The Ising Model I [tsc18]

The model named after Ernst Ising (pronounced "easing") was introduced in 1925 to explain ferromagnetism based on a (postulated) interaction that was discovered a year later: the exchange interaction.

The Hamiltonian of the Ising model on a $\mathcal{D}$-dimensional lattice of any type with sites labeled i is often rendered in the general form,

$$\mathcal{H} = -\sum_{\langle ij \rangle} J_{ij}\sigma_i\sigma_j - \sum_i H_i\sigma_i.$$

where $\langle ij \rangle$ are nearest-neighbor pairs of sites. The degrees of freedom are characterized by binary variables $\sigma_i = \pm 1$, each coupled to its nearest neighbors via J_{ij} and to a local external field H_i.

Ising magnet:

The primary interpretation of the σ_i is that of localized electron spins with a strongly uniaxial exchange coupling.

For the case of a uniform coupling and a uniform external field parallel to the easy axis, the simplified Hamiltonian reads,

$$\mathcal{H} = -J\sum_{\langle ij \rangle} \sigma_i\sigma_j - H\sum_i \sigma_i \quad \begin{cases} J > 0 & : \text{ ferromagnet} \\ J < 0 & : \text{ antiferromagnet} \end{cases}$$

Canonical partition function:

$$Z_N = \mathrm{Tr}\big[e^{-\beta\mathcal{H}}\big] = \sum_{\sigma_1,\ldots,\sigma_N} \exp\left(\beta J\sum_{\langle ij \rangle} \sigma_i\sigma_j + \beta H\sum_i \sigma_i\right).$$

Gibbs free energy: $G(T,H,N) = -k_{\mathrm{B}}T\ln Z_N(T,H)$.

Enthalpy: $E(T,H,N) = -\dfrac{\partial}{\partial\beta}\ln Z_N = \dfrac{1}{Z_N}\mathrm{Tr}\big[\mathcal{H}e^{-\beta\mathcal{H}}\big]$.

Entropy: $S(T,H,N) = \dfrac{1}{T}(E-G)$.

Magnetization: $M(T,H,N) = -\left(\dfrac{\partial G}{\partial H}\right)_{TN} = \dfrac{1}{Z_N}\mathrm{Tr}\left[\sum_i \sigma_i e^{-\beta\mathcal{H}}\right] = \sum_i \langle\sigma_i\rangle$.

Heat capacity: $C_H(T,H,N) = k_{\mathrm{B}}\beta^2\dfrac{\partial^2}{\partial\beta^2}\ln Z_N$.

Susceptibility: $\chi_T(T,H,N) = \beta^{-1}\dfrac{\partial^2}{\partial H^2}\ln Z_N$.

Ising lattice gas:

Consider a volume V in $\mathcal{D}$-dimensional space and superimpose an imaginary lattice of cell size $v_{\rm c}$. The (fixed) number of cells is $N = V/v_{\rm c}$.

Each cell is large enough to contain one molecule of a one-component fluid. The hard-core repulsion between molecules prohibits multiple cell occupancy. Molecules in nearest-neighbor cells experience an attractive contact force.

Potential energy between particles in cells i and j:

$$V_{ij} = \begin{cases} \infty & \text{if } i = j, \\ -u & \text{if } i, j \text{ are nearest}-\text{neighbor cells}, \\ 0 & \text{otherwise.} \end{cases}$$

Cell occupancy: $\tau_i = 0, 1$ (lattice gas variable).

The lattice gas neglects the kinetic energy of particles, which does not imply zero pressure even in the absence of an interaction.

Lattice gas Hamiltonian: $\mathcal{H} = -u \sum_{\langle ij \rangle} \tau_i \tau_j$.

Canonical partition function: $Z_{N_{\rm p}} = \sum_{\tau_1, \ldots, \tau_N} \exp\left(\beta u \sum_{\langle ij \rangle} \tau_i \tau_j \right) \delta_{N_{\rm p}, \sum_i \tau_i}$.

A switch of ensemble removes the constraint $\sum_i \tau_i = N_{\rm p}$.

Grand partition function:

$$Z = \sum_{N_{\rm p}=0}^{\infty} e^{\beta \mu N_{\rm p}} Z_{N_{\rm p}} = \sum_{\tau_1, \ldots, \tau_N} \exp\left(\beta u \sum_{\langle ij \rangle} \tau_i \tau_j + \beta \mu \sum_i \tau_i \right).$$

The number of cells, $N = V/v_{\rm c}$, is fixed, whereas the number $N_{\rm p}$ of particles (or occupied cells) is controlled by the chemical potential μ.

Grand potential: $\Omega(T, V, \mu) = -k_{\rm B} T \ln Z(T, V, \mu)$.

Pressure: $p = -\left(\frac{\partial \Omega}{\partial V} \right)_{T\mu}$.

Average number of particles: $N_{\rm p} = -\left(\frac{\partial \Omega}{\partial \mu} \right)_{TV}$.

Entropy: $S = -\left(\frac{\partial \Omega}{\partial T} \right)_{V\mu}$.

Mapping between Ising lattice gas and Ising magnet:

Variable transformation: $\tau_i = \frac{1}{2}(1-\sigma_i) \quad \Leftrightarrow \quad \sigma_i = 1 - 2\tau_i$.

Coordination number: z (each cell has z nearest neighbors).

$$
\begin{aligned}
Z &= \sum_{\sigma_1,\ldots,\sigma_N} \exp\left(\frac{1}{4}\beta u \sum_{\langle ij\rangle}\Big[\sigma_i\sigma_j - (\sigma_i+\sigma_j) + 1\Big] + \frac{1}{2}\beta\mu\sum_i\Big[1-\sigma_i\Big]\right). \\
&= \sum_{\sigma_1,\ldots,\sigma_N} \exp\left(\frac{1}{4}\beta u\sum_{\langle ij\rangle}\sigma_i\sigma_j - \left[\frac{1}{4}\beta z u + \frac{1}{2}\beta\mu\right]\sum_i\sigma_i\right) \\
&\qquad\qquad \times \exp\left(\left[\frac{1}{8}\beta u z + \frac{1}{2}\beta\mu\right]N\right),
\end{aligned}
$$

where we have used $\displaystyle\sum_{\langle ij\rangle}\sigma_i = \frac{1}{2}z\sum_i\sigma_i, \quad \sum_{\langle ij\rangle} = \frac{1}{2}zN.$

Set $\displaystyle\frac{1}{4}u = J, \quad -\left[\frac{1}{4}zu + \frac{1}{2}\mu\right] = H \quad \Rightarrow \ \frac{1}{8}uz + \frac{1}{2}\mu = -H - \frac{1}{2}zJ.$

$$
Z(T,V,\mu) = e^{-\beta N(H+\frac{1}{2}zJ)} \underbrace{\sum_{\sigma_1,\ldots,\sigma_N} \exp\left(\beta J\sum_{\langle ij\rangle}\sigma_i\sigma_j + \beta H\sum_i\sigma_i\right)}_{Z_N(T,H)}.
$$

- Relation between grand partition function $Z(T,V,\mu)$ of Ising lattice gas and canonical partition function $Z_N(T,H)$ of Ising ferromagnet.
- The degrees of freedom (subject to interactions) are particles, i.e. occupied cells, in the lattice gas and spins in the magnet.
- The average number N_p of particles is controlled by the chemical potential μ, whereas the number N of spins is fixed.
- The extensivity of the system is encoded in the volume $V = Nv_\mathrm{c}$ of the lattice gas and in the number N of spins in the magnet.
- The primary thermodynamic potentials are the grand potential Ω for the lattice gas and the Gibbs free energy G for the magnet.
- Ideal lattice gas [tex172]: $u = 0 \quad \Rightarrow \ Z = \big[1 + e^{\beta\mu}\big]^{V/v_\mathrm{c}}$.
- Langevin/Brillouin paramagnet [tex85]: $u = 0 \quad \Rightarrow \ M = N\tanh H$.

Transfer matrix solution of the Ising magnet in $\mathcal{D} = 1$:

The Ising magnet in $\mathcal{D} = 1$ (a linear chain of N sites) is a perfect model for a gentle introduction to the transfer matrix method of exact analysis.

Hamiltonian: $\mathcal{H} = -\sum_{l+1}^{N} \left[J\sigma_l\sigma_{l+1} + \frac{1}{2}H(\sigma_l + \sigma_{l+1}) \right]$.

Periodic boundary conditions: $\sigma_{N+1} \equiv \sigma_1$.

Scaled parameters: $\hat{J} \doteq \beta J, \quad \hat{H} \doteq \beta H$.

Canonical partition function:

$$\begin{aligned} Z_N &= \sum_{\sigma_1,\ldots,\sigma_N} \exp\left(\sum_{l=1}^{N} \left[\hat{J}\sigma_l\sigma_{l+1} + \frac{1}{2}\hat{H}(\sigma_L + \sigma_{l+1}) \right] \right) \\ &= \sum_{\sigma_1,\ldots,\sigma_N} V(\sigma_1,\sigma_2)V(\sigma_2,\sigma_3)\cdots V(\sigma_N,\sigma_1), \end{aligned}$$

where the functions,

$$V(\sigma_l,\sigma_{l+1}) = \exp\left(\hat{J}\sigma_l\sigma_{l+1} + \frac{1}{2}\hat{H}(\sigma_l + \sigma_{l+1}) \right),$$

are the elements, $\langle\sigma_l|\mathbf{V}|\sigma_{l+1}\rangle$, of the transfer matrix,

$$\mathbf{V} = \begin{pmatrix} V(+1,+1) & V(+1,-1) \\ V(-1,+1) & V(-1,-1) \end{pmatrix} = \begin{pmatrix} e^{\hat{J}+\hat{H}} & e^{-\hat{J}} \\ e^{-\hat{J}} & e^{\hat{J}-\hat{H}} \end{pmatrix}.$$

Consider $N = 2$: Summing $V(\sigma_1,\sigma_2)V(\sigma_2,\sigma_1)$ over σ_2 yields the diagonal elements of $\mathbf{V}\cdot\mathbf{V} = \mathbf{V}^2$. Summing over σ_1 yields the trace $\mathrm{Tr}[\mathbf{V}^2]$.

The N-fold sum in Z_N is equivalent to an N-fold multiplication of identical matrices $\mathbf{V}$ and the evaluation of the trace of the product matrix:

$$Z_N = \mathrm{Tr}\big[\mathbf{V}^N\big].$$

Diagonalization of symmetric matrix $\mathbf{V}$ by orthogonal matrix $\mathbf{O}$ [tex185]:

$$\mathbf{O}^{-1}\cdot\mathbf{V}\cdot\mathbf{O} = \begin{pmatrix} \lambda_+ & 0 \\ 0 & \lambda_- \end{pmatrix}, \quad \mathbf{O} \doteq \begin{pmatrix} \cos\phi & -\sin\phi \\ \sin\phi & \cos\phi \end{pmatrix}.$$

The matrix $\mathbf{O}^{-1}\cdot\mathbf{V}\cdot\mathbf{O}$ is diagonal if $\cot(2\phi) = e^{2\hat{J}}\sinh\hat{H}$.

Eigenvalues: $\lambda_\pm = e^{\hat{J}}\left[\cosh\hat{H} \pm \sqrt{\sinh^2\hat{H} + e^{-4\hat{J}}} \right]$.

Partition function dominated by largest eigenvalue λ_+ of transfer matrix:

$$Z_N = \lambda_+^N + \lambda_-^N = \lambda_+^N \left[1 + (\lambda_-/\lambda_+)^N\right] \overset{N\to\infty}{\rightsquigarrow} \lambda_+^N.$$

Gibbs free energy in the thermodynamic limit:

$$G(T,H,N) = -J - Nk_{\mathrm{B}}T \ln\Big(\cosh\hat{H} + \sqrt{\sinh^2\hat{H} + e^{-4\hat{J}}}\Big).$$

The magnetization $M(T,H,N)$ and entropy $S(T,H,N)$ are first derivatives of G. The enthalpy $E(T,H,N) = G+TS$ and the internal energy $U(T,H,N) = E + HM$ follow directly [tex185]

The response functions $C_H(T,H,N)$ (heat capacity) and $\chi_T(T,H,N)$ (susceptibility) are second derivatives of G [tex185].

Expectation values via transfer matrix:

Joint probability distribution:

$$P(\sigma_1,\ldots,\sigma_N) = \frac{1}{Z_N} e^{-\beta\mathcal{H}} = \frac{1}{Z_N} V(\sigma_1,\sigma_2)V(\sigma_2,\sigma_3)\cdots V(\sigma_N,\sigma_1).$$

Magnetization per site, previously derived from $G(T,H,N)$, here derived as an expectation value:

$$\bar{M}(T,H) = \langle\sigma_i\rangle = \sum_{\sigma_1,\ldots,\sigma_N} \sigma_i P(\sigma_1,\ldots,\sigma_N).$$

The periodic boundary conditions make $\langle\sigma_i\rangle$ site-independent, facilitating the matrix representation,

$$\langle\sigma_i\rangle = \frac{1}{Z_N}\mathrm{Tr}\big[\mathbf{S}\cdot\mathbf{V}^N\big], \quad \mathbf{S} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

The transformation $\mathbf{O}$ which diagonalized $\mathbf{V}$ makes $\mathbf{S}$ nondiagonal. The gain far outweighs the loss. We infer [tex189]:

$$\mathbf{O}^{-1}\cdot\mathbf{S}\cdot\mathbf{O} = \begin{pmatrix} \cos 2\phi & -\sin 2\phi \\ -\sin 2\phi & -\cos 2\phi \end{pmatrix},$$

$$\begin{aligned}\langle\sigma_i\rangle &= \lim_{N\to\infty}\frac{1}{Z_N}\mathrm{Tr}\left[\begin{pmatrix} \cos 2\phi & -\sin 2\phi \\ -\sin 2\phi & -\cos 2\phi \end{pmatrix}\cdot\begin{pmatrix} \lambda_+^N & 0 \\ 0 & \lambda_-^N \end{pmatrix}\right] \\ &= \lim_{N\to\infty}\cos 2\phi\frac{\lambda_+^N - \lambda_-^N}{\lambda_+^N + \lambda_-^N} = \cos 2\phi,\end{aligned}$$

in agreement with the result obtained previously in [tex189].

Correlation functions via transfer matrix:

The two-spin correlation function is of primary interest and our focus here:

$$\langle \sigma_i \sigma_j \rangle = \sum_{\sigma_1,\ldots,\sigma_N} \sigma_i \sigma_j P(\sigma_1,\ldots,\sigma_N).$$

The periodic boundary conditions make $\langle \sigma_i \sigma_{i+n} \rangle$ independent of site i, which facilitates the following matrix representation:

$$\langle \sigma_i \sigma_{i+n} \rangle = \frac{1}{Z_N} \mathrm{Tr}\big[\mathbf{S} \cdot \mathbf{V}^n \cdot \mathbf{S} \cdot \mathbf{V}^{N-n}\big].$$

The combination of diagonalizing N matrices $\mathbf{V}$ and undiagonalizing two matrices $\mathbf{S}$ keeps the matrix product manageable [tex189]:

$$\begin{aligned}
\langle \sigma_i \sigma_{i+n} \rangle = \frac{1}{Z_N} \Bigg[& \begin{pmatrix} \cos 2\phi & -\sin 2\phi \\ -\sin 2\phi & -\cos 2\phi \end{pmatrix} \cdot \begin{pmatrix} \lambda_+^n & 0 \\ 0 & \lambda_-^n \end{pmatrix} \\
& \cdot \begin{pmatrix} \cos 2\phi & -\sin 2\phi \\ -\sin 2\phi & -\cos 2\phi \end{pmatrix} \cdot \begin{pmatrix} \lambda_+^{N-n} & 0 \\ 0 & \lambda_-^{N-n} \end{pmatrix} \Bigg] \\
= \cos^2 2\phi \, & \frac{\lambda_+^N - \lambda_-^N}{\lambda_+^N + \lambda_-^N} + \sin^2 2\phi \, \frac{\lambda_-^n \lambda_+^{N-n} + \lambda_+^n \lambda_-^{N-n}}{\lambda_+^N + \lambda_-^N} \\
\stackrel{N\to\infty}{\longrightarrow} \; & \cos^2 2\phi + \left(\frac{\lambda_-}{\lambda_+}\right)^n \sin^2 2\phi.
\end{aligned}$$

The covariance is a function that decays to zero for $n \to \infty$ even in the presence of a non-vanishing magnetization $\langle \sigma_i \rangle$ [tex189]:

$$C(n) \doteq \langle \sigma_i \sigma_{i+n} \rangle - \langle \sigma_i \rangle \langle \sigma_{i+n} \rangle = \left[1 + e^{4\hat{J}} \sinh^2 \hat{H}\right]^{-1} \left(\frac{\lambda_-}{\lambda_+}\right)^n.$$

Dominant long-distance asymptotics: $C(n) \sim e^{-n/\xi}$.

Correlation length: $\xi(T,H) \doteq [\ln(\lambda_+/\lambda_-)]^{-1}$.

Ising lattice gas in $\mathcal{D} = 1$:

We employ the mapping established earlier in this module for the transcription of the transfer matrix solution:

$$Z(T,V,\mu) = e^{-N\beta(H+J)} Z_N(T,H) = e^{-N\hat{H}} \left[\cosh(\hat{H}) + \sqrt{\sinh^2(\hat{H}) + e^{-4\hat{J}}}\right]^N,$$

$$J = \frac{u}{4}, \quad H = -\frac{u+\mu}{2}, \quad V = N v_\mathrm{c}, \quad \hat{H} \doteq \beta H, \quad \hat{J} \doteq \beta J.$$

Here u is the interaction energy between occupied cells of volume v_c and μ the chemical potential, which controls cell occupancy.

Ideal gas limit:

We use the limit $u = 0$ as a benchmark for the study of interaction effects.

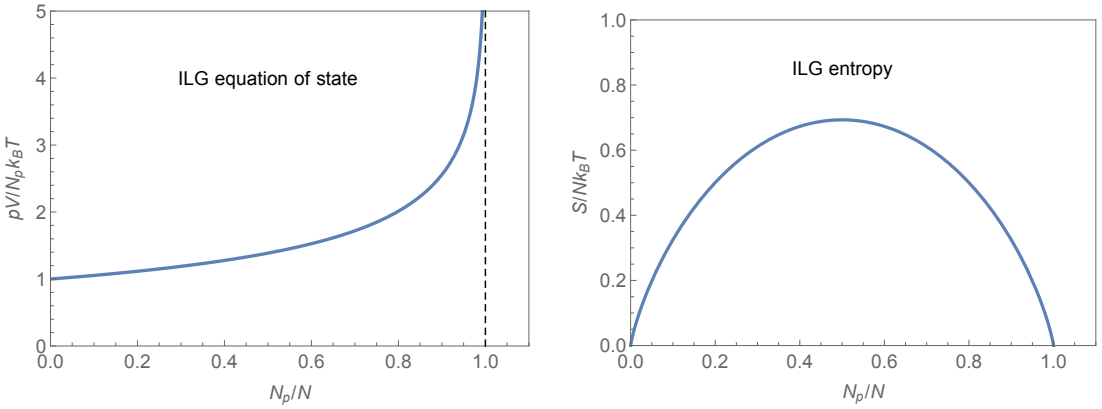
$$Z = e^{-N\beta H}\left[2\cosh(\beta H)\right]^N = \left[1 + e^{\beta\mu}\right]^{V/v_c}$$

$$\Rightarrow\ \Omega(T, V, \mu) = -pV = -k_B T \ln Z = -\frac{V}{v_c} k_B T \ln\left(1 + e^{\beta\mu}\right).$$

From first derivatives we extract explicit expressions for the equation of state and the entropy [tex172]:

$$\frac{pV}{N_p k_B T} = -\frac{N}{N_p} \ln\left(1 - \frac{N_p}{N}\right),$$

$$\frac{S}{N k_B} = -\frac{N_p}{N} \ln\frac{N_p}{N} - \left(1 - \frac{N_p}{N}\right) \ln\left(1 - \frac{N_p}{N}\right).$$



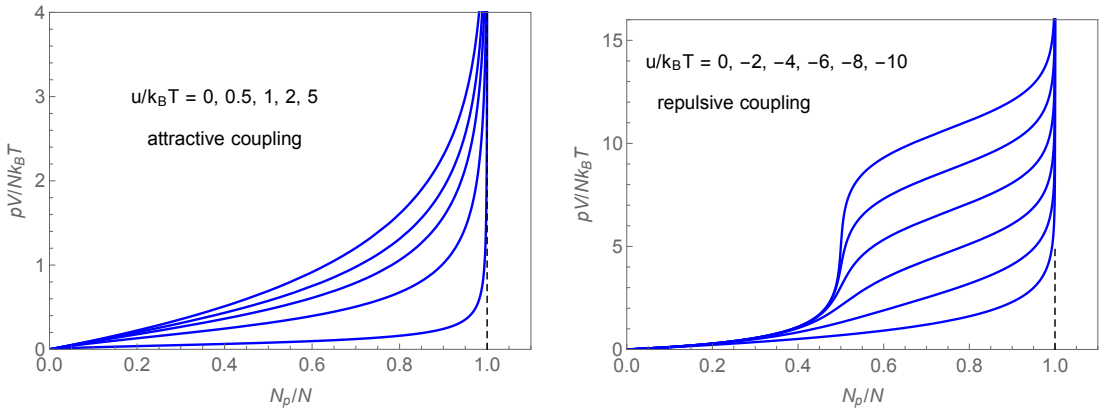
- Average lattice-gas density: N_p/N.
- Classical ideal gas limit: $N_p/N \to 0 \quad \Rightarrow\ pV \to N k_B T$.
- The excess pressure of the ILG is due to the fact that each particle occupies a nonzero volume v_c. The pressure diverges when the lattice is fully occupied.
- The entropy rises from zero as N_p/N increases from zero, reaches a maximum at $N_p/N = \frac{1}{2}$, and returns to zero as $N_p/N \to 1$.
- The curve has a particle/hole mirror symmetry.
- The empty lattice and the fully occupied lattice have zero entropy.
- The half-full lattice comprises the largest number of microstates, which produces the entropy maximum.

Ising lattice gas equation of state in $\mathcal{D} = 1$:

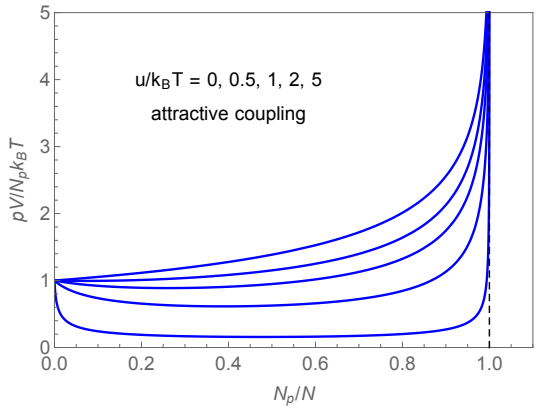
The thermodynamic equation of state of the Ising lattice gas can be inferred directly from the grand partition function in paramagnetic form [tex194]:

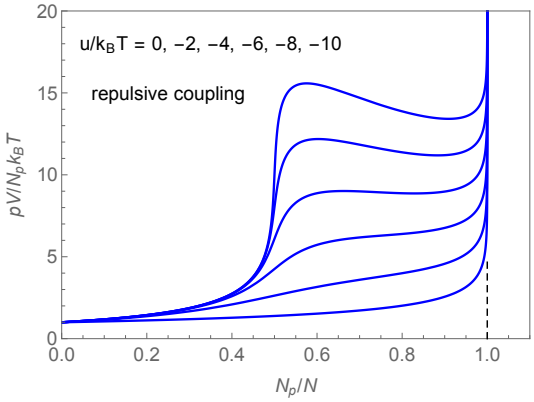
$$\frac{pV}{Nk_BT} = w + \ln\left(\cosh w + \sqrt{\sinh^2 w + e^{-\beta u}}\right),$$
$$\frac{N_{\mathrm{p}}}{N} = \frac{1}{2}\left[1 + \frac{\sinh w}{\sqrt{\sinh^2 w + e^{-\beta u}}}\right],$$

where $w = \frac{1}{2}\beta(u + \mu)$ is the parameter. The explicit ILG result is readily recovered in the limit $u \to 0$ [tex194].



- For attractive coupling ($u > 0$), the ILG curve is the highest. For repulsive coupling ($u > 0$), it is the lowest.
- At fixed volume and temperatures, the curves represent a measure of pressure per cell.
- All curves are monotonic. Each occupied cell adds pressure, irrespective of interaction.
- An attractive particle interaction slows down the rise of pressure when particles are added.
- Near saturation, the pressure rises steeply and diverges irrespective of interaction. This is a steric effect.
- The effect of a repulsive particle interaction is very weak at low density.
- The repulsive interaction quickly gains traction around half filling when nearest-neighbor occupied cells are harder to avoid.
- For strong repulsive interaction, a high plateau develops at more than half filling.

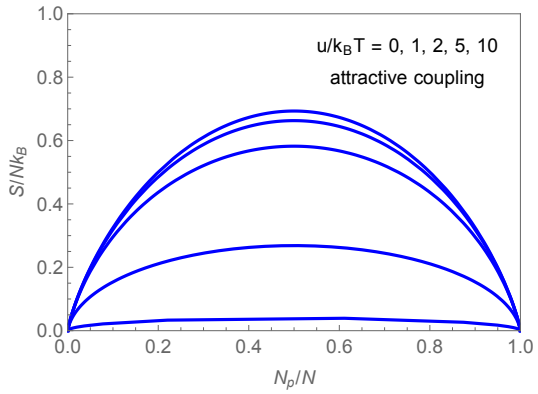


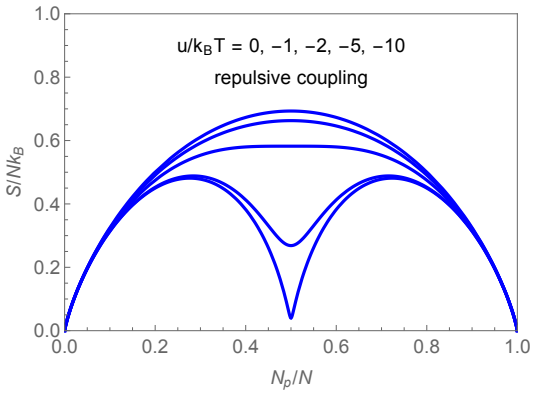


- At fixed volume and temperatures, these curves represent a measure of pressure per particle.
- For attractive coupling ($u > 0$), the ILG curve is again the highest and for repulsive coupling ($u > 0$) the lowest.
- Adding particles at low density reduces the pressure per particle when they attract one another sufficiently strongly.
- Adding particles at more than half filling reduces the pressure per particle when they repel one another sufficiently strongly.
- in the low-density limit, $N_\mathrm{p}/N \to 0$, the result $pV/N_\mathrm{p}k_BT = 1$ for the classical ideal gas is recovered irrespective of interaction.

Ising lattice gas entropy in $\mathcal{D} = 1$:

A parametric expression for the entropy, $\{S(w)/Nk_B, N_\mathrm{p}/N\}$, is readily derived from the grand partition function in a similar fashion [tex195].





– At fixed particle density, both attractive and repulsive interactions of increasing strength reduce the entropy. However, the entropy reduction is associated with different kinds of ordering tendencies.

– In the ILG limit $u \to 0$, the entropy is dominated by the distribution of occupied (vacant) cells below (above) half filling.

– Attractive coupling between occupied cells favors clusters below half filling and (effectively) clusters of vacant cells above half filling.

– Coupled clusters act like compound particles or compound vacancies. Their number decreases as the (attractive) coupling strength increases. The highest entropy is realized at half filling.

– A repulsive interaction between occupied cells suppresses clustering of particles below half filling and (effectively) vacancies above half filling.

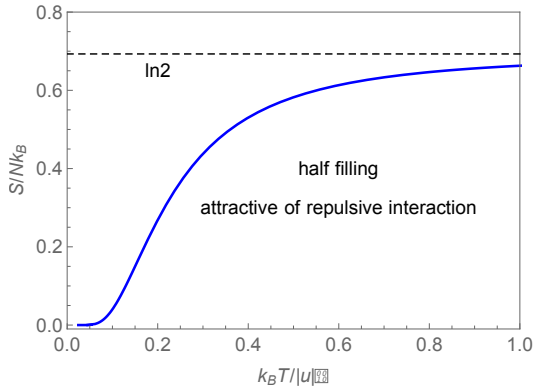
– For low densities of particles or vacancies, the effect of a repulsive interaction is very small. Randomly placed particles or vacancies at low density produce few nearest neighbors.

– The highest impact of a repulsive interaction is realized at half filling. Here the only microstates which avoid clustering of particles are ordered states where occupied and vacant cells alternate.

– The particle-hole symmetry of occupied and vacant cells is differently manifest for attractive and repulsive interaction.

– An additional symmetry makes the dependence of S/Nk_B on u/k_BT independent of the sign of u at half filling.

The entropy per cell as a function scaled temperature $k_BT/|u|$ is then the same monotonic function for attractive interaction ($u > 0$) and repulsive interaction ($u > 0$) [tex201]. The entropy of the ideal lattice gas ($u = 0$) is independent of temperature.



Ising lattice gas internal energy in $\mathcal{D} = 1$:

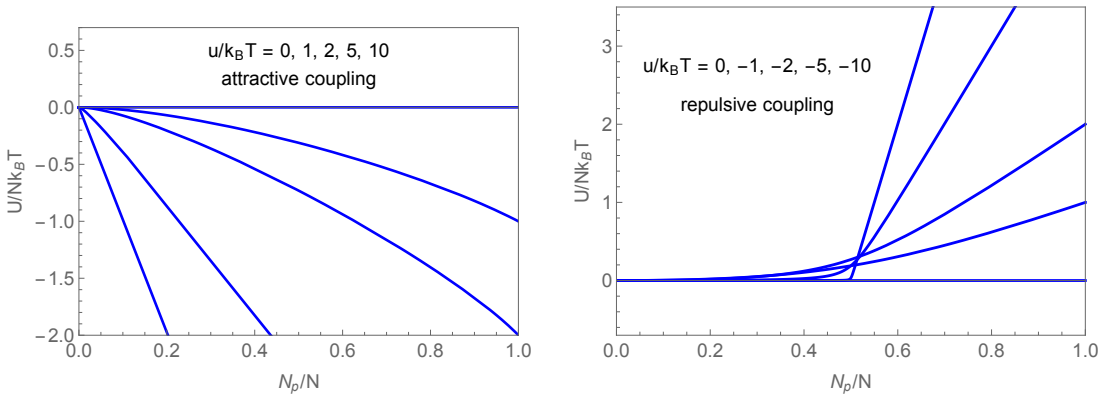
A parametric expression for the internal energy can be constructed via Euler's equation,

$$U = TS - pV + \mu N_{\rm p} \quad \Rightarrow \frac{U}{Nk_BT} = \frac{S}{Nk_B} - \frac{pV}{Nk_BT} + \left(2w - \frac{u}{k_BT}\right)\frac{N_{\rm p}}{N},$$

from the expressions established earlier:

$$\frac{U}{Nk_BT} = -\frac{\beta u}{2}\frac{[\sinh w + \cosh w][\sinh w + \sqrt{\sinh^2 w + e^{-\beta u}}]}{\sqrt{\sinh^2 w + e^{-\beta u}}[\cosh w + \sqrt{\sinh^2 w + e^{-\beta u}}]},$$

$$\frac{N_{\rm p}}{N} = \frac{1}{2}\left[1 + \frac{\sinh w}{\sqrt{\sinh^2 w + e^{-\beta u}}}\right],$$



- An attractive coupling produces a negative internal energy of significant magnitude even for relatively small densities due to clustering.
- A repulsive interaction makes configurations with occupied nearest-neighbor sites energetically unfavorable.
- If less then half the lattice sites are occupied, nearest-neighbor repulsion is readily avoided by strong repusive coupling.