Thomas-Fermi Calculation

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June 2025

1 Equation Derivation

$$\epsilon[n(r)] = \epsilon_H + \epsilon_{ext} + \epsilon_{xc} \tag{1}$$

$$= \frac{e^2}{2}\int_{\mathbf{r}_1\mathbf{r}_2} n(\mathbf{r_1})V(\mathbf{r}_1,\mathbf{r}_2)n(\mathbf{r}_2) - e\int_{\mathbf{r}}\Phi(\mathbf{r})n(\mathbf{r}) + \int_{\mathbf{r}} E_{xc}(n(\mathbf{r})) \tag{2}$$

$$= \frac{1}{2A}\sum_{\mathbf{q}} V(\mathbf{q})n(\mathbf{q})n(-\mathbf{q}) + \sum_{\mathbf{r}}\Phi(\mathbf{r})n(\mathbf{r})dA + \sum_{\mathbf{r}} E_{xc}(n(\mathbf{r})dA \tag{3}$$

The first term is the Hartree Energy, where $V(\mathbf{r}_1,\mathbf{r}_2) = \frac{1}{4\pi\epsilon|\mathbf{r}_1-\mathbf{r}_2|}$. Second term is the external potential energy, and the last part is the exchange energy. Keep in mind that energies are integrated within the plane. Each of them is defined as follows. Definition of the Fourier Transformation:

$$n(\mathbf{q}) = \sum_{\mathbf{r}} n(\mathbf{r})e^{-i\frac{2\pi}{N}(\mathbf{q}\cdot\mathbf{r})}dA \tag{4}$$

Screened Fourier-Transformed Coulomb Interaction:

$$V(\mathbf{q}) = \frac{e^2}{4\pi\epsilon_{hBN}}\frac{4\pi\sinh\left(\beta d_t|\mathbf{q})|\sinh\left(\beta d_b|\mathbf{q}|\right)}{\sinh\left(\beta(d_t+d_b)|\mathbf{q}|\right)|\mathbf{q}|} \tag{5}$$

Screened Fourier-Transformed external electric potential:

$$\Phi(\mathbf{q}) = -eV_t(\mathbf{q})\frac{\sinh\left(\beta d_b|\mathbf{q}|\right)}{\sinh\left(\beta(d_t+d_b)|\mathbf{q}|\right)} - eV_B\frac{d_t}{d_t+d_b} \tag{6}$$

Gaussian convolution of the density to incorporate the effect of the magnetic field:

$$\tilde{n}(\mathbf{r}) = \mathcal{N}^{-1}\sum_{\mathbf{r}'} n(\mathbf{r}')e^{-|\mathbf{r}-\mathbf{r}'|^2/2l_B^2} \tag{7}$$

1.1 Derivation of the Green's function

Definition of the Fourier Transformation:

$$\varphi(\mathbf{q},z) = \int_{\mathbb{R}^2} d^2\mathbf{r}\; e^{-i\mathbf{q}\cdot\mathbf{r}}\;\varphi(\mathbf{r},z), \qquad \mathbf{r}=(x,y),\ \mathbf{q}=(q_x,q_y). \tag{8}$$

Poisson's equation:

$$\nabla\cdot(\hat{\varepsilon}\nabla\varphi)(\mathbf{r},z) = -\rho(\mathbf{r},z), \quad \hat{\varepsilon} = \begin{pmatrix} \varepsilon_{\parallel} & 0 & 0 \\ 0 & \varepsilon_{\parallel} & 0 \\ 0 & 0 & \varepsilon_{\perp} \end{pmatrix}. \tag{9}$$

where $\rho(\mathbf{r},z)$ is the electron density.

Write down:

$$\varepsilon_{\parallel}\nabla_{\parallel}^2\varphi(\mathbf{r},z) + \varepsilon_{\perp}\frac{\partial^2}{\partial z^2}\varphi(\mathbf{r},z) = -\rho(\mathbf{r},z) \tag{10}$$

Inverse Fourier Transform by inserting $\varphi(\mathbf{r},z) = \frac{1}{2\pi}\int d\mathbf{q}e^{i\mathbf{q}\cdot\mathbf{r}}\varphi(\mathbf{q},z)$ and $\rho(\mathbf{r},z) = \frac{1}{2\pi}\int d\mathbf{q}e^{i\mathbf{q}\cdot\mathbf{r}}\rho(\mathbf{q},z)$

$$\varepsilon_{\parallel}q^2\varphi(\mathbf{q},z) = \varepsilon_{\perp}\frac{\partial^2}{\partial z^2}\varphi(\mathbf{q},z) + \rho(\mathbf{q},z).$$

For simplicity, $\beta^2 = \frac{\varepsilon_{\parallel}}{\varepsilon_{\perp}},\ \alpha = \beta q,\ \varphi(\mathbf{q},z) \to \varphi(z),\ \rho(\mathbf{q},z) \to \rho(z)$

$$\alpha^2\varphi(z) = \frac{\partial^2}{\partial z^2}\varphi(z) + \frac{1}{\epsilon_{\perp}}\rho(z). \tag{11}$$

Here, instead of solving the Poisson's equation, let us use the differential equation of the Green's function that suffices the following equations (where $\mathbf{R} = (\mathbf{r},z)$)

$$\hat{\varepsilon}\mathcal{G}(\mathbf{R},\mathbf{R}') = \frac{1}{4\pi|\mathbf{R}-\mathbf{R}'|} + \chi(\mathbf{R},\mathbf{R}') \tag{12}$$

where $\Delta\chi = 0$,

$$\varphi(\mathbf{R}) = \int \mathcal{G}(\mathbf{R},\mathbf{R}')\rho(\mathbf{R}')d\mathbf{R}' \tag{13}$$

$$(\frac{\partial^2}{\partial z^2} - \alpha^2)\mathcal{G}(\mathbf{q},\mathbf{q}';z,z') = -\frac{1}{\epsilon_{\perp}}\delta(z-z') \tag{14}$$

with Dirichlet's boundary condition (z_t and z_b mean the thickness of the top and bottom hBNs:

$$\mathcal{G}(z=d_t,z') = 0, \quad \mathcal{G}(z=-d_B,z') = 0 \tag{15}$$

In the following equations, we divide into the two cases. Here we mention that z' satifies the following equation: $-d_b \le z' \le d_t$

(i) $z \neq z'$

$$\frac{\partial^2}{\partial z^2}\mathcal{G} = \alpha^2\mathcal{G}$$

$$\mathcal{G}(z,z') = Ae^{\alpha z} + Be^{-\alpha z} \tag{16}$$

(a) $z > z'$

From eq. (15),

$$\mathcal{G}(d_t, z') = 0 \rightarrow B = -Ae^{2\alpha d_t}$$

Therefore,

$$\mathcal{G}(z, z') = Ae^{\alpha d_t}(e^{\alpha(d_t - z)} + e^{-\alpha(d_t - z)}) \rightarrow A\sinh(\alpha(d_t - z)) \quad (17)$$

is obtained by replacing the $2Ae^{\alpha d_t}$ with A at the arrow. Likewise,

(b) $z < z'$

$$\mathcal{G}(z, z') = B\sinh(\alpha(z + d_B)) \quad (18)$$

(ii) $z = z'$

First, since $\mathcal{G}$ should be continuous at $z = z'$, by using the eq.(17) and eq.(18),

$$A\sinh(\alpha(d_t - z')) = B\sinh(\alpha(z' + d_B)) \quad (19)$$

Second, by integrating once the eq.(14) between $z' - \Delta$ and $z' + \Delta$,which is an infinitesimal value, using the Heaviside step function,

$$\int_{z=z'-\Delta}^{z=z'+\Delta} (\frac{\partial^2}{\partial z^2}\mathcal{G}(z) - \alpha^2\mathcal{G}(z)) = \int_{z=z'-\Delta}^{z=z'+\Delta} -\varepsilon_\perp \delta(z - z')dz$$

$$[\frac{d\mathcal{G}}{dz}]_{z'-\Delta}^{z'+\Delta} - \alpha \int_{z=z'-\Delta}^{z=z'+\Delta} \mathcal{G}(z)dz = -\frac{1}{\varepsilon_\perp}[\Theta(z - z')]_{z'-\Delta}^{z'+\Delta}$$

Second term should vanishes at the limit of $\Delta \rightarrow +0$ since Green's function should be continuous again,

$$\frac{d\mathcal{G}}{dz}(z' + \Delta) - \frac{d\mathcal{G}}{dz}(z' - \Delta) = -\frac{1}{\varepsilon_\perp} \quad (20)$$

By differentiating the eq.(17) and eq.(18), inserting $z = z' + \Delta$ and $z = z' - \Delta$, and taking the limit of the $\Delta \rightarrow +0$,

$$A\alpha\cosh(\alpha(d_t - z')) + B\alpha\cosh(\alpha(z' + d_\beta)) = \frac{1}{\varepsilon_\perp} \quad (21)$$

From (i) and (ii), A and B are determined by solving the simultaneous equations (17) and (19) .

$$A = \frac{\sinh(\beta q(z' + d_b))}{\sinh(\beta q(d_t + d_b))}\frac{1}{\varepsilon_\parallel q},\ B = \frac{\sinh(\beta q(d_t - z'))}{\sinh(\beta q(d_t + d_b))}\frac{1}{\varepsilon_\parallel q} \quad (22)$$

Therefore,

$$\mathcal{G}(q; z, z') = \begin{cases} \frac{\sinh(\beta q(d_t - z))\sinh\left(\beta q(z' + d_b)\right))}{\sinh(\beta q(d_t + d_b))}\frac{1}{\varepsilon_\parallel q} & z > z', \\ \frac{\sinh\left(\beta q(d_t - z')\right)\sinh\left(\beta q(z' + d_b)\right)}{\sinh(\beta q(d_t + d_b))}\frac{1}{\varepsilon_\parallel q} & z = z', \\ \frac{\sinh(\beta q(z + d_B))\sinh\left(\beta q(d_t - z')\right)}{\sinh(\beta q(d_t + d_b))}\frac{1}{\varepsilon_\parallel q} & z < z' \end{cases} \quad (23)$$

1.2 2D-discrete-Fourier-Transformation of the Hartree term

$$
\begin{aligned}
\epsilon_H &= \frac{e^2}{2}\int_{\mathbf{r_1}\mathbf{r_2}} n(\mathbf{r_1})V(\mathbf{r}_1,\mathbf{r}_2)n(\mathbf{r}_2) \\
&= \frac{e^2}{2}\sum_{x_i,y_i,x_j,y_j} n(x_i,y_i)V(x_i,y_i,x_j,y_j)n(x_j,y_j)(d\cdot d)^2
\end{aligned}
$$

where N is the number of grid, L is the length of this system, A is the area of the system, hence $A = L^2$ and $d = N/L$,

$$
= \frac{e^2A^2}{2N^4}\sum_{n'_x,n'_y,n_x,n_y=0}^{N-1} n(dn'_x,dn'_y)V(dn'_x,dn'_y,dn_x,dn_y)n(dn_x,dn_y)
$$

by inserting the inverse discrete fourier transform of the density and the interaction, namely

$$
\begin{aligned}
n(d((n)-(n'))&= \frac{1}{A}\sum_{k_x=0}^{N-1}\sum_{k_x=0}^{N-1}\tilde{n}(\frac{k_x}{d},\frac{k_y}{d})e^{i\frac{2\pi}{N}(k_xn_x+k_yn_y)} \\
V(d(\mathbf{n_1},\mathbf{n_2}) &= \frac{1}{e^2A}\sum_{k_x^V=0}^{N-1}\sum_{k_y^V=0}^{N-1}\tilde{V}(\frac{k_x^V}{d},\frac{k_y^V}{d})e^{i\frac{2\pi}{N}(k_x^V(n_x-n'_x)+k_y^V(n_y-n'_y))}
\end{aligned}
$$

Therefore,

$$
\begin{aligned}
&= \frac{e^2A^2}{2N^4}\frac{1}{e^2A^3}\sum_{k_x,k_y,k'_x,k'_y,k_x^V,k_y^V=0}^{N-1}\ \sum_{n'_x,n'_y,n_x,n_y=0}^{N-1}\tilde{n}(\frac{k_x}{d},\frac{k_y}{d})\tilde{V}(\frac{k_x^V}{d},\frac{k_y^V}{d})\tilde{n}(\frac{k'_x}{d},\frac{k'_y}{d}) \\
&\times e^{i\frac{2\pi}{N}(n_x(k_x+k_x^V)+n_y(k_y+k_y^V))}e^{i\frac{2\pi}{N}(n'_x(k_x-k_x^V)+n'_y(k'_y-k_y^V))} \\
&= \frac{1}{2N^4A}\sum_{\mathbf{k},\mathbf{k^V},\mathbf{k'}}\tilde{n}(\frac{\mathbf{k}}{d})\tilde{V}(\frac{\mathbf{k^V}}{d})\tilde{n}(\frac{\mathbf{k'}}{d})N\delta_{k_x,-k_x^V}N\delta_{k_y,-k_y^V}N\delta_{k'_x,k_x^V}N\delta_{k'_y,k_y^V} \\
&= \frac{1}{2A}\sum_{\mathbf{k}}\tilde{n}(\frac{-\mathbf{k}}{d})\tilde{V}(\frac{\mathbf{k}}{d})\tilde{n}(\frac{\mathbf{k'}}{d}) \\
&= \frac{1}{2A}\sum_{\mathbf{q}}\tilde{n}(-\mathbf{q})\tilde{V}(\mathbf{q})\tilde{n}(\mathbf{q})
\end{aligned}
$$

1.3 Derivation of Eq.(5)

Actually, since the definition of the Green's function here eq.(12) is the same for the definition of the interaction potential in eq.(2) namely, $V(\mathbf{r}_1,\mathbf{r}_2) =$

$\frac{1}{4\pi\epsilon|\mathbf{r}_1-\mathbf{r}_2|}$, gate screened 2d-fourier-transformed interaction potential is the eq.(23) that satisfies $z = z' = 0$, that is,

$$\mathcal{G}(q;0,0) = \frac{\sinh(\beta q d_t)\sinh(\beta q d_b)}{\sinh\left(\beta q(d_t+d_b)\right)}\frac{1}{\varepsilon_{\parallel} q} \tag{24}$$

Therefore,

$$V(\mathbf{q}) = e^2\mathcal{G}(q;0,0) = \frac{e^2}{4\pi\epsilon_{hBN}}\frac{4\pi\sinh\left(\beta d_t|\mathbf{q}\right)|\sinh\left(\beta d_b|\mathbf{q}|\right)}{\sinh\left(\beta(d_t+d_b)|\mathbf{q}|\right)|\mathbf{q}|} \tag{25}$$