Coulomb Lattice Summation

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October 17, 2012

API functions

```
double cls::coul_matrix(const FSolidModel& solid,
        const FOpMatrix& den_mat,
        FOpMatrix& coul_mat);
```

- output `coul_matrix`

$$\tilde{V}^{0J}_{\mu\nu} = \langle \mu^0 | \tilde{V} | \nu^J \rangle = \int \mu^0(\mathbf{r}) \tilde{V}(\mathbf{r}) \nu^J(\mathbf{r}) d\mathbf{r}^3 \tag{1}$$

$$\tilde{V}(\mathbf{r}) = \int \frac{\tilde{\rho}(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}'^3, \quad \tilde{\rho} = \rho - \frac{N}{\Omega} \tag{2}$$

- return: the energy in terms of the actual electron density ρ and the modified potential $\tilde{V}$

$$\varepsilon = \int_{\mathbf{r} \in C} \rho(\mathbf{r}) \tilde{V}(\mathbf{r}) d\mathbf{r} \tag{3}$$

Algorithm

- modified density $\tilde{\rho}(\mathbf{r})$ at each real space grid

$$\tilde{\rho} = \rho - \frac{N}{\Omega}$$

- use DFT to transform $\tilde{\rho}(\mathbf{r})$ in one unit cell, then solve the Poisson equation in **k**-space

$$\tilde{\rho}(\mathbf{r}) \rightarrow \tilde{\rho}(\mathbf{k}) \rightarrow \tilde{V}(\mathbf{k}) = \frac{\tilde{\rho}(\mathbf{k})}{k^2}$$

- use inversed DFT to transform $\tilde{V}(\mathbf{k})$

$$\tilde{V}(\mathbf{k}) \rightarrow \tilde{V}(\mathbf{r})$$

- $V_{\mu\nu}^{0J}$

formulation

$$\tilde{\rho}(\mathbf{r}) = \sum_{\mu\nu IJ} D^{IJ}_{\mu\nu} \mu^I(\mathbf{r}) \nu^J(\mathbf{r}) - \rho_0 \tag{4}$$

- Translation symmetry of density matrix D

$$D^{IJ}_{\mu\nu} = D^{0,J-I}_{\mu\nu}, \quad \mathbf{R}^{J-I} = \mathbf{R}^J - \mathbf{R}^I$$

- periodic basis function

$$\mu^I(\mathbf{r}) = \mu^0(\mathbf{r} - \mathbf{R}^I) \tag{5}$$

- formula of density in code

$$\tilde{\rho}(\mathbf{r}) = \sum_{\mu\nu IJ} D^{I,I+J}_{\mu\nu} \mu^I(\mathbf{r}) \nu^{I+J}(\mathbf{r}) - \rho_0 = \sum_I \rho^I(\mathbf{r}) - \rho_0 \tag{6}$$

$$\rho^I(\mathbf{r}) = \sum_{\mu\nu J} D^{0J}_{\mu\nu} \mu^I(\mathbf{r}) \nu^{I+J}(\mathbf{r}) = \sum_{\mu\nu J} D^{0J}_{\mu\nu} \mu^0(\mathbf{r} - \mathbf{R}^I) \nu^0(\mathbf{r} - \mathbf{R}^{I+J}) \tag{7}$$