объединенный
институт
ядерных
исследований
дубна

E17-87-380

N.S.Tonchev

FINITE-SIZE EFFECTS IN A QUANTUM EXACTLY SOLUBLE MODEL FOR STRUCTURAL PHASE TRANSITION

Submitted to "Physica A"

1987

I. INTRODUCTION

A great deal of interest has recently arisen in exploring the finite-size scaling effects on the basis of exactly solvable models [1-8]. However, all the efforts in this direction are concentrated on the classical critical phenomena. Here, we consider a model whose finite-size critical behaviour can be studied exactly both in <u>classical</u> and <u>quantum</u> limits. The Hamiltonian of this model system, reads

$$\mathcal{H}=\frac{1}{2}\sum_{\ell}\left(\frac{\hat{P}_{\ell}^{2}}{m}-A\hat{Q}_{\ell}^{2}\right)+\frac{1}{4}\sum_{\langle\ell,\ell'\rangle}\Phi(\ell,\ell')(\hat{Q}_{\ell}-\hat{Q}_{\ell'})^{2}+\frac{B}{4N}\left(\sum_{\ell}\hat{Q}_{\ell}^{2}\right)^{2}. \quad (1)$$

Here, $\hat{Q}_{\ell}$ and $\hat{P}_{\ell}$ are the operators of displacement and momentum of the particle of mass m at site ℓ of a d-dimensional hypercubical lattice of size $L\equiv N^{\frac{1}{d}}$. The parameter $A\equiv\nu_{0}^{2}m>0$ determines the frequency of a mode unstable in the harmonic approximation, and the parameter $B>0$ "switches on" an anharmonic interaction, this being inversely proportional to the particle number N. The harmonic strength constant $\Phi(\ell,\ell')$ is nonsero only for finite numbers of neighbours on the lattice.

In the theory of structural phase transitions, models of this kind attract interest because for them the self-consistent phonon approximation turns out to be exact in the thermodynamic limit [9-11]. In [9] it was shown that in its bulk critical properties, in the classical limit, the model (1) belongs to the universality class of the Berlin-Kac spherical model. In refs [10,11], using the approximating hamiltonian method and some finite-size arguments, both the classical and quantum critical behaviour of the model (1) is studied exactly.

For a given system, because of the dimensional crossover rule* between its classical and quantum bulk critical behaviours, some relations between its finite-size properties in this limits also must exist. In the present study, a step in this direction is made. Using the method of refs.[10,11] the fully finite susceptibilities for the model (1) at the bulk critical temperature T_c are obtained in quantum and classical limits

2. THE BASIC EQUATION

Under periodic boundary conditions the inverted susceptibility of the system per particle $\Delta = \chi^{-1}(q\to 0, T) = \Omega^{-2}_{q=0}(\Delta)$ (see the notation and eqs.(4),(5) in ref. [11]) obeys the following self-consistency equation

$$1+\Delta = \frac{\lambda}{L^d}\sum_q \frac{1}{2\Omega_q(\Delta)}\coth\frac{\lambda\Omega_q(\Delta)}{2t} . \qquad (2)$$

In eq.(2) the dimensionless temperature $t=T/4E_0$ and the quantum parameter $\lambda=\hbar\nu_0/4E_0$, ($E_0=A^2/4B$ is the barrier height of the double-well potential in (1)), are introduced. The trial harmonic frequency $\Omega_q(\Delta)$ has the form:

$$\Omega^2_q(\Delta) = \Delta + s^\sigma\Big(\sum_{i=1}^{d} q_i^2\Big)^{\frac{\sigma}{2}} ,$$

with $\sigma=2$ for the short-range, and $0<\sigma<2$ for the long-range interaction of the particles in (1).

*For a review, see, e.g. ref. [12].

Separating the term with $q=0$ in eq.(2) and changing the sum over $q_i=(2\pi/L)n_i$, $n_i=\pm1,\pm2,\dots,+L/2$ with an integral over $x_i=(\alpha/L)n_i$, $\alpha=2\pi s$ we get

$$1+\Delta = \frac{\lambda}{2L^d\Delta^{\frac12}}\coth\frac{\lambda\Delta^{\frac12}}{2t} + \frac{\lambda}{2}\frac{S_d}{\alpha^d}\int_{x_1}^{x_D}\frac{x^{d-1}}{(\Delta+x^\sigma)^{\frac12}}\coth\frac{\lambda(\Delta+x^\sigma)^{\frac12}}{2t}\,dx, \quad (3)$$

where $S_d = 2(\pi)^{\frac{d}{2}}/\Gamma(d/2)$ is the surface of the d-dimensional unit sphere and $x_1=\alpha/L$, $x_D=\alpha(L_D/L)$, $L_D=L(d/S_d)^{\frac1d}$. The mathematical correctness of the change of eq.(2) by eq.(3), for large L, may be established by using the Euler-Maclaurin summation formula. A similar mathematical procedure is used for studying some asymptotic properties of the lattice sums in the theory of the random-walk on a lattice[13] . When parameter σ in eq.(2) is noninteger ($0<\sigma<2$), this approach has some advantage in comparison with those based on the Poisson summation formula.

3. FINITE-SIZE BEHAVIOUR OF THE SUSCEPTIBILITY AT T_c AND λ_c

We shall consider eq.(3) in two limiting cases: A) classical, when the bulk critical temperature $T_c>0$ and quantum parameter $\lambda=0$ (see ref.[10]); B) quantum, when the phase transition in the bulk system driven by a variation of λ occurs at some $\lambda_c>0$, and $T=0$ (see ref.[11]).

A) In the classical limit, and for d and σ not necessary integer numbers it is possible to express the integral in the r.h.s. of eq.(3) in terms of the hypergeometric function, i.e.

$$1+\Delta=\frac{t}{L^d\Delta}+\frac{tS_d}{d\,\alpha^d}\Big[\frac{X_D^d}{X_D^\sigma+\Delta}F\Big(1,1;1+\frac{d}{\sigma};\frac{X_D^\sigma}{X_D^\sigma+\Delta}\Big)-\frac{X_1^d}{X_1^\sigma+\Delta}F\Big(1,1;1+\frac{d}{\sigma};\frac{X_1^\sigma}{X_1^\sigma+\Delta}\Big)\Big]. \qquad (4)$$

The following asymptotic expressions for the susceptibility at the dimensionless bulk critical temperature $t_c=\alpha^d(d-\sigma)/S_d X_D^{(d-\sigma)}>0$ can be deduced after some algebra from eq.(4):

a) $$\chi_L^d(q=0,t_c)\sim\Delta_0^{-1}L^\sigma, \qquad (\sigma<d<2\sigma), \qquad (5)$$

where Δ_0 obeys the equation

$$\frac{t_c}{\Delta_0}\approx\frac{\alpha^d}{X_D^{(d-\sigma)}(\alpha^\sigma+\Delta_0)}F\Big(1,1;2-\frac{d}{\sigma};\frac{\Delta_0}{\alpha^\sigma+\Delta_0}\Big) \qquad (6)$$

b) $$\chi_L^d(q=0,t_c)\sim(\sigma/X_D^\sigma t_c)^{\frac{1}{2}}L^\sigma(\ln L)^{\frac{1}{2}}, \qquad (d=2\sigma) \qquad (7)$$

c) $$\chi_L^d(q=0,t_c)\sim t_c^{-\frac{1}{2}}L^{\frac{d}{2}}, \qquad (d>2\sigma). \qquad (8)$$

B) From eq.(3) in the quantum limit instead of eq.(4) we have

$$1+\Delta=\frac{\lambda}{2L^d\Delta^{\frac{1}{2}}}+\frac{\lambda S_d}{2d\,\alpha^d}\Big[\frac{X_D^d}{(X_D^\sigma+\Delta)^{\frac{1}{2}}}F\Big(1,\frac{1}{2};1+\frac{d}{\sigma};\frac{X_D^\sigma}{X_D^\sigma+\Delta}\Big)-\frac{X_1^d}{(X_1^\sigma+\Delta)^{\frac{1}{2}}}F\Big(1,\frac{1}{2};1+\frac{d}{\sigma};\frac{X_1^\sigma}{X_1^\sigma+\Delta}\Big)\Big]. \qquad (9)$$

At the bulk critical value of the parameter $\lambda_c=2\alpha^d(d-\frac{\sigma}{2})/S_d X_D^{(d-\frac{\sigma}{2})}>0$ one can obtain the following asymptotic expressions for the susceptibility:

a) $$\chi_L^d(q=0,\lambda_c)\sim\Delta_0^{-1}L^\sigma, \qquad (\tfrac{\sigma}{2}<d<\tfrac{3}{2}\sigma), \qquad (10)$$

where Δ_0 obeys the equation

$$\frac{\lambda_c}{2\Delta_0^{\frac{1}{2}}}\approx\frac{\alpha^d}{X_D^{(d-\frac{\sigma}{2})}(\alpha^\sigma+\Delta_0)^{\frac{1}{2}}}F\Big(1,\frac{1}{2};\frac{3}{2}-\frac{d}{\sigma};\frac{\Delta_0}{\alpha^\sigma+\Delta_0}\Big), \qquad (11)$$

b) $$\chi_L^d(q=0,\lambda_c)\sim(2\sigma/X_D^\sigma\lambda_c)^{\frac{2}{3}}L^\sigma(\ln L)^{\frac{2}{3}}, \qquad (d=\tfrac{3}{2}\sigma). \qquad (12)$$

c) $$\chi_L^d(q=0,\lambda_c)\sim(2/\lambda_c)^{\frac{2}{3}}L^{\frac{2}{3}d}, \qquad (d>\tfrac{3}{2}\sigma). \qquad (13)$$

4. DISCUSSION

In the thermodynamic limit it is possible to show that the critical behaviour of the system (1) obeys the dimensional crossover rule, i.e. the critical behaviour of the d-dimensional system at $T_c=0$ is equivalent to the behaviour of the classical $(d+\frac{\sigma}{2})$-dimensional system at $\lambda=0$. (for details see ref.[11], where the case $\sigma=2$ is studied).

Finite-size scaling states (see,e.g.[1]) that in the vicinity of T_c, $\chi_L(T)\sim L^{\gamma/\nu}$, where ν and γ are the bulk exponents measuring the divergence of the correlation length and susceptibility. Because of the dimensional crossover rule it is natural to suppose the same asymptotic behaviour of $\chi_L(\lambda)$ near λ_c.

In the case under consideration: $\gamma=\sigma/(d-\sigma)$, $\nu=1/(d-\sigma)$ in the classical limit and for $d_\ell^{cl}(\equiv\sigma)<d<d_u^{cl}(\equiv 2\sigma)$; $\gamma=2\sigma/(2d-\sigma)$, $\nu=2/(2d-\sigma)$ in the quantum limit and for $d_\ell^{q}(\equiv\frac{1}{2}\sigma)<d<d_u^{q}(\equiv\frac{3\sigma}{2})$. From eqs.(5) and (10) it is easy to verify that finite-size scaling is valid in both the classical and quantum cases, and in the former the finite-size critical behaviour of the model (1) is identical with that of the mean spherical model [1-7]. By eqs. (6),(7) and (11),(12) one can carry out a detailed investigation of the borderline cases $d=d_u(\equiv d_u^{cl}$ or $\equiv d_u^{q})$. In the classical limit we obtain essentially the same results as for the mean spherical model [1,6]. The solutions of eqs.(6) and (11) are singular in $\varepsilon=(d_u-d)\to 0^+$ like $\Delta\sim\varepsilon^{-\frac{1}{2}}$ in the classical and like $\Delta\sim\varepsilon^{-\frac{2}{3}}$ in the quantum limit. In $d=d_u$ there is a breakdown of hyperscaling, and finite-size scaling does not hold in its simplest form (cf.[1,6]). In more than $d=d_u$ dimensions a dangerous irrelevant variable must be involved in a manner similar to that of ref.[6] to explain the conformity of eqs.(8) and (13) with the finite-size scaling. It is interesting to note that for $d>d_u$ the parameter σ does not govern the divergence of χ_L.

The dimensional crossover makes it possible to express the asymptotic behaviour of the susceptibility in the classical and quantum limit (see eqs.(5)-(14) in a unified fashion

$$\chi_N(q=0,\zeta_c)\sim\begin{cases}\Delta_0 N^{\frac{\sigma}{d}}, & (d_\ell<d<d_u),\\ \left(\dfrac{\sigma}{d X_D^{\sigma}\zeta_c}\right)^{\frac{\sigma}{d_u}}(N\ \ln N)^{\frac{\sigma}{d_u}}, & (d=d_u)\\ \zeta^{-\frac{\sigma}{d_u}} N^{\frac{\sigma}{d_u}}, & (d>d_u)\end{cases}\qquad(14)$$

and

$$\frac{\zeta_c}{\Delta_0^{\frac{d_\ell}{\sigma}}}\simeq\frac{\alpha^d}{X_D^{(d-d_\ell)}(\alpha^\sigma+\Delta_0)^{\frac{d_\ell}{\sigma}}}F\left(1,1,\frac{d_u-d}{\sigma};\frac{\Delta_0}{\alpha^\sigma+\Delta_0}\right),\qquad(15)$$

when the only difference between both the cases is reflected in $d_u\equiv(d_u^{cl}$ or $d_u^{q})$, $d_\ell\equiv(d_\ell^{cl}$ or $d_\ell^{q})$ because $\zeta_c\equiv(t_c$, or $\lambda_c/2)=\alpha^d(d-d_\ell)/S_d X_D^{(d-d_\ell)}$.

It should also be mentioned that in the framework of the model (1) it is not difficult to compute the other physical quantities of interest for the quantum finite-size critical phenomena.

REFERENCES

1. E.Brezin, J.Physique 43 (1982) 15.
2. J.M.Luck, Phys.Rev. B31 (1985) 3069.
3. S.Singh and R.K.Pathria, Phys.Rev. B31(1985) 4483.
4. S.Singh and R.K.Pathria, Phys.Rev. B32 (1985) 4618.
5. S.Singh, R.K.Pathria and M.E.Fisher, Phys.Rev. B33 (1986) 6415.
6. J.Shapiro and J.Rudnick, Journ. of Stat.Phys. 43 (1986) 51.
7. M.E.Fisher and V.Privman, Comm.Math.Phys. 103 (1986) 527.
8. Yu.M.Ivanchenko, A.A.Lisiansky, A.Z.Filipov, Teor. Mat.Fiz. (USSR) 67 (1986) 143.
9. T.Schneider, E.Stoll and H.Beck, Physica 79A (1975) 201.
10. N.M.Plakida and N.S.Tonchev, Teor.Mat.Fiz. (USSR) 63 (1985) 270.

11. N.M.Plakida and N.S.Tonchev, Physica 136A (1986) 176.

12. G.Busiello, L.De Cesare and I.Rabuffo, Physica 117A (1983) 445.

13. E.W. Montroll and G.H. Weiss, J.Math.Phys. 6(1975) 167.

Received by Publishing Department
on June 3, 1987.

Тончев Н.С. E17-87-380

Конечноразмерные эффекты в одной квантовой точно решаемой модели структурного фазового перехода

На примере точно решаемой модели структурного фазового перехода проверены некоторые следствия конечноразмерного скейлинга. В частности вычислена восприимчивость системы в квантовом и классических режимах. Показано, что в обоих случаях восприимчивость имеет одинаковое скейлинговое поведение.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

Препринт Объединенного института ядерных исследований. Дубна 1987

Tonchev N.S. E17-87-380

Finite-Size Effects in a Quantum Exactly Soluble Model for Structural Phase Transition

Some consequences of finite-size scaling are examined within an axactly soluble model of structural phase transition. Explicit expressions for the susceptibility for classical and quantum limits are derived. It is shown that both the cases have the same scaling behaviour.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

Preprint of the Joint Institute for Nuclear Research. Dubna 1987