PC5203 Advanced Solid State Physics

Weeks 4-6, due Thursday 16 Sep 2021

[main concepts to cover: molecular vibrations, normal modes, phonons, creation and annihilation operators, tight-binding models, electron band structures.]

1. A water molecule has 9 degrees of freedom (need 9 coordinates to describe the positions of O and two H as point particles in three dimensions). However, 6 of them represent rigid space translation and rotation, so the vibrational degrees of freedom are the remaining 3. If we choose the changes of two bond lengths as Δr_1 and Δr_2 and the angle between them as $\Delta\theta$, the potential energy *V* is given on the slide 5 of week 2. Based on this information, (a) determine the kinetic energy K due to molecular vibration. Note that the masses of hydrogen and oxygen are 1 and 16 u, respectively. (b) Derive the equations of motion of the molecular vibration. (c) Determine the three vibrational frequencies, expressing the result in the traditional units of cm^{-1}. Determine the normal mode for each frequency and draw pictures to indicate their vibrational modes.

2. Using the Jordan-Wigner transform defined on slide 9 of week 3 for the matrix representation as $2^N \times 2^N$ matrices C_k and $C_k^\dagger$ for the fermion annihilation and creation operators, show that the three anti-commutation relations (c and c, $c^\dagger$ and $c^\dagger$ as well c and $c^\dagger$) for *N* fermions are all satisfied. [Hint: work out first how two direct-product matrices multiply according to the usual rule of matrix multiplication.]

3. Using the nearest neighbor tight-binding model of graphene for the π-orbitals as defined on page 10 of slides of week 3, and the Fourier transform convention on the same slide to $\boldsymbol{k} = (k_x, k_y)$, (a) show that the single particle Hamiltonian in $\boldsymbol{k}$ space is $H(\boldsymbol{k}) = \begin{pmatrix} 0 & f^* \\ f & 0 \end{pmatrix}$, with $f = -t\left[\exp\left(i\frac{k_y a}{\sqrt{3}}\right) + 2\cos\left(\frac{k_x a}{2}\right)\exp\left(-i\frac{k_y a}{2\sqrt{3}}\right)\right]$. Here $a = |\boldsymbol{a}_1| = |\boldsymbol{a}_2|$ is the lattice constant. (b) Determine the eigenvalues and ortho-normal eigenvectors of $H(\boldsymbol{k})$. (c) Expand the Hamiltonian at K or K' Dirac point, show that it is given by a massless Dirac model $H(\boldsymbol{k}) = \hbar v_F\left(\sigma_x \Delta k_x + \sigma_y \Delta k_y\right) + O(\Delta k^2)$, $\Delta\boldsymbol{k} = \boldsymbol{k} - \boldsymbol{K}$. Given that the hopping $t = 2.8$ eV, carbon-carbon bond length is 0.14 nm, evaluate the Fermi velocity v_F in units of m/s. (d) Determine the density of state $D(E)$ near the Dirac point.