Phase Coexistence in Confined Ising Systems: a Density Matrix Renormalization Approach[1]

Enrico Carlon[2,4] and Andrzej Drzewiński[3]

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[2] Institute for Theoretical Physics, Katholieke Universiteit Leuven, B-3001 Leuven, Belgium

[3] Institute for Low Temperature and Structure Research, Polish Academy of Sciences, P.O.Box 937, 50-950 Wrocław 2, Poland

[4] To whom correspondence should be addressed

Abstract

Using a density matrix renormalization approach we have calculated the phase diagram of a two dimensional Ising model confined between two infinite walls, with opposing surface fields and a bulk field which grows linearly as function of the distance from the walls and models the effect of gravity on a confined fluid. In absence of gravity two phase coexistence is restricted to temperatures below the wetting temperature as pointed out by Parry and Evans [*Phys. Rev. Lett.* **64**, 439 (1990)]. We find that the competing effect of gravity and surface fields restores the "ordinary" finite size scaling to the bulk critical point, in agreement with previous mean-field results. We have calculated the exponents related to the shift towards the critical point in the limit $L \to \infty$, where L is the distance between the walls and we have found good agreement with previous scaling assumptions. Magnetization profiles calculated from a solid-on-solid hamiltonian agree well with density matrix renormalization results for temperatures not too close to the bulk critical temperature.

KEY WORDS: finite size scaling, liquid-liquid equilibria, statistical mechanics, vapor-liquid equilibria, wetting.

1. INTRODUCTION

Finite size and surface effects may have a strong influence on the thermodynamics of a physical system. A well known example is a fluid confined between two parallel plates where liquid-vapor condensation occurs at lower pressure than in the bulk, a phenomenon known as capillary condensation [1].

A familiar and simple model that mimics this effect is the Ising model confined between two identical parallel walls separated by a finite distance L [2]. Surface fields acting on the spins at the walls model the wall-fluid interaction. The two phase coexistence line is shifted to finite values of the bulk magnetic field h (see Fig. 1(a)). One can distinguish two situations: the scaling of the finite system critical point $(h_c(L), T_c(L))$ towards the bulk critical point and the scaling of the coexistence bulk field $h_0(L)$ at fixed $T < T_c$ towards the $h = 0$ axis. The finite size scaling in these two situations is governed by different critical exponents, shown in Fig. 1(a).

Parry and Evans [3] analyzed the case of opposing (i.e. antiparallel) surface fields where one wall favors the phase with positive magnetization (or, say, the liquid) and the other the phase with negative magnetization (vapor). They found that two phase coexistence is restricted to temperatures below the interface delocalization transition temperature $T_d(L)$, which, very surprisingly, does not scale to the bulk critical point, but to the wetting temperature T_w as illustrated in Fig. 1(b). On the basis of a mean-field and scaling analysis Parry and Evans concluded that the interface delocalization temperature scales as [3]:

$$T_d(L) - T_w \sim \frac{1}{L^{1/\beta_s}} \tag{1}$$

with β_s the exponent which describes the divergence of the wetting layer for a semi-infinite system. Monte Carlo simulations, performed to test the validity of this scenario, confirm Parry and Evans' results [4,5].

In trying to clarify the effect of the opposing surface fields in the confined geometry Rogiers and Indekeu [6] included a bulk field which models the effect of gravity on the fluid.

Their results are based on a mean-field approach and show that the ordinary finite size scaling to the bulk critical point is recovered in an extended parameter space where gravity is included.

In this article we analyze the effect of opposing walls and gravity on a two dimensional Ising strip using the density matrix renormalization group (DMRG), a method invented by White [8] for the study of quantum spin chains and later adapted by Nishino [9] for two dimensional classical systems. The DMRG is a very accurate method and it allows the study of very large systems, beyond the mean-field approximation. The spin space is truncated in a very efficient manner so that effective transfer matrices, of small (i.e. numerically tractable) dimensions, but which describes large systems can be constructed.

We recall that for an Ising $L \times \infty$ strip the transfer matrix has dimension $2^L \times 2^L$ that grows exponentially fast with L. This limits the largest size available for numerical computations to $L \approx 15 - 20$. The DMRG algorithm consists of several iterations that, starting from an exact transfer matrix of a small system, enlarge the strip width until the effective transfer matrix of the wanted size is generated. The accuracy is very high, several order of magnitudes with respect of that of a typical Monte Carlo simulation [8]. More details of the implementation of the method for the present model will be presented elsewhere [10].

Our results for the confined Ising model with opposing surface fields and gravity essentially confirm the mean-field scenario presented in [6]. We have calculated the finite size scaling exponents in the temperature and gravitational field directions and we have found good agreement with previous scaling assumptions [2,7].

2. THE MODEL

We consider a two dimensional ($L \times \infty$) strip with the following Hamiltonian [6]:

$$H = -J \sum_{i,j} s_{i,j} s_{i+1,j} - J \sum_{i,j} s_{i,j} s_{i,j+1} + h_1 s_{1,j} - h_1 s_{L,j} + g \sum_j \sum_{i=1}^{L} (2i - 1 - L) s_{i,j} \qquad (2)$$

where $s_{i,j} = \pm 1$ and $1 \leq i \leq L$. The bulk "gravitational" field is chosen antisymmetric with respect to the center of the strip. The competing effect of surface and bulk fields (which

occurs in (2) when h_1 and g have the same sign) restores phase coexistence up to the bulk critical temperature, as the competing effect between parallel surface fields and a constant bulk field restores the two phase coexistence in the capillary condensation problem.

For given values of the strip width L and surface fields h_1 we have calculated the phase boundaries between the two phase and the one phase coexistence region [11]. We recall that no true criticality occurs in a $L \times \infty$ system for finite values of L; pseudo-critical points can be detected from e.g. specific heat maxima [11]. The finite-size scaling of pseudo-critical points in two dimensional confined systems have been considered before in the study of the effect of identical and opposing walls in absence of gravity [3,4]. We have tested the accuracy of the method, in absence of gravity, by calculating the interface delocalization transition temperature $T_d(L)$ for various values of the surface fields. We have found a finite size scaling in good agreement with the scaling relation (1) with the two dimensional Ising exponent $\beta_s = 1$ (see inset of Fig. 3); the extrapolation of the numerical data for $L \to \infty$ gives very accurate estimates of the wetting temperature in good agreement with the exact results [12]. Details will be presented elsewhere [10].

Fig. 2 shows the phase boundaries between the one and two-phase coexistence regions for two different values of the surface fields ($h_1 = 0.2$ and $h_1 = 0.5$). As the system size increases the two phase coexistence region becomes very narrow and the phase boundary maximum ($g_{\max}$,$T_{\max}$) scales to the bulk critical point $T = T_c$, $g = 0$. In the temperature direction we find a good agreement with the scaling law [2]:

$$T_{\max}(L) - T_c \sim \frac{1}{L^{1/\nu}}, \tag{3}$$

with $\nu = 1$ for the two dimensional Ising model.

The situation is more complicated along the gravitational field direction. Fig. 3 shows a plot of $\ln(g_{\max}(L))$ vs. $\ln(L)$ for four values of h_1, from 0.1 to 0.99 and $J = 1$ (We restrict ourselves to $h_1 < J$ for which wetting occurs at non-zero temperatures: $T_w > 0$). Van Leeuwen and Sengers [7] considered the influence of gravity on the bulk properties of a fluid and conjectured a scaling exponent for the gravitational constant g; on a finite strip their

analysis implies that [6]:

$$g_{\max}(L) \sim L^{-(1+y_H)}. \tag{4}$$

where y_H is the magnetic exponent ($y_H = 1.875$ for the two dimensional Ising model).

For the largest surface field considered ($h_1 = 0.99$) and $L \geq 20$ a fit of the DMRG data gives an exponent 2.86(2) in very good agreement with the scaling relation (4). At small surface fields, as shown in Fig. 3, the data clearly deviate from the scaling relation (4), possibly due to large corrections to scaling. The interplay with a scaling to the first order line $T < T_c$, $g = 0$, which differently from the capillary condensation case is of type $1/L^2$ [10] may be the cause of the observed deviations from (4).

Fig. 4 shows some magnetization profiles calculated by DMRG for $L = 40$, $J = 1$, $h_1 = 0.5$ and for different values of g and T. Notice the difference between the profile in the two phase coexistence region (a) and the profiles in the single phase region (b,c) where an interface is present. The dashed lines are magnetization profiles calculated from a solid-on-solid interface hamiltonian, which is discussed in some details in the following section. Results are in good agreement with the DMRG profiles, especially at low temperatures where the solid-on-solid approximation is very good.

3. SOLID-ON-SOLID INTERFACE HAMILTONIAN

In a solid-on-solid approach the interface is approximated by a continuous single valued function $l(y)$, where y is the coordinate along the wall and l denotes the shift of the interface position from the center of the strip. The partition function takes the form:

$$Z = \int \mathcal{D}\left[l(y)\right] \; e^{-\beta H(l(y))} \tag{5}$$

where $\mathcal{D}\left[l(y)\right]$ denotes a functional integration over all possible interface configurations and β is the inverse temperature. The hamiltonian is given by:

$$H = \int dy \left\{ \frac{\sigma_0}{2} \left(\frac{dl}{dy} \right)^2 + U(l(y)) \right\} \tag{6}$$

where σ_0 is the surface tension and $U(l)$ the potential of the interface. Using a transfer matrix approach [13] the problem can be mapped onto a one dimensional quantum problem, which amounts to solving the following Schrödinger equation:

$$\left\{-\frac{1}{2\sigma_0\beta^2}\frac{d^2}{dl^2}+U(l)\right\}\psi_n(l)=E_n\psi_n(l) \tag{7}$$

where the ground state energy E_0 corresponds to the interface free energy and $|\psi_0(l)|^2$, the ground state wavefunction squared, equals the probability of finding the interface at a position l. From the microscopic hamiltonian (2) one can easily calculate the potential $U(l)$, which, neglecting the effects of the walls, is simply quadratic as function of the distance from the center of the strip: $U(l) = 2gm_0l^2$; in the calculation we have assumed that all the spins to the left or right side of the interface are equal to $+m_0$ and $-m_0$, the bulk magnetization of the two dimensional Ising model in absence of gravity, which is known exactly. In this approximation (7) becomes the Schrödinger equation for a one dimensional harmonic oscillator; the ground state wavefunction is:

$$\psi_0(l)=\frac{e^{-l^2/(2\xi^2)}}{\pi^{1/4}\sqrt{\xi}} \tag{8}$$

and the parameter ξ measures the average interface width and is given by:

$$\xi=\sqrt{\frac{1}{2\beta\sqrt{\sigma_0 m_0|g|}}} \tag{9}$$

Notice that the effect of the walls can be safely neglected if $\xi \ll L$, when g, m_0 and σ_0 are sufficiently large and at not too high temperatures. The magnetization profile as a function of l takes the form:

$$m(l)=m_0\left\{\int_{-\infty}^{l}ds\left|\psi_0^2(s)\right|-\int_{l}^{\infty}ds\left|\psi_0^2(s)\right|\right\}=\frac{2m_0}{\sqrt{\pi}}\int_0^{l/\xi}dt\ e^{-t^2} \tag{10}$$

Gravity localizes the interface within a width approximately equal to ξ; if g becomes small and at higher temperatures, when $\xi \approx L$, one has to include the effect of the confining potential in the calculation.

4. CONCLUSION

We have used the DMRG method to study the competing effects of opposing surface fields and of a bulk "gravitational" field in a two dimensional Ising model. Gravity restores the ordinary finite-size scaling to the bulk critical point, as concluded in [6] on the basis of a mean-field approach. A finite size scaling analysis along the temperature and gravitational field directions yields exponents in agreement with previous scaling assumptions [2,7].

As pointed out by White [8] the DMRG method works the best when open boundary conditions are used, while results are poorer with periodic boundary conditions. This makes the method suited to study the effet of walls and confinement in two dimensional lattice models of fluids with short range interactions.

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FIGURE CAPTIONS

Fig. 1: (a) Phase diagram of the Ising model confined between two parallel identical walls with positive surface fields; for positive surface fields the phase coexistence line (thick dashed line) is shifted to negative bulk field value. The scaling of the capillary critical point $h_c(L)$ and $T_c(L)$ towards the bulk critical point $h = 0$, $T = T_c$ is governed by the magnetic $y_H = d - \beta/\nu$ and thermal $y_T = 1/\nu$ critical exponents. The scaling of the coexistence field to the first order line for $T < T_c$ is of type: $h_0(L) \sim 1/L$. (b) Phase diagram for the strip with antiparallel surface fields [3]. The two phase coexistence region is restricted to temperatures below the interface delocalization transition temperature $T_d(L)$.

Fig. 2: Phase diagram of the model in presence of gravity calculated by means of DMRG methods for $J = 1$, $h_1 = 0.2$ and $h_1 = 0.5$ and for different values of L. (a) $L = 14$ (diamonds), $L = 20$ (squares), $L = 30$ (crosses) and $L = 40$ (triangles); (b) $L = 12$ (diamonds), $L = 14$ (squares), $L = 20$ (crosses) and $L = 40$ (triangles). The area below the curves is the two phase coexistence region. As the width increases the two phase coexistence region shrinks and shifts towards the $g = 0$ axis; the maxima of the phase boundaries shift to the bulk critical point $T = T_c$, $g = 0$.

Fig. 3: Scaling of $\ln(g_{\max}(L))$ as function of $\ln L$ for $h_1 = 0.1$ (circles), $h_1 = 0.2$ (diamonds), $h_1 = 0.5$ (squares), $h_1 = 0.99$ (triangles). The dotted lines correspond to an exponent $1 + y_H = 2.875$ and are drawn as guide to the eye. Inset: Scaling of $T_{\max}(L)$ and $T_d(L)$ for $h_1 = 0.5$; results are in agreement with the two dimensional Ising model exponents $\nu = 1$ and $\beta_s = 1$.

Fig. 4: Magnetization profiles calculated with the DMRG method for $L = 40$ and $h_1 = 0.5$ in the two phase coexistence region (a) and in the single phase region (b) and (c). The dashed lines are the profiles given by the formula (10).

FIGURES

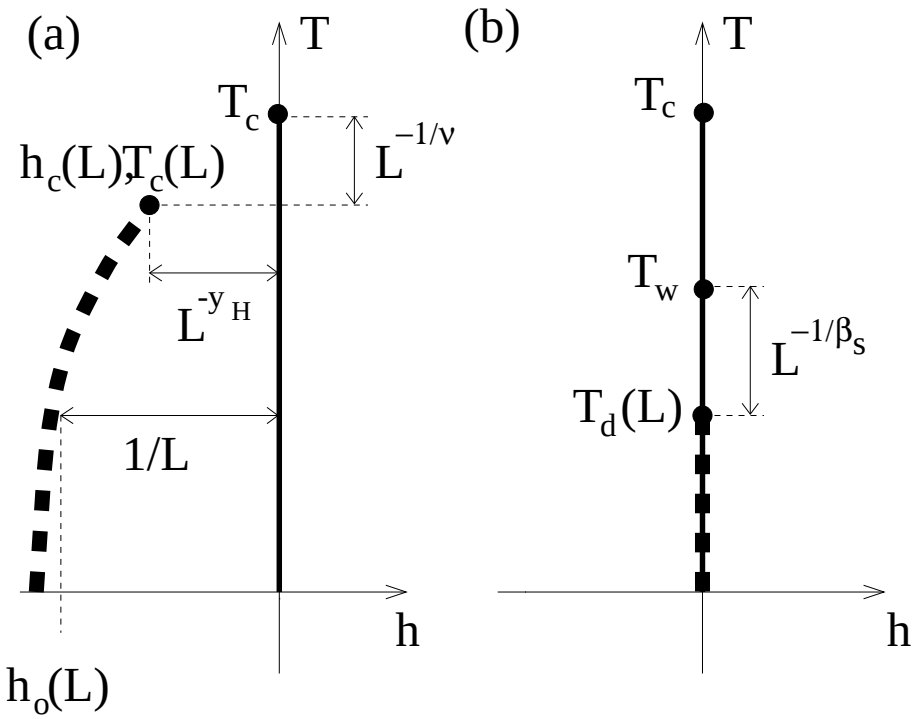


FIG. 1.

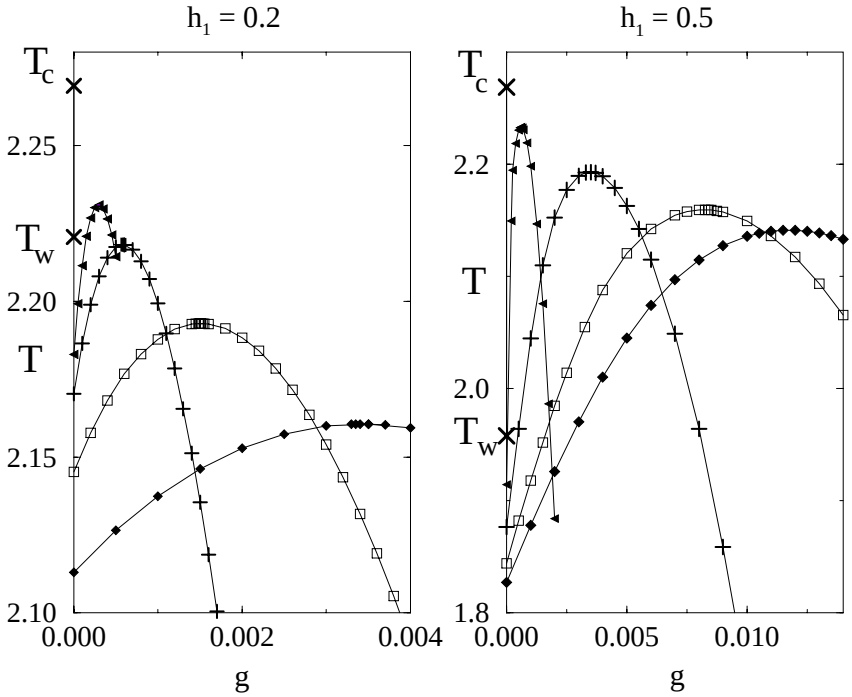
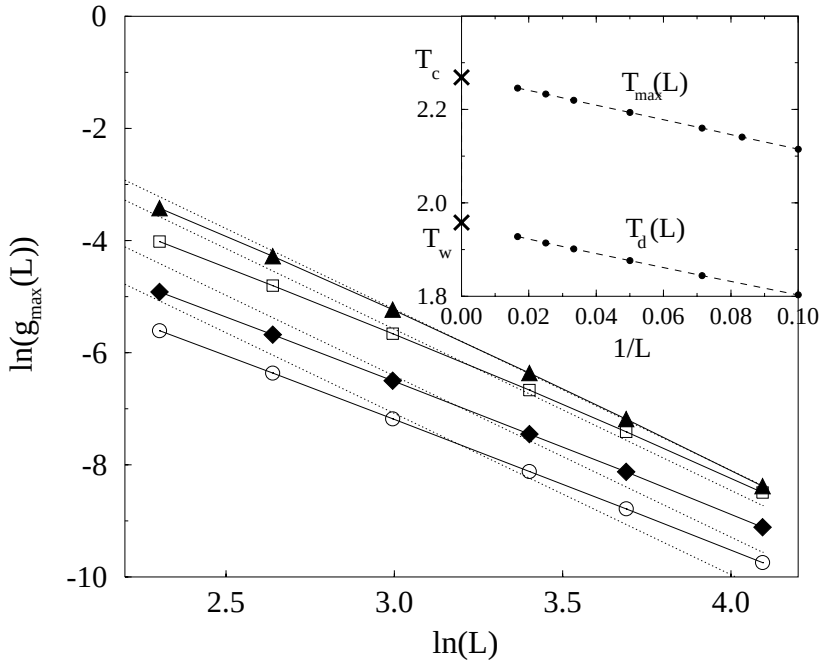


FIG. 2.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-6
-8
-10
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3.0
3.5
4.0
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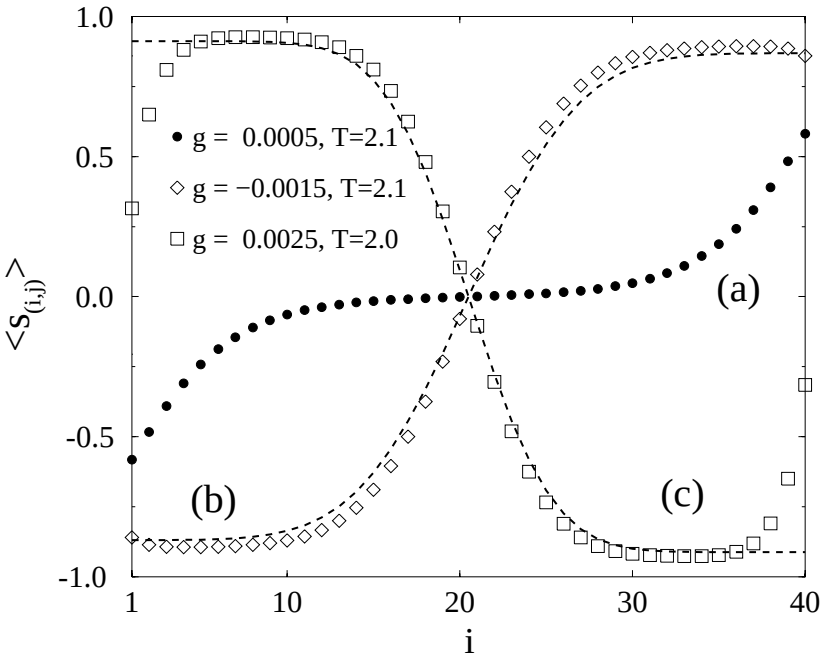
ln(g_max(L))
T_c
2.2
2.0
T_w
1.8
T_max(L)
T_d(L)
0.00
0.02
0.04
0.06
0.08
0.10
1/L

FIG. 3.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0.0
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-1.0
1
10
20
30
40
i
<s_(i,j)>
g = 0.0005, T=2.1
g = −0.0015, T=2.1
g = 0.0025, T=2.0
(a)
(b)
(c)

FIG. 4.