Statistical Physics and Computer Simulations
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Exercise Sheet 4

1. **The 1D Potts Model**
Consider the one–dimensional Potts model with Hamiltonian

$$H = -J \sum_{i=1}^{N} \delta(S_i, S_{i+1}).$$

Here $J > 0$ is the coupling constant, while the Potts variables (generalized "spins") can take the values $S = 0, 1, 2, \ldots, q$ (so–called q–state Potts model). $\delta(x, y)$ denotes the Kronecker delta, i. e. $\delta(x, y) = 1$ if $x = y$ and zero otherwise. First consider the special case $q = 2$ and show by means of a variable transformation that this corresponds to the Ising model. Then solve the statistical mechanics of the model for arbitrary values of q, using the transfer matrix method. Plot the specific heat as a function of temperature for $q = 2, 3, 4$.

Hints:

- Show that the transfer matrix can be written as a multiple of the unit matrix, plus a matrix whose entries are one throughout.
- Consider this latter matrix. By guessing one eigenvector, show that q is an eigenvalue. Calculate the other eigenvalues by showing that the matrix is positive–definite, and considering the trace.
- From this, conclude the eigenvalues of the full transfer matrix.

2. **The Virial Theorem**
Consider a d–dimensional fluid of N particles which interact via a pair potential:

$$H = \sum_i \frac{\vec{p}_i^{\,2}}{2m} + \sum_{i<j} U\left(|\vec{r}_i - \vec{r}_j|\right).$$

Assume this system is in a cubic box with periodic boundary conditions of volume $V = L^d$. Within the framework of the canonical ensemble, show the virial theorem for the pressure

$$PV = NT + \frac{1}{d} \sum_{i<j} \left\langle \vec{r}_{ij} \cdot \vec{F}_{ij} \right\rangle,$$

where $\vec{r}_{ij} = \vec{r}_i - \vec{r}_j$ and $\vec{F}_{ij}$ is the interparticle force.

Hint:
It is useful to transform to reduced coordinates $\vec{s}_i$ via $\vec{r}_i = L\vec{s}_i$. This allows us to study straightforwardly how the partition function changes upon changing the volume (i. e. we keep the $\vec{s}_i$ fixed).

3. **The Constant–Pressure Ensemble**
Starting from the observation that a Laplace transformation of a partition functions will, in the thermodynamic limit, always induce the corresponding Legendre transformation, give the partition function of a system in the (N, P, T) ensemble.