



**MathsNET**

A joined up approach to  
teaching and learning  
mathematics

# The cluster expansion

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- Write an expression for the Hamiltonian of a system of particles that interact through a two-body potential and that do not sit on lattice sites.
- Explain why when this Hamiltonian is inserted into our expression for the canonical partition function the resulting integral separates into a product of an integral over the momentum coordinates and a integral over the position coordinates. Discuss how one the integral over the momentum coordinates can be solved exactly.
- Explain how the cluster expansion allows one to rewrite the integral over the position coordinates introduced in the above as a sum of integrals.
- Discuss the result that you obtain if you truncate the expansion introduced in the previous part and only include the first term



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- If the sum of integral that you have introduced is truncated after the second term what assumption are you making about the interactions between the particles
- Discuss how the second term in the cluster expansion integral is solved in general and what assumptions are made about the interaction during the derivation
- Describe the shape of the hard spheres potential and show that  $\int_0^\infty f_{12} r^2 dr = -A + \beta B$  for this potential. How are the values of  $A$  and  $B$  calculated from the parameters of the hard sphere potential?
- Give an expression for the free energy of the van der Waals gas and explain how this quantity is derived from the partition function for a system of hard spheres



- Show how the equation of state for the van-der-Waals gas can be derived from the partition function for a system of hard spheres and explain the various assumptions made during this derivation