Research Statement

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During my Ph.D. research at the University of Rochester, I have been studying critical behavior and phase transitions in statistical systems by various importance sampling simulation methods. Specifically, I have worked and been working on the following three projects:

1. **Structural and morphological transitions in gold nanorods**. Gold nanorods with thousands of atoms were heated up continuously from 5K to above melting temperature (T_m) by constant temperature molecular dynamics. Intermediate metastable shorter and wider states have been observed below T_m. The structural change of the interior from fcc to hcp-dominated is accompanied with the shape change. These simulation results are consistent with experimental observations.

   This work was done under the supervision of Prof. Christoph Dellago in the Chemistry Department. In January 2003 Prof. Dellago moved to a new position in Vienna and I transfered to the research group of Prof. Steve Teitel in the Physics Department. Prof. Teitel showed interest in the gold project and we three continued to work on the project below.

2. **Melting and equilibrium shape of icosahedral gold nanoparticles**. Gold nanoclusters with $1,000$ - $5,000$ atoms were cooled down slowly by Andersen thermostat from above T_m to 100K. Mackay icosahedra with missing central atom have been observed to be the preferred solid structure. The particles were then heated up slowly by constant temperature molecular dynamics towards T_m, when the behavior of the surface atoms has been tracked. We find that although the surface remains ordered up to T_m, the increasing mobility of vertex and edge atoms softens the stable fcc $< 111 >$ surface structure significantly at about 100K below T_m, smears sharp vertices and edges presented at low temperatures, leads to interlayer and intralayer diffusion, and shrinks the average facet size.

   After this project I started to work on Prof. Teitel's 2D superconducting network simulations.

3. **Non-equilibrium phase diagram of a driven two dimensional vortex lattice**. The driven 2D lattice Coulomb gas has been used as a model for vortices in superconducting networks. An enhanced continuous time Monte Carlo simulation method ensures us to obtain physical results for driven lattices. The nearest neighbors are found through Voronoi Diagram / Delaunay Triangulation. This project is ongoing to reach the final goal of understanding the phase transitions between driven non-equilibrium steady states.

In addition to the methods applied in our projects, such as microcanonical and canonical molecular dynamics, Andersen thermostat, Metropolis and continuous time Monte Carlo methods, I practiced some advanced methods like parallel tempering, umbrella sampling, and transition path sampling. I also have knowledge of simulated annealing, genetic algorithms, and multicanonical ensemble sampling.

During these projects, my knowledge of programming and electronics enables me to implement algorithms professionally, and settle down computer related problems quickly. Good readability, reusability and easy maintenance is provided by object oriented programming with C++. I also built a 16-node RedHat linux cluster and performed a parallel tempering program to locate the exact melting temperature of a gold nanocluster with 603 atoms.

For my future research work, I will be happy to continue working on any interesting problems in theoretical chemical or condensed matter physics. I also have a broad interest in the connection between condensed matter physics and other fields, such as optics, biophysics, quantum computing, graph theory, etc.