# The Liouville equation for high harmonic generation in solid: the electromagnetic gauge dependence and the Bloch/Wannier representation

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(Dated: 25 October 2017)

## Abstract

We provide a derivation of of the Liouville equation in various representations and gauges .

## Appendix A: Fundamental formulas

$$
\begin{aligned}
< n\mathbf{k}|\hat{\mathbf{x}}|n''\mathbf{k}'' > &= < n\mathbf{k}|\{-i\nabla_{\mathbf{k}''}e^{i\mathbf{k}''\cdot\hat{\mathbf{x}}}\}|u_{n''\mathbf{k}''} > \\
&= -i\nabla_{\mathbf{k}''} < n\mathbf{k}|n''\mathbf{k}'' > +i < u_{n\mathbf{k}}|e^{-i(\mathbf{k}-\mathbf{k}'')\cdot\hat{\mathbf{x}}}|\nabla_{\mathbf{k}''}u_{n''\mathbf{k}''} > \\
&= -i\nabla_{\mathbf{k}''} < n\mathbf{k}|n''\mathbf{k}'' > +\delta(\mathbf{k}-\mathbf{k}'')\mathbf{d}_{nn''}(\mathbf{k}) \qquad \text{(A1)}\\
< n''\mathbf{k}''|\hat{\mathbf{x}}|n'\mathbf{k}' > &= < u_{n''\mathbf{k}''}|\{i\nabla_{\mathbf{k}''}e^{-i\mathbf{k}''\cdot\hat{\mathbf{x}}}\}|n'\mathbf{k}' > \\
&= i\nabla_{\mathbf{k}''} < n''\mathbf{k}''|n'\mathbf{k}' > -i < \nabla_{\mathbf{k}"}u_{n''\mathbf{k}''}|e^{-i(\mathbf{k}''-\mathbf{k}')\cdot\hat{\mathbf{x}}}|u_{n'\mathbf{k}'} > \\
&= i\nabla_{\mathbf{k}''} < n''\mathbf{k}''|n'\mathbf{k}' > +\delta(\mathbf{k}''-\mathbf{k}')\mathbf{d}_{n''n'}(\mathbf{k}') \qquad \text{(A2)}
\end{aligned}
$$

$$
\begin{aligned}
i < u_{n\mathbf{k}}|e^{-i(\mathbf{k}-\mathbf{k}'')\cdot\hat{\mathbf{x}}}|\nabla_{\mathbf{k}''}u_{n''\mathbf{k}''} > &= \frac{iN}{\Omega} < u_{n\mathbf{K}}|e^{-i(\mathbf{K}-\mathbf{K}'')\cdot\hat{\mathbf{x}}}|\nabla_{\mathbf{K}''}u_{n''\mathbf{K}''} > \\
&= \frac{iN}{\Omega}\int d\mathbf{x} < u_{n\mathbf{K}}|\mathbf{x}>< \mathbf{x}|\nabla_{\mathbf{K}''}u_{n''\mathbf{K}''} > e^{-i(\mathbf{K}-\mathbf{K}'')\cdot\mathbf{x}} \\
&= \frac{iN}{\Omega}\sum_{\mathbf{R}} e^{-i(\mathbf{K}-\mathbf{K}'')\cdot\mathbf{R}}\int_{BL} d\mathbf{y} < u_{n\mathbf{K}}|\mathbf{y}>< \mathbf{y}|\nabla_{\mathbf{K}''}u_{n''\mathbf{K}''} > e^{-i(\mathbf{K}-\mathbf{K}'')\cdot\mathbf{y}} \\
&= \frac{iN^2}{\Omega}\delta_{KK''}\int_{BL} d\mathbf{y} < u_{n\mathbf{K}}|\mathbf{y}>< \mathbf{y}|\nabla_{\mathbf{K}}u_{n''\mathbf{K}} > \\
&= i\Omega\delta(\mathbf{k}-\mathbf{k}'')\int_{BL} d\mathbf{y} < u_{n\mathbf{k}}|\mathbf{y}>< \mathbf{y}|\nabla_{\mathbf{k}}u_{n\mathbf{k}} > \\
&= \frac{i\Omega}{N}\delta(\mathbf{k}-\mathbf{k}'')\int d\mathbf{x} < u_{n\mathbf{k}}|\mathbf{x}>< \mathbf{x}|\nabla_{\mathbf{k}}u_{n''\mathbf{k}} > \\
&= \delta(\mathbf{k}-\mathbf{k}'')\{\frac{i\Omega}{N} < u_{n\mathbf{k}}|\nabla_{\mathbf{k}}u_{n''\mathbf{k}} >\} \\
&\equiv \delta(\mathbf{k}-\mathbf{k}'')\mathbf{d}_{nn''}(\mathbf{k}) \qquad \text{(A3)}
\end{aligned}
$$

$$
\begin{aligned}
i < \nabla_{\mathbf{k}"}u_{n''\mathbf{k}''}|e^{-i(\mathbf{k}''-\mathbf{k}')\cdot\hat{\mathbf{x}}}|u_{n'\mathbf{k}'} > &= \frac{iN}{\Omega} < \nabla_{\mathbf{K}''}u_{n''\mathbf{K}''}|e^{-i(\mathbf{K}''-\mathbf{K}')\cdot\hat{\mathbf{x}}}|u_{n'\mathbf{K}'} > \\
&= \frac{iN}{\Omega}\int d\mathbf{x} < \nabla_{\mathbf{K}''}u_{n''\mathbf{K}''}|\mathbf{x}>< \mathbf{x}|u_{n'\mathbf{K}'} > e^{-i(\mathbf{K}''-\mathbf{K}')\cdot\mathbf{x}} \\
&= \frac{iN}{\Omega}\sum_{\mathbf{R}} e^{-i(\mathbf{K}''-\mathbf{K}')\cdot\mathbf{R}}\int_{BL} d\mathbf{y} < \nabla_{\mathbf{K}''}u_{n''\mathbf{K}''}|\mathbf{y}>< \mathbf{y}|u_{n'\mathbf{K}'} > e^{-i(\mathbf{K}''-\mathbf{K}')\cdot\mathbf{y}} \\
&= \frac{iN^2}{\Omega}\delta_{K''K'}\int_{BL} d\mathbf{y} < \nabla_{\mathbf{K}'}u_{n''\mathbf{K}'}|\mathbf{y}>< \mathbf{y}|u_{n'\mathbf{K}'} > \\
&= i\Omega\delta(\mathbf{k}''-\mathbf{k}')\int_{BL} d\mathbf{y} < \nabla_{\mathbf{k}'}u_{n''\mathbf{k}'}|\mathbf{y}>< \mathbf{y}|u_{n'\mathbf{k}'} > \\
&= \frac{i\Omega}{N}\delta(\mathbf{k}''-\mathbf{k}')\int d\mathbf{x} < \nabla_{\mathbf{k}'}u_{n''\mathbf{k}'}|\mathbf{x}>< \mathbf{x}|u_{n'\mathbf{k}'} >
\end{aligned}
$$

$$
\begin{aligned}
&= \delta(\mathbf{k}'' - \mathbf{k}')\{\frac{i\Omega}{N} < \nabla_{\mathbf{k}'} u_{n''\mathbf{k}'}|u_{n'\mathbf{k}'} >\} \\
&= -\delta(\mathbf{k}'' - \mathbf{k}')\{\frac{i\Omega}{N} < u_{n''\mathbf{k}'}|\nabla_{\mathbf{k}'} u_{n'\mathbf{k}'} >\} \\
&\equiv -\delta(\mathbf{k}'' - \mathbf{k}')\mathbf{d}_{n''n'}(\mathbf{k}')
\end{aligned} \tag{A4}
$$

$$
\begin{aligned}
0 &= i\nabla_{\mathbf{k}} < u_{n\mathbf{k}}|u_{n'\mathbf{k}} > \\
&= i < \nabla_{\mathbf{k}} u_{n\mathbf{k}}|u_{n'\mathbf{k}} > + i < u_{n\mathbf{k}}|\nabla_{\mathbf{k}} u_{n'\mathbf{k}} > \\
&= -(i < u_{n'\mathbf{k}}|\nabla_{\mathbf{k}} u_{n\mathbf{k}} >)^* + i < u_{n\mathbf{k}}|\nabla_{\mathbf{k}} u_{n'\mathbf{k}} > \\
&= -\mathbf{d}^*_{n'n}(\mathbf{k}) + \mathbf{d}_{nn'}(\mathbf{k}).
\end{aligned} \tag{A5}
$$

$$
\begin{aligned}
&< nk|[\hat{x},\hat{\rho}]|n'k' > \\
&\quad = \sum_{n''} \int dk''(< nk|\hat{x}|n''k'' >< n''k''|\hat{\rho}|n'k' > - < nk|\hat{\rho}|n''k'' >< n''k''|\hat{x}|n'k' >) \\
&\quad = \sum_{n''} \int dk''[\{-i\nabla_{\mathbf{k}''} < n\mathbf{k}|n''\mathbf{k}'' > + \delta(\mathbf{k} - \mathbf{k}'')\mathbf{d}_{nn''}(\mathbf{k})\} < n''k''|\hat{\rho}|n'k' > \\
&\qquad - < nk|\hat{\rho}|n''k'' > \{i\nabla_{\mathbf{k}''} < n''\mathbf{k}''|n'\mathbf{k}' > + \delta(\mathbf{k}'' - \mathbf{k}')\mathbf{d}_{n''n'}(\mathbf{k}')\}] \\
&\quad = i(\nabla_{\mathbf{k}} + \nabla_{\mathbf{k}'}) < nk|\hat{\rho}|n'k' > + \sum_{n''}\{\mathbf{d}_{nn''}(\mathbf{k}) < n''k|\hat{\rho}|n'k' > - < nk|\hat{\rho}|n''k' > \mathbf{d}_{n''n'}(\mathbf{k}')\}
\end{aligned} \tag{A6}
$$

$$
\begin{aligned}
&<nk|[\hat{x},[\hat{x},\hat{\rho}]]|n'k' > \\
&= \sum_{n'''} \int dk''' < nk|\hat{x}|n'''k''' >< n'''k'''|[\hat{x},\hat{\rho}]|n'k' > - < nk|[\hat{x},\hat{\rho}]|n'''k''' >< n'''k'''|\hat{x}|n'k' >) \\
&= \sum_{n'''} \int dk'''\{-i\nabla_{k'''} < nk|n'''k''' > + \delta(\mathbf{k} - \mathbf{k}''')\mathbf{d}_{nn'''}(k)\} \\
&\quad \times [i(\nabla_{k'''} + \nabla_{k'}) < n'''k'''|\hat{\rho}|n'k' > + \sum_{n''} \mathbf{d}_{n'''n''}(\mathbf{k}''') < n''k'''|\hat{\rho}|n'k' > - < n'''k'''|\hat{\rho}|n''k' > \mathbf{d}_{n''n'}(\mathbf{k}')\}] \\
&\quad -[i(\nabla_k + \nabla_{k'''}) < nk|\hat{\rho}|n'''k''' > + \sum_{n''} \mathbf{d}_{nn''}() < n''k|\hat{\rho}|n'''k''' > - < nk|\hat{\rho}|n''k''' > \mathbf{d}_{n''n'''}(k''')] \\
&\quad \times\{i\nabla_{k'''} < n'''k'''|n'k' > + \delta(k''' - k')\mathbf{d}_{n'''n'}(k')\} \\
&= -(\nabla_k + \nabla_{k'})^2 < nk|\hat{\rho}|n'k' > + 2i(\nabla_k + \nabla_{k'})\{\sum_{n''} \mathbf{d}_{nn''}(k) < n''k|\hat{\rho}|n'k' > - < nk|\hat{\rho}|n''k' > \mathbf{d}_{n''n'}(k')\} \\
&\quad + \sum_{n''n'''} [d_{nn''}(k)d_{n''n'''}(k) < n'''k|\hat{\rho}|n'k' > -2d_{nn''}(k) < n''k|\hat{\rho}|n'''k' > d_{n'''n'}(k') + < nk|\hat{\rho}|n''k' > d_{n''n'''}(k')d_{n'''n'}(k')]
\end{aligned} \tag{A7}
$$

$$[\hat{\mathbf{x}}, \hat{H}_0] = [\hat{\mathbf{x}}, \frac{\hat{\mathbf{p}}}{2m}] = \frac{i\hbar}{m}\hat{\mathbf{p}} \tag{A8}$$

$$\begin{aligned} < n\mathbf{k}|\hat{\mathbf{p}}|n'\mathbf{k}' > &= i\frac{m(\epsilon_{n\mathbf{k}} - \epsilon_{n'\mathbf{k}'})}{\hbar} < n\mathbf{k}|\hat{\mathbf{x}}|n'\mathbf{k}' > \\ &= \begin{cases} \frac{m}{\hbar}(\epsilon_{n\mathbf{k}} - \epsilon_{n'\mathbf{k}'})\{-\nabla_{\mathbf{k}} < n\mathbf{k}|n'\mathbf{k}' > + i\delta(\mathbf{k}-\mathbf{k}')\mathbf{d}_{nn'}(\mathbf{k})\} \\ \frac{m}{\hbar}(\epsilon_{n\mathbf{k}} - \epsilon_{n'\mathbf{k}'})\{\nabla_{\mathbf{k}'} < n\mathbf{k}|n'\mathbf{k}' > + i\delta(\mathbf{k}-\mathbf{k}')\mathbf{d}_{nn'}(\mathbf{k})\} \end{cases} \end{aligned} \tag{A9}$$

$$\begin{aligned} < n\mathbf{k}|\hat{\mathbf{p}}|n\mathbf{k} > &= \frac{m}{i\hbar} < n\mathbf{k}|[\hat{\mathbf{x}}, \hat{H}_0]|n\mathbf{k} > \\ &= \frac{m}{i\hbar}\{< u_{n\mathbf{k}}|(i\nabla_{\mathbf{k}} e^{-i\mathbf{k}\cdot\hat{\mathbf{x}}})\hat{H}_0|n\mathbf{k} > - < n\mathbf{k}|\hat{H}_0(-i\nabla_{\mathbf{k}} e^{i\mathbf{k}\cdot\hat{\mathbf{x}}})|u_{n\mathbf{k}} >\} \\ &= \frac{m}{\hbar}\{\nabla_{\mathbf{k}} < n\mathbf{k}|\hat{H}_0|n\mathbf{k} > - < \nabla_{\mathbf{k}} u_{n\mathbf{k}}|e^{-i\mathbf{k}\cdot\hat{\mathbf{x}}}\hat{H}_0|n\mathbf{k} > - < n\mathbf{k}|\hat{H}_0 e^{i\mathbf{k}\cdot\hat{\mathbf{x}}}|\nabla_{\mathbf{k}} u_{n\mathbf{k}} >\} \\ &= \frac{m}{\hbar}\{\nabla_{\mathbf{k}}\epsilon_{n\mathbf{k}} - \epsilon_{n\mathbf{k}}\nabla_{\mathbf{k}} < u_{n\mathbf{k}}|u_{n\mathbf{k}} >\} \\ &= \frac{m}{\hbar}\nabla_{\mathbf{k}}\epsilon_{n\mathbf{k}} \end{aligned} \tag{A10}$$

### Appendix B: Bloch-basis and length gauge

### Appendix C: velocity/current and position

$$\begin{aligned} J &= -e\frac{\partial}{\partial t}tr(\hat{\rho}\hat{\mathbf{x}}) \\ &= -e\, tr(\frac{\partial\hat{\rho}}{\partial t}\hat{\mathbf{x}}) \\ &= -\frac{e}{i\hbar}tr([\hat{H}, \hat{\rho}]\hat{\mathbf{x}}) \\ &= -\frac{e}{i\hbar}tr\{\hat{\rho}(\hat{\mathbf{x}}\hat{H} - \hat{H}\hat{\mathbf{x}})\} \\ &= -\frac{e}{i\hbar}tr\{\hat{\rho}[\hat{\mathbf{x}}, \hat{H}]\} \\ &= -\frac{e}{m}tr\{\hat{\rho}(\hat{\mathbf{p}} - e\mathbf{A})\} \\ &= -\frac{e}{m}\sum_{nn'}\int d\mathbf{k}\int d\mathbf{k}' < n\mathbf{k}|\hat{\rho}|n'\mathbf{k}' >< n'\mathbf{k}'|\hat{\mathbf{p}}|n\mathbf{k} > + \frac{e^2\mathbf{A}}{m}tr(\hat{\rho}) \\ &= -\frac{e}{\hbar}\sum_{nn'}\int d\mathbf{k}\int d\mathbf{k}' < n\mathbf{k}|\hat{\rho}|n'\mathbf{k}' > (\epsilon_{n'\mathbf{k}'} - \epsilon_{n\mathbf{k}})\{\nabla_{\mathbf{k}} < n'\mathbf{k}'|n\mathbf{k} > + i\delta(\mathbf{k}'-\mathbf{k})\mathbf{d}_{n'n}(\mathbf{k})\} \end{aligned}$$

$$
\begin{aligned}
&+\frac{e^2\mathbf{A}}{m}tr(\hat{\rho}) \\
&= +\frac{e}{\hbar}\sum_{nn'}\int d\mathbf{k}\int d\mathbf{k}'\nabla_{\mathbf{k}}\{< n\mathbf{k}|\hat{\rho}|n'\mathbf{k}' > (\epsilon_{n'\mathbf{k}'}-\epsilon_{n\mathbf{k}})\} < n'\mathbf{k}'|n\mathbf{k} > \\
&-\frac{e}{\hbar}\sum_{nn'}\int d\mathbf{k} < n\mathbf{k}|\hat{\rho}|n'\mathbf{k} > (\epsilon_{n'\mathbf{k}}-\epsilon_{n\mathbf{k}})\{i\mathbf{d}_{n'n}(\mathbf{k})\} + \frac{e^2\mathbf{A}}{m}tr(\hat{\rho}) \\
&= -\frac{e}{\hbar}\sum_{n}\int d\mathbf{k} < n\mathbf{k}|\hat{\rho}|n\mathbf{k} > \nabla_{\mathbf{k}}\epsilon_{n\mathbf{k}} - \frac{e}{\hbar}\sum_{nn'}\int d\mathbf{k} < n\mathbf{k}|\hat{\rho}|n'\mathbf{k} > (\epsilon_{n'\mathbf{k}}-\epsilon_{n\mathbf{k}})\{i\mathbf{d}_{n'n}(\mathbf{k})\} + \frac{e^2\mathbf{A}}{m}tr(\hat{\rho})
\end{aligned} \tag{C1}
$$

$$
\begin{aligned}
J^2 &= -\frac{e}{\hbar}\int d\mathbf{k}(< v\mathbf{k}|\hat{\rho}|v\mathbf{k} > \nabla_{\mathbf{k}}\epsilon_{v\mathbf{k}} + < c\mathbf{k}|\hat{\rho}|c\mathbf{k} > \nabla_{\mathbf{k}}\epsilon_{c\mathbf{k}}) + \frac{e^2\mathbf{A}}{m}tr(\hat{\rho}) \\
&-\frac{e}{\hbar}\int d\mathbf{k}[< v\mathbf{k}|\hat{\rho}|c\mathbf{k} > (\epsilon_{c\mathbf{k}}-\epsilon_{v\mathbf{k}})\{i\mathbf{d}_{cv}(\mathbf{k})\} + < c\mathbf{k}|\hat{\rho}|v\mathbf{k} > (\epsilon_{v\mathbf{k}}-\epsilon_{c\mathbf{k}})\{i\mathbf{d}_{vc}(\mathbf{k})\}] \\
&= -\frac{e}{\hbar}\int d\mathbf{k}(< v\mathbf{k}|\hat{\rho}|v\mathbf{k} > \nabla_{\mathbf{k}}\epsilon_{v\mathbf{k}} + < c\mathbf{k}|\hat{\rho}|c\mathbf{k} > \nabla_{\mathbf{k}}\epsilon_{c\mathbf{k}}) + \frac{e^2\mathbf{A}}{m}tr(\hat{\rho}) \\
&+\frac{e}{\hbar}\int d\mathbf{k}(\epsilon_{c\mathbf{k}}-\epsilon_{v\mathbf{k}})\mathbf{Im}[< v\mathbf{k}|\hat{\rho}|c\mathbf{k} > \mathbf{d}_{vc}]
\end{aligned} \tag{C2}
$$

$$
\begin{aligned}
\mathbf{x} &= tr(\hat{\rho}\hat{\mathbf{x}}) \\
&= \sum_{nn'}\int d\mathbf{k}\int d\mathbf{k}' < n\mathbf{k}|\hat{\rho}|n'\mathbf{k}' >< n'\mathbf{k}'|\hat{\mathbf{x}}|n\mathbf{k} > \\
&= \sum_{nn'}\int d\mathbf{k}\int d\mathbf{k}' < n\mathbf{k}|\hat{\rho}|n'\mathbf{k}' > \{\frac{1}{2i}(\nabla_{\mathbf{k}}-\nabla_{\mathbf{k}'}) < n'\mathbf{k}'|n\mathbf{k} > +\delta(\mathbf{k}'-\mathbf{k})\mathbf{d}_{n'n}(\mathbf{k})\} \\
&= \sum_{nn'}\int d\mathbf{k} < n\mathbf{k}|\hat{\rho}|n'\mathbf{k} > \mathbf{d}_{n'n}(\mathbf{k})
\end{aligned} \tag{C3}
$$

$$
\mathbf{x}^2 = \int d\mathbf{k}\{< v\mathbf{k}|\hat{\rho}|v\mathbf{k} > \mathbf{d}_{vv}(\mathbf{k}) + < c\mathbf{k}|\hat{\rho}|c\mathbf{k} > \mathbf{d}_{cc}(\mathbf{k}) + 2\mathbf{Re}\{< v\mathbf{k}|\hat{\rho}|c\mathbf{k} > \mathbf{d}^*_{vc}(\mathbf{k})\}] \tag{C4}
$$

### Appendix D: Wannier basis

$n$ is the band index, $\mathbf{k}$ is the crystal momentum, $\mathbf{R}$ is the Bravais Lattice The Bloch states $\{|n\mathbf{k}>\}$ and Wannier states $\{|n\mathbf{R}>\}$ are related by the Fourier expansion.

$$
\begin{aligned}
|n\mathbf{R}> &= \frac{1}{\sqrt{N}}\sum_{\mathbf{K}} exp(-i\mathbf{K}\cdot\mathbf{R})|n\mathbf{K}> \\
&= \frac{1}{\sqrt{\Omega}}\int_{BZ} d\mathbf{k}\, exp(-i\mathbf{k}\cdot\mathbf{R})|n\mathbf{k}>
\end{aligned}
$$

$$= \frac{1}{\sqrt{\Omega}} \int_{BZ} d\mathbf{k}\, exp\{-i\mathbf{k}\cdot(\mathbf{R}-\hat{\mathbf{x}})\}|u_{n\mathbf{k}}> \tag{D1}$$

$$<\mathbf{x}|n\mathbf{R}> = \frac{1}{\sqrt{\Omega}} \int_{BZ} d\mathbf{k}\, exp\{-i\mathbf{k}\cdot(\mathbf{R}-\mathbf{x})\} <\mathbf{x}|u_{n\mathbf{k}}> \tag{D2}$$

$$|n\mathbf{K}> = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}} \; exp(i\mathbf{k}\cdot\mathbf{R})|n\mathbf{R}> \tag{D3}$$

$$\begin{aligned} |n\mathbf{k}> &= \sqrt{\frac{N}{\Omega}}|n\mathbf{K}> \\ &= \frac{1}{\sqrt{\Omega}} \sum_{\mathbf{R}} \; exp(i\mathbf{k}\cdot\mathbf{R})|n\mathbf{R}> \end{aligned} \tag{D4}$$

$$\int_{BZ} d\mathbf{k} = \frac{\Omega}{N}\sum_{\mathbf{K}} \tag{D5}$$

$$\sum_{\mathbf{K}} |n\mathbf{K}><n\mathbf{K}| = \int_{BZ} d\mathbf{k}|n\mathbf{k}><n\mathbf{k}| \tag{D6}$$

$$\delta_{KK'} =<n\mathbf{K}|n\mathbf{K}'> = \frac{\Omega}{N} <n\mathbf{k}|n\mathbf{k}'>= \frac{\Omega}{N}\delta(\mathbf{k}-\mathbf{k}') \tag{D7}$$

$$\nabla_{\mathbf{k}} = \nabla_{\mathbf{K}} \tag{D8}$$

$$\begin{aligned} <n\mathbf{R}|n'\mathbf{R}'> &= \frac{1}{\Omega}\int\int_{BZ} d\mathbf{k}d\mathbf{k}' exp\{i(\mathbf{k}\cdot\mathbf{R}-\mathbf{k}'\cdot\mathbf{R}')\} <n\mathbf{k}|n'\mathbf{k}'> \\ &= \frac{\delta_{nn'}}{\Omega}\int_{BZ} d\mathbf{k}\, exp\{i\mathbf{k}\cdot(\mathbf{R}-\mathbf{R}')\} \\ &= \delta_{nn'}\delta_{\mathbf{R}\mathbf{R}'} \end{aligned} \tag{D9}$$

$$\begin{aligned} |n\mathbf{R}> &= \frac{1}{\Omega}\int_{BZ} d\mathbf{k}\, exp(-i\mathbf{k}\cdot\mathbf{R})|n\mathbf{k}> \\ &= \frac{1}{\Omega}\sum_{\mathbf{R}'}\int_{BZ} d\mathbf{k}\, exp\{-i\mathbf{k}\cdot(\mathbf{R}-\mathbf{R}')\}|n\mathbf{R}'> \\ &= \sum_{\mathbf{R}'}\delta_{\mathbf{R}\mathbf{R}'}|n\mathbf{R}'> \\ &= |n\mathbf{R}> \end{aligned} \tag{D10}$$

$$\begin{aligned} \int_{BZ} d\mathbf{k}' <n\mathbf{k}|n'\mathbf{k}'> &= \frac{1}{\Omega}\sum_{\mathbf{R}\mathbf{R}'}\int_{BZ} d\mathbf{k}' exp\{i(\mathbf{k}\cdot\mathbf{R}-\mathbf{k}'\cdot\mathbf{R}')\} <n\mathbf{R}|n'\mathbf{R}'> \\ &= \frac{\delta_{nn'}}{\Omega}\sum_{\mathbf{R}}\int_{BZ} d\mathbf{k}' exp\{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}\} \\ &= \frac{\delta_{nn'}}{N}\sum_{\mathbf{R}\mathbf{K}'} exp\{i(\mathbf{K}-\mathbf{K}')\cdot\mathbf{R}\} \\ &= \frac{\delta_{nn'}}{N}\sum_{\mathbf{R}} 1 \\ &= \delta_{nn'} \end{aligned} \tag{D11}$$

$$\begin{aligned} |n\mathbf{k}> &= \frac{1}{\sqrt{\Omega}}\sum_{\mathbf{R}} \; exp(i\mathbf{k}\cdot\mathbf{R})|n\mathbf{R}> \\ &= \frac{1}{\Omega}\sum_{\mathbf{R}}\int_{BZ} d\mathbf{k}'\; exp\{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}\}|n\mathbf{k}'> \end{aligned}$$

$$
\begin{aligned}
&= \frac{1}{\sqrt{N\Omega}} \sum_{\mathbf{R}\mathbf{K}'} exp\{i(\mathbf{K}-\mathbf{K}')\cdot\mathbf{R}\}|n\mathbf{K}'> \\
&= \sqrt{\frac{N}{\Omega}} \sum_{\mathbf{K}'} \delta_{\mathbf{K}\mathbf{K}'}|n\mathbf{K}'> \\
&= \sqrt{\frac{N}{\Omega}} |n\mathbf{K}> \\
&= |n\mathbf{k}> \qquad \text{(D12)}
\end{aligned}
$$

$$
\begin{aligned}
<\mathbf{x}|u_{n\mathbf{k}}> &= exp(-i\mathbf{k}\cdot\mathbf{x}) <\mathbf{x}|n\mathbf{k}> \\
&= \frac{1}{\sqrt{\Omega}} \sum_{\mathbf{R}} exp\{-i\mathbf{k}\cdot(\mathbf{x}-\mathbf{R})\} <\mathbf{x}|n\mathbf{R}> \qquad \text{(D13)} \\
\nabla_{\mathbf{k}} <\mathbf{x}|u_{n\mathbf{k}}> &= \frac{-i}{\sqrt{\Omega}} \sum_{\mathbf{R}} (\mathbf{x}-\mathbf{R}) exp\{-i\mathbf{k}\cdot(\mathbf{x}-\mathbf{R})\} <\mathbf{x}|n\mathbf{R}> \qquad \text{(D14)}
\end{aligned}
$$

where $N$ is number of Bravais lattice points, and $\Omega$ is the volume of a Brillouin Zone. The matrix element of an operator $\hat{O}$ is transferred to

$$
\begin{aligned}
<n\mathbf{R}|\hat{O}|n'\mathbf{R}'> &= \frac{1}{\Omega} \int\int_{BZ} d\mathbf{k}d\mathbf{k}' exp[i(\mathbf{k}\cdot\mathbf{R}-\mathbf{k}'\cdot\mathbf{R}')] <n\mathbf{k}|\hat{O}|n'\mathbf{k}'> \qquad \text{(D15)} \\
\widetilde{o}(\mathbf{R}) &= \frac{1}{\Omega} \int_{BZ} d\mathbf{k} exp(-i\mathbf{k}\cdot\mathbf{R}) o(\mathbf{k}) \\
&= \frac{1}{N} \sum_{\mathbf{K}} exp(-i\mathbf{K}\cdot\mathbf{R}) o(\mathbf{K}) \qquad \text{(D16)}
\end{aligned}
$$

$$
\begin{aligned}
<n\mathbf{R}|\hat{H}_0|n'\mathbf{R}'> &= \frac{1}{\Omega} \int\int_{BZ} d\mathbf{k}\, d\mathbf{k}' exp\{i(\mathbf{k}\cdot\mathbf{R}-\mathbf{k}'\cdot\mathbf{R}')\} <n\mathbf{k}|\hat{H}_0|n'\mathbf{k}'> \\
&= \frac{1}{\Omega} \int d\mathbf{k}\, exp\{i\mathbf{k}\cdot(\mathbf{R}-\mathbf{R}')\} \delta_{nn'}\epsilon_{n\mathbf{k}} \\
&= \delta_{nn'} \widetilde{\epsilon}_n(\mathbf{R}'-\mathbf{R}) \qquad \text{(D17)}
\end{aligned}
$$

Assuming the 1-dimensional tight-binding model: $\epsilon_{n\mathbf{k}} = E_n^0 + \Delta E_n\{1 - cos(\mathbf{ka})\}$, where $\mathbf{a}$ is lattice constant,

$$
\begin{aligned}
\widetilde{\epsilon}_n(\mathbf{R}) &= \frac{1}{\Omega} \int d\mathbf{k}\, exp(-i\mathbf{k}\cdot\mathbf{R}) \epsilon_{n\mathbf{k}} \\
&= \frac{1}{\Omega} \int d\mathbf{k}\, exp(-i\mathbf{k}\cdot\mathbf{R}) [E_n^0 + \Delta E_n\{1 - cos(ka)\}] \\
&= (E_n^0 + \Delta E_n)\delta_{\mathbf{R}\mathbf{0}} - \frac{\Delta E_n}{2}\{\delta_{\mathbf{R}\mathbf{a}} + \delta_{\mathbf{R}(-\mathbf{a})}\} \qquad \text{(D18)}
\end{aligned}
$$

(D19)

$$
\begin{aligned}
< n\mathbf{R}|[\hat{H}_0,\hat{\rho}]|n'\mathbf{R}' >=& \sum_{n''\mathbf{R}''} (< n\mathbf{R}|\hat{H}_0|n''\mathbf{R}'' >< n''\mathbf{R}''|\hat{\rho}|n'\mathbf{R}' > - < n\mathbf{R}|\hat{\rho}|n''\mathbf{R}'' >< n''\mathbf{R}''|\hat{H}_0|n'\mathbf{R}' >)\\
=& \sum_{n''\mathbf{R}''} \{\delta_{nn''}\widetilde{\epsilon}_n(\mathbf{R}''-\mathbf{R}) < n''\mathbf{R}''|\hat{\rho}|n'\mathbf{R}' > - < n\mathbf{R}|\hat{\rho}|n''\mathbf{R}'' > \delta_{n''n'}\widetilde{\epsilon}_{n'}(\mathbf{R}'-\mathbf{R}'')\}\\
=&\sum_{\mathbf{R}''}\{\widetilde{\epsilon}_n(\mathbf{R}''-\mathbf{R}) < n\mathbf{R}''|\hat{\rho}|n'\mathbf{R}' > - < n\mathbf{R}|\hat{\rho}|n'\mathbf{R}'' > \widetilde{\epsilon}_{n'}(\mathbf{R}'-\mathbf{R}'')\}
\end{aligned}
\tag{D20}
$$

$$
\begin{aligned}
< n\mathbf{R}|\hat{\mathbf{x}}|n'\mathbf{R}' >=&\frac{1}{\Omega}\int\int_{BZ} d\mathbf{k}\, d\mathbf{k}' exp\{i(\mathbf{k}\cdot\mathbf{R}-\mathbf{k}'\cdot\mathbf{R}')\} < n\mathbf{k}|\hat{\mathbf{x}}|n'\mathbf{k}' >\\
=&\frac{1}{\Omega}\int\int_{BZ} d\mathbf{k}\, d\mathbf{k}' exp\{i(\mathbf{k}\cdot\mathbf{R}-\mathbf{k}'\cdot\mathbf{R}')\}\{i\nabla_{\mathbf{k}} < n\mathbf{k}|n'\mathbf{k}' > +\delta(\mathbf{k}-\mathbf{k}')\mathbf{d}_{nn'}(\mathbf{k})\}\\
=&\frac{1}{\Omega}\int d\mathbf{k}\, exp\{i\mathbf{k}\cdot(\mathbf{R}-\mathbf{R}')\}\{\delta_{nn'}\mathbf{R}+\mathbf{d}_{nn'}(\mathbf{k})\} && \text{(D21)}\\
=&\delta_{nn'}\delta_{\mathbf{R}\mathbf{R}'}\mathbf{R}+\widetilde{\mathbf{d}}_{nn'}(\mathbf{R}'-\mathbf{R}) && \text{(D22)}
\end{aligned}
$$

(D23)

$$
\begin{aligned}
\widetilde{\mathbf{d}}_{nn'}(\mathbf{R}-\mathbf{R}') =&\frac{1}{\Omega}\int d\mathbf{k}\, exp\{-i\mathbf{k}\cdot(\mathbf{R}-\mathbf{R}')\}\mathbf{d}_{nn'}(\mathbf{k})\\
=&\frac{1}{\Omega}\int d\mathbf{k}\, exp\{-i\mathbf{k}\cdot(\mathbf{R}-\mathbf{R}')\}\{\frac{i\Omega}{N} < u_{n\mathbf{k}}|\nabla_{\mathbf{k}}u_{n'\mathbf{k}} >\}\\
=&i\int_{BL} d\mathbf{y}\int d\mathbf{k}\, exp\{-i\mathbf{k}\cdot(\mathbf{R}-\mathbf{R}')\} < u_{n\mathbf{k}}|\mathbf{y} > (\nabla_{\mathbf{k}} < \mathbf{y}|u_{n'\mathbf{k}} >)\\
=&\frac{1}{\Omega}\int_{BL} d\mathbf{y}\int d\mathbf{k}\, exp\{-i\mathbf{k}\cdot(\mathbf{R}-\mathbf{R}')\}\\
&\times[\sum_{\mathbf{R}''} exp\{i\mathbf{k}\cdot(\mathbf{y}-\mathbf{R}'')\} < n\mathbf{R}''|\mathbf{y} >][\sum_{\mathbf{R}'''}(\mathbf{y}-\mathbf{R}''')exp\{-i\mathbf{k}\cdot(\mathbf{y}-\mathbf{R}''')\} < \mathbf{y}|n'\mathbf{R}''' >]\\
=&\frac{1}{\Omega}\sum_{\mathbf{R}''\mathbf{R}'''}\int_{BL} d\mathbf{y}(\mathbf{y}-\mathbf{R}''')\int d\mathbf{k}\, exp\{-i\mathbf{k}\cdot(\mathbf{R}-\mathbf{R}'+\mathbf{R}''-\mathbf{R}''')\} < n\mathbf{R}''|\mathbf{y} >< \mathbf{y}|n'\mathbf{R}''' >\\
=&\sum_{\mathbf{R}''}\int_{BL} d\mathbf{y}(\mathbf{y}-\mathbf{R}+\mathbf{R}'-\mathbf{R}'') < n\mathbf{R}''|\mathbf{y} >< \mathbf{y}|n'(\mathbf{R}-\mathbf{R}'+\mathbf{R}'') >
\end{aligned}
$$

$$
\begin{aligned}
< \mathbf{x}|u_{n\mathbf{k}} >=&exp(-i\mathbf{k}\cdot\mathbf{x}) < \mathbf{x}|n\mathbf{k} >\\
=&\frac{1}{\sqrt{\Omega}}\sum_{\mathbf{R}} exp\{-i\mathbf{k}\cdot(\mathbf{x}-\mathbf{R})\} < \mathbf{x}|n\mathbf{R} > && \text{(D24)}\\
\nabla_{\mathbf{k}} < \mathbf{x}|u_{n\mathbf{k}} >=&\frac{-i}{\sqrt{\Omega}}\sum_{\mathbf{R}}(\mathbf{x}-\mathbf{R})exp\{-i\mathbf{k}\cdot(\mathbf{x}-\mathbf{R})\} < \mathbf{x}|n\mathbf{R} > && \text{(D25)}\\
< \mathbf{x}|n\mathbf{R} >=&\frac{1}{\sqrt{\Omega}}\int_{BZ} d\mathbf{k}\, exp\{-i\mathbf{k}\cdot(\mathbf{R}-\mathbf{x})\} < \mathbf{x}|u_{n\mathbf{k}} > && \text{(D26)}
\end{aligned}
$$

$$
\begin{aligned}
< n\mathbf{R}|[\hat{\mathbf{x}},\hat{\rho}]|n'\mathbf{R}' >=& \sum_{n''\mathbf{R}''} (< n\mathbf{R}|\hat{\mathbf{x}}|n''\mathbf{R}'' >< n''\mathbf{R}''|\hat{\rho}|n'\mathbf{R}' > - < n\mathbf{R}|\hat{\rho}|n''\mathbf{R}'' >< n''\mathbf{R}''|\hat{\mathbf{x}}|n'\mathbf{R}' >) \\
=& \sum_{n''\mathbf{R}''} [\{\delta_{nn''}\delta_{\mathbf{R}\mathbf{R}''}\mathbf{R} + \widetilde{\mathbf{d}}_{nn''}(\mathbf{R}'' - \mathbf{R})\} < n''\mathbf{R}''|\hat{\rho}|n'\mathbf{R}' > \\
& - < n\mathbf{R}|\hat{\rho}|n''\mathbf{R}'' > \{\delta_{n''n'}\delta_{\mathbf{R}''\mathbf{R}'}\mathbf{R}' + \widetilde{\mathbf{d}}_{n''n'}(\mathbf{R}' - \mathbf{R}'')\}] \\
=& (\mathbf{R} - \mathbf{R}') < n\mathbf{R}|\hat{\rho}|n'\mathbf{R}' > \\
& + \sum_{n''\mathbf{R}''} \{\widetilde{\mathbf{d}}_{nn''}(\mathbf{R}'' - \mathbf{R})\} < n''\mathbf{R}''|\hat{\rho}|n'\mathbf{R}' > - < n\mathbf{R}|\hat{\rho}|n''\mathbf{R}'' > \widetilde{\mathbf{d}}_{n''n'}(\mathbf{R}' - \mathbf{R}'')\}]
\end{aligned}
\tag{D27}
$$

$$
\begin{aligned}
i\hbar < n\mathbf{R}|\hat{\rho}|n'\mathbf{R}' >=& \sum_{n''\mathbf{R}''} (< n\mathbf{R}|\hat{H}_0 - e\mathbf{E}\cdot\hat{\mathbf{x}}|n''\mathbf{R}'' >< n''\mathbf{R}''|\hat{\rho}|n'\mathbf{R}' > - < n\mathbf{R}|\hat{\rho}|n''\mathbf{R}'' >< n''\mathbf{R}''|\hat{H}_0 - e\mathbf{E}\cdot\hat{\mathbf{x}}|n'\mathbf{R}' >) \\
=& \sum_{\mathbf{R}''} \{\widetilde{\epsilon}_n(\mathbf{R}'' - \mathbf{R}) < n\mathbf{R}''|\hat{\rho}|n'\mathbf{R}' > - < n\mathbf{R}|\hat{\rho}|n'\mathbf{R}'' > \widetilde{\epsilon}_{n'}(\mathbf{R}' - \mathbf{R}'')\} \\
& - e\mathbf{E}\cdot(\mathbf{R} - \mathbf{R}') < n\mathbf{R}|\hat{\rho}|n'\mathbf{R}' > \\
& - e\mathbf{E}\cdot \sum_{n''\mathbf{R}''} \{\widetilde{\mathbf{d}}_{nn''}(\mathbf{R}'' - \mathbf{R})\} < n''\mathbf{R}''|\hat{\rho}|n'\mathbf{R}' > - < n\mathbf{R}|\hat{\rho}|n''\mathbf{R}'' > \widetilde{\mathbf{d}}_{n''n'}(\mathbf{R}' - \mathbf{R}'')\}]
\end{aligned}
\tag{D28}
$$

## Appendix E: the Chern topology

revisited in the wannier basis (2-dimension)

$$
C_1 = \frac{i}{2\pi} \int d\mathbf{k}\, \nabla_{\mathbf{k}} \times < u_{n\mathbf{k}}|\nabla_{\mathbf{k}} u_{n\mathbf{k}} >
\tag{E1}
$$


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