Ongoing Projects and New Project for 2016

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1. Sublimation and Melting in a Mobile Potts Model

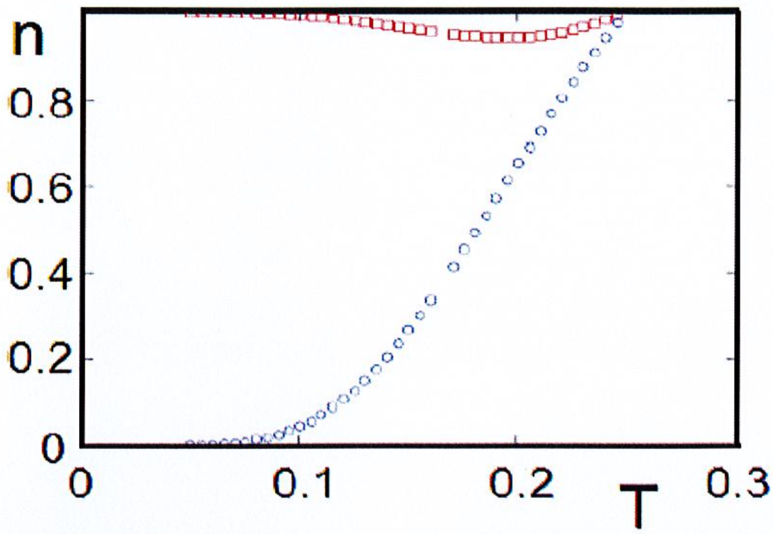
During the 2015 visit professor Kaufman collaborated with professor Diep and his PhD students on a couple of projects: 1. the mobile 6-state Potts model: 2. spin 1 (BEG model) on a finite width slab. The two models can be unified and generalized as explained below. We propose to further study this unified model using mean-field approximation and Monte Carlo simulations.

The space is divided in M equal volume v cells centered on the sites of a Bravais (cubic for example) lattice. Any cell is either vacant or occupied by a single particle characterized by a q value spin. Neighboring particles that have the same spin value get a lower energy –J than if they have different spin values. Zero energy is assigned to neighboring cells that have at least a vacancy. We assign an energy –K to neighboring cells that are occupied irrespective of their spin values. In the grand canonical ensemble we allow for fluctuating number of particles and include in the Hamiltonian a single site (cell) term proportional to the chemical potential H if there is a particle at the cell. This model can be described by assigning at each site a q + 1 Potts spin σ = 0, 1 … q. The zero value corresponds to vacancy while the values 1, 2 … q correspond to a particle having a spin. The Hamiltonian is:

$$(1-\delta(\sigma j,0))$$
$$\text{¿}$$
$$(1-\delta(\sigma i,0))\text{¿}$$
$$(1-\delta(\sigma j,0))+K\sum_{i,j}\text{¿}$$
$$\frac{-H}{k_B T}=J\sum_{i,j}\delta(\sigma i,\sigma j)(1-\delta(\sigma i,0))\text{¿}$$

(1)

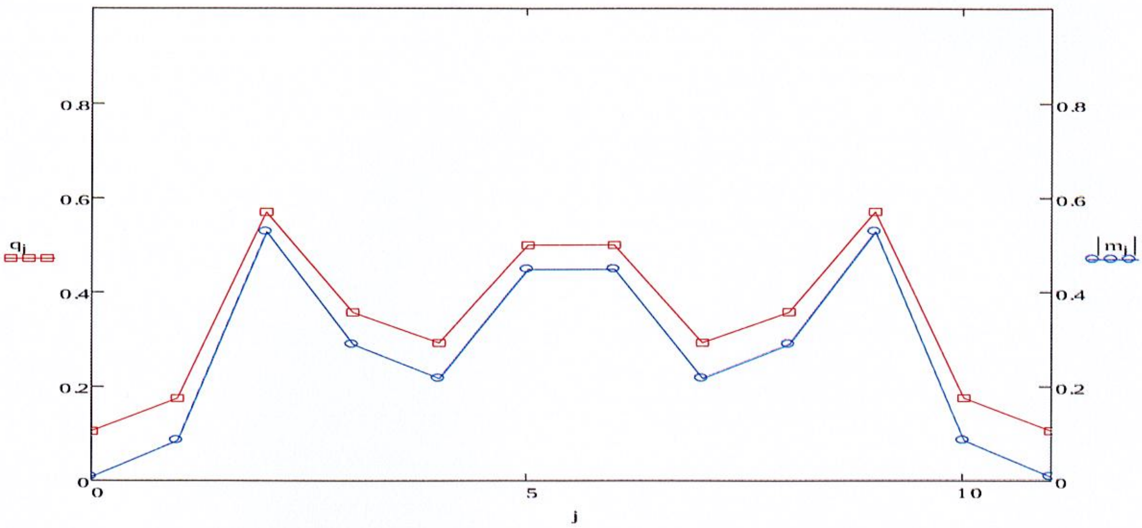
In our 2015 collaboration (Bulk Transition and Surface Sublimation of a Mobile Potts Model, A. Bailly-Reyre, H. T. Diep, M. Kaufman submitted Phys Rev E) we have studied this model for q = 6 with K = 0. In this model the solid (ordered phase) sublimates into the gas (disordered) phase. The phase diagram in the temperature T, concentration n plane is shown below:



The solid (the high n branch, red)) coexists with the gas (the low n branch, blue).
By allowing a non-zero K the phase diagram will now include a **disordered high density** phase that we identify to be the liquid phase. We then anticipate getting phase diagrams that include melting (solid – liquid transition) and vaporization (liquid- gas transitions). It is interesting to study this for slabs on N layers.

2. BEG in Mean-Field

The model in Eq 1 in the case of $q = 2$ reduces to the BEG model which is used to describe the phase diagram of superfluid He4-He3 mixtures. We started to study this for slabs of finite depth. The mean field results, that still need Monte Carlo confirmation, are quite interesting as one can get for particular choices of the parameters oscillations in the superfluid order parameter m as function of the location. There may be an important application for such oscillations as one can then have sandwiches of normal ($m = 0$) and superfluid ($m \neq 0$) slabs built by just choosing the correct total width.



N = 12

J = 0.6 K = 0.6 $\Delta = 3.2$

msurface = 4.78395×10^{-13} qsurface = 0.092356

It is interesting to also study the profiles of the order parameter for other choices of the parameters for which the bulk system is tricritical or at a critical-end point.

3. Two-group conflicts: a statistical physics model

We collaborate with Dr. Sanda Kaufman[1] on a "social physics" project applying statistical physics techniques to model two-group conflict. We consider two disputing groups. Each individual i in each of the two groups has a preference s_i regarding the way in which the conflict should be resolved. The individual preferences (corresponding to spins) span a range between +S (prone to settlement) and -S (prone to protracted conflict). The noise in this system is quantified by a "social temperature" T. Individuals interact within their group and with individuals of the other group. A pair of individuals i, j within a group contributes $-s_i * s_j$ to the energy. The inter-group

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energy of individual i is taken to be proportional to the product between s_i and the mean value of the preferences (spins) from the other group's members. We consider an equivalent-neighbor network where everyone interacts with everyone. We explore effects of the network topology on the qualitative behavior of this model. Then we analyze some examples of realistic situations where the strength of interactions diminishes with (social or geographic) distance between individuals.