Notes on a paper 'Closest Wannier functions to a given set of localized orbitals'

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The technical notes provide detailed derivations of the equations presented in the paper [T. Ozaki, Phys. Rev. B 110, 125115 (2024)].

I. EQ. (1) IN THE PAPER

By operating the identity relation for $|Q_{\mathbf{R}p}\rangle$, we have

$$|Q_{\mathbf{R}p}\rangle = \frac{1}{N_{\rm BC}} \sum_{\mathbf{k}\mu} |\phi_{\mathbf{k}\mu}\rangle\langle\phi_{\mathbf{k}\mu}|Q_{\mathbf{R}p}\rangle. \tag{N.1}$$

The integral is evaluated as

$$\begin{aligned}\langle\phi_{\mathbf{k}\mu}|Q_{\mathbf{R}p}\rangle &= \int dr^3 \phi^*_{\mathbf{k}\mu}(\mathbf{r}) Q_{\mathbf{R}p}(\mathbf{r}),\\ &= \int dr^3 \phi^*_{\mathbf{k}\mu}(\mathbf{r}) Q_{\mathbf{0}p}(\mathbf{r}-\mathbf{R}),\\ &= \int dr'^3 \phi^*_{\mathbf{k}\mu}(\mathbf{r}'+\mathbf{R}) Q_{\mathbf{0}p}(\mathbf{r}'),\\ &= {\rm e}^{-i\mathbf{k}\cdot\mathbf{R}} \int dr'^3 \phi^*_{\mathbf{k}\mu}(\mathbf{r}') Q_{\mathbf{0}p}(\mathbf{r}'),\\ &= {\rm e}^{-i\mathbf{k}\cdot\mathbf{R}} \langle\phi_{\mathbf{k}\mu}|Q_{\mathbf{0}p}\rangle. \end{aligned}\tag{N.2}$$

Inserting Eq. (N.2) into Eq. (N.1), and introducing the window function w, we define L as

$$|L_{\mathbf{R}p}\rangle = \frac{1}{N_{\rm BC}} \sum_{\mathbf{k},\mu} {\rm e}^{-i\mathbf{k}\cdot\mathbf{R}} |\phi_{\mathbf{k}\mu}\rangle w(\varepsilon_{\mathbf{k}\mu}) \langle\phi_{\mathbf{k}\mu}|Q_{\mathbf{0}p}\rangle. \tag{N.3}$$

II. EQ. (7) IN THE PAPER

The distance measure function is explicitly calculated as

$$\begin{aligned}F[B] &= \sum_p \langle R_{\mathbf{0}p}|R_{\mathbf{0}p}\rangle,\\ &= \sum_p \Big(\langle L_{\mathbf{0}p}| - \langle W_{\mathbf{0}p}|\Big)\Big(|L_{\mathbf{0}p}\rangle - |W_{\mathbf{0}p}\rangle\Big),\\ &= \sum_p \Big(\langle L_{\mathbf{0}p}|L_{\mathbf{0}p}\rangle - \langle L_{\mathbf{0}p}|W_{\mathbf{0}p}\rangle\\ &\quad -\langle W_{\mathbf{0}p}|L_{\mathbf{0}p}\rangle + \langle W_{\mathbf{0}p}|W_{\mathbf{0}p}\rangle\Big).\end{aligned}\tag{N.4}$$

The inner products in Eq. (N.4) can be evaluated as, e.g.,

$$\begin{aligned}\sum_p \langle L_{\mathbf{0}p}|L_{\mathbf{0}p}\rangle &= \sum_p \left(\frac{1}{N_{\rm BC}} \sum_{\mathbf{k},\mu} a^*_{\mathbf{k}\mu,p}\langle\phi_{\mathbf{k}\mu}|\right)\\ &\quad\times\left(\frac{1}{N_{\rm BC}} \sum_{\mathbf{k}',\mu'} |\phi_{\mathbf{k}'\mu'}\rangle a_{\mathbf{k}'\mu',p}\right),\\ &= \frac{1}{N_{\rm BC}} \sum_{\mathbf{k}} \sum_{p,\mu} a^*_{\mathbf{k}\mu,p} a_{\mathbf{k}\mu,p},\\ &= \frac{1}{N_{\rm BC}} \sum_{\mathbf{k}} {\rm tr}\left[A^\dagger(\mathbf{k})A(\mathbf{k})\right].\end{aligned}\tag{N.5}$$

The other inner products can be obtained as well. So, we arrive at the following equation.

$$F[B] = \frac{1}{N_{\rm BC}} \sum_{\mathbf{k}} X[B,\mathbf{k}]. \tag{N.6}$$

with

$$X[B,\mathbf{k}] = {\rm tr}\left[\left(A^\dagger(\mathbf{k}) - B^\dagger(\mathbf{k})\right)\left(A(\mathbf{k}) - B(\mathbf{k})\right)\right], \tag{N.7}$$

III. EQ. (10) IN THE PAPER

$X[U]$ is calculated as

$$\begin{aligned}X[U] &= {\rm tr}\left[\left(A^\dagger - U^\dagger\right)(A-U)\right],\\ &= {\rm tr}\left[A^\dagger A - A^\dagger U - U^\dagger A + U^\dagger U\right],\\ &= {\rm tr}\left[A^\dagger A - 2P + I\right].\end{aligned}\tag{N.8}$$

As well, $X[B]$ is calculated as

$$\begin{aligned}X[B] &= {\rm tr}\left[\left(A^\dagger - B^\dagger\right)(A-B)\right],\\ &= {\rm tr}\left[A^\dagger A - A^\dagger B - B^\dagger A + B^\dagger B\right],\\ &= {\rm tr}\left[A^\dagger A - A^\dagger B - B^\dagger A + I\right].\end{aligned}\tag{N.9}$$

So, we have

$$\begin{aligned}X[U] - X[B] &= 2{\rm tr}\left[\frac{1}{2}\left(A^\dagger B + B^\dagger A\right) - P\right],\\ &= 2{\rm tr}\left[\frac{1}{2}\left(V\Sigma V^\dagger UB + B^\dagger UV^\dagger\Sigma V\right) - V\Sigma V^\dagger\right],\\ &= 2{\rm tr}\left[\Sigma D - \Sigma\right],\\ &= 2\sum_n \sigma_n\left(d_{nn} - 1\right)\end{aligned}\tag{N.10}$$

with

$$D = \frac{1}{2}\left(V^\dagger U^\dagger B V + V^\dagger B^\dagger U V\right). \tag{N.11}$$

IV. EQ. (14) IN THE PAPER

Inserting $A = W\Sigma V^\dagger$ and $P = V\Sigma V^\dagger$ into Eq. (N.8), we have

$$\begin{aligned} X[U] &= \mathrm{tr}\left[A^\dagger A - 2P + I\right], \\ &= \mathrm{tr}\left[V\Sigma W^\dagger W \Sigma V^\dagger - 2V\Sigma V^\dagger + I\right], \\ &= \mathrm{tr}\left[\Sigma^2 - 2\Sigma + I\right], \\ &= \sum_p (\sigma_p - 1)^2 . \end{aligned} \tag{N.12}$$

Inserting Eq. (N.12) into Eq. (N.6) and considering the k-dependency, we obtain

$$F[U] = \frac{1}{N_{\mathrm{BC}}} \sum_{\mathbf{k},p} (\sigma_{\mathbf{k}p} - 1)^2 , \tag{N.13}$$

V. EQ. (15) IN THE PAPER

Using Eq. (2) in the paper and noting that $\sum_{\mathbf{R}} \mathrm{e}^{\mathrm{i}(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}} = N_{\mathrm{BC}}\delta_{\mathbf{k}\mathbf{k}'}$, one can evaluate the Fourier transform of the overlap integrals for $\{L\}$ as

$$\begin{aligned} \sum_{\mathbf{R}} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{R}} \langle L_{\mathbf{0}p} | L_{\mathbf{R}q}\rangle &= \sum_{\mathbf{R}} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{R}} \left(\frac{1}{N_{\mathrm{BC}}} \sum_{\mathbf{k}',\mu} a^*_{\mathbf{k}'\mu,p} \langle \phi_{\mathbf{k}'\mu}| \right) \\ &\quad \times \left(\frac{1}{N_{\mathrm{BC}}} \sum_{\mathbf{k}'',\nu} \mathrm{e}^{-\mathrm{i}\mathbf{k}''\cdot\mathbf{R}} |\phi_{\mathbf{k}''\nu}\rangle a_{\mathbf{k}''\nu,q} \right), \\ &= \frac{1}{N_{\mathrm{BC}}} \sum_{\mathbf{k}',\mu} \left(\sum_{\mathbf{R}} \mathrm{e}^{\mathrm{i}(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}} \right) a^*_{\mathbf{k}'\mu,p} a_{\mathbf{k}'\mu,q}, \\ &= \sum_{\mu} a^*_{\mathbf{k}\mu,p} a_{\mathbf{k}\mu,q}, \end{aligned} \tag{N.14}$$

VI. EQ. (18) IN THE PAPER

Noting the KS hamiltonian is given by

$$\hat{H}_{\mathrm{KS}} = \frac{1}{N_{\mathrm{BC}}} \sum_{\mathbf{k},\mu} |\phi_{\mathbf{k}\mu}\rangle \varepsilon_{\mathbf{k}\mu} \langle \phi_{\mathbf{k}\mu}|, \tag{N.15}$$

and using Eq. (5) at $B = U$ in the paper, we can evaluate the matrix element of the KS hamiltonian with respect to the CWFs as

$$\begin{aligned} t_{\mathbf{0}p,\mathbf{R}q} &= \langle W_{\mathbf{0}p} | \hat{H}_{\mathrm{KS}} | W_{\mathbf{R}q} \rangle, \\ &= \left(\frac{1}{N_{\mathrm{BC}}} \sum_{\mathbf{k}',\mu} u^*_{\mathbf{k}'\mu,p} \langle \phi_{\mathbf{k}'\mu}| \right) \left(\frac{1}{N_{\mathrm{BC}}} \sum_{\mathbf{k},\mu} |\phi_{\mathbf{k}\mu}\rangle \varepsilon_{\mathbf{k}\mu} \langle \phi_{\mathbf{k}\mu}|, \right) \\ &\quad \times \left(\frac{1}{N_{\mathrm{BC}}} \sum_{\mathbf{k}'',\nu} \mathrm{e}^{-\mathrm{i}\mathbf{k}''\cdot\mathbf{R}} |\phi_{\mathbf{k}''\nu}\rangle u_{\mathbf{k}''\nu,q} \right), \\ &= \frac{1}{N_{\mathrm{BC}}} \sum_{\mathbf{k},\mu} \varepsilon_{\mathbf{k}\mu} u^*_{\mathbf{k}\mu,p} u_{\mathbf{k}\mu,q} \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{R}}. \end{aligned} \tag{N.16}$$