CALCULATIONS OF THE CRITICAL INDICES FOR THREE-DIMENSIONAL SYSTEMS BY THE PERTURBATION METHOD

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A new method for the calculation of critical indices near the critical point (CP) has been proposed. The method is based on the insertion of small parameters into the equations of the fluctuation theory of phase transitions. The values obtained by this method for the critical indices of a three-dimensional system are confirmed experimentally, being closest to the results calculated in the framework of the Ising model.

Researches of the critical phenomena in liquids [1–4] belong to the actual problems of the condensed matter physics. As a result, the calculations of the critical indices, which define the power-law behaviors of various properties of a substance along critical directions, also remain challenging. The fluctuation theory of phase transitions (FTPT) [2–4] does not provide numerical values for these parameters, but only determines relations between them. Namely,

$$\beta = \gamma/(\delta-1) = d\nu - \beta\delta, \quad \gamma = 2\beta\delta - d\nu,$$

$$d\xi - 1 = 1/\delta, \quad \eta = 2 - d(\delta-1)/(\delta+1),$$

$$\alpha_t = 2 - d\nu, \quad \alpha_\mu = 2/(\beta\delta) - d\xi. \qquad (1)$$

Various model approximations — the solution of three- and two-dimensional Ising models, the ε-expansion method, the solution of the renormalization group equations [2–4], the method of collective variables [5] — are used to determine the numerical values of critical indices. Within this direction of researches, some features in the behavior of the equilibrium and kinetic properties of inhomogeneous systems in a gravitational field near the CP have been used in works [6, 7] to accomplish the task concerned. In particular, these features include the nonmonotonous temperature dependences of the scattered light intensity $I(h,t) \sim (\partial\rho/\partial\mu)_T(h,t)$ and the compressibility $(\partial\rho/\partial\mu)_T(h,t)$ at the constant field $h = \rho_k g\Delta z/P_k$ [8], as well as that of the equilibration time $\tau_p(t)$ [9] of the inhomogeneous system in the gravitational field h. The analysis of these dependences for inhomogeneous systems in the gravitational field leads to the following inequalities which couple the critical indices [6, 7]:

$$3\xi - 2/(\beta\delta) < 0, \quad \beta\delta - \nu - 1 < 0. \qquad (2)$$

Relations (2) bring about a number of important inequalities for the magnitudes of some critical indices of the FTPT:

$$\nu < 2/3, \quad \xi > 2/5, \quad \gamma < 4/3, \quad \delta < 5, \quad \beta > 1/3. \qquad (3)$$

These inequalities do not contradict relations (1) of the FTPT [2–4], being confirmed by the analysis of numerous experimental data in the vicinity of the CP [10–16].

On the basis of these inequalities, one can introduce, in addition to the critical indices of the FTPT (1), other small parameters which are defined by the relations

$$\nu_0 = \frac{2}{3} - \nu \ll \nu, \quad \xi_0 = \xi - \frac{2}{5} \ll \xi, \quad \gamma_0 = \frac{4}{3} - \gamma \ll \gamma,$$

$$\delta_0 = 5 - \delta \ll \delta; \quad \beta_0 = \beta - \frac{1}{3} \ll \beta. \qquad (4)$$

The results of experimental and theoretical researches [10–16] of the magnitudes of critical indices [2, 3] enable the new parameters (4) to be ranged in the following order:

$$\delta_0 \gg \gamma_0 > \alpha_t > \alpha_\mu \approx \eta \gg \nu_0 \gg \xi_0 \approx \beta_0 \approx (3 \div 4)10^{-3}. \qquad (5)$$

The assumption about the approximate equality between the small parameters ξ_0 and β_0, taking their smallness into account, insignificantly affects the calculation accuracy for the magnitudes of the critical indices [2]. However, this assumption, which was made on the basis of the FTPT equations (1), enables a number of relations between the small indices α_t, α_μ, η, ν_0, ξ_0, etc. for three-dimensional systems to be obtained. For example,

$$\eta = (25/2)\xi_0 + [(25/2)\xi_0]^2, \quad \alpha_t = 3\nu_0,$$

$$\nu_0 \approx (25/4)\xi_0, ... \tag{6}$$

These relations allow one to determine the interrelations between the critical indices for the correlation length, the correlation function, and the heat capacity which with an error of no more that 1%, look like

$$\nu^2 = \xi, \tag{7}$$

$$\alpha_t = 3/4(\alpha_\mu + \eta). \tag{8}$$

Solving the system of equations (6)—(8), we obtain the following values for the small parameters of the correlation length: $\nu_0 = 0.0303$ and $\xi_0 = 0.0049$.

Taking the amplitudes of these small parameters into account, one can calculate, on the basis of Eqs. (1) and (4), all the critical indices of the FTPT [2–4] for three-dimensional systems:

$$\nu = 0.6363, \quad \xi = 0.4049, \quad \beta = 3\nu - 1/\nu = 0.3373,$$

$$\gamma = 2/\nu - 3\nu = 1.234, \quad \delta = 1/(3\nu^2 - 1) = 4.659,$$

$$\eta = 5 - 2/\nu^2 = 0.0602,$$

$$\alpha_t = 2 - 3\nu = 0.0911, \quad \alpha_\mu = 2\nu - 3\nu^2 = 0.05797. \tag{9}$$

Moreover, proceeding from Eqs. (6)—(8), one can also find the relations between all the small indices (4), as well as the numerical values for the latter. Table 1 quotes these relations in the linear approximation.

The introduction of the small parameters (4) and the use of relations (6)—(8) allow one to find a new system of relations between all the critical indices of the FTPT as well [2–4]. These relations, in the linear approximation, are presented in Table 2. They can serve as the basis for finding the set of quadratic equations, which determine the numerical values of all the critical indices of the FTPT [2–4]:

$$\nu^2 + 0.096\nu - 0.464 = 0; \quad \xi^2 - 0.937\xi + 0.215 = 0;$$

$$\delta^2 + 7.92\delta - 58.2 = 0; \quad \gamma^2 + 2.31\gamma - 4.37 = 0;$$

$$\beta^2 - 0.916\beta + 0.195 = 0; \quad \alpha_t^2 - 4.482\alpha_t + 0.4 = 0;$$

$$\eta^2 - 2.99\eta + 0.178 = 0. \tag{10}$$

The roots of these equations are listed in the last column of Table 2.

T a b l e 1

	ξ_0	ν_0	δ_0	γ_0	β_0	α_t	η	Calculation by Eqs. (4)—(8)
ξ_0	—	$\frac{12}{75}\nu_0$	$\frac{1}{75}\delta_0$	$\frac{18}{325}\gamma_0$	$\frac{72}{75}\beta_0$	$\frac{4}{75}\alpha_t$	$\frac{6}{75}\eta$	0.0049
ν_0	$\frac{25}{4}\xi_0$	—	$\frac{1}{12}\delta_0$	$\frac{3}{10}\gamma_0$	$6\beta_0$	$\frac{1}{3}\alpha_t$	$\frac{1}{2}\eta$	0.0303
δ_0	$75\xi_0$	$12\nu_0$	—	$\frac{18}{5}\gamma_0$	$72\beta_0$	$4\alpha_t$	6η	0.364
γ_0	$\frac{325}{18}\xi_0$	$\frac{10}{3}\nu_0$	$\frac{5}{18}\delta_0$	—	$\frac{52}{3}\beta_0$	$\frac{10}{9}\alpha_t$	$\frac{5}{3}\eta$	0.101
β_0	$\frac{75}{72}\xi_0$	$\frac{1}{6}\nu_0$	$\frac{1}{72}\delta_0$	$\frac{3}{52}\gamma_0$	—	$\frac{1}{18}\alpha_t$	$\frac{1}{12}\eta$	0.005
α_t	$\frac{75}{4}\xi_0$	$3\nu_0$	$\frac{1}{4}\delta_0$	$\frac{9}{10}\gamma_0$	$18\beta_0$	—	$\frac{3}{2}\eta$	0,091
η	$\frac{25}{2}\xi_0$	$2\nu_0$	$\frac{1}{6}\delta_0$	$\frac{3}{5}\gamma_0$	$12\beta_0$	$\frac{2}{3}\alpha_t$	—	0,0607
α_μ	$0.1333–15.5\xi_0$	$0.1333–2.48\nu_0$	$0.1333–0.207\delta_0$	$0.1333–0.744\gamma_0$	$0.1333–14.88\beta_0$	$0.1333–0.827\alpha_t$	$0.1333–1,24\eta$	0.0589

T a b l e 2

	ν	ξ	δ	γ	β	α_t	η	Solution of Eqs. (10)
ν	—	$\frac{58-125\xi}{12}$	$\frac{3+\delta}{12}$	$\frac{9\gamma+8}{30}$	$\frac{8-18\beta}{3}$	$\frac{4-2\alpha_t}{6}$	$\frac{4-3\eta}{6}$	0.6349
ξ	$\frac{58-12\nu}{125}$	—	$\frac{35-\delta}{75}$	$\frac{174-18\gamma}{375}$	$\frac{72\beta+6}{75}$	$\frac{30+4\alpha_t}{75}$	$\frac{6\eta+30}{75}$	0,403
δ	$12\nu - 3$	$35 - 75\xi$	—	$\frac{18\gamma+1}{5}$	$29 - 72\beta$	$5 - 4\alpha_t$	$5 - 6\eta$	4,635
γ	$\frac{30\nu-8}{9}$	$\frac{174-375\xi}{18}$	$\frac{5\delta-1}{18}$	—	$8 - 20\beta$	$\frac{12-10\alpha_t}{9}$	$\frac{4-5\eta}{3}$	1.233
β	$\frac{8-3\nu}{18}$	$\frac{75\xi-6}{72}$	$\frac{29-\delta}{72}$	$\frac{24-3\gamma}{60}$	—	$\frac{\alpha_t+6}{18}$	$\frac{4+\eta}{12}$	0.337
α_t	$\frac{4-6\nu}{2}$	$\frac{75\xi-30}{4}$	$\frac{5-\delta}{4}$	$\frac{12-9\gamma}{10}$	$18\beta - 6$	—	$\frac{3}{2}\eta$	0.091
η	$\frac{4-6\nu}{3}$	$\frac{25\xi-10}{2}$	$\frac{5-\delta}{6}$	$\frac{4-3\gamma}{5}$	$12\beta - 4$	$\frac{2}{3}\alpha_t$	—	0.0608
α_μ	$2\nu - 3\nu^2$	$2\xi^{1/2} - 3\xi$	$\frac{(3+\delta)^2}{48} - \frac{3+\delta}{6}$	$\frac{(9\gamma+8)^2}{300} - \frac{9\gamma+8}{15}$	$\frac{(8+18\beta)^2}{3} - 2\frac{8+18\beta}{3}$	$\frac{(4-2\alpha_t)^2}{12} - \frac{4-2\alpha_t}{3}$	$\frac{(4-2\eta)^2}{12} - \frac{4-3\eta}{3}$	0.0605

Basing on the inequality $\nu < 2/3$ and the obtained relation (7), the following simple empirical formulas for calculating the numerical values of the critical indices can be proposed:

$$(\nu < 2/3) = 2/\pi = 0.637; \quad \xi = \nu^2 \approx (2/\pi)^2 = 0.405;$$

$$\beta \approx 6/\pi - \pi/2 = 0.339;$$

$$\gamma = \pi - 6/\pi = 1.232; \quad \delta = \pi^2/(12 - \pi^2) = 4.63;$$

$$\alpha_t \approx 2 - 6/\pi = 0.09; \quad \eta = 5 - \pi^{2/2} = 0.065;$$

$$\alpha_\mu = 3(2/\pi)^2[\pi/3 - 1] = 0.0574(\pi \approx 3.142). \quad (11)$$

It is evident that the results of calculations by these formulas almost coincide with the solutions of Eqs. (9) and (10).

Thus, the introduction of small parameters has allowed us to find the set of equations, which determine the numerical values for the critical indices of the FTPT [2–4]. The results obtained are confirmed by numerous experimental data in the vicinity of the CP. One can see that the magnitudes of the critical indices are closest to the results of calculations obtained in the framework of the three-dimensional Ising model and by the method of ε-expansion [2].

1. *Landau L.D., Lifshits E.M.* Statistical Physics. — Oxford: Pergamon Press, 1969.
2. *Patashinski A.Z., Pokrovski V.L.* Fluctuation Theory of Phase Transitions. — Oxford: Pergamon Press, 1982.
3. *Wilson K.G., Kogut J.* // Phys. Repts. — 1974. — **12**, N 2. — P. 75 — 199.
4. *Stanley H.E.* Introduction to Phase Transitions and Critical Phenomena. — Oxford: Oxford University Press, 1971.
5. *Yukhnovskii I.R.* Phase Transitions of the Second Order: Collective Variables Method. — Singapore: World Scientific, 1987.
6. *Alekhin O.D.* // Visn. Kyiv. Univ. Ser. Fiz. Mat. Nauk. — 2002. — N 4. — P. 340 — 343.
7. *Alekhin O.D.* // Ibid. — 2003. — N 2. — P. 319 — 321.
8. *Alekhin A.D., Krupskii N.P., Chalyi A.V.* // Zh. Eksp. Teor. Fiz. — 1972. — **63**, N 4(10). — P. 1417 — 1420.
9. *Alekhin A.D.* // Ukr. Fiz. Zh. — 1986. — **31**, N 5. — P. 720 — 722.
10. *Golik A.Z., Shimanskii Yu.I. et al.* // The Equation of State for Gases and Liquids (to the Centenary of the Van der Waals Equation). — Moscow: Nauka, 1975. — P. 189—217 (in Russian).
11. *Artyukhovskaya L.M., Shimanskaya E.T., Shimanskii Yu.I.* // Ukr. Fiz. Zh. — 1970. — **15**, N 2. — P. 1974 — 1981.
12. *Artyukhovskaya L.M., Shimanskaya E.T., Shimanskii Yu.I.* // Zh. Eksp. Teor. Fiz. — 1970. — **59**, N 3(9). — P. 688.
13. *Artyukhovskaya L.M., Shimanskaya E.T., Shimanskii Yu.I.* // Ibid. — 1972. — **68**, N 6(12). — P. 2159.
14. *Bulavin L.A.* Properties of Liquids in the Critical Range. — Kyiv: Kyiv Univ. Publ. House, 2002 (in Russian).
15. *Alekhin O.D., Rudnikov E.G.* // Zh. Fiz. Dosl. — 2004. — N1.
16. *Anisimov M.A.* Critical Phenomena in Liquids and Liquid Crystals. — Philadelphia: Gordon and Breach, 1991.

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РОЗРАХУНКИ КРИТИЧНИХ ПОКАЗНИКІВ ТРИВИМІРНИХ СИСТЕМ МЕТОДОМ МАЛОГО ПАРАМЕТРА

О.Д. Альохін

Р е з ю м е

Запропоновано новий метод розрахунків критичних показників поблизу критичної точки (КТ), оснований на введенні малих параметрів в рівняння флуктуаційної теорії фазових переходів. Одержані цим методом величини критичних показників для тривимірних систем підтверджуються експериментально і найбільш близькі до розрахунків, проведених на основі моделі Ізінга.