# 4012 Condensed Matter Theory: Tutorial 3

1. Consider the following interacting Hamiltonian for the $H_2$ molecule, known as the U-V model

$$H_{\rm UV} = t\sum_{\sigma}(c^{\dagger}_{1\sigma}c_{2\sigma} + c^{\dagger}_{2\sigma}c_{1\sigma}) + U\sum_{\mu=1}^{2}\hat{n}_{\mu\uparrow}\hat{n}_{\mu\downarrow} + V\hat{n}_1\hat{n}_2 \ ,$$

where $c^{\dagger}_{\mu\sigma}$ ($c_{\mu\sigma}$) is the creation (annihilation) operator for an electron at site $\mu$ with spin $\sigma$, $\hat{n}_{\mu\sigma} = c^{\dagger}_{\mu\sigma}c_{\mu\sigma}$ and $\hat{n}_{\mu} = \hat{n}_{\mu\uparrow} + \hat{n}_{\mu\downarrow}$. Here $t < 0$ is the usual hopping integral while $U$ and $V$ are the local and non-local Hubbard terms, respectively.

   (a) Write the anti-commutation relations between the creation and annihilation operators. By using such anti-commutation relations demonstrate that the first term in the Hamiltonian (proportional to $t$) transfers an electron from one atom in the molecule to the other without changing its spin.

   (b) Derive the mean field approximation of the Hamiltonian $H_{\rm UV}$, where all the operators product of density fluctuations are neglected.

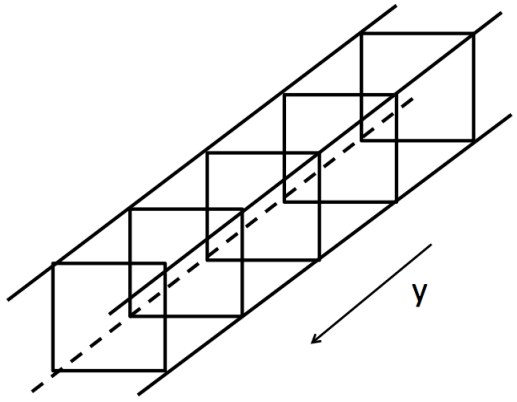
   (c) Write the Hamiltonian matrix corresponding to the mean field approximation of $H_{\rm UV}$ over a convenient basis set (hint: this is now a single-particle problem).

   (d) Calculate the eigenvalues and eigenvectors of the mean field Hamiltonian and the total energy in the case there are two electrons on the molecule.

2. Consider an infinite 2D simple cubic lattice of Hydrogen atoms with lattice spacing $a = 1$. The electronic structure of such solid can be described by using a set of orthonormal functions $|\mathbf{R}\rangle$, where the vector $|\mathbf{R}\rangle$ represents a 1s orbital placed at the position $\mathbf{R}$.

   (a) Calculate the band-structure of this system in the case the interaction extends to second nearest-neighbours. Use $\epsilon_0$ as on-site energy and $t_1$ and $t_2$, respectively as first and second nearest-neighbour hopping parameters.

   (b) Now cut the 2D lattice along the $y$-direction in strip 4-site wide and roll it up to form a nanotube (see figure).




   Calculate the band-structure of the nanotube, by explicitly writing down the expression for the different one-dimensional bands arising from the quantization along the $x$-direction. Draw the band-structure along the corresponding 1D Brillouin zone and also draw the associated density of states. For the plots use the following values $\epsilon_0$=0 and $t_1 = 2t_2 = 2t$ ($t < 0$).

   (c) For one of the nanotube sub-bands calculate the quantum mechanical probability to find an electron at one arbitrary atomic position.

(d) Calculate all the Fermi wave-vectors in the case the Fermi energy is $E_{\rm F} = 4t$. Furthermore calculate the value of the possible group velocities at the Fermi energy (Fermi velocities). [Use the same on-site energy and the hoping parameters as those at point b)].