Computation of the electron density

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The nanotube model is made by replicating the central unit cell N times according to the helical symmetry principles. Each unit cell is labelled with an $\mathbf{R}$ vector that points to its center from the central unit cell. For the central unit cell, $\mathbf{R} = (0, 0)$, and there are other cells in both directions, i.e., with both $\mathbf{R}$ and $-\mathbf{R}$. The pth basis vector in the $\mathbf{R}$ unit cell is labelleled as $|\chi_p^{\mathbf{R}}\rangle$. Then we transform the basis functions from the real ($\mathbf{R}$) space to the reciprocal ($\mathbf{k}$) space to produce Bloch-orbital basis:

$$|\chi_p^{\mathbf{k}}\rangle = \frac{1}{\sqrt{N}} \sum_{-\mathbf{R}}^{\mathbf{R}} e^{i\mathbf{k}\mathbf{R}} |\chi_p^{\mathbf{R}}\rangle \tag{1}$$

There is one $\mathbf{k}$ vector corresponding to each $\mathbf{R}$. The Fock matrix built in the $|\chi_p^{\mathbf{k}}\rangle$ basis is block diagonal, one block for each $\mathbf{k}$. The electronic orbitals are labelled with $\mathbf{k}$ as well. If we diagonalize the Fock matrix, we obtain the $c_{p,m}^{\mathbf{k}}$ values, the coefficient of the pth Bloch-basis in the mth orbital for a given $\mathbf{k}$.

We do not compute the full electron density, but we are interested in the density for the individual orbitals. The "density matrix" in the reciprocal space for a given $\mathbf{k}$ point ant the mth orbital:

$$P_{pq}^{(\mathbf{k},m)} = (c_{p,m}^{\mathbf{k}})^* c_{q,m}^{\mathbf{k}} \tag{2}$$

Then we transform it to the real space for each $\mathbf{R}$ vector. The matrix element for the pth basis in the $\mathbf{R}$ unit cell and qth basis in the central unit cell is

$$P_{pq}^{\mathbf{R0}(\mathbf{k},m)} = e^{i\mathbf{k}\mathbf{R}} P_{pq}^{(\mathbf{k},m)}. \tag{3}$$

The contribution of the central unit cell to the electron density is

$$\rho^{(\mathbf{k},m)}(\mathbf{r}) = \sum_{-\mathbf{R}}^{\mathbf{R}} \sum_{p,q} P_{pq}^{\mathbf{R0}(\mathbf{k},m)} \chi_p^{\mathbf{R}}(\mathbf{r}) \chi_q^{\mathbf{0}}(\mathbf{r}), \tag{4}$$

where we take one basis function from the central unit cell and the other one from the whole nanotube. It is important to rotate the basis functions as they are rolled up on the surface of the nanotube's cylinder. The total electron density will be the sum of the contributions of all unit cells in the nanotube, computed the same way as the position of the atoms.

$$\rho_{\text{tot}}^{(\mathbf{k},m)}(\mathbf{r}) = \rho^{(\mathbf{k},m)}(\mathbf{r}) + \sum_{\mathbf{R}} \rho^{(\mathbf{k},m)}(\mathbf{r} - \mathbf{R}) + \sum_{-\mathbf{R}} \rho^{(\mathbf{k},m)}(\mathbf{r} + \mathbf{R}) \tag{5}$$

The program computes the electron density of the central unit cell for a large number of grid points in space, and the $\rho^{(\mathbf{k},m)}(\mathbf{r} \pm \mathbf{R})$ values are computed with 3D linear interpolation.