The Ising model – Summary of L12

Aim: Study connections between macroscopic phenomena and the underlying microscopic world for a ferromagnet.
How: Study the simplest possible model of a ferromagnet containing the essential physics: the Ising model.
Objective: Gain qualitative understanding of the physics governing the phenomena and reveal possible universal behaviour.

Collection of interacting spins $s_i = \pm 1, i = 1, 2, \ldots, N$ placed on a regular lattice of N sites $\mathbf{r}_i$.

$$\begin{aligned} E_{\{s_i\}} &= \text{spin-spin interactions} + \text{spin-external field interactions} \\ &= -J \sum_{\langle ij \rangle} s_i s_j - H \sum_{i=1}^{N} s_i \quad \textbf{Ising model}. \end{aligned}$$

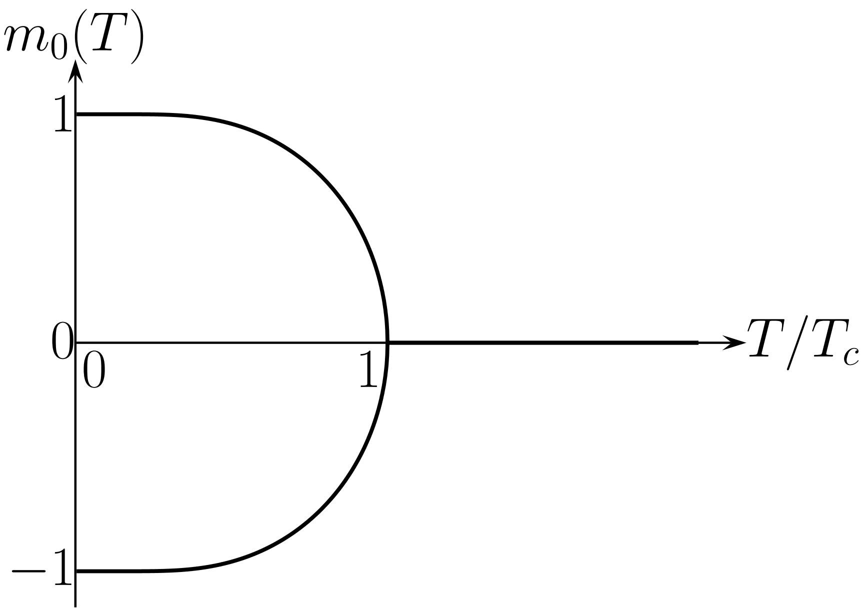
Order parameter: The average magnetisation per spin

$$m(T, H) = \sum_{\{s_i\}} p_{\{s_i\}} m_{\{s_i\}} = \frac{1}{Z} \sum_{\{s_i\}} \exp(-\beta E_{\{s_i\}}) m_{\{s_i\}},$$

with $m_{\{s_i\}} = \frac{1}{N} \sum_{i=1}^{N} s_i$ and the partition function

$$Z = \sum_{\{s_i\}} \exp(-\beta E_{\{s_i\}}).$$

The magnetisation in zero external field $m_0(T) = \lim_{H \to 0^\pm} m(T, H)$ for the Ising model in $d \geq 2$.



The Ising model – Summary of L13

Objective: Gain qualitative understanding of the phase transition in the Ising model: N lattice spins $s_i = \pm 1$ with positive nearest-neighbour interaction J placed in an external field H,

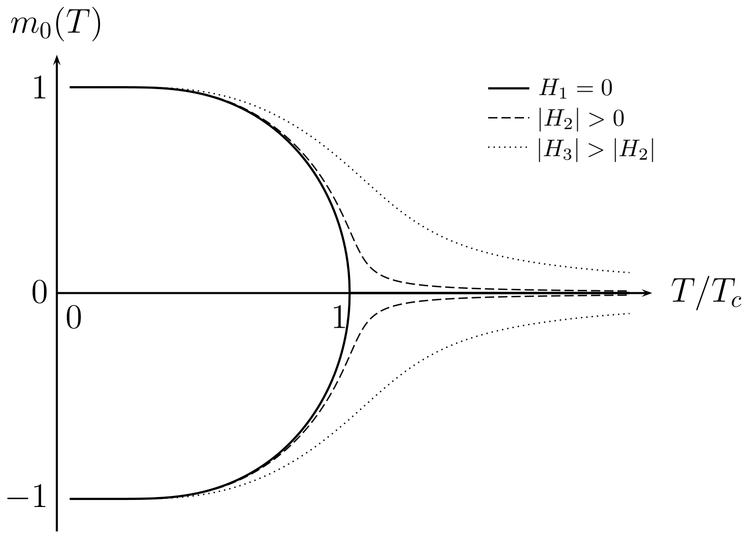
$$E_{\{s_i\}} = -J \sum_{\langle ij \rangle} s_i s_j - H \sum_{i=1}^{N} s_i.$$

In equilibrium, the spin system will minimise the **free energy**

$$F = \langle E \rangle - TS.$$

Assume zero external field $H = 0$. The order parameter is the average magnetisation per spin $m_0(T) = \lim_{H \to 0^\pm} m(T, H)$.

- When $J/(k_B T) \ll 1$, the free energy is minimised by maximising the entropy. Spins are randomly orientated, $m_0(T) = 0$.
- When $J/(k_B T) \gg 1$, the free energy is minimised by minimising the energy. Spins are aligning, $m_0(T) \neq 0$.



The correlation length $\xi(T, H)$ sets the scale of typical largest fluctuations away from the microstates with (a) randomly orientated spins when $T > T_c$ (b) fully aligned spins when $T < T_c$.

- Trivially self-similar states with $\xi(T, 0) = 0$ at $T = \infty$ and $T = 0$.
- Non-trivially self-similar states with $\xi(T_c, 0) = \infty$ at $T = T_c$.

The Ising model – Summary of L14

Ising model in $d = 1$: Interacting spins $s_i = \pm 1$ with pbc.

$$E_{\{s_i\}} = -J \sum_{i=1}^{N} s_i s_{i+1} - H \sum_{i=1}^{N} s_i$$

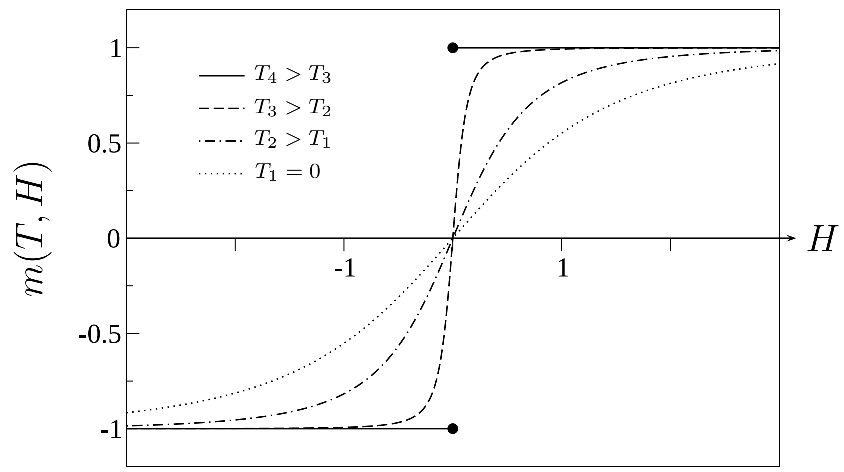
$$Z = \sum_{\{s_i\}} e^{\beta\left[J\sum_{i=1}^{N} s_i s_{i+1} + \frac{H}{2}\sum_{i=1}^{N}(s_i + s_{i+1})\right]}$$

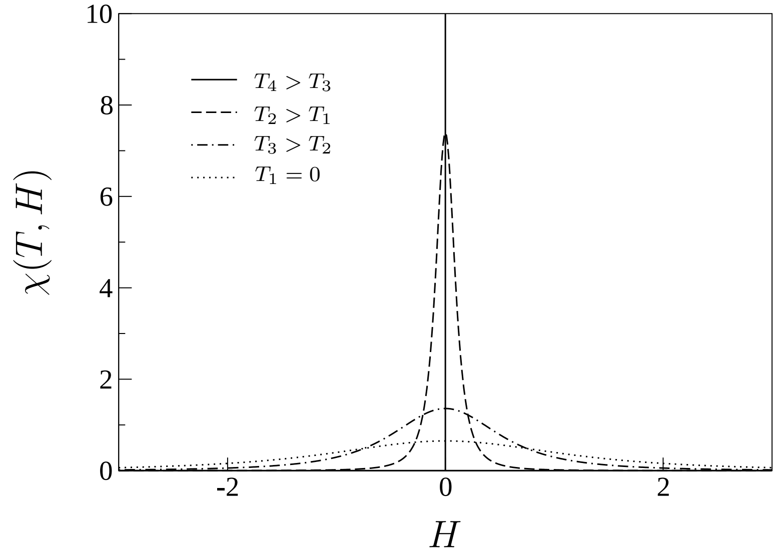
$$= \sum_{\{s_i\}} T_{s_1 s_2} T_{s_2 s_3} T_{s_3 s_4} T_{s_4 s_5} \ldots T_{s_{N-1} s_N} T_{s_N s_1}$$

$$= \lambda_+^N + \lambda_-^N \qquad \text{Eigenvalues of } \mathbf{T}\text{, i.e., } |\mathbf{T} - \lambda \mathbf{I}| = 0$$

$$F = -k_b T \ln Z \rightarrow -N k_b T \ln \lambda_+ \quad \text{for } N \rightarrow \infty$$

$$m(T, H) = -\left(\frac{\partial f}{\partial H}\right)_T = \frac{\sinh(\beta H)}{\sqrt{\sinh^2(\beta H) + e^{-4J\beta}}}.$$





The Ising model – Summary of L15

Ising model in $d = 1$: Interacting spins $s_i = \pm 1$ with pbc.

$$E = -J \sum_{i=1}^{N} s_i s_{i+1} - H \sum_{i=1}^{N} s_i.$$

The spin-spin correlation function

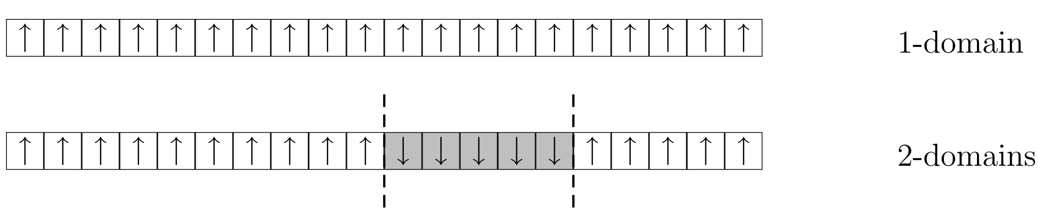
$$\begin{aligned} g(\mathbf{r}_i, \mathbf{r}_j) &= \langle\, (s_i - \langle s_i \rangle)\,(s_j - \langle s_j \rangle)\,\rangle \\ &= \langle s_i s_j \rangle - \langle s_i \rangle \langle s_j \rangle \\ &= \begin{cases} 0 & \text{for } T = 0 \\ \langle s_i s_{i+r} \rangle & \text{for } T > 0 \end{cases} \\ &= \begin{cases} 0 & \text{for } T = 0 \\ \exp(-r/\xi) & \text{for } T > 0. \end{cases} \end{aligned}$$

witht the correlation length

$$\xi = -\frac{1}{\ln[\tanh(\beta J)]} \to \begin{cases} 0 & \text{for } T \to \infty \\ \frac{1}{2}\exp(2\beta J) & \text{for } T \to 0. \end{cases}$$

The correlation function is related to the susceptibility per spin

$$\sum_{\mathbf{r}_j} g(\mathbf{r}_i, \mathbf{r}_j) = k_B T \chi = \frac{\langle M^2 \rangle - \langle M \rangle^2}{N}.$$



The free energy $F = \langle E \rangle - TS = \langle E \rangle - k_B T \ln \Omega$ so

$$F_{\text{2-domains}} - F_{\text{1-domain}} = 4J - k_B T \ln N(N-1).$$

A single domain of aligned spins is unstable against thermal fluctuations for finite T for large enough N since $F_{\text{2-domains}} < F_{\text{1-domain}}$.
In the $d = 1$ Ising model, $T_c = 0$.

Ising Model – Summary of L16

Mean-field approach ignores correlations between spins.

$$E_{\{s_i\}} = NJzm^2/2 - (Jzm + H)\sum_{i=1}^{N} s_i.$$

Model of N noninteracting spins in an effective field $Jzm + H$, where each spin feels an average internal field Jzm from the z nearest neighbour spins in addition to the external field H.

The partition function is readily calculated analytically

$$Z = \exp(-\beta NJzm^2/2)\,[2\cosh(\beta Jzm + \beta H)]^N .$$

The free energy per spin is a function of T and H,

$$f = Jzm^2/2 - k_BT\ln[2\cosh(\beta Jzm + \beta H)] .$$

The magnetisation per spin minimises the free energy and satisfies

$$m = \tanh(\beta Jzm + \beta H) \qquad (\star).$$

Letting $T_c = Jz/k_B$, Equation $(\star)$ in zero external field reads

$$m_0(T) = \tanh(\frac{T_c}{T}m_0(T)) \qquad (\star\star).$$

For $T \geq T_c$ the solution $m_O(T) = 0$ is unique and stable. For $T < T_c$ the trivial solution becomes unstable but two new stable non-zero solutions appear for the first time, therefore

$$m_0(T) = \begin{cases} 0 & \text{for } T \geq T_c \\ \pm\sqrt{3/T_c}(T_c - T)^{\beta} & \text{for } T \to T_c^- . \end{cases}$$

The susceptibility per spin

$$\chi(T,0) = (\partial m/\partial H)_T|_{H=0} = \Gamma_{\pm}|T - T_c|^{-\gamma^{\pm}} \quad \text{for } T \to T_c^{\pm}$$

with exponents $\gamma^{\pm} = 1$ and amplitudes $\Gamma_+ = 1/k_B, \Gamma_- = 1/(2k_B)$.

The magnetisation per spin at $T = T_c$

$$m(T_c, H) \propto \text{sign}(H)|H|^{1/\delta} \quad \text{for } |H| \to 0$$

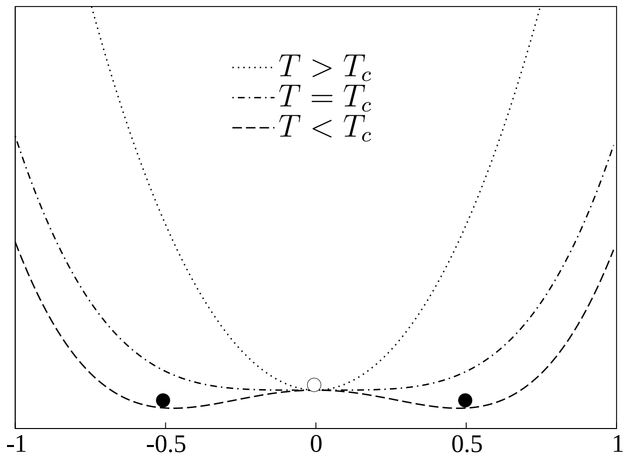
with ciritcal exponent $\delta = 3$.

The Ising model – Summary of L17

Landau theory for the Ising model. Expanding the free energy per spin in powers of the order parameter m:

$$f = f_0 - Hm + a_2(T - T_c)m^2 + a_4 m^4 \quad a_2, a_4 > 0.$$

The magnetisation m is determined by minimising the free energy, so it must



satisfy the equation $\left(\frac{\partial f}{\partial m}\right)_{T,H} = 0$ implying

$$-H + 2a_2(T - T_c)m + 4a_4 m^3 = 0.$$

The magnetisation in zero external field ($\beta = 1/2$)

$$m_0(T) = \begin{cases} 0 & \text{for } T \geq T_c \\ \pm\sqrt{\frac{a_2}{2a_4}(T_c - T)} & \text{for } T \to T_c^-. \end{cases}$$

The susceptibility per spin in zero external field ($\gamma^\pm = 1$)

$$\chi(T, 0) = \left(\frac{\partial m}{\partial H}\right)_T\bigg|_{H=0} = \begin{cases} \frac{1}{k_B}(T - T_c)^{-1} & \text{for } T \to T_c^+ \\ \frac{1}{2k_B}(T_c - T)^{-1} & \text{for } T \to T_c^-. \end{cases}$$

The magnetisation at $T = T_c$ in small external fields ($\delta = 3$)

$$m(T_c, H) \propto \text{sign}(H)|H|^{1/\delta} \quad \text{for } T = T_c \text{ and } |H| \to 0.$$

The specific heat capacity in zero external field ($\alpha^\pm = 0$)

$$c(T, 0) = \left(\frac{\partial \epsilon}{\partial T}\right)_H\bigg|_{H=0} = \begin{cases} 0 & \text{for } T \to T_c^+ \\ \frac{3}{2}k_B & \text{for } T \to T_c^-. \end{cases}$$

The Ising model – Summary of L18

Widom scaling ansatz for the magnetisation per spin

$$m(t,h) = |t|^{\beta}\mathcal{M}_{\pm}(h/|t|^{\Delta}) \quad \text{for } t \to 0^{\pm} \text{ and } |h| \to 0,$$

where β and Δ (the so called gap exponent) are universal critical exponents and $\mathcal{M}_{\pm}$ universal scaling functions that must satisfy

$$\begin{aligned}
&m(t,h) = -m(t,-h) && \Leftrightarrow \mathcal{M}_{\pm}(x) = -\mathcal{M}_{\pm}(-x) \\
&m(t,h) = \pm|t|^{\beta} \quad \text{for } t \to 0^{-} && \Leftrightarrow \mathcal{M}_{-}(0) = \pm\text{non-zero constant} \\
&m(t,h) = 0 \quad \text{for } t > 0 && \Leftrightarrow \mathcal{M}_{+}(0) = 0 \\
&m(0,h) \propto \text{sign}(h)|h|^{1/\delta} && \Leftrightarrow M_{\pm}(x) \propto \text{sign}(x)|x|^{1/\delta} \quad \text{for } x \to \pm\infty, \Delta = \beta\delta
\end{aligned}$$

The susceptibility per spin

$$\chi(t,h) = |t|^{\beta-\Delta}\mathcal{M}'_{\pm}(h/|t|^{\Delta})$$

so taking the limit $h \to 0$ we find

$$\Delta = \beta + \gamma \quad \text{and} \quad \mathcal{M}'_{\pm}(0) = \text{non-zero constants}$$

Widom scaling ansatz for the singular part of the free energy per spin

$$f_s(t,h) = |t|^{2-\alpha}\mathcal{F}_{\pm}\left(h/|t|^{\Delta}\right) \quad \text{for } t \to 0^{\pm} \text{ and } |h| \to 0.$$

and by taking derivatives with respect to the external field we find

$$\begin{aligned}
m(t,h) &\propto |t|^{2-\alpha-\Delta}\ \mathcal{F}'_{\pm}\left(h/|t|^{\Delta}\right) \quad \text{for } t \to 0^{\pm} \text{ and } |h| \to 0 \\
\chi(t,h) &\propto |t|^{2-\alpha-2\Delta}\mathcal{F}''_{\pm}\left(h/|t|^{\Delta}\right) \quad \text{for } t \to 0^{\pm} \text{ and } |h| \to 0.
\end{aligned}$$

The Widom scaling ansatz for the free energy per spin and the correlation function (see Exercise 2.5) implies scaling relations

$$\begin{aligned}
\beta\delta &= \beta + \gamma && \text{Widom scaling law} \\
\alpha + 2\beta + \gamma &= 2 && \text{Rushbrook scaling law} \\
d\nu &= 2 - \alpha && \text{Josephson scaling law} \\
\gamma &= \nu(2-\eta) && \text{Fisher scaling law.}
\end{aligned}$$

The exponents take the same value for $t \to 0^{\pm}$. There are only two independent critical exponents.

The Ising model – Summary of L19

Defining the dimensionless reduced temperature $t = (T - T_c)/T_c$ and external field $h = H/k_B T$, the Widom scaling ansatz for the free energy per spin and the correlation function when $t \to 0^{\pm}$, $|h| \to 0$ are

$$f_s(t,h) = |t|^{2-\alpha}\mathcal{F}_{\pm}\left(h/|t|^{\Delta}\right) \tag{1}$$

$$g(\mathbf{r},t,h) = |\mathbf{r}|^{-(d-2+\eta)}\mathcal{G}_{\pm}\left(|\mathbf{r}|/|t|^{-\nu}, h/|t|^{\Delta}\right). \tag{2}$$

The origin of scaling is intimately related to the existence of only one relevant length scale ξ which diverges at the critical point $(T_c, 0)$. Spins are correlated over scales up to ξ leading Kadanoff to introduce the idea of real-space transformation.

- Divide the system into blocks I each with b^d spins.
- Coarse-grain system by replacing all spins in block I with a block spin S_I.
- Rescale all length scales by factor b.

The renormalisation implies $N' = b^{-d}N, t' = b^{y_t}t, h' = b^{y_h}h$ and

$$Z(N,t,h) = \sum_{\{s_I\}} \sum_{\substack{\{s_i\}\text{ consistent}\\ \text{with }\{s_I\}}} \exp(-\beta E_{\{s_i\}}) = \sum_{\{s_I\}} \exp(-\beta E'_{\{s_I\}}) = Z(N',t',h')$$

The partition function is invariant but the free energy per spin satisfies

$$f(t,h) = b^{-d}f(t',h') = b^{-d}f(b^{y_t}t, b^{y_h}h) \quad \text{for all } b < \xi$$

which by letting $b = |t|^{-1/y_t}$ is equivalent with Equation (1).
Similarly, one can show the correlation function satisfies

$$g(|\mathbf{r}|,t,h) = |b|^{-2\beta/\nu}g(|\mathbf{r}'|,t',h') = |b|^{-2\beta/\nu}g(|\mathbf{r}|/b, b^{y_t}t, b^{y_h}h) \quad \text{for all } b < \xi$$

which by letting $b = |t|^{-1/y_t}$ is equivalent with Equation (2).
Kadanoff block spin real-space renormalisation transformation gives heuristic explanation for the Widom scaling ansatz for the free energy and the correlation function.

The Ising model – Summary of L20

Renormalisation in $d = 1$. The reduced energy for the Ising model

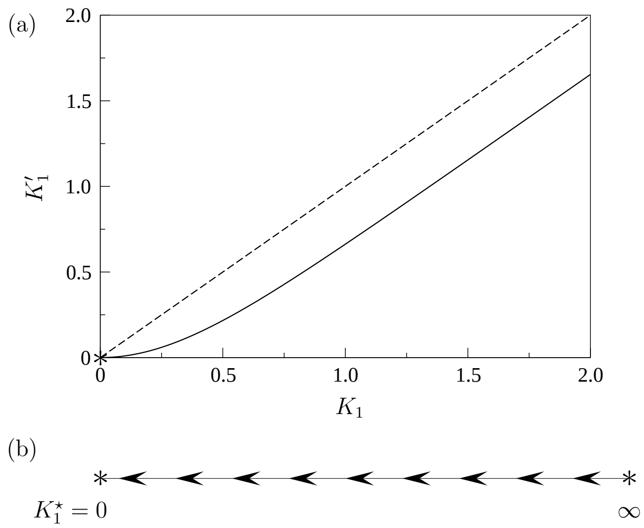
$$\beta E_{\{s_i\}} = -\frac{J}{k_B T}\sum_{\langle ij\rangle} s_i s_j - \frac{H}{k_B T}\sum_{i=1}^{N} s_i = -K_1 \sum_{\langle ij\rangle} s_i s_j - h\sum_{i=1}^{N} s_i.$$

The partition function (in zero external field, $h = 0$) in $d = 1$:

$$\begin{aligned} Z(K_1, N) &= \sum_{\langle ij\rangle} \exp\left(K_1 \sum_{i=1}^{N} s_i s_{i+1}\right) \\ &= \sum_{\text{odd spins}} \sum_{\text{even spins}} \exp\left(K_1[s_1 s_2 + s_2 s_3]\right)\cdots\exp\left(K_1[s_{N-1}s_N + s_N s_1]\right) \\ &= \sum_{\text{odd spins}} \exp\left(K_0' + K_1' s_1 s_3\right)\cdots\exp\left(K_0' + K_1' s_{N-1} s_1\right) \\ &= \exp(N' K_0') Z(K_1', N'), \end{aligned}$$

where the renormalised coupling constants and number of spins

$$\begin{aligned} K_0' &= 2\sqrt{\cosh 2K_1} \\ K_1' &= \frac{1}{2}\ln\left(\cosh 2K_1\right) \\ N' &= N/2. \end{aligned}$$



In the renormalised lattice, nn spins couple with strength $K_1' < K_1$. For $0 < K_1 < \infty$, the renormalisation induces a flow from the unstable fixed point $K_1^\star = \infty$ (spins fully aligned) towards the stable fixed point $K_1^\star = 0$ (spins noninteracting): No phase transition in $d = 1$ for $(t, h) \neq (0, 0)$.