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ON THE FINITE-SIZE SCALING IN THE PRESENCE OF QUANTUM FLUCTUATIONS

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1. INTRODUCTION

The idea of finite-size scaling (FSS) as formulated by Fisher[1] in 1971 and further developed by a number of authors concerns classical systems undergoing a phase transition[2]. It is well known from the theory of critical phenomena of bulk systems[3] that for $T_c > 0$ quantum fluctuations are negligible near the critical point. However, quantum systems may have critical points at temperature T=0. This would change the usual (classical) FSS in the low-temperature region.

In principle, there are four length scales if quantum effects are taken into consideration: the finite geometry characteristic size L, the correlation length ξ which diverges at the critical point, the microscopic range of the interactions a, and the thermal De Broglie wavelength λ_D which diverges at T=0 determining the "weight" of the quantum fluctuations in the process of phase transformation. Thus the various thermodynamic quantities must depend on the dimensionless ratios ξ/a, L/a and λ_D/a. According to the FSS hypothesis the <u>microscopic</u> length a must drop out from the expressions for the thermodynamic quantities close to the critical point $T=T_c$ of the bulk system. For example, for some physical quantity A (the finite-size susceptibility, the correlation length, etc.), FSS hypothesis states that

$$A_L(t) = A_\infty(t) f\left(L/\xi\,,\ L/\lambda_D\right)\,; \qquad (1)$$

where $t = (T-T_c)/T_c$ is the reduced temperature.

It is the purpose of the present article to verify the hypothesis (1).

2. THE MODEL

We use the statistical distribution $\exp(-H(\Psi))$ with the following quantum Landau-Ginzburg-Wilson functional[3-5]:

$$H(\psi)=\int_0^{\beta\hbar}d\tau\int d^dx\left[\frac{1}{2}\left(\frac{\partial}{\partial\tau}\psi(x,\tau)\right)^2+\frac{1}{2}\left(\nabla\psi(x,\tau)\right)^2+\frac{ta^{-2}}{2}\psi^2(x,\tau)+\frac{ga^{d-3}}{4!}\psi^4(x,\tau)\right]. \quad (2)$$

Here $\beta = 1/T$.

The parameters t and g are dimensionless, the microscopic distance **a** appears as an explicit dimensional factor, while the dimension of $\psi(x,\tau)$ is $L^{(1-d)/2}$.

In a fully finite (block) geometry and under periodic boundary conditions we expand the n-component order parameter $\psi(x,\tau)$ in Fourrier modes

$$\psi(x,\tau)=\sqrt{\frac{T}{\hbar V}}\sum_{k,\omega}e^{ik\cdot x+i\omega\tau}\psi(k,\omega). \quad (3)$$

In eq.(3) each component of k runs over discrete values specified by

$$k=(2\pi n_1/L,\dots,2\pi n_d/L),\ L=N_0 a,\ V=N_0^d a^d,\ n_i=0,\pm1,\pm2,\dots \quad (4)$$

and it is cut-off at a^{-1}. The Matsubara frequencies of the fluctuation field $\psi(k,\omega)\equiv\psi(q)$ are $\omega_\ell=2\pi\ell T/\hbar=2\pi\ell/\lambda_D,(\ell=0,\pm1,\dots)$, where for the thermal De Broglie wavelength we have $\lambda_D=\hbar/T$ in units consistent with (1). The substitution of eq.(3) in eq.(2) yields

$$H(\psi)=\frac{1}{2}\sum_{\substack{\alpha\\ q=(k,\omega)}}(\omega_\ell^2+k^2+ta^{-2})\psi_\alpha^2(q)+\frac{ga^{d-3}}{4!L^d\lambda_D}\sum_{\substack{\alpha,\beta\\ q_1,q_2,q_3}}\psi_\alpha(q_1)\psi_\beta(q_2)\psi_\alpha(q_3)\psi_\beta(q_1+q_2-q_3). \quad (5)$$

Splitting as usual the zero-momentum components $\psi_\alpha=\psi_\alpha(q=0)$ and tracing out all non-zero q [6,7], we obtain the effective distribution

$$\exp(-H_{eff}(\psi))=\sum_{\{\psi(q)\}}{}'\exp(-H(\psi_\alpha(q))), \quad (6)$$

which is the basis for calculating the finite-size effects in the low-temperature (quantum) region. In this case an extra "dimension" (being periodic with a finite-size $\lambda_D\sim L\gg1$) appears in comparison with the pure classical case.

3. FINITE-SIZE SCALING AND QUANTUM FLUCTUATIONS.

For $d>d_u$ (d_u is the upper critical dimensionality), the loop corrections can be ignored altogether and the effective distribution takes the form

$$\exp\left[\beta\hbar L^d\left(\frac{1}{2}ta^{-2}\psi^2+\frac{g}{4!}a^{d-3}\psi^4\right)\right]. \quad (7)$$

From eq.(7) for the susceptibility $\beta\hbar L^d\langle\psi^2\rangle$, we obtain

$$\chi=\xi^2G\left((L/a)^{d/2}(\lambda_D/a)^{1/2}(a/\xi)^2\right)=a^2t^{-1}F(xz), \quad (8)$$

where $x=\lambda_D/L$ and $z=t(L/a)^{(d+1)/2}/g^{1/2}$. In eq. (8) the microscopic distance **a** appears explicitly for $d>3$ manifesting the break_down of the scaling form (1).

For $d<d_u$, it is important to take into account the loop corrections. Let us consider the universal scaling variable

$$z=\tilde{t}(L/a)^{(d+1)/2}/\tilde{g}^{1/2}, \quad (9)$$

where

$$\tilde{t} = t_R + t_L \tag{10a}$$

and

$$\tilde{g} = g_R + g_L \tag{10b}$$

are the shifted dimensionless temperature and the coupling constant to one-loop order, respectively. The ψ^2 insertion counterterm renormalizes t to

$$t_R = t\, Z_{\psi^2} \quad , \tag{11}$$

where to one-loop order in the minimal subtraction scheme

$$Z_{\psi^2} = 1 + \frac{(n+2)}{6}\, g\, t\, \frac{1}{8\pi^2 \varepsilon} \tag{12}$$

Now the counterterm of the massless theory includes integration over the Matsubara frequency ω

$$\mathcal{U}(p,\Omega) = \frac{K_d}{2\pi} \int_{-\infty}^{\infty} d\omega \int d^d k \; \frac{1}{(k^2+\omega^2)\left[(k+p)^2+(\omega+\Omega)^2\right]} \tag{13a}$$

(cf. the classical case [6]).

The above function has a pole at d=3, while for d=3 - ε we have

$$\mathcal{U}(p,\Omega) = \frac{\Gamma(\frac{d}{2})\Gamma(2-\frac{d}{2})}{3-d} + O(\varepsilon) \cong \frac{1}{8\pi^2 \varepsilon} \quad , \; \varepsilon = 3-d \ll 1 . \tag{13b}$$

In eq.(13a) $K_d^{-1} = 2^{d-1}\pi^{d/2}\,\Gamma(d/2)$ is the area of the d-dimensional unit sphere.

The second term t_L in eq.(10) has the form (cf. [6])

$$t_L a^{-2} = \frac{(n+2)}{6}\, g\, a^{d-3} \frac{T}{\hbar L^d} \sum_{\omega_\ell}{}' \sum_{\underset{\sim}{k}}{}' \frac{1}{\underset{\sim}{k}^2 + \omega_\ell^2 + t a^{-2}} =$$

$$= \left(\frac{TL}{\hbar}\right)\left(\frac{L}{a}\right)^{1-d} \frac{g a^{-2}}{4\pi^2} \int_0^\infty du \left\{ A\left[\left(\frac{TL}{\hbar}\right)^2 u\right] A^d(u) - 1 \right\} e^{-\left(t\left(\frac{L}{a}\right)^2/4\pi^2\right)u} , \tag{14}$$

where $A(u) = \sum_{n=-\infty}^{n=+\infty} e^{-un^2}$ and the prime in the d-fold sum denotes that the term with a zero summation index has been omitted. The integral in the r.h.s. of eq.(14) has an ultraviolet divergence for d>1. Adding and subtracting the small-u asymptotic behaviour of $A\left[\left(\frac{TL}{\hbar}\right)^2 u\right] A^d(u)$ and after analytical continuation in d, we obtain the same pole as in eq. (11) but with an opposite sign.

The pole of t_L cancels the pole of t_R and for eq.(10a) we obtain

$$\tilde{t} = t + \frac{n+2}{12}\, \hat{g}\, t \ln t + \frac{n+2}{3} \left(\frac{TL}{\hbar}\right)\left(\frac{a}{L}\right)^2 \hat{g} \int_0^\infty du \left\{ A\left[\left(\frac{TL}{\hbar}\right)^2 u\right] A^3(u) - \right. \tag{15}$$

$$\left. - 1 - \left(\frac{TL}{\hbar}\right)^{-1}\left(\frac{\pi}{u}\right)^2 \right\} e^{-\left(t\left(\frac{L}{a}\right)^2/4\pi^2\right)u} + O(\hat{g}^2)$$

with

$$\hat{g} = \left.\frac{g}{2^d\, \pi^{(d+1)/2}\, \Gamma\left(\frac{d+1}{2}\right)}\right|_{d=3-\varepsilon} = \frac{g}{8\pi^2} + O(\varepsilon) . \tag{16}$$

Similar calculations to one-loop order for the renormalised coupling constant $\tilde{g}$ (eq.(10b)) lead to

$$\tilde{g} = g\left\{ 1 + \frac{n+8}{12}\, \hat{g}\,(1+\ln t) - \frac{n+8}{12}\, \frac{\hat{g}}{\pi^2} \left(\frac{TL}{\hbar}\right) \int_0^\infty du \; u \,\cdot \right. \tag{17}$$

$$\left. \cdot \left\{ A\left[\left(\frac{TL}{\hbar}\right)^2 u\right] A^3(u) - 1 - \left(\frac{TL}{\hbar}\right)^{-1}\left(\frac{\pi}{u}\right)^2 \right\} e^{-\left(t\left(\frac{L}{a}\right)^2/4\pi^2\right)u} + O(\hat{g}^2) \right\} .$$

In order to test the FSS hypothesis (1) in the vicinity below d_u let us consider the scaling variable z at the fixed point (f.p.). Here it is important to note that in the low-temperature region the upper critical dimensionality varies continuously from $d_u=4$ (classical case) to $d_u=3$ (quantum case)[3]. This in conjecture with the fact that $\tilde{t}$ and $\tilde{g}$ have been calculated near d=3 allows us to use the quantum fixed point value $\hat{g}^* = 6\varepsilon/(n+8)$, where $\varepsilon = 3-d$. After some algebra we have up to $O(\varepsilon^2)$

$$
\begin{aligned}
z\big|_{f.p.} &= \tilde{t}\left(\frac{L}{a}\right)^{(d+1)/2} \tilde{g}^{-1/2}\big|_{f.p.} = \\
&= (g^*)^{-1/2}\Big\{ y - \frac{\varepsilon}{4}y + \frac{(n-4)}{4(n+8)}\varepsilon y \ln y + \frac{2(n+2)}{(n+8)}\varepsilon x \int_0^\infty du \Big[A(x^2u)A^d(u) - 1 - \\
&\quad - \frac{1}{x}\left(\frac{\pi}{u}\right)^{(d+1)/2}\Big] e^{-(y/4\pi^2)u} + \frac{\varepsilon}{4\pi^2} xy \int_0^\infty du\, u \Big[A(x^2u)A^d(u) - 1 - \\
&\quad - \frac{1}{x}\left(\frac{\pi}{u}\right)^{(d+1)/2}\Big] e^{-(y/4\pi^2)u} + O(\varepsilon^2)\Big\}
\end{aligned}
\tag{18}
$$

or, inashort form

$$
z\big|_{f.p.} = z(x,y). \tag{19}
$$

To obtain the above expression, we used the quantum critical exponent $\nu = \frac{1}{2} + \frac{n+2}{4(n+8)}\varepsilon$ and the fact that the terms proportional to $\ln(L/a)$ cancel up to order ε^1 exactly. For convenience, in eq.(18) a new characteristic variable $y = t\left(\frac{L}{a}\right)^{1/\nu} = \left(\frac{L}{\xi}\right)^{1/\nu}$ is introduced. The result (19) verifies the FSS hypothesis(1).

4. CONCLUDING REMARKS

An eventual application of the FSS ideas to low-temperature (quantum) systems has been proposed by Cardy[2] (see the introduction of Ch. 1 therein). Certain progress along this line has been achieved on the basis of a lattice quantum model for structural phase transitions[8]. In ref. (9) the finite-size effects in quantum Heisenberg antiferromagnets (the nonlinear σ -model) in two and three dimensions have been analysed.

In the present study the finite-size scaling hypothesis in the presence of quantum fluctuations is verified by means of the ε - analysis. We used the ε -expansion approach of Brezin and Zinn-Justin[6] and Rudnick et al.[7] for studing the quantum FSS in the framework of a field theoretical model commonly used in the theory of structural phase transitions.

The crucial point in our calculations is the cancellation of the pole in the one-loop counterterm (see eq.(12)) with the pole of the finite-size correction (see eq.(14)). This is in close analogy to the pure classical case[6]. Let us note however that in the low-temperature region this cancellation takes place for $d=3-\varepsilon$ (see eqs.(15) and (17)). Hertz[3] was the first to note that in the low-temperature region quantum fluctuations reduce <u>continuously</u> the upper critical dimensionality from d_u to d_u-z (z is the dynamical exponent: for model (2) z is equal to 1 and $d_u=4$). From the latter it follows that for $T \to 0^+$ one may verify the FSS using the quantum (T=0) fixed point values for the coupling constants given by the dimensional crossover rule. This is done in the calculation of the universal scaling quantity z at the fixed point (see eq.(18)) and, hence, the validity of relation (18) is restricted to $d < 3$.

The appearance of an additional (in comparison with the pure classical case) variable $x = \lambda_D / L$ in eq.(1) is a consequence of the fact that except as a hypercube of linear size L, the system under consideration may be regarded as hyperparallelepiped of linear size L in d directions and of linear size $\lambda_D = \hbar/T$ in one direction with periodic boundary conditions. This anisotropy is in the origin of the complication of the FSS relation (1).

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