Defect fugacity, Spinwave Stiffness and T_c of the 2-d Planar Rotor Model

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February 1, 2008

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Abstract

We obtain precise values for the fugacities of vortices in the 2-d planar rotor model from Monte Carlo simulations in the sector with *no* vortices. The bare spinwave stiffness is also calculated and shown to have significant anharmonicity. Using these as inputs in the KT recursion relations, we predict the temperature $T_c = 0.925$, using linearised equations, and $T_c = 0.899 \pm .005$ using next higher order corrections, at which vortex unbinding commences in the unconstrained system. The latter value, being in excellent agreement with all recent determinations of T_c, demonstrates that our method 1) constitutes a stringent measure of the relevance of higher order terms in KT theory and 2) can be used to obtain transition temperatures in similar systems with modest computational effort.

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Introduction: The phase behaviour of isotropic magnets and related systems in two dimensions is a particular challenge since famous theorems exclude long-range order[1], but nevertheless phase transitions occur in models such as the two- dimensional XY ferromagnet[2] or the planar rotor model ($S_i^x = \cos \phi_i, S_i^y = \sin \phi_i$, where $\mathbf{S_i}$ is a two component spin at the site i with unit magnitude and orientation $0 \leq \phi_i < 2\pi$),

$$\beta\mathcal{H} = -\frac{1}{T} \sum_{<ij>} \cos(\phi_i - \phi_j), \tag{1}$$

the sum extends once over all nearest neighbor pairs of the (square) lattice, and T is the reduced temperature (the Boltzmann constant $k_B = \beta^{-1}T$ is taken to be 1 throughout). Originally[2] it was proposed that a critical temperature T_c occurs where the correlation length ξ describing the decay of the correlation function $g(\mathbf{r}) =< \mathbf{S(0)S(r)} >$ with distance $\mathbf{r}$, and the susceptiblity $\chi = \sum_\mathbf{r} < \mathbf{S}(0) \cdot \mathbf{S(r)} > /T$ diverge according to power laws,

$$\xi \sim t^{-\nu}, \chi \sim t^{-\gamma}, t \equiv T/T_c - 1 \tag{2}$$

ν, γ being the usual critical exponents. However, Kosterlitz and Thouless (KT)[3, 4] developed a completely different scenario, based on the unbinding of vortex- antivortex pairs, yielding an essential singularity,

$$\begin{aligned} \ln \xi &= \ln \xi_0 + bt^{-\bar{\nu}}, \\ \chi &\propto \xi^{2-\eta} \end{aligned} \tag{3}$$

where ξ_0, b are nonuniversal constants, while an approximate renormalization group treatment[3, 4] predicted that the exponents $\bar{\nu}, \eta$ take the universal values,

$$\begin{aligned} \bar{\nu} &= 1/2, \\ \eta &= 1/4. \end{aligned} \tag{4}$$

For $T < T_c$, spin-wave theory remains essentially valid and $g(r) \sim r^{-\eta(T)}$ where $\eta(T)$ increases smoothly with increasing temperature from $\eta(T = 0) = 0$ upto $\eta(T_c) \equiv \eta = 1/4$. The spinwave stiffness $K(T)$ (in which we have absorbed a factor of $1/T$ as in Eq.(1)) smoothly decreases and also involves a universal ratio at $T_c, K(T_c) = 2/\pi[4, 5]$. A related critical behaviour

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is predicted for the superfluid- normal fluid transition of helium in two-dimensions[5], for the roughening transition of interfaces[6], transitions of adsorbed layers on surfaces to modulated structures incommensurate with the substrate periodicity, etc. Thus, this problem has found widespread interest[7]. A particularly interesting —- but also still controversial—- extension deals with two- dimensional melting [8, 9, 10].

However, both the physical mechanism for the vortex- antivortex pair dissociation at T_c and the resulting predictions have been questioned many times (eg.[11, 12]). The theory[3, 4, 5, 13, 14, 15, 16, 17, 18] involves problematic assumptions such as the decoupling of vortex and spinwave excitations; and numerical analyses[12, 19, 20, 21, 22, 23, 24, 25, 26] often are not fully convincing although usually the KT theory is favoured. Monte Carlo studies are difficult since ξ increases so strongly as t gets small (eg. $\xi > 40$ lattice spacings for $t \leq .1$), and so it is questionable whether the asymptotic critical region is reached. Even studies for very large lattices (1200×1200) still reveal problems with Eq.(4)[23], and the simulation data can well be fitted to Eq.(2) if (albeit rather large) corrections to scaling are taken into account[23]. The most recent analyses, in fact, point towards the need of considering logarithmic corrections[25, 26].

In the present paper we hence follow a different strategy for a Monte Carlo test of the KT renormalization approach, avoiding the brute force methods of Refs.[12, 19, 20, 21, 22, 23, 24, 25, 26]. Namely we test the KT scenario by obtaining the proper input parameters for the renormalization group flow equations, which then are solved numerically. In this way a stringent consistency test is possible which is different from all previous approaches to the problem.

Monte Carlo estimation of input parameters to the KT theory The KT theory[3, 4, 5, 6, 7] can be cast in the framework of a two parameter renormalization flow for the spinwave stiffness $K(l)$ and the fugacity of vortices $y(l)$, where l is related to the considered length scale as $l = \ln(r/a)$, where a is the lattice spacing. These flow equations in terms of the scaled variables $x = (2 - \pi K)$ and $y' = 4\pi y$ and upto next to leading order[17] are,

$$\frac{dx}{dl} = y'^2 - y'^2 x, \tag{5}$$

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$$\frac{dy'}{dl} = xy' + \frac{5}{4}y'^3.$$

Using a linearised version of these equations (i.e. keeping only the first terms on the right hand side of these equations) and using the approximate initial conditions $y(l = 0) \simeq \exp(-10.2/2T)$ and $K(l = 0) = 1/T$ – a result from harmonic spin wave theory strictly valid at $T \to 0$, Kosterlitz[4] found that a non- trivial fixed point $K(l = \infty) = 2/\pi, y(l = \infty) = 0)$ exists (cf. Eq. (3) above) but the resulting estimate for $T_c \simeq 1.35$ is rather different from the current best estimates $T_c = 0.895 \pm .005$ [22, 24, 25]. Does this discrepancy mean that the KT scenario does not work?

Such a conclusion would clearly be premature, however, because the above assumption implies that even at $T = T_c$ one can still take the unrenormalized zero temperature value of the spin wave stiffness as a starting value for the recursion, Eq.(5). To test this assumption we have obtained K (and y) from Monte Carlo simulations. Two sets of simulations are carried out. The first set uses the full Hamiltonian, Eq.(1), while the second set uses the constraint that neither vortices nor antivortices can form[27]. Note that an elementary plaquette of the square lattice contains a vortex or an antivortex, if the angles ϕ_i of the spins $1, 2, 3, 4$ at the corners of the plaquette (labelled anticlockwise) satisfy the condition $\sum_{i=1}^{4} \Delta\phi_i = \pm 2\pi$, where we have defined $\Delta\phi_i = \phi_{i+1} - \phi_i, \phi_5 = \phi_1$. If there are only spin wave excitations in the system,$\sum_{i=1}^{4} \Delta\phi_i = 0$ for all plaquettes. Hence the no- vorticity constraint in the Monte Carlo elementary step (which involves an attempt to replace ϕ_i by a randomly chosen ϕ'_i, with $0 \le \phi'_i < 2\pi$) considers whether $\sum_{i=1}^{4} \Delta\phi_i = 0$ is still true for this trial configuration for all the four adjoining plaquettes to which the site i belongs. If the constraint is not true, the trial move is automatically rejected. Note that we always start the simulation from a vortex free initial fully aligned state ($\cos\phi_i = 1$ for all i).

Fig.1 gives a plot of the inverse stiffness constant $K^{-1} = 4\pi \ln < M^2 >$ $/ \ln N$, where $< M^2 >= T\chi_N$. Note that while K^{-1} diverges in the unconstrained system at T_c, it stays finite in the constrained system and finite size effects are negligible even at T_c since the constrained system is not at a critical point there. Therefore K can be obtained very precisely – the constrained system was equilibrated using 2×10^3 Monte Carlo Steps (MCS) per site and a further averaging over 3×10^3 MCS was sufficient to obtain high quality data. Fig. 1 shows that indeed the harmonic theory result for $K^{-1}(= T)$ is poor near T_c.

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Next we wish to estimate $y(l = 0)$ from simulations as accurately as possible. This was done in two ways: (i) the concentration n_v of vortex pair excitations was measured in the unconstrained simulations of Eq.(1), (ii) the rejection rate p of Monte Carlo moves that were rejected was measured in the constrained simulations (Fig. 2.). The chemical potential μ of the vortices could be obtained from the slope of $-\ln n_v$ or $-\ln p$ as a function of T^{-1}. We see that again our data for p in the constrained simulations were of much superior quality because of the absence of a phase transition. Our estimate for $y(l = 0) = \exp(-\mu/T)$ can now be used together with our value for $K^{-1}(l = 0)(\simeq T + T^2/2$ from numerical fits to the data) in the recursion relations Eq.(5) to obtain the renormalized rigidity modulus K_R and hence T_c.

The recursion relations Eq.(5) are solved numerically to obtain the renormalized modulus and fugacity. Using only the linearized equations (which can be solved analytically) we obtain $T_c = 0.925$ which is considerably closer to the experimental value than the KT estimate of 1.35 but there is still a significant discrepancy. However, this discrepancy vanishes when the full equations incorporating leading order correction terms (which do not affect universal behaviour and hence usually omitted) are used. Taking leading order correction terms into account, we obtain $T_c = 0.899 \pm 0.005$ in excellent agreement with the brute force simulations! Fig.3 presents the resulting flow diagram, which displays the importance of these correction terms directly.

In addition, our results offer a simple way of calculating the nonuniversal critical amplitude b (note that Fig. 3 implies that Eq.(4) holds, of course). Critical amplitudes are usually notoriously difficult quantities to estimate directly from simulations. Following Ref.[17] we define y_0 as the intercept of the flows for $T > T_c$ with the $y'-$axis (see Fig. 3). The leading order behaviour of the correlation length $\xi \sim \pi/y_0$. Using the fact that y_0^2 has an expansion $y_0^2 = \sum_i a_i t^i$ with $t = (T - T_c)/T_c$ (see Fig. 4), we get $b = \pi/\sqrt{a_1} = 1.534 \pm .002$ which is in excellent agreement with the estimate $b = 1.585(9)$ obtained by Olsson[24] by directly fitting the behaviour of the dielectric function $\epsilon(t) = K/K_R$.

<u>Discussion and conclusions</u> Our analysis demonstrates that the planar rotor model is fully consistent with the KT theory, but for a quantitatively accurate description of the transition (especially for nonuniversal quantities)

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it is indispensible that the higher order terms in the recursion relations Eq.(5) are taken into account. This finding implies that far away from T_c significant corrections to Eq.(3) are expected — this offers an explanation why the direct simulations [12, 20, 21, 22, 23, 24, 26] have difficulties in extracting the correct critical behaviour unambiguously. In contrast, our method yields critical properties with comparatively modest computational effort. We expect that analogous methods can be applied to other models that are expected to show KT transitions; in fact, we are currently undertaking an extension of our approach to the controversial issue of two- dimensional melting.

References

[1] Mermin N.D. and Wagner H. Phys. Rev. Lett. **17**, 1133 (1966); Hohenberg P. C. Phys. Rev. **158**, 383 (1967).

[2] Stanley H. E. and Kaplan T. A. Phys. Rev. Lett. **17**, 913 (1966)

[3] Kosterlitz J. M. and Thouless D. J., J. Phys. C **6**, 1181 (1973).

[4] Kosterlitz J. M., J. Phys. C **7**, 1046 (1974).

[5] Nelson D. R. and Kosterlitz J. M., Phys. Rev. Lett. **39**, 1201 (1977).

[6] Chui S. T. and Weeks J. D., Phys. Rev. B **14**, 4978 (1976).

[7] For reviews, see Minnhagen P. Rev. Mod. Phys. **59**, 1001 (1987); Kleinert H. *Gauge Fields in Condensed Matter* (World Scientific, Singapore 1989) Vol. 1.

[8] Halperin B. I. and Nelson D. R. Phys. Rev. Lett. **41**, 121 (1978).

[9] Strandburg K. J., Rev. Mod. Phys. **60**, 161 (1988).

[10] Weber H., Marx D. and Binder K. Phys. Rev. B **51**, 14636 (1995); Jaster A. Europhys. Lett. **42**, 277 (1988).

[11] Zittartz J., Z. Physik B **23** 55,63 (1976); Luther A. and Scalapino D. J., Phys. Rev. B **16**, 1356 (1977); Fucito F. and Solomon S. Phys. Lett. B **134**, 235 (1984).

[12] Patrascioiu A. and Seiler E. Phys. Rev. Lett. **60**, 875 (1988).

[13] José J. V., Kadanoff L. P., Kirkpatrick S. and Nelson D. R., Phys. Rev. B **16**, 1217 (1977).

[14] Ohta T. and Kawasaki K. Progr. Theor. Phys. **60**, 365 (1978).

[15] Nakayama I. and Tsuneto T. Progr. Theor. Phys. **63**, 402 (1980).

[16] Cardy J. L. and Parga N., J. Phys. C **13**, 571 (1980).

[17] Amit D. J., Goldschmidt Y. Y. and Grinstein G., J. Phys. A **13**, 585 (1980).

[18] Kadanoff L. P. and Zisook A. B., Nucl. Phys. B **180**[FS2] 61 (1981).

[19] Shugard W. J., Weeks J. D. and Gilmer G. H., Phys. Rev. Lett. **41**, 1399 (1978).

[20] Tobochnik J. and Chester G.V., Phys. Rev. B **20**, 3761 (1979).

[21] Van Himbergen J. E. and Chakravarty S. Phys. Rev. B **23** 359 (1981).

[22] Gupta R. and Baillie C.F., Phys. Rev. B **45**, 2883 (1992).

[23] Janke W. and Nather K., Phys. Rev. **B48**, 7419 (1993).

[24] Olsson P., Phys. Rev. Lett. **73**, 3339 (1994)

[25] Kim J.-K. Phys. Lett. A, **223**, 261 (1996)

[26] Janke W. , Phys. Rev. **B55**, 3580 (1997).

[27] Ben-Av R. and Solomon S., Phys. Rev. B **37**, 9817 (1988).

FIGURE CAPTIONS

Fig 1. The inverse spinwave stiffness $K^{-1}(T)$ plotted vs. temperature, for two types of simulations: (i) The unconstrained system of $L \times L$ lattices with $L = 100$ ($\diamond$); (ii) The constrained (vortex free) system for $L = 30(\times), 60(+)$ and $100(\square)$, respectively. The dashed straight line represents the result of harmonic theory ($K^{-1} = T$) while the full curve is a fit to the form $T + aT^2$ with $a = .50 \pm .01$.

Fig. 2. Plot of $-\ln(n_v)$ and $-\ln(p)$ vs. the inverse temperature. The vortex concentration n_v ($\diamond$) is calculated in the unconstrained simulation of Eq.(1) for $L \times L$ lattices ($L = 100$). The rejection ratio p in the constrained simulation was calculated for $L = 60(+)$ and $L = 100(\square)$ respectively. The dotted line is a fit to the latter data (near the transition temperature) yielding $2\mu = c = 6.55 \pm .03$.

Fig. 3. Flows of $x = (2 - \pi K)$ and $y = \exp(-\mu/T)$ under the action of the renormalisation group starting from a set of initial conditions ($\circ$) obtained from our simulations of the XY model. The dotted lines ($y = \pm x$) are the separatrix for the linearized flow equations valid for flows near the fixed point $x = 0, y = 0$, the thick lines are the actual separatrix for the nonlinear equations Eq. (5). Note that these curves separate flows that terminate on the critical line $x < 0, y = 0$ (ordered phase) from flows towards $y \to \infty$ (disordered phase). Arrows give the direction of the flow.

Fig. 4. Square of the intercept y_0, of the flows (Fig. 3.) with the $y'-$axis as a function of $t = (T - T_c)/T_c$ for $T > T_c$. The data points ($\diamond$) are fitted to a straight line $y' = a_1 t$. The critical amplitude b for the correlation length $\xi \sim \exp(bt^{-1/2})$, is given by $b = \pi/\sqrt{a_1} = 1.534 \pm .002$.
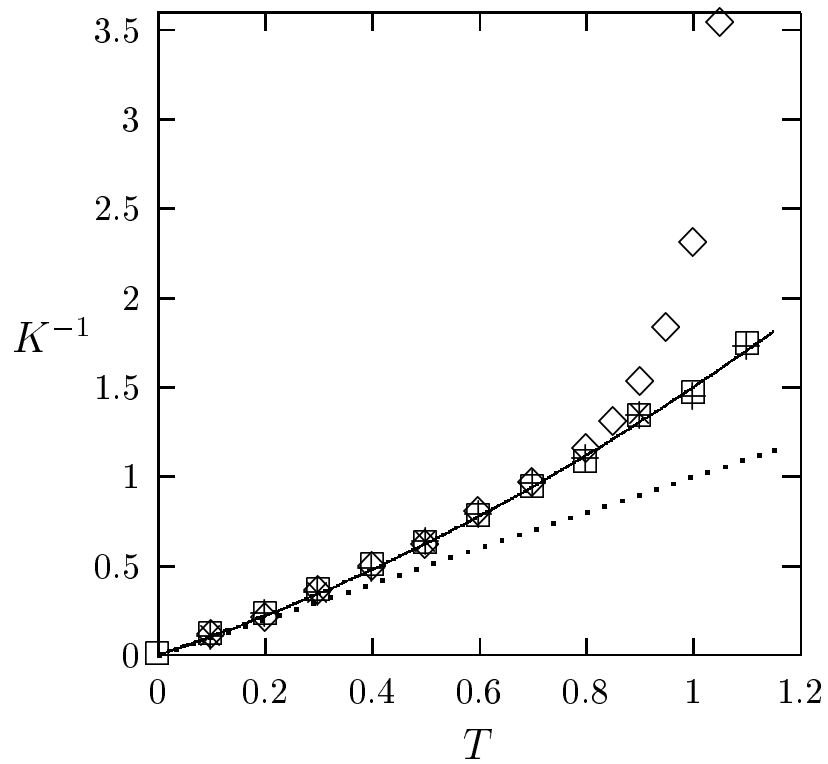
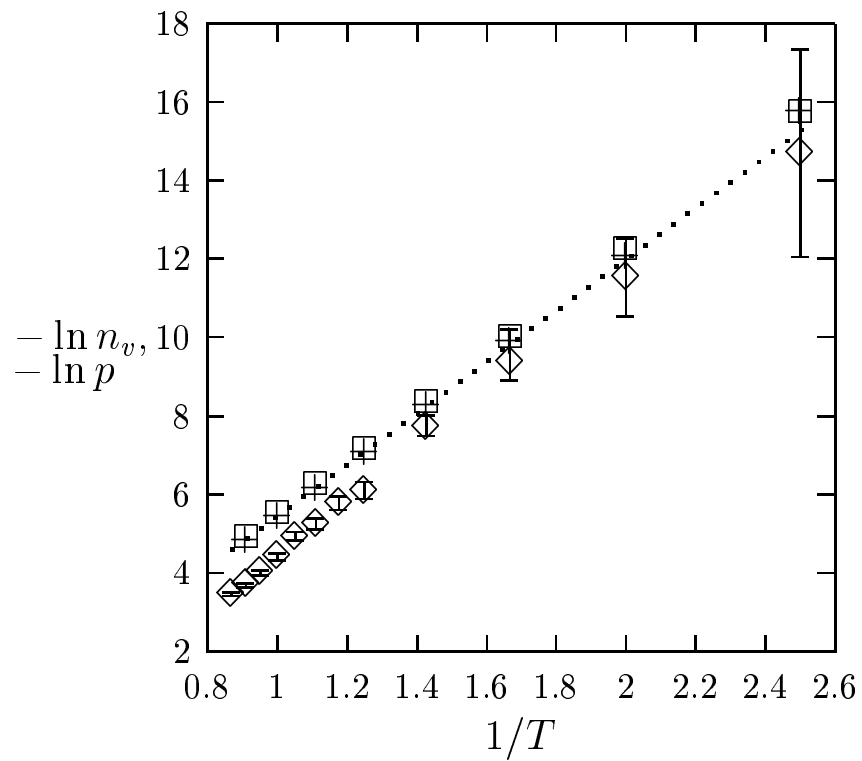**Figure 1:**
(Sengupta, Nielaba , Binder; Euro. Phys. Lett.)

Figure 2:
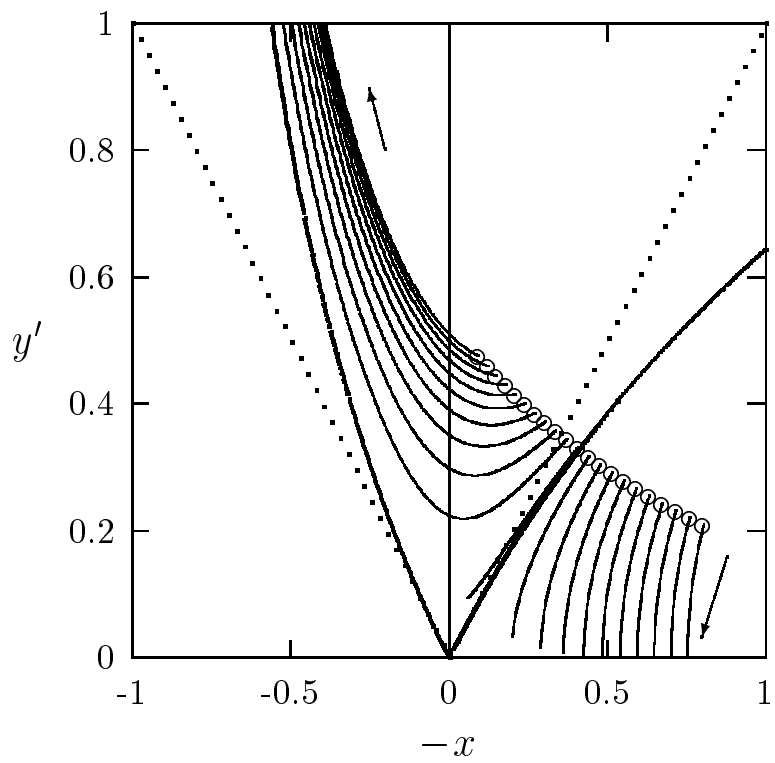(Sengupta, Nielaba , Binder; Euro. Phys. Lett.)
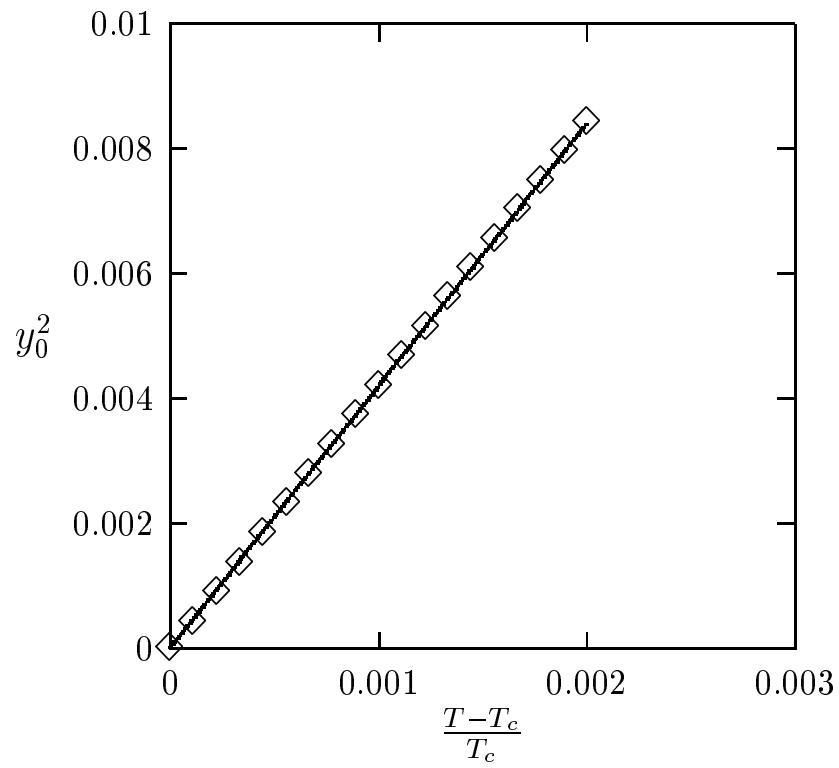
Figure 3:
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Figure 4:
(Sengupta, Nielaba , Binder; Euro. Phys. Lett.)