Henley group research opportunities

My research interests are spread over several distinct subjects. All involve interesting spatial dependences – symmetries or complicated patterns.

I divide them into four quadrants:
- The NSF grant (quadrants 1 and 2) mostly covers interacting, many-body quantum systems.
- The DOE grant (quadrants 3 and 4) is more materials-oriented, covering atomic or macromolecular structures in classical systems.

1. Strongly interacting fermions (NSF)

I work with simplified models, in the spirit of the Hubbard model. My aim is to work the borderline between analytic and computational physics, figuring out how to detect interesting (perhaps exotic) behaviors from exact diagonalizations (An example of an exotic behavior spontaneous currents, see Fig. 1).

S.A. Cheong's Ph.D. thesis (1/2006), worked out ways to use the reduced density matrix of a small cluster of sites for such purposes. [See e.g. S. A. Cheong and CLH, Phys. Rev. B 74, 165121 (2006).] I have tentative collaborations with Dr. Andreas Läuchli (Switz.) and Prof. Jan von Delft (Cornell PhD '95, Germany) to apply the notion of "correlation density matrix" (which contains all kinds of correlation present, even unanticipated ones).

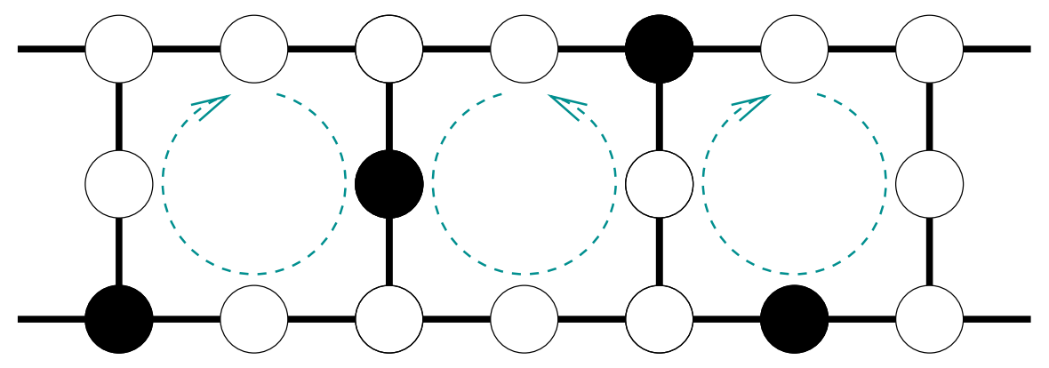

Fig. 1. A ladder lattice with spinless fermions (filled circles), obeying neighbor exclusion; arrows show possible spontaneous currents (from a proposal). Such (hidden) symmetry breakings have been conjectured to characterize the pseudogap phase in high-T_c's. We're writing a paper to elucidate which features of a toy model favor such a phase [with Sumiran Pujari].

My future activities under this head may include collaborating with Prof. Garnet Chan (Cornell, Chemistry), a computational chemist who hopes ambitiously to develop renormalization-group algorithms for interacting systems in $d > 1$ dimensions. There is the possibility of us sharing a (physics) student.

We're involved in simple phenomenology to help analyze the Séamus Davis group's STM data on high-T_c cuprates: (i) coupling of some phonon modes to the superconductivity [Sumiran Pujari] (ii) effect of spatial modulation of the superconducting order parameter on STM spectrum [Debo Olaosebikan, Ron Maimon].

2. Frustrated antiferromagnets (NSF)

We study (quantum) spins on *highly frustrated* lattices. That means there is no single ground state in which all the interactions are simultaneously minimized, but instead a large number of practically degenerate states.

I'm interested in devising effective Hamiltonians $\mathcal{H}_{\mathrm{eff}}$ which express the small energy differences among the states due e.g. to the zero-point spin fluctuations around a classical ground state (Fig. 2); this was the thesis of Uzi Hizi (Ph.D. June 2006). We found neat ways to express $\mathcal{H}_{\mathrm{eff}}$ in terms which are products of the spins around a loop, i.e. it has the functional form of an "Ising gauge theory".

When the spins are length 1/2, frustrated systems are promising places to find interesting exotic phases, such as "spin liquids" or fractional-charge states.

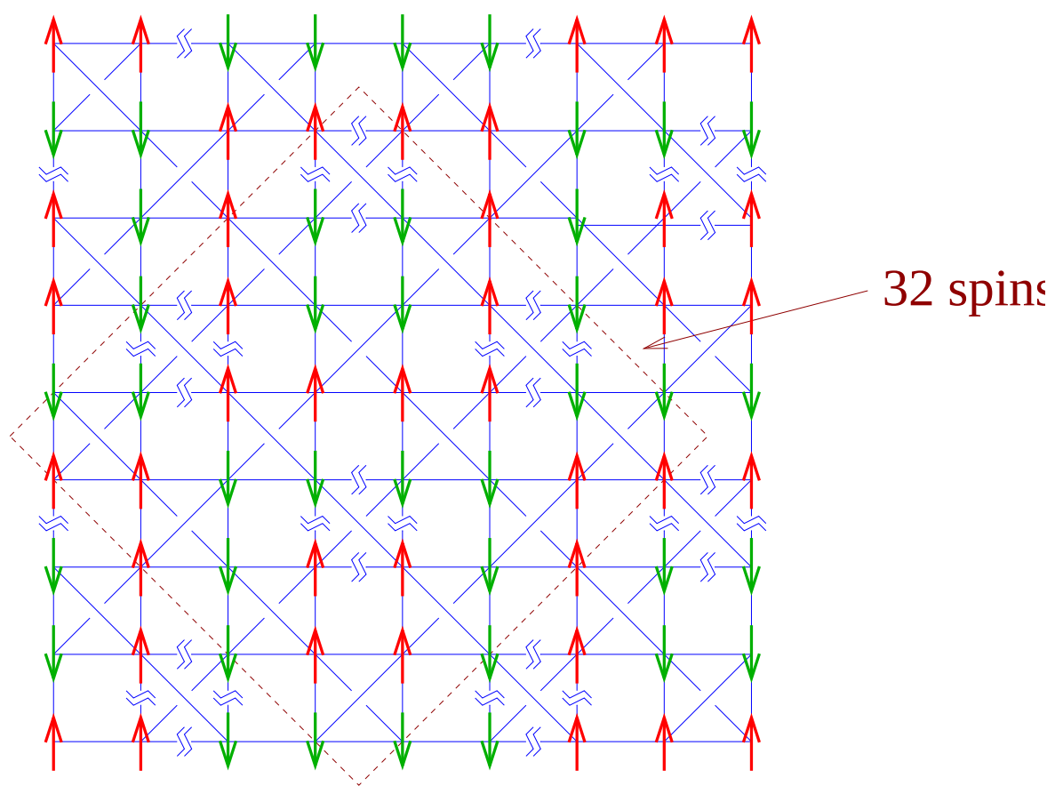

Fig. 2. The simplest ground state minimizing (harmonic order) spin-wave zero-point energy, for spins of large length S on the pyrochlore lattice [U. Hizi and CLH, Phys. Rev. B 73, 054403 (2006).] There appear to be of $O(e^L)$ states with this one in a system of $O(L^3)$ spins, i.e. the entropy of ground states is infinite but not extensive.

My aim for the future is the role of disorder (impurities) in highly frustrated magnets. To start, we're working on quantum antiferromagnets at percolation [Srivatsan Chakram] – currently studying the composition law of normal modes. (Percolation refers to the critical behavior when a system is diluted to the threshold where it becomes disconnected.)

Another topic is "non-abelian height models", a simple way to realize "topological order."
This exotic property was mainly known in quantum-many-body states such as the quantized Hall effect, However, a baby version of it is realized in some classical systems; we're working on simulations [John Papaioannou, undergrad].

3. Quasicrystal structures (DOE)

A quasicrystal has a symmetry (most often 5-fold or 10-fold) which is incompatible with crystal periodicity, yet it retains a high degree of translational order (as seen in Bragg diffraction peaks) as well as local chemical order. A longstanding dispute is unresolved, whether there are "Penrose matching rules" that dictate a virtually unique ground state, or whether the order emerges from a "random tiling" (ensemble of nearly degenerate configurations).

I continue this materials modeling with Marek Mihalkovič (Slovakia) and with undergraduates [currently Sejoon Lim.] We predict the microscopic structure (using effective interatomic potentials derived from ab-initio calculations) and do statistical physics of the random-tiling state. Last year we discovered a semi-realistic model in which microscopic pair interactions implement Penrose matching rules!

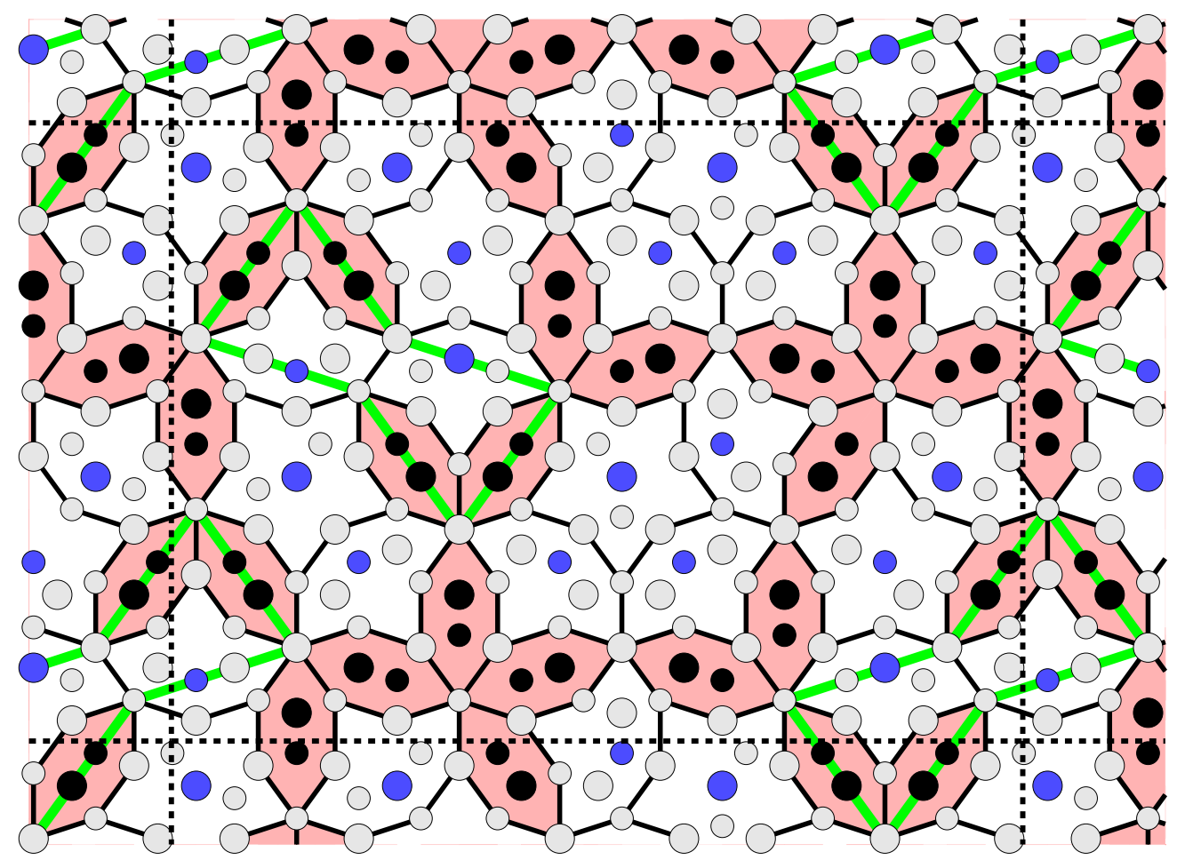

Fig. 3. End result of a simulation of $Al_{0.70}Ni_{0.21}Co_{0.09}$ decagonal quasicrystal. [M. Mihalkovič et al, Phys. Rev. B 65, 104205 (2002)]. Large and small circles are atoms from the two layers; gray=Al, blue=Co, black=Ni. "Hexagon", "boat", and "star" tiles can be seen at two different scales.

Along with this, I'm interested in the mathematical problem of optimum packings of spheres with two sizes.

4. Biological physics (DOE)

I'm interested in problems from biological physics which heavily involve symmetry, geometry, and the packing of identical units.
We [Steve Hicks] are modeling the formation of the "capsid" (shell) of viruses, which is built from many copies of the same proteins. Our aim is to understand what really fixes the capsid's size, to compare the ensemble of shapes and sizes to imaging experiments, and to extract coarse-grained elastic constants from protein simulations. We interact some with the Vogt group in Molecular Biology (retroviruses).

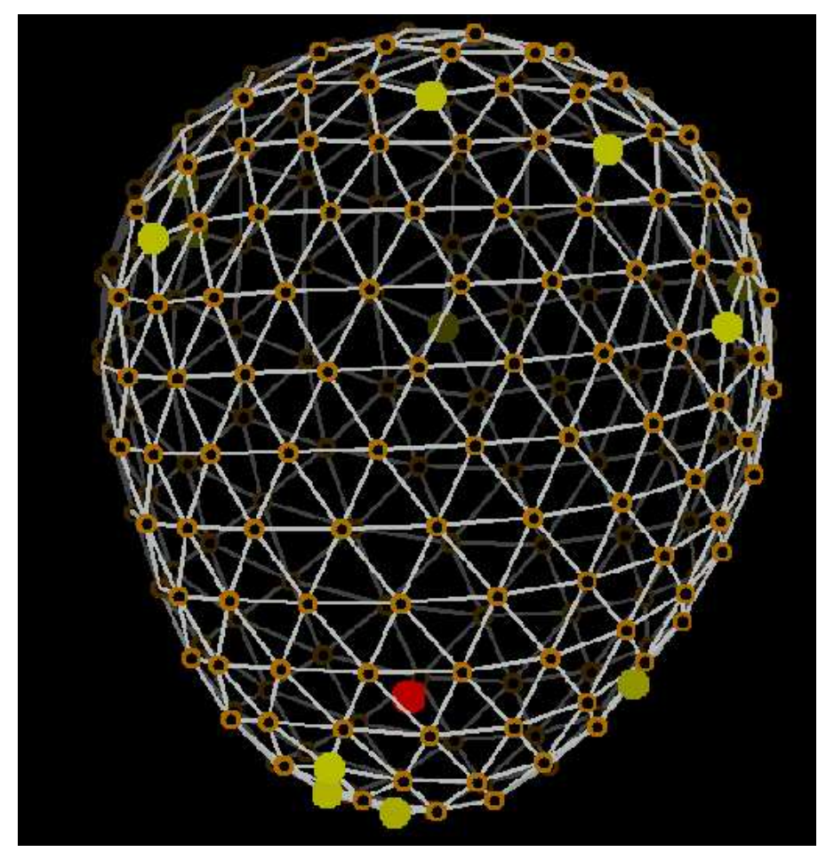

Fig. 4. Model for an HIV capsid. Triangular units accrete at random in a fashion that is biased, but hardly guaranteed, to form a closed shell. [S. D. Hicks and CLH, Phys. Rev. E 74, 031912 (2006).] In this run we tried to capture the peculiar "ice-cream cone" asymmetric shape of HIV

A project I'd like to start soon: how does the well-known *microscopic* handedness of proteins get propagated to the *macroscopic* handedness seen in *plants* (the screw twist of climbing vines) and *animals* (asymmetry of the heart etc. in vertebrates). That's nontrivial, since development uses some sort of diffusion, but that is independent of the molecule's handedness. The mechanism should involve long helical fibers – specifically microtubules. The animal side leads to modeling the motions of cilia, but I'm likely to focus on plants which are less understood. This research will lean on hydrodynamics and elastic theory; it could be appropriate for an IGERT first-summer project.