ICCP/PHY480: Project 3 - Due Friday May 3.

Choose one of the following four options

Option 1. Tight binding model of electronic structure: Calculate single particle electron energy levels using tight binding models: The tight binding Hamiltonian we use is,

$$H = \sum_{ij} t_{ij} |i><j| + \sum_i \epsilon_i |i><i| = \sum_{ij} t_{ij} c_i^\dagger c_j + \sum_i \epsilon_i n_i. \tag{1}$$

where $c_i^\dagger, c_i, n_i$ are the electron creation, annihilation and number operator at site "i". (i) Calculate and display the energy dispersion relations of graphene, showing the Dirac points; (ii) Find the density of states and inverse participation ratio of disordered square lattice using Anderson model. Look at the effect of lattice size and disorder. Find a partner and each use a different programming package or language, chosen from: Mathematica, Matlab, Python, C++, Fortran...

Option 2. Exact ground state and mass gap of a quantum spin system: Calculate the lowest energy levels of the many body quantum spin Hamiltonian the transverse Ising model for a one dimensional chain with L sites and periodic boundary conditions.

$$H = -J \sum_{i=1}^{L} \sigma_i^z \sigma_{i+1}^z + \lambda \sum_{i=1}^{L} \sigma_i^x \tag{2}$$

where σ_i^z, σ_i^x are Pauli matrices. You should calculate the ground state magnetization and the "mass gap", which is the energy gap between the ground state and the first excited state, as a function of λ/J and L. Use exact diagonalization of the $2^L \times 2^L$ Hamiltonian matrix. Find a partner and each use a different programming package or language, chosen from: Mathematica, Matlab, Python, C++, Fortran etc. Note that space matrix storage and extreme eigenvalue routines are required.

Option 3. Time evolution of a quantum particle incident on a barrier: Numerically solve the dynamics of a wave packet using the time dependent Schrodinger equation in the presence of

scattering barriers described by a potential $V(\vec{r})$;

$$i\hbar\frac{\partial\psi(\vec{r},t)}{\partial t} = [-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})]\psi(\vec{r},t) \tag{3}$$

First solve this in one dimension and illustrate the interaction of a wave packet with a barrier as a function of the barrier width and height, and the energy and width of the wavepacket. For example you can calculate the transmission probability as a function of energy. Then solve the Schrodinger equation in two dimensions and illustrate double slit interference and diffraction. Write three subroutines with different solvers: (i) Simple Euler; (ii) Runge-Kutta; (iii) Choose either the Crank-Nicholson or the Split operator method. Find a partner and each use a different programming package or language, chosen from: Mathematica, Matlab, Python, C++, Fortran...

Option 4. Lattice Boltzmann method: The Boltzman equation, for the one particle distribution function $f(\vec{r},\vec{p},t)$

$$f(t+\delta t,\vec{x}+\delta\vec{x},\vec{v}+\delta\vec{v}) - f(t,\vec{x},\vec{v}) \rightarrow= \frac{\partial f}{\partial t}|_{collision}\delta t \tag{4}$$

can be used to derive the equations of hydrodynamics. The discretized version of this equation must preserve the known mass and momentum conservation laws, and also energy conservation if the system is not dissipative. Lattice Boltzmann is a discretized version of the Boltzmann equation that has these properties. The positions are placed on a lattice and a discrete set of particle velocities is allowed. Rules for how particles move and velocities change along with the correct boundary conditions are required to carry out the simulation. The calculations should start with using a triangular lattice and non-slip boundary conditions to reproduce Poiseuille flow. This is being offered by Jos, so if you want to work with a dutch partner on this it is better. I have not programmed this but we can probably figure it out if someone really wants to do it without a dutch partner.