlo (MC) data for the 3D Ising model with free b.c. The qualitative and quantitative differences between MC data for periodic and free b.c. are well explained by the theory. The applicability of our theory to finite-size effects near the gas-liquid critical point of $^3$He is briefly discussed.

## 1. Introduction

Because of gravity effects, the theoretical and experimental study of finite-size effects near critical points of fluids has been restricted in the past to the $\lambda$-transition of $^4$He [1]. Recently the opportunity of using a microgravity environment has opened up the prospect of exploring finite-size effects also near gas-liquid critical points [2]. So far no quantitative theoretical predictions exist for this case. One expects that strong finite-size effects are exhibited by the compressibility $\chi$. Here we present preliminary results of a renormalization-group (RG) calculation of $\chi$ for $T \geq T_c$ within the $\varphi^4$ model in cubic geometry with *non-periodic* boundary conditions (b.c.). The results are tested by comparison with new Monte Carlo (MC) data for the susceptibility $\chi$ of the three-dimensional (3D) Ising model with free b.c.

## 2. Susceptibility for $T \geq T_c$

Our theory is based on the $\varphi^4$ model,

$$\mathcal{H} = \int_V \left[\frac{r_0}{2}\varphi^2 + \frac{1}{2}(\nabla\varphi)^2 + u_0\varphi^4\right] + \int_S \frac{c_0}{2}\varphi^2 , \quad (1)$$

for a one-component field $\varphi(\mathbf{x})$ in a $L^d$ cube with periodic b.c. in $d-1$ ($\mathbf{y}$) directions and a surface interaction $\sim c_0$ at the two surfaces $S$ perpendicular to the $z$-direction. We shall consider the leading deviation $\sim 1/c_0$ from Dirichlet b.c. ($c_0 = \infty, \varphi = 0$ at $S$). For this case the susceptibility $\chi_{c_0}(T, L) = V^{-1}\int_V d^d\mathbf{x} d^d\mathbf{x}' \langle\varphi(\mathbf{x})\varphi(\mathbf{x}')\rangle$ for $T \geq T_c$ has the structure

$$\chi_{c_0} = L^{-1}(1 + 2c_0^{-1}\partial/\partial L_z)(L_z\chi_\infty)|_{L_z=L} , \quad (2)$$

where $\chi_\infty$ is the susceptibility for D.b.c. Thus it suffices to study $\chi_\infty$. For $T \geq T_c$ we decompose $\varphi(\mathbf{x}) = \varphi_1 \sin(\pi z/L) + \sum' \sigma_{\mathsf{n},\mathbf{m}}(\mathbf{y}, z)$, where $\varphi_1$ is the lowest-mode amplitude and $\sigma_{\mathsf{n},\mathbf{m}}$ describe the higher modes [3]. The integers $\mathsf{n}$ and $\mathbf{m}$ are assigned to D.b.c. and p.b.c. , respectively. The sum $\sum'$ over $\mathsf{n}$ and $\mathbf{m}$ excludes the lowest mode ($\mathsf{n} = 1, \mathbf{m} = \mathbf{0}$).

We have determined $\chi_\infty$ in terms of averages $\langle(\varphi_1)^n\rangle$, $n$=2,4,6, apart from higher orders, where the weight of $\langle\ \rangle$ is $\exp\{-\mathcal{H}^{eff}\}$. The effective Hamiltonian $\mathcal{H}^{eff}(\varphi_1)$ is obtained from $\int \mathcal{D}\sigma\, e^{-\mathcal{H}}$ and reads to leading order

$$\mathcal{H}^{eff} = V\left[r_0^{eff}\varphi_1^2/2 + u_0^{eff}\varphi_1^4\right] + \mathcal{O}(\varphi_1^6) , \quad (3)$$

$$r_0^{eff}(r_0) = r_0 + \frac{\pi^2}{L^2} + 12\frac{u_0}{V}\sum{}' \left[p_{\mathsf{n},\mathbf{m}} + \frac{1}{2}p_{1,\mathbf{m}}\right] \quad (4)$$

with $p_{\mathsf{n},\mathbf{m}} = \left(r_0 + \frac{\pi^2}{L^2}(\mathsf{n}^2 + 4\mathbf{m}^2)\right)^{-1}$ and $u_0^{eff} = 3u_0/2 - 9u_0^2 V^{-1}\sum'(4p_{\mathsf{n},\mathbf{m}}^2 + 5p_{1,\mathbf{m}}^2 - 2p_{\mathsf{n},\mathbf{m}}p_{\mathsf{n}+2,\mathbf{m}})$ .

It is appropriate to introduce the temperature variable $s_0 = r_0 - r_{0c}(L)$, where $r_{0c}(L)$ incorporates a shift of the temperature scale relative to the case of p.b.c. Thus we define $r_{0c}(L)$ by requiring $[r_0^{eff}(r_{0c})]_{Dbc} - [r_0^{eff}(0)]_{pbc} = 0$. To describe the critical behaviour we turn to RG theory using minimal subtraction at $d = 3$ [4]. The renormalized counterpart $s(l)$ of $s_0$ [5] serves to determine the flow parameter $l(t, L)$ according to $s(l) = \xi_0^{-2}l^2$, where $\xi_0$ is the bulk amplitude of the correlation length $\xi = \xi_0 t^{-\nu}$, $t = (T - T_c)/T$. The deviation from D.b.c. is described by $c(l) = A_c l^{-\phi/\nu}$ with $\phi \approx 0.7$ [6]. Here the nonuniversal coupling $c_0$ enters via $A_c$ which is treated as adjustable parameter. The asymptotic ($L \gg \xi_0$, $t \ll 1$) result for $\chi_{c_0}$ reads

$$\chi_{c_0}(T,L) = L^{\gamma/\nu} P(x) \left[1 + 2A_c^{-1} L^{-\phi/\nu} g(x)\right] \qquad (5)$$

with $x = tL^{1/\nu}$. $g(x)$ is determined by $P(x)$ according to (2). The scaling function $P(x)$ is plotted in Fig. 1 (solid line). The non-negligible effect of the higher modes $\sigma_{n,m}$ is exhibited by the difference between the solid and the dot-dashed lines. Both curves differ significantly from $P_\chi^+(x)$ for p.b.c. (dashed line) [7]. We anticipate that $P(x)$ will exhibit a maximum below $T_c$ ($x < 0$) which can be included in the theory by extending $p_{n,m}$ to $p_{n,m}(\varphi_1)$ [8].

### 3. Comparison with Monte Carlo Data

In order to test our theory we have performed MC simulations of $\chi_{fbc}$ for the 3D Ising model for $L = 24, 56$ with f.b.c. in one direction. The nonperiodic b.c. were realized using a modified multi-spin-coding technique [9]. In the scaling plot (Fig. 1)

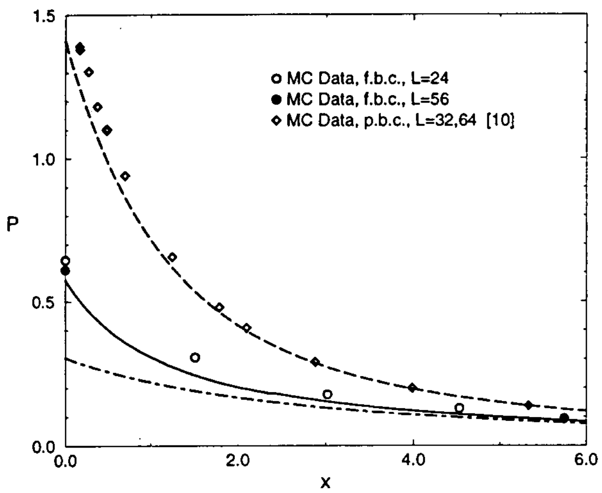


Figure 1: Theoretical prediction of the scaling function $P$ of $\chi_\infty$ vs $x = tL^{1/\nu}$ (solid line) in units of the lattice constant. Dot-dashed line: renormalized lowest-mode approximation for $\chi_\infty$, dashed line: $P_\chi^+$ of $\chi_{pbc}$ [7]. MC data of $\chi_{fbc}$ for $L = 24, 56$.

the significant suppression of $\chi_\infty$ (relative to $\chi_{pbc}$) predicted by the theory is consistent with the MC data for $\chi_{fbc}$. The latter agree with [11]. The systematic deviation of the $\chi_{fbc}$ data from $\chi_\infty$ indicates the necessity of including a finite $0 < c_0 < \infty$. In Fig. 2 this is taken into account by adjusting $A_c = 0.33$. Also shown is the asymptotic bulk curve [12] in order to demonstrate the fundamental difference between periodic and non-periodic b.c. In contrast to $\chi_{pbc}$, both $\chi_{c_0}$ and $\chi_\infty$ deviate from $\chi_{bulk}$ even for $\xi \ll L$ because of a power-law behaviour $\chi_{bulk} - \chi_\infty \sim t^{-\gamma-\nu}$. Thus this surface effect may be detectable well away from $T_c$, even if finite-size effects closer to $T_c$ are masked, e.g. , by gravity.

Possible applications to the liquid-gas critical point of $^3$He [2] would require to extend the $\varphi^4$ model to finite ordering field $h \neq 0$ in order to describe the entire vicinity of $(T_c, P_c)$ in the $(T, P)$ plane of the fluid phase diagram. The present results at $h = 0$, $T \geq T_c$ correspond only to a path in continuation of the coexistence line. It remains to be seen whether the (nonuniversal) properties of confined liquid $^3$He near a solid surface can be described within the $\varphi^4$ model of the type (1) with $0 < c_0 < \infty$.

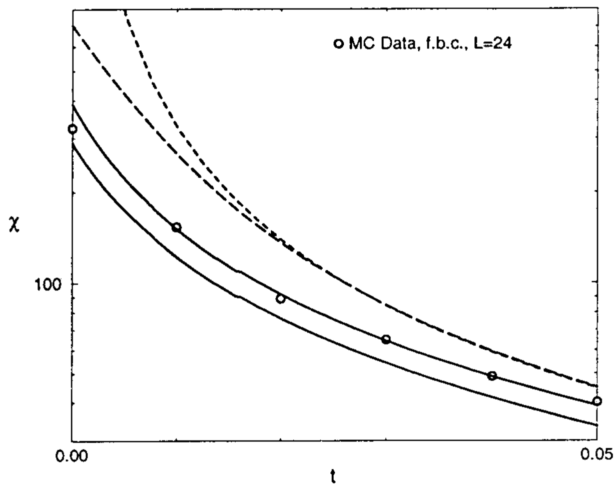


Figure 2: Theoretical prediction and MC data of the susceptibility $\chi$ for $L = 24$ vs t. From bottom to top: $\chi_\infty$, $\chi_{c_0}$ ($A_c = 0.33$), $\chi_{pbc}$ [7], $\chi_{bulk}$ [12].

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