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

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Abstract

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

Appendix A: Fundamental formulas

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

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

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

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

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

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

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

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

$$\begin{aligned}
< n\mathbf{k}|[\hat{\mathbf{x}}, \hat{H}_0]|n'\mathbf{k}' > &= (\epsilon_{n'\mathbf{k}'} - \epsilon_{n\mathbf{k}}) < n\mathbf{k}|\hat{\mathbf{x}}|n'\mathbf{k}' > \\
&= \begin{cases} (\epsilon_{n'\mathbf{k}'} - \epsilon_{n\mathbf{k}})\{i\nabla_{\mathbf{k}} < n\mathbf{k}|n'\mathbf{k}' > +\delta(\mathbf{k}-\mathbf{k}')\mathbf{d}_{nn'}(\mathbf{k})\} \\ (\epsilon_{n'\mathbf{k}'} - \epsilon_{n\mathbf{k}})\{-i\nabla_{\mathbf{k}'} < n\mathbf{k}|n'\mathbf{k}' > +\delta(\mathbf{k}-\mathbf{k}')\mathbf{d}_{nn'}(\mathbf{k})\} \end{cases}
\end{aligned}$$

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

$$\begin{aligned}
< n\mathbf{k}|\hat{\mathbf{p}}|n\mathbf{k} > &= \frac{m}{i\hbar} < n\mathbf{k}|[\hat{\mathbf{x}}, \hat{H}_0]|n\mathbf{k} > \\
&= \frac{m}{i\hbar}\{< u_{n\mathbf{k}}|(i\nabla_{\mathbf{k}}e^{-i\mathbf{k}\cdot\hat{\mathbf{x}}})\hat{H}_0|n\mathbf{k} > - < n\mathbf{k}|\hat{H}_0(-i\nabla_{\mathbf{k}}e^{i\mathbf{k}\cdot\hat{\mathbf{x}}})|u_{n\mathbf{k}} >\} \\
&= \frac{m}{\hbar}\{\nabla_{\mathbf{k}} < n\mathbf{k}|\hat{H}_0|n\mathbf{k} > - < \nabla_{\mathbf{k}}u_{n\mathbf{k}}|e^{-i\mathbf{k}\cdot\hat{\mathbf{x}}}\hat{H}_0|n\mathbf{k} > - < n\mathbf{k}|\hat{H}_0e^{i\mathbf{k}\cdot\hat{\mathbf{x}}}|\nabla_{\mathbf{k}}u_{n\mathbf{k}} >\} \\
&= \frac{m}{\hbar}\{\nabla_{\mathbf{k}}\epsilon_{n\mathbf{k}} - \epsilon_{n\mathbf{k}}\nabla_{\mathbf{k}} < u_{n\mathbf{k}}|u_{n\mathbf{k}} >\} \\
&= \frac{m}{\hbar}\nabla_{\mathbf{k}}\epsilon_{n\mathbf{k}}
\end{aligned} \tag{A10}$$

Appendix B: Bloch-basis and length gauge

$$\begin{aligned}
&i\hbar\frac{\partial}{\partial t}< n\mathbf{k}|\hat{\rho}|n'\mathbf{k}' > \\
&=\sum_{n''}\int_{BZ} dk''(< n\mathbf{k}|\hat{H}_0 - e\mathbf{E}\cdot\hat{\mathbf{x}}|n''\mathbf{k}'' >< n''\mathbf{k}''|\hat{\rho}|n'\mathbf{k}' > \\
&\quad - < n\mathbf{k}|\hat{\rho}|n''\mathbf{k}'' >< n''\mathbf{k}''|\hat{H}_0 - e\mathbf{E}\cdot\hat{\mathbf{x}}|n'\mathbf{k}' >) \\
&=(\epsilon_{n\mathbf{k}} - \epsilon_{n'\mathbf{k}'}) < n\mathbf{k}|\hat{\rho}|n'\mathbf{k}' > \\
&\quad -e\mathbf{E}\cdot\sum_{n''}\int_{BZ} dk''(< n\mathbf{k}|\hat{\mathbf{x}}|n''\mathbf{k}'' >< n''\mathbf{k}''|\hat{\rho}|n'\mathbf{k}' > - < n\mathbf{k}|\hat{\rho}|n''\mathbf{k}'' >< n''\mathbf{k}''|\hat{\mathbf{x}}|n'\mathbf{k}' >) \\
&=(\epsilon_{n\mathbf{k}} - \epsilon_{n'\mathbf{k}'}) < n\mathbf{k}|\hat{\rho}|n'\mathbf{k}' > \\
&\quad -e\mathbf{E}\cdot[i(\nabla_{\mathbf{k}} + \nabla_{\mathbf{k}'}) < n\mathbf{k}|\hat{\rho}|n'\mathbf{k}' > + \sum_{n''}\{\mathbf{d}_{nn''}(\mathbf{k}) < n''\mathbf{k}|\hat{\rho}|n'\mathbf{k}' > -\mathbf{d}_{n''n'}(\mathbf{k}') < n\mathbf{k}|\hat{\rho}|n''\mathbf{k}' >\}]
\end{aligned} \tag{B1}$$

$$
\begin{aligned}
& i\hbar\frac{\partial}{\partial t} < v\mathbf{k}|\hat{\rho}|v\mathbf{k}> \\
& \quad = -e\mathbf{E}\cdot[i\nabla_{\mathbf{k}} < v\mathbf{k}|\hat{\rho}|v\mathbf{k}> + \{\mathbf{d}_{vc}(\mathbf{k}) < c\mathbf{k}|\hat{\rho}|v\mathbf{k}> - \mathbf{d}_{cv}(\mathbf{k}) < v\mathbf{k}|\hat{\rho}|c\mathbf{k}>\}] \\
& \quad = -e\mathbf{E}\cdot[i\nabla_{\mathbf{k}} < v\mathbf{k}|\hat{\rho}|v\mathbf{k}> - 2i\mathbf{Im}\{\mathbf{d}^{*}_{vc}(\mathbf{k}) < v\mathbf{k}|\hat{\rho}|c\mathbf{k}>\}]
\end{aligned} \tag{B2}
$$

$$
\begin{aligned}
& i\hbar\frac{\partial}{\partial t} < c\mathbf{k}|\hat{\rho}|c\mathbf{k}> \\
& \quad = -e\mathbf{E}\cdot[i\nabla_{\mathbf{k}} < c\mathbf{k}|\hat{\rho}|c\mathbf{k}> + \{\mathbf{d}_{cv}(\mathbf{k}) < v\mathbf{k}|\hat{\rho}|c\mathbf{k}> - \mathbf{d}_{vc}(\mathbf{k}) < c\mathbf{k}|\hat{\rho}|v\mathbf{k}>\}] \\
& \quad = -e\mathbf{E}\cdot[i\nabla_{\mathbf{k}} < c\mathbf{k}|\hat{\rho}|c\mathbf{k}> + 2i\mathbf{Im}\{\mathbf{d}^{*}_{vc}(\mathbf{k}) < v\mathbf{k}|\hat{\rho}|c\mathbf{k}>\}]
\end{aligned} \tag{B3}
$$

$$
\begin{aligned}
& i\hbar\frac{\partial}{\partial t} < v\mathbf{k}|\hat{\rho}|c\mathbf{k}> \\
& \quad = (\epsilon_{v\mathbf{k}} - \epsilon_{c\mathbf{k}}) < v\mathbf{k}|\hat{\rho}|c\mathbf{k}> \\
& \qquad - e\mathbf{E}\cdot[i\nabla_{\mathbf{k}} < v\mathbf{k}|\hat{\rho}|c\mathbf{k}> + \sum_{n''}\{\mathbf{d}_{vn''}(\mathbf{k}) < n''\mathbf{k}|\hat{\rho}|c\mathbf{k}> - \mathbf{d}_{n''c}(\mathbf{k}) < v\mathbf{k}|\hat{\rho}|n''\mathbf{k}>\}] \\
& \quad = -(\epsilon_{c\mathbf{k}} - \epsilon_{v\mathbf{k}}) < v\mathbf{k}|\hat{\rho}|c\mathbf{k}> - ie\mathbf{E}\cdot\nabla_{\mathbf{k}} < v\mathbf{k}|\hat{\rho}|c\mathbf{k}> \\
& \qquad - e\mathbf{E}\cdot[-\{\mathbf{d}_{cc}(\mathbf{k}) - \mathbf{d}_{vv}(\mathbf{k})\} < v\mathbf{k}|\hat{\rho}|c\mathbf{k}> + \mathbf{d}_{vc}(\mathbf{k})\{< c\mathbf{k}|\hat{\rho}|c\mathbf{k}> - < v\mathbf{k}|\hat{\rho}|v\mathbf{k}>\}]
\end{aligned} \tag{B4}
$$

$$
\begin{aligned}
H_L &= tr\{\hat{\rho}(\hat{H}_0 - e\mathbf{E}\cdot\hat{\mathbf{x}})\} \\
&= \sum_n \int d\mathbf{k} < n\mathbf{k}|\hat{\rho}|n\mathbf{k}> \epsilon_{n\mathbf{k}} - e\mathbf{E}\cdot\{\sum_{nn'}\int d\mathbf{k}\int d\mathbf{k}' < n\mathbf{k}|\hat{\rho}|n'\mathbf{k}'>< n'\mathbf{k}'|\hat{\mathbf{x}}|n\mathbf{k}>\} \\
&= \sum_n \int d\mathbf{k} < n\mathbf{k}|\hat{\rho}|n\mathbf{k}> \epsilon_{n\mathbf{k}} \\
&\quad - e\mathbf{E}\cdot[\sum_{nn'}\int d\mathbf{k}\int d\mathbf{k}' < n\mathbf{k}|\hat{\rho}|n'\mathbf{k}'> \{\frac{1}{2i}(\nabla_{\mathbf{k}} - \nabla_{\mathbf{k}'}) < n'\mathbf{k}'|n\mathbf{k}> + \delta(\mathbf{k}'-\mathbf{k})\mathbf{d}_{n'n}(\mathbf{k})\}] \\
&= \sum_n \int d\mathbf{k} < n\mathbf{k}|\hat{\rho}|n\mathbf{k}> \epsilon_{n\mathbf{k}} \\
&\quad - e\mathbf{E}\cdot\{\sum_n \int d\mathbf{k}\,\mathbf{Im}(\nabla_{\mathbf{k}} < n\mathbf{k}|\hat{\rho}|n\mathbf{k}>) + \sum_{nn'}\int d\mathbf{k} < n\mathbf{k}|\hat{\rho}|n'\mathbf{k}> \mathbf{d}_{n'n}(\mathbf{k})\} \\
&= \sum_n \int d\mathbf{k} < n\mathbf{k}|\hat{\rho}|n\mathbf{k}> \epsilon_{n\mathbf{k}} - e\mathbf{E}\cdot\{\sum_{nn'}\int d\mathbf{k} < n\mathbf{k}|\hat{\rho}|n'\mathbf{k}> \mathbf{d}_{n'n}(\mathbf{k})\}
\end{aligned} \tag{B5}
$$

$$
\begin{aligned}
H_L^2 &= \sum_n \int d\mathbf{k} < n\mathbf{k}|\hat{\rho}|n\mathbf{k}> \epsilon_{n\mathbf{k}} - e\mathbf{E}\cdot\{\sum_{nn'}\int d\mathbf{k} < n\mathbf{k}|\hat{\rho}|n'\mathbf{k}> \mathbf{d}_{n'n}(\mathbf{k})\} \\
&= \int d\mathbf{k}(< v\mathbf{k}|\hat{\rho}|v\mathbf{k}> \epsilon_{v\mathbf{k}} + < c\mathbf{k}|\hat{\rho}|c\mathbf{k}> \epsilon_{c\mathbf{k}}) \\
&\quad - e\mathbf{E}\cdot\int d\mathbf{k}[< v\mathbf{k}|\hat{\rho}|v\mathbf{k}> \mathbf{d}_{vv}(\mathbf{k}) + < c\mathbf{k}|\hat{\rho}|c\mathbf{k}> \mathbf{d}_{cc}(\mathbf{k}) + 2\mathbf{Re}\{< v\mathbf{k}|\hat{\rho}|c\mathbf{k}> \mathbf{d}^{*}_{vc}(\mathbf{k})\}]
\end{aligned} \tag{B6}
$$

Appendix C: Bloch-basis and velocity gauge

$$\begin{aligned}
& i\hbar\frac{\partial}{\partial t} < n\mathbf{k}|\hat{\rho}|n'\mathbf{k}' > \\
&= \sum_{n''}\int d\mathbf{k}''(< n\mathbf{k}|\hat{H}_0 - \frac{e\mathbf{A}\cdot\hat{\mathbf{p}}}{m}|n''\mathbf{k}'' >< n''\mathbf{k}''|\hat{\rho}|n'\mathbf{k}' > \\
&\quad - < n\mathbf{k}|\hat{\rho}|n''\mathbf{k}'' >< n''\mathbf{k}''|\hat{H}_0 - \frac{e\mathbf{A}\cdot\hat{\mathbf{p}}}{m}|n'\mathbf{k}' >) \\
&= (\epsilon_{n\mathbf{k}} - \epsilon_{n'\mathbf{k}'}) < n\mathbf{k}|\hat{\rho}|n'\mathbf{k}' > \\
&\quad - \frac{e\mathbf{A}}{m}\cdot\sum_{n''}\int d\mathbf{k}''\{< n\mathbf{k}|\hat{\mathbf{p}}|n''\mathbf{k}'' >< n''\mathbf{k}''|\hat{\rho}|n'\mathbf{k}' > - < n\mathbf{k}|\hat{\rho}|n''\mathbf{k}'' >< n''\mathbf{k}''|\hat{\mathbf{p}}|n'\mathbf{k}' >\} \\
&= (\epsilon_{n\mathbf{k}} - \epsilon_{n'\mathbf{k}'}) < n\mathbf{k}|\hat{\rho}|n'\mathbf{k}' > \\
&\quad - \frac{e\mathbf{A}}{\hbar}\cdot\sum_{n''}\int d\mathbf{k}''[(\epsilon_{n\mathbf{k}} - \epsilon_{n''\mathbf{k}''})\{\nabla_{\mathbf{k}''} < n\mathbf{k}|n''\mathbf{k}'' > + i\delta(\mathbf{k}-\mathbf{k}'')\mathbf{d}_{nn''}(\mathbf{k})\} < n''\mathbf{k}''|\hat{\rho}|n'\mathbf{k}' > \\
&\quad - < n\mathbf{k}|\hat{\rho}|n''\mathbf{k}'' > (\epsilon_{n''\mathbf{k}''} - \epsilon_{n'\mathbf{k}'})\{-\nabla_{\mathbf{k}''} < n''\mathbf{k}''|n'\mathbf{k}' > + i\delta(\mathbf{k}''-\mathbf{k}')\mathbf{d}_{n''n'}(\mathbf{k}')\}] \\
&= (\epsilon_{n\mathbf{k}} - \epsilon_{n'\mathbf{k}'}) < n\mathbf{k}|\hat{\rho}|n'\mathbf{k}' > \\
&\quad - \frac{e\mathbf{A}}{\hbar}\cdot(\nabla_{\mathbf{k}}\epsilon_{n\mathbf{k}} - \nabla_{\mathbf{k}'}\epsilon_{n'\mathbf{k}'}) < n\mathbf{k}|\hat{\rho}|n'\mathbf{k}' > \\
&\quad - \frac{ie\mathbf{A}}{\hbar}\cdot\sum_{n''}[(\epsilon_{n\mathbf{k}} - \epsilon_{n''\mathbf{k}})\mathbf{d}_{nn''}(\mathbf{k}) < n''\mathbf{k}|\hat{\rho}|n'\mathbf{k}' > - (\epsilon_{n''\mathbf{k}'} - \epsilon_{n'\mathbf{k}'}) < n\mathbf{k}|\hat{\rho}|n''\mathbf{k}' > \mathbf{d}_{n''n'}(\mathbf{k}')]
\end{aligned} \tag{C1}$$

$$\begin{aligned}
& i\hbar\frac{\partial}{\partial t} < v\mathbf{k}|\hat{\rho}|v\mathbf{k} > \\
&= -\frac{ie\mathbf{A}}{\hbar}\cdot\{(\epsilon_{v\mathbf{k}} - \epsilon_{c\mathbf{k}})\mathbf{d}_{vc}(\mathbf{k}) < c\mathbf{k}|\hat{\rho}|v\mathbf{k} > - (\epsilon_{c\mathbf{k}} - \epsilon_{v\mathbf{k}}) < v\mathbf{k}|\hat{\rho}|c\mathbf{k} > \mathbf{d}_{cv}(\mathbf{k})\} \\
&= +\frac{ie\mathbf{A}}{\hbar}\cdot[2(\epsilon_{c\mathbf{k}} - \epsilon_{v\mathbf{k}})\mathbf{Re}\{\mathbf{d}^*_{vc}(\mathbf{k}) < v\mathbf{k}|\hat{\rho}|c\mathbf{k} >\}]
\end{aligned} \tag{C2}$$

$$\begin{aligned}
& i\hbar\frac{\partial}{\partial t} < c\mathbf{k}|\hat{\rho}|c\mathbf{k} > \\
&= -\frac{ie\mathbf{A}}{\hbar}\cdot\{(\epsilon_{c\mathbf{k}} - \epsilon_{v\mathbf{k}})\mathbf{d}_{cv}(\mathbf{k}) < v\mathbf{k}|\hat{\rho}|c\mathbf{k} > - (\epsilon_{v\mathbf{k}} - \epsilon_{c\mathbf{k}}) < c\mathbf{k}|\hat{\rho}|v\mathbf{k} > \mathbf{d}_{vc}(\mathbf{k})\} \\
&= -\frac{ie\mathbf{A}}{\hbar}\cdot[2(\epsilon_{c\mathbf{k}} - \epsilon_{v\mathbf{k}})\mathbf{Re}\{\mathbf{d}^*_{vc}(\mathbf{k}) < v\mathbf{k}|\hat{\rho}|c\mathbf{k} >\}]
\end{aligned} \tag{C3}$$

$$\begin{aligned}
& i\hbar\frac{\partial}{\partial t} < v\mathbf{k}|\hat{\rho}|c\mathbf{k} > \\
&= (\epsilon_{v\mathbf{k}} - \epsilon_{c\mathbf{k}}) < v\mathbf{k}|\hat{\rho}|c\mathbf{k} > - \frac{e\mathbf{A}}{\hbar}\cdot\{(\nabla_{\mathbf{k}}\epsilon_{v\mathbf{k}} - \nabla_{\mathbf{k}}\epsilon_{c\mathbf{k}}) < v\mathbf{k}|\hat{\rho}|c\mathbf{k} >\} \\
&\quad - \frac{ie\mathbf{A}}{\hbar}\cdot\{(\epsilon_{v\mathbf{k}} - \epsilon_{c\mathbf{k}})\mathbf{d}_{vc}(\mathbf{k}) < c\mathbf{k}|\hat{\rho}|c\mathbf{k} > - (\epsilon_{v\mathbf{k}} - \epsilon_{c\mathbf{k}}) < v\mathbf{k}|\hat{\rho}|v\mathbf{k} > \mathbf{d}_{vc}(\mathbf{k})\} \\
&= -(\epsilon_{c\mathbf{k}} - \epsilon_{v\mathbf{k}}) < v\mathbf{k}|\hat{\rho}|c\mathbf{k} > + \frac{e\mathbf{A}}{\hbar}\cdot\{(\nabla_{\mathbf{k}}\epsilon_{c\mathbf{k}} - \nabla_{\mathbf{k}}\epsilon_{v\mathbf{k}}) < v\mathbf{k}|\hat{\rho}|c\mathbf{k} >\} \\
&\quad + \frac{ie\mathbf{A}}{\hbar}\cdot\{(\epsilon_{c\mathbf{k}} - \epsilon_{v\mathbf{k}})\mathbf{d}_{vc}(\mathbf{k})(< c\mathbf{k}|\hat{\rho}|c\mathbf{k} > - < v\mathbf{k}|\hat{\rho}|v\mathbf{k} >)\}
\end{aligned} \tag{C4}$$

$$
\begin{aligned}
H_V &= tr\{\hat{\rho}(\hat{H}_0 - \frac{e\mathbf{A}\cdot\hat{\mathbf{p}}}{m})\} \\
&= \sum_n \int d\mathbf{k} < n\mathbf{k}|\hat{\rho}|n\mathbf{k} > \epsilon_{n\mathbf{k}} - \frac{e\mathbf{A}}{m}\cdot\{\sum_{nn'}\int d\mathbf{k}\int d\mathbf{k}' < n\mathbf{k}|\hat{\rho}|n'\mathbf{k}' >< n'\mathbf{k}'|\hat{\mathbf{p}}|n\mathbf{k} >\} \\
&= \sum_n \int d\mathbf{k} < n\mathbf{k}|\hat{\rho}|n\mathbf{k} > \epsilon_{n\mathbf{k}} \\
&\quad -\frac{e\mathbf{A}}{\hbar}\cdot[\sum_{nn'}\int d\mathbf{k}\int d\mathbf{k}'(\epsilon_{n'\mathbf{k}'} - \epsilon_{n\mathbf{k}}) < n\mathbf{k}|\hat{\rho}|n'\mathbf{k}' > \{\nabla_{\mathbf{k}} < n'\mathbf{k}'|n\mathbf{k} > + i\delta(\mathbf{k}' - \mathbf{k})\mathbf{d}_{n'n}(\mathbf{k})\}] \\
&= \sum_n \int d\mathbf{k} < n\mathbf{k}|\hat{\rho}|n\mathbf{k} > \epsilon_{n\mathbf{k}} \\
&\quad -\frac{e\mathbf{A}}{\hbar}\cdot[\sum_n \int d\mathbf{k}\nabla_{\mathbf{k}}\epsilon_{n\mathbf{k}} < n\mathbf{k}|\hat{\rho}|n\mathbf{k} > + i\sum_{n\neq n'}\int d\mathbf{k} < n\mathbf{k}|\hat{\rho}|n'\mathbf{k} > (\epsilon_{n'\mathbf{k}'} - \epsilon_{n\mathbf{k}})\mathbf{d}_{n'n}(\mathbf{k})]
\end{aligned} \tag{C5}
$$

$$
\begin{aligned}
H_V^2 = &\int d\mathbf{k}(< v\mathbf{k}|\hat{\rho}|v\mathbf{k} > \epsilon_{v\mathbf{k}} + < c\mathbf{k}|\hat{\rho}|c\mathbf{k} > \epsilon_{c\mathbf{k}}) \\
&-\frac{e\mathbf{A}}{\hbar}\cdot\int d\mathbf{k}(< v\mathbf{k}|\hat{\rho}|v\mathbf{k} > \nabla_{\mathbf{k}}\epsilon_{v\mathbf{k}} + < c\mathbf{k}|\hat{\rho}|c\mathbf{k} > \nabla_{\mathbf{k}}\epsilon_{c\mathbf{k}}) \\
&+\frac{2e\mathbf{A}}{\hbar}\cdot\int d\mathbf{k}(\epsilon_{c\mathbf{k}} - \epsilon_{v\mathbf{k}})\mathbf{Im}\{< v\mathbf{k}|\hat{\rho}|c\mathbf{k} > \mathbf{d}^*_{vc}(\mathbf{k})\}
\end{aligned} \tag{C6}
$$

Appendix D: velocity/current and position

$$
\begin{aligned}
J &= -e\frac{\partial}{\partial t}tr(\hat{\rho}\hat{\mathbf{x}}) \\
&= -e\, tr(\frac{\partial\hat{\rho}}{\partial t}\hat{\mathbf{x}}) \\
&= -\frac{e}{i\hbar}tr([\hat{H},\hat{\rho}]\hat{\mathbf{x}}) \\
&= -\frac{e}{i\hbar}tr(\hat{H}\hat{\rho}\hat{\mathbf{x}} - \hat{\rho}\hat{H}\hat{\mathbf{x}}) \\
&= -\frac{e}{i\hbar}tr\{\hat{\rho}(\hat{\mathbf{x}}\hat{H} - \hat{H}\hat{\mathbf{x}})\} \\
&= -\frac{e}{i\hbar}tr\{\hat{\rho}[\hat{\mathbf{x}},\hat{H}]\}
\end{aligned} \tag{D1}
$$

$$
\hat{H}^L_{int} = -e\mathbf{E}\cdot\hat{\mathbf{x}}, \tag{D2}
$$

$$
\hat{H}^V_{int} = \frac{-2e\mathbf{A}\cdot\hat{\mathbf{p}} + e^2|\mathbf{A}|^2}{2m}. \tag{D3}
$$

$$
\begin{aligned}
J^L &= -\frac{e}{i\hbar} tr\{\hat{\rho}[\hat{\mathbf{x}}, \hat{H^L}]\} \\
&= -\frac{e}{i\hbar} tr\{\hat{\rho}[\hat{\mathbf{x}}, (\hat{H}_0 - e\mathbf{E}\cdot\hat{\mathbf{x}})]\} \\
&= -\frac{e}{i\hbar} tr\{\hat{\rho}[\hat{\mathbf{x}}, \hat{H}_0]\} \\
&= -\frac{e}{i\hbar} \sum_{nn'} \int d\mathbf{k} \int d\mathbf{k}' < n\mathbf{k}|\hat{\rho}|n'\mathbf{k}' >< n'\mathbf{k}'|[\hat{\mathbf{x}}, \hat{H}_0]|n\mathbf{k} > \\
&= -\frac{e}{i\hbar} \sum_{nn'} \int d\mathbf{k} \int d\mathbf{k}' < n\mathbf{k}|\hat{\rho}|n'\mathbf{k}' > (\epsilon_{n'\mathbf{k}'} - \epsilon_{n\mathbf{k}})\{-i\nabla_{\mathbf{k}} < n'\mathbf{k}'|n\mathbf{k} > +\delta(\mathbf{k}' - \mathbf{k})\mathbf{d}_{n'n}(\mathbf{k})\} \\
&= -\frac{e}{\hbar} \sum_{n} \int d\mathbf{k} < n\mathbf{k}|\hat{\rho}|n\mathbf{k} > \nabla_{\mathbf{k}}\epsilon_{n\mathbf{k}} + \frac{e}{\hbar} \sum_{nn'} \int d\mathbf{k} < n\mathbf{k}|\hat{\rho}|n'\mathbf{k} > (\epsilon_{n'\mathbf{k}} - \epsilon_{n\mathbf{k}})\{i\mathbf{d}_{n'n}(\mathbf{k})\}
\end{aligned}
\tag{D4}
$$

$$
\begin{aligned}
J^V &= -\frac{e}{i\hbar} tr\{\hat{\rho}[\hat{\mathbf{x}}, \hat{H^V}]\} \\
&= -\frac{e}{i\hbar} tr\{\hat{\rho}[\hat{\mathbf{x}}, (\hat{H}_0 + \frac{-2e\mathbf{A}\cdot\hat{\mathbf{p}} + e^2|\mathbf{A}|^2}{2m})]\} \\
&= -\frac{e}{i\hbar} tr\{\hat{\rho}[\hat{\mathbf{x}}, \hat{H}_0]\} + \frac{e^2}{im\hbar}\mathbf{A} tr\{\hat{\rho}[\hat{\mathbf{x}}, \hat{\mathbf{p}}]\} \\
&= -\frac{e}{i\hbar} tr\{\hat{\rho}[\hat{\mathbf{x}}, \hat{H}_0]\} + \frac{e^2}{m}\mathbf{A} tr(\hat{\rho}) \\
&= -\frac{e}{m} \sum_{nn'} \int d\mathbf{k} \int d\mathbf{k}' < n\mathbf{k}|\hat{\rho}|n'\mathbf{k}' >< n'\mathbf{k}'|\hat{\mathbf{p}}|n\mathbf{k} > + \frac{e^2\mathbf{A}}{m} tr(\hat{\rho}) \\
&= -\frac{e}{\hbar} \sum_{nn'} \int d\mathbf{k} \int d\mathbf{k}' < n\mathbf{k}|\hat{\rho}|n'\mathbf{k}' > (\epsilon_{n'\mathbf{k}'} - \epsilon_{n\mathbf{k}})\{\nabla_{\mathbf{k}} < n'\mathbf{k}'|n\mathbf{k} > +i\delta(\mathbf{k}' - \mathbf{k})\mathbf{d}_{n'n}(\mathbf{k})\} \\
&\quad + \frac{e^2\mathbf{A}}{m} tr(\hat{\rho}) \\
&= +\frac{e}{\hbar} \sum_{nn'} \int d\mathbf{k} \int d\mathbf{k}' \nabla_{\mathbf{k}}\{< n\mathbf{k}|\hat{\rho}|n'\mathbf{k}' > (\epsilon_{n'\mathbf{k}'} - \epsilon_{n\mathbf{k}})\} < n'\mathbf{k}'|n\mathbf{k} > \\
&\quad - \frac{e}{\hbar} \sum_{nn'} \int d\mathbf{k} < n\mathbf{k}|\hat{\rho}|n'\mathbf{k} > (\epsilon_{n'\mathbf{k}} - \epsilon_{n\mathbf{k}})\{i\mathbf{d}_{n'n}(\mathbf{k})\} + \frac{e^2\mathbf{A}}{m} tr(\hat{\rho}) \\
&= \frac{e}{\hbar} \sum_{n} \int d\mathbf{k} < n\mathbf{k}|\hat{\rho}|n\mathbf{k} > \nabla_{\mathbf{k}}\epsilon_{n\mathbf{k}} - \frac{e}{\hbar} \sum_{nn'} \int d\mathbf{k} < n\mathbf{k}|\hat{\rho}|n'\mathbf{k} > (\epsilon_{n'\mathbf{k}} - \epsilon_{n\mathbf{k}})\{i\mathbf{d}_{n'n}(\mathbf{k})\} + \frac{e^2\mathbf{A}}{m} tr(\hat{\rho})
\end{aligned}
\tag{D5}
$$

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

$$
\begin{aligned}
&= -\frac{e}{\hbar}\int d\mathbf{k}(< v\mathbf{k}|\hat{\rho}|v\mathbf{k}> \nabla_{\mathbf{k}}\epsilon_{v\mathbf{k}} + < c\mathbf{k}|\hat{\rho}|c\mathbf{k}> \nabla_{\mathbf{k}}\epsilon_{c\mathbf{k}}) + \frac{e^2\mathbf{A}}{m}tr(\hat{\rho}) \\
&\quad + \frac{e}{\hbar}\int d\mathbf{k}(\epsilon_{c\mathbf{k}} - \epsilon_{v\mathbf{k}})\mathbf{Im}[< v\mathbf{k}|\hat{\rho}|c\mathbf{k}> \mathbf{d}_{vc}]
\end{aligned}
\tag{D6}
$$

$$
\begin{aligned}
J^L &= -e\frac{\partial}{\partial t}tr(\hat{\rho}\hat{\mathbf{x}}) \\
&= -e\, tr(\frac{\partial\hat{\rho}}{\partial t}\hat{\mathbf{x}}) \\
&= -\frac{e}{i\hbar}tr([\hat{H}_0 - e\mathbf{E}\cdot\hat{\mathbf{x}}, \hat{\rho}]\hat{\mathbf{x}})
\end{aligned}
\tag{D7}
$$

$$
\begin{aligned}
\mathbf{x} &= tr(\hat{\rho}\hat{\mathbf{x}}) \\
&= \sum_{nn'}\int d\mathbf{k}\int d\mathbf{k}' < n\mathbf{k}|\hat{\rho}|n'\mathbf{k}' >< n'\mathbf{k}'|\hat{\mathbf{x}}|n\mathbf{k}> \\
&= \sum_{nn'}\int d\mathbf{k}\int d\mathbf{k}' < n\mathbf{k}|\hat{\rho}|n'\mathbf{k}' > \{\frac{1}{2i}(\nabla_{\mathbf{k}} - \nabla_{\mathbf{k}'}) < n'\mathbf{k}'|n\mathbf{k}> + \delta(\mathbf{k}' - \mathbf{k})\mathbf{d}_{n'n}(\mathbf{k})\} \\
&= \sum_{nn'}\int d\mathbf{k} < n\mathbf{k}|\hat{\rho}|n'\mathbf{k}> \mathbf{d}_{n'n}(\mathbf{k})
\end{aligned}
\tag{D8}
$$

$$
\mathbf{x}^2 = \int d\mathbf{k}\{< v\mathbf{k}|\hat{\rho}|v\mathbf{k}> \mathbf{d}_{vv}(\mathbf{k}) + < c\mathbf{k}|\hat{\rho}|c\mathbf{k}> \mathbf{d}_{cc}(\mathbf{k}) + 2\mathbf{Re}\{< v\mathbf{k}|\hat{\rho}|c\mathbf{k}> \mathbf{d}^*_{vc}(\mathbf{k})\}] \tag{D9}
$$

Appendix E: 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.

$$
\begin{aligned}
|n\mathbf{R}> &= \frac{1}{\sqrt{N}}\sum_{\mathbf{K}} exp(-i\mathbf{K}\cdot\mathbf{R})|n\mathbf{K}> \\
&= \frac{1}{\sqrt{\Omega}}\int_{BZ} d\mathbf{k}\, exp(-i\mathbf{k}\cdot\mathbf{R})|n\mathbf{k}> \\
&= \frac{1}{\sqrt{\Omega}}\int_{BZ} d\mathbf{k}\, exp\{-i\mathbf{k}\cdot(\mathbf{R} - \hat{\mathbf{x}})\}|u_{n\mathbf{k}}>
\end{aligned}
\tag{E1}
$$

$$
< \mathbf{x}|n\mathbf{R}> = \frac{1}{\sqrt{\Omega}}\int_{BZ} d\mathbf{k}\, exp\{-i\mathbf{k}\cdot(\mathbf{R} - \mathbf{x})\} < \mathbf{x}|u_{n\mathbf{k}}> \tag{E2}
$$

$$
|n\mathbf{K}> = \frac{1}{\sqrt{N}}\sum_{\mathbf{R}} exp(i\mathbf{k}\cdot\mathbf{R})|n\mathbf{R}> \tag{E3}
$$

$$
\begin{aligned}
|n\mathbf{k}> &= \sqrt{\frac{N}{\Omega}}|n\mathbf{K}> \\
&= \frac{1}{\sqrt{\Omega}}\sum_{\mathbf{R}}\ exp(i\mathbf{k}\cdot\mathbf{R})|n\mathbf{R}>
\end{aligned} \tag{E4}
$$

$$
\int_{BZ} d\mathbf{k} = \frac{\Omega}{N}\sum_{\mathbf{K}} \tag{E5}
$$

$$
\sum_{\mathbf{K}} |n\mathbf{K}><n\mathbf{K}| = \int_{BZ} d\mathbf{k}|n\mathbf{k}><n\mathbf{k}| \tag{E6}
$$

$$
\delta_{KK'} =<n\mathbf{K}|n\mathbf{K}'> = \frac{\Omega}{N}<n\mathbf{k}|n\mathbf{k}'>= \frac{\Omega}{N}\delta(\mathbf{k}-\mathbf{k}') \tag{E7}
$$

$$
\nabla_{\mathbf{k}} = \nabla_{\mathbf{K}} \tag{E8}
$$

$$
\begin{aligned}
<n\mathbf{R}|n'\mathbf{R}'> &= \frac{1}{\Omega}\int\int_{BZ} d\mathbf{k}d\mathbf{k}' exp\{i(\mathbf{k}\cdot\mathbf{R}-\mathbf{k}'\cdot\mathbf{R}')\}<n\mathbf{k}|n'\mathbf{k}'> \\
&= \frac{\delta_{nn'}}{\Omega}\int_{BZ} d\mathbf{k}\, exp\{i\mathbf{k}\cdot(\mathbf{R}-\mathbf{R}')\} \\
&= \delta_{nn'}\delta_{\mathbf{R}\mathbf{R}'}
\end{aligned} \tag{E9}
$$

$$
\begin{aligned}
|n\mathbf{R}> &= \frac{1}{\Omega}\int_{BZ} d\mathbf{k}\ exp(-i\mathbf{k}\cdot\mathbf{R})|n\mathbf{k}> \\
&= \frac{1}{\Omega}\sum_{\mathbf{R}'}\int_{BZ} d\mathbf{k}\ exp\{-i\mathbf{k}\cdot(\mathbf{R}-\mathbf{R}')\}|n\mathbf{R}'> \\
&= \sum_{\mathbf{R}'}\delta_{\mathbf{R}\mathbf{R}'}|n\mathbf{R}'> \\
&= |n\mathbf{R}>
\end{aligned} \tag{E10}
$$

$$
\begin{aligned}
\int_{BZ} d\mathbf{k}'<n\mathbf{k}|n'\mathbf{k}'> &= \frac{1}{\Omega}\sum_{\mathbf{R}\mathbf{R}'}\int_{BZ} d\mathbf{k}' exp\{i(\mathbf{k}\cdot\mathbf{R}-\mathbf{k}'\cdot\mathbf{R}')\}<n\mathbf{R}|n'\mathbf{R}'> \\
&= \frac{\delta_{nn'}}{\Omega}\sum_{\mathbf{R}}\int_{BZ} d\mathbf{k}' exp\{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}\} \\
&= \frac{\delta_{nn'}}{N}\sum_{\mathbf{R}\mathbf{K}'} exp\{i(\mathbf{K}-\mathbf{K}')\cdot\mathbf{R}\} \\
&= \frac{\delta_{nn'}}{N}\sum_{\mathbf{R}} 1 \\
&= \delta_{nn'}
\end{aligned} \tag{E11}
$$

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

$$= |n\mathbf{k}> \tag{E12}$$

$$\begin{aligned}
<\mathbf{x}|u_{n\mathbf{k}}> &= exp(-i\mathbf{k}\cdot\mathbf{x}) <\mathbf{x}|n\mathbf{k}> \\
&= \frac{1}{\sqrt{\Omega}} \sum_{\mathbf{R}} exp\{-i\mathbf{k}\cdot(\mathbf{x}-\mathbf{R})\} <\mathbf{x}|n\mathbf{R}> && \text{(E13)} \\
\nabla_{\mathbf{k}} <\mathbf{x}|u_{n\mathbf{k}}> &= \frac{-i}{\sqrt{\Omega}} \sum_{\mathbf{R}} (\mathbf{x}-\mathbf{R}) exp\{-i\mathbf{k}\cdot(\mathbf{x}-\mathbf{R})\} <\mathbf{x}|n\mathbf{R}> && \text{(E14)}
\end{aligned}$$

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

$$\begin{aligned}
< n\mathbf{R}|\hat{O}|n'\mathbf{R}' > &= \frac{1}{\Omega} \int\int_{BZ} d\mathbf{k}d\mathbf{k}' exp[i(\mathbf{k}\cdot\mathbf{R} - \mathbf{k}'\cdot\mathbf{R}')] < n\mathbf{k}|\hat{O}|n'\mathbf{k}' > && \text{(E15)} \\
\widetilde{o}(\mathbf{R}) &= \frac{1}{\Omega} \int_{BZ} d\mathbf{k} exp(-i\mathbf{k}\cdot\mathbf{R}) o(\mathbf{k}) \\
&= \frac{1}{N} \sum_{\mathbf{K}} exp(-i\mathbf{K}\cdot\mathbf{R}) o(\mathbf{K}) && \text{(E16)}
\end{aligned}$$

$$\begin{aligned}
< n\mathbf{R}|\hat{H}_0|n'\mathbf{R}' > &= \frac{1}{\Omega} \int\int_{BZ} d\mathbf{k}\, d\mathbf{k}' exp\{i(\mathbf{k}\cdot\mathbf{R} - \mathbf{k}'\cdot\mathbf{R}')\} < n\mathbf{k}|\hat{H}_0|n'\mathbf{k}' > \\
&= \frac{1}{\Omega} \int d\mathbf{k}_{BZ}\, exp\{i\mathbf{k}\cdot(\mathbf{R}-\mathbf{R}')\} \delta_{nn'} \epsilon_{n\mathbf{k}} \\
&= \delta_{nn'} \widetilde{\epsilon}_n(\mathbf{R}'-\mathbf{R}) && \text{(E17)}
\end{aligned}$$

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,

$$\begin{aligned}
\widetilde{\epsilon}_n(\mathbf{R}) &= \frac{1}{\Omega} \int d\mathbf{k}\, exp(-i\mathbf{k}\cdot\mathbf{R}) \epsilon_{n\mathbf{k}} \\
&= \frac{1}{\Omega} \int d\mathbf{k}\, exp(-i\mathbf{k}\cdot\mathbf{R}) [E_n^0 + \Delta E_n\{1 - cos(ka)\}] \\
&= (E_n^0 + \Delta E_n)\delta_{\mathbf{R0}} - \frac{\Delta E_n}{2}\{\delta_{\mathbf{Ra}} + \delta_{\mathbf{R(-a)}}\} && \text{(E18)} \\
& && \text{(E19)}
\end{aligned}$$

$$\begin{aligned}
< n\mathbf{R}|[\hat{H}_0, \hat{\rho}]|n'\mathbf{R}' > &= \sum_{n''\mathbf{R}''} (< n\mathbf{R}|\hat{H}_0|n''\mathbf{R}'' >< n''\mathbf{R}''|\hat{\rho}|n'\mathbf{R}' > - < n\mathbf{R}|\hat{\rho}|n''\mathbf{R}'' >< n''\mathbf{R}''|\hat{H}_0|n'\mathbf{R}' >) \\
&= \sum_{n''\mathbf{R}''} \{\delta_{nn''} \widetilde{\epsilon}_n(\mathbf{R}''-\mathbf{R}) < n''\mathbf{R}''|\hat{\rho}|n'\mathbf{R}' > - < n\mathbf{R}|\hat{\rho}|n''\mathbf{R}'' > \delta_{n''n'} \widetilde{\epsilon}_{n'}(\mathbf{R}'-\mathbf{R}'')\} \\
&= \sum_{\mathbf{R}''} \{\widetilde{\epsilon}_n(\mathbf{R}''-\mathbf{R}) < n\mathbf{R}''|\hat{\rho}|n'\mathbf{R}' > - < n\mathbf{R}|\hat{\rho}|n'\mathbf{R}'' > \widetilde{\epsilon}_{n'}(\mathbf{R}'-\mathbf{R}'')\}
\end{aligned} \tag{E20}$$

$$
\begin{aligned}
< n\mathbf{R}|\hat{\mathbf{x}}|n'\mathbf{R}' > =& \frac{1}{\Omega}\int\int_{BZ} d\mathbf{k}\, d\mathbf{k}' exp\{i(\mathbf{k}\cdot\mathbf{R}-\mathbf{k}'\cdot\mathbf{R}')\} < n\mathbf{k}|\hat{\mathbf{x}}|n'\mathbf{k}' > \\
=& \frac{1}{\Omega}\int\int_{BZ} d\mathbf{k}\, d\mathbf{k}' exp\{i(\mathbf{k}\cdot\mathbf{R}-\mathbf{k}'\cdot\mathbf{R}')\}\{i\nabla_{\mathbf{k}} < n\mathbf{k}|n'\mathbf{k}' > +\delta(\mathbf{k}-\mathbf{k}')\mathbf{d}_{nn'}(\mathbf{k})\} \\
=& \frac{1}{\Omega}\int d\mathbf{k}\, exp\{i\mathbf{k}\cdot(\mathbf{R}-\mathbf{R}')\}\{\delta_{nn'}\mathbf{R}+\mathbf{d}_{nn'}(\mathbf{k})\} && \text{(E21)} \\
=& \delta_{nn'}\delta_{\mathbf{R}\mathbf{R}'}\mathbf{R}+\widetilde{\mathbf{d}}_{nn'}(\mathbf{R}'-\mathbf{R}) && \text{(E22)}
\end{aligned}
$$

(E23)

$$
\begin{aligned}
\widetilde{\mathbf{d}}_{nn'}(\mathbf{R}) =& \frac{1}{\Omega}\int d\mathbf{k}\, exp(-i\mathbf{k}\cdot\mathbf{R})\mathbf{d}_{nn'}(\mathbf{k}) \\
=& \frac{1}{\Omega}\int d\mathbf{k}\, exp(-i\mathbf{k}\cdot\mathbf{R})\{\frac{i\Omega}{N} < u_{n\mathbf{k}}|\nabla_{\mathbf{k}}u_{n'\mathbf{k}} >\} \\
=& \frac{i}{N}\int d\mathbf{x}\int d\mathbf{k}\, exp(-i\mathbf{k}\cdot\mathbf{R}) < u_{n\mathbf{k}}|\mathbf{x} > (\nabla_{\mathbf{k}} < \mathbf{x}|u_{n'\mathbf{k}} >) \\
=& \frac{1}{N\Omega}\int d\mathbf{x}\int d\mathbf{k}\, exp(-i\mathbf{k}\cdot\mathbf{R}) \\
& \times[\sum_{\mathbf{R}'} exp\{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{R}')\} < n\mathbf{R}'|\mathbf{y} >][\sum_{\mathbf{R}''}(\mathbf{x}-\mathbf{R}'')exp\{-i\mathbf{k}\cdot(\mathbf{x}-\mathbf{R}'')\} < \mathbf{x}|n'\mathbf{R}'' >] \\
=& \frac{1}{N\Omega}\sum_{\mathbf{R}'\mathbf{R}''}\int d\mathbf{x}(\mathbf{x}-\mathbf{R}'')\int d\mathbf{k}\, exp\{-i\mathbf{k}\cdot(\mathbf{R}-\mathbf{R}'+\mathbf{R}'')\} < n\mathbf{R}'|\mathbf{x} >< \mathbf{x}|n'\mathbf{R}'' > \\
=& \frac{1}{N}\sum_{\mathbf{R}''}\int d\mathbf{x}(\mathbf{x}-\mathbf{R}'') < n(\mathbf{R}+\mathbf{R}'')|\mathbf{x} >< \mathbf{x}|n'\mathbf{R}'' > \\
=& \frac{1}{N}\sum_{\mathbf{R}''}\int d\mathbf{x}'\mathbf{x}' < n(\mathbf{R}+\mathbf{R}'')|\mathbf{x}'+\mathbf{R}'' >< \mathbf{x}+\mathbf{R}''|n'\mathbf{R}'' > \\
=& \int d\mathbf{x}'\mathbf{x}' < n\mathbf{R}|\mathbf{x}' >< \mathbf{x}|n'\mathbf{0} > ? && \text{(E24)}
\end{aligned}
$$

(E25)

$$
\begin{aligned}
\widetilde{\mathbf{d}}^{*}_{nn'}(\mathbf{R}) =& \frac{1}{\Omega}\int d\mathbf{k}\, exp(i\mathbf{k}\cdot\mathbf{R})\mathbf{d}^{*}_{nn'}(\mathbf{k}) \\
=& \frac{1}{\Omega}\int d\mathbf{k}\, exp(i\mathbf{k}\cdot\mathbf{R})\mathbf{d}_{n'n}(\mathbf{k}) \\
=& \widetilde{\mathbf{d}}_{n'n}(-\mathbf{R}) && \text{(E26)}
\end{aligned}
$$

$$
< n\mathbf{R}|[\hat{\mathbf{x}},\hat{\rho}]|n'\mathbf{R}' > = \sum_{n''\mathbf{R}''}(< n\mathbf{R}|\hat{\mathbf{x}}|n''\mathbf{R}'' >< n''\mathbf{R}''|\hat{\rho}|n'\mathbf{R}' > - < n\mathbf{R}|\hat{\rho}|n''\mathbf{R}'' >< n''\mathbf{R}''|\hat{\mathbf{x}}|n'\mathbf{R}' >)
$$

$$
\begin{aligned}
&= \sum_{n''\mathbf{R}''} [\{\delta_{nn''}\delta_{\mathbf{R}\mathbf{R}''}\mathbf{R} + \widetilde{\mathbf{d}}_{nn''}(\mathbf{R}''-\mathbf{R})\} < n''\mathbf{R}''|\hat{\rho}|n'\mathbf{R}' > \\
&\quad - < n\mathbf{R}|\hat{\rho}|n''\mathbf{R}'' > \{\delta_{n''n'}\delta_{\mathbf{R}''\mathbf{R}'}\mathbf{R}' + \widetilde{\mathbf{d}}_{n''n'}(\mathbf{R}'-\mathbf{R}'')\}] \\
&=(\mathbf{R}-\mathbf{R}') < n\mathbf{R}|\hat{\rho}|n'\mathbf{R}' > \\
&\quad + \sum_{n''\mathbf{R}''} \{\widetilde{\mathbf{d}}_{nn''}(\mathbf{R}''-\mathbf{R})\} < n''\mathbf{R}''|\hat{\rho}|n'\mathbf{R}' > - < n\mathbf{R}|\hat{\rho}|n''\mathbf{R}'' > \widetilde{\mathbf{d}}_{n''n'}(\mathbf{R}'-\mathbf{R}'')\}]
\end{aligned}
\tag{E27}
$$

$$
\begin{aligned}
i\hbar < n\mathbf{R}|\hat{\rho}|n'\mathbf{R}' >=& \sum_{n''\mathbf{R}''} (< n\mathbf{R}|\hat{H}_0 - e\mathbf{E}\cdot\hat{\mathbf{x}}|n''\mathbf{R}'' >< n''\mathbf{R}''|\hat{\rho}|n'\mathbf{R}' > - < n\mathbf{R}|\hat{\rho}|n''\mathbf{R}'' >< n''\mathbf{R}''|\hat{H}_0 - e\mathbf{E}\cdot\hat{\mathbf{x}}|n'\mathbf{R}' >) \\
=& \sum_{\mathbf{R}''} \{\widetilde{\epsilon}_n(\mathbf{R}''-\mathbf{R}) < n\mathbf{R}''|\hat{\rho}|n'\mathbf{R}' > - < n\mathbf{R}|\hat{\rho}|n'\mathbf{R}'' > \widetilde{\epsilon}_{n'}(\mathbf{R}'-\mathbf{R}'')\} \\
&-e\mathbf{E}\cdot(\mathbf{R}-\mathbf{R}') < n\mathbf{R}|\hat{\rho}|n'\mathbf{R}' > \\
&-e\mathbf{E}\cdot \sum_{n''\mathbf{R}''} \{\widetilde{\mathbf{d}}_{nn''}(\mathbf{R}''-\mathbf{R})\} < n''\mathbf{R}''|\hat{\rho}|n'\mathbf{R}' > - < n\mathbf{R}|\hat{\rho}|n''\mathbf{R}'' > \widetilde{\mathbf{d}}_{n''n'}(\mathbf{R}'-\mathbf{R}'')\}]
\end{aligned}
\tag{E28}
$$

$$
\begin{aligned}
i\hbar < v\mathbf{R}|\hat{\rho}|v\mathbf{R}' >=& \sum_{\mathbf{R}''} \{\widetilde{\epsilon}_v(\mathbf{R}''-\mathbf{R}) < v\mathbf{R}''|\hat{\rho}|v\mathbf{R}' > - < v\mathbf{R}|\hat{\rho}|v\mathbf{R}'' > \widetilde{\epsilon}_v(\mathbf{R}'-\mathbf{R}'')\} \\
&-e\mathbf{E}\cdot(\mathbf{R}-\mathbf{R}') < v\mathbf{R}|\hat{\rho}|v\mathbf{R}' > \\
&-e\mathbf{E}\cdot \sum_{n''\mathbf{R}''} \{\widetilde{\mathbf{d}}_{vn''}(\mathbf{R}''-\mathbf{R})\} < n''\mathbf{R}''|\hat{\rho}|v\mathbf{R}' > - < v\mathbf{R}|\hat{\rho}|n''\mathbf{R}'' > \widetilde{\mathbf{d}}_{n''v}(\mathbf{R}'-\mathbf{R}'')\}]
\end{aligned}
\tag{E29}
$$

$$
\begin{aligned}
\rho_{init} =& \frac{1}{\Omega}\int d\mathbf{k}|v\mathbf{k} >< v\mathbf{k}|? \\
=& \frac{1}{N}\sum_{\mathbf{K}} |v\mathbf{K} >< v\mathbf{K}|? \\
=& \frac{1}{N}\sum_{\mathbf{K}} |v\mathbf{R} >< v\mathbf{R}|??
\end{aligned}
\tag{E30}
$$

$$
\begin{aligned}
\mathbf{x} &= tr(\hat{\rho}\hat{\mathbf{x}}) \\
&= \sum_{nn'\mathbf{R}\mathbf{R}'} < n\mathbf{R}|\hat{\rho}|n'\mathbf{R}' >< n'\mathbf{R}'|\hat{\mathbf{x}}|n'\mathbf{R}' > \\
&= \sum_{nn'\mathbf{R}\mathbf{R}'} < n\mathbf{R}|\hat{\rho}|n'\mathbf{R}' > \{\delta_{nn'}\delta_{\mathbf{R}\mathbf{R}'}\mathbf{R} + \widetilde{\mathbf{d}}_{nn'}(\mathbf{R}'-\mathbf{R})\} \\
&= \sum_{n\mathbf{R}} < n\mathbf{R}|\hat{\rho}|n\mathbf{R} > \mathbf{R} + \sum_{nn'\mathbf{R}\mathbf{R}'} < n\mathbf{R}|\hat{\rho}|n'\mathbf{R}' > \widetilde{\mathbf{d}}_{nn'}(\mathbf{R}'-\mathbf{R})
\end{aligned}
\tag{E31}
$$

$$
\begin{aligned}
J^L &= -e\frac{\partial}{\partial t}tr(\hat{\rho}\hat{\mathbf{x}}) \\
&= -e\sum_{nn'\mathbf{R}\mathbf{R}'} < n\mathbf{R}|\frac{\partial\hat{\rho}}{\partial t}|n'\mathbf{R}' >< n'\mathbf{R}'|\hat{\mathbf{x}}|n'\mathbf{R}' > \\
&= -\frac{e}{i\hbar}\sum_{nn'\mathbf{R}\mathbf{R}'} < n\mathbf{R}|[H_0 - e\mathbf{E}\cdot\hat{\mathbf{x}},\rho]|n'\mathbf{R}' >< n'\mathbf{R}'|\hat{\mathbf{x}}|n'\mathbf{R}' > \\
&= -\frac{e}{i\hbar}\sum_{nn'\mathbf{R}\mathbf{R}'\mathbf{R}''} \{\widetilde{\epsilon}_n(\mathbf{R}''-\mathbf{R}) < n\mathbf{R}''|\hat{\rho}|n'\mathbf{R}' > - < n\mathbf{R}|\hat{\rho}|n'\mathbf{R}'' > \widetilde{\epsilon}_{n'}(\mathbf{R}'-\mathbf{R}'')\} - e\mathbf{E}\cdot(\mathbf{R}-\mathbf{R}') < n\mathbf{R}|\hat{\rho}|n'\mathbf{R}' > \\
&\quad + \sum_{n''\mathbf{R}''}\{\widetilde{\mathbf{d}}_{nn''}(\mathbf{R}''-\mathbf{R})\} < n''\mathbf{R}''|\hat{\rho}|n'\mathbf{R}' > - < n\mathbf{R}|\hat{\rho}|n''\mathbf{R}'' > \widetilde{\mathbf{d}}_{n''n'}(\mathbf{R}'-\mathbf{R}'')\}]]\{\delta_{nn'}\delta_{\mathbf{R}\mathbf{R}'}\mathbf{R} + \widetilde{\mathbf{d}}_{nn'}(\mathbf{R}-\mathbf{R})\}
\end{aligned}
\tag{E32}
$$

Appendix F: the Chern topology

revisited in the wannier basis. The first Chern number in two dimension is

$$
C_1 = \frac{i}{2\pi}\int d^2\mathbf{k}(< \nabla_{\mathbf{kx}}u_{n\mathbf{k}}|\nabla_{\mathbf{ky}}u_{n\mathbf{k}} > - < \nabla_{\mathbf{ky}}u_{n\mathbf{k}}|\nabla_{\mathbf{kz}}u_{n\mathbf{k}} >)
\tag{F1}
$$

If the we take the periodic gauge for the Bloch basis (i.e. $|u_{n\mathbf{k}} >= |u_{n(\mathbf{k}+\mathbf{K})} >$) and assume the smooth gauge (i.e. the derivative of Bloch basis $\nabla_{\mathbf{k}}|u_{n\mathbf{k}} >$ exists for any $\mathbf{k}$.), then the first Chern number C_1 vanishes, since

$$
\begin{aligned}
\int d^2\mathbf{k} < \nabla_{\mathbf{kx}}u_{n\mathbf{k}}|\nabla_{\mathbf{ky}}u_{n\mathbf{k}} > &= \int d^2\mathbf{k}\int d^2\mathbf{r}(\nabla_{\mathbf{kx}} < u_{n\mathbf{k}}|\mathbf{r} >)(\nabla_{\mathbf{ky}} < \mathbf{r}|u_{n\mathbf{k}} >) \\
&= \frac{1}{\Omega}\int d^2\mathbf{k}\int d^2\mathbf{r}[\sum_{\mathbf{R}}(\mathbf{x}-\mathbf{R_x})exp\{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{R})\} < n\mathbf{R}|\mathbf{r} >] \\
&\quad \times[\sum_{\mathbf{R}'}(\mathbf{y}-\mathbf{R}'_{\mathbf{y}})exp\{-i\mathbf{k}\cdot(\mathbf{r}-\mathbf{R}')\} < \mathbf{r}|n\mathbf{R}' >] \\
&= \frac{1}{\Omega}\sum_{\mathbf{R}\mathbf{R}'}\int d^2\mathbf{k}\int d^2\mathbf{r}(\mathbf{x}-\mathbf{R_x})(\mathbf{y}-\mathbf{R}'_{\mathbf{y}})exp\{-i\mathbf{k}\cdot(\mathbf{R}-\mathbf{R}')\} < n\mathbf{R}|\mathbf{r} >< \mathbf{r}|n\mathbf{R}' > \\
&= \sum_{\mathbf{R}}\int d^2\mathbf{r}(\mathbf{x}-\mathbf{R_x})(\mathbf{y}-\mathbf{R_y}) < n\mathbf{R}|\mathbf{r} >< \mathbf{r}|n\mathbf{R} > \\
&= \int d^2\mathbf{k} < \nabla_{\mathbf{ky}}u_{n\mathbf{k}}|\nabla_{\mathbf{kx}}u_{n\mathbf{k}} > .
\end{aligned}
\tag{F2}
$$

Conversely if the first Chern number C_1 vanishes, then we can construct a Bloch basis satisfying the periodic and smooth gauge. (prove)

If we define a gauge-invariant? curvature $P_{nn'}$ as follows

$$
P_{nn'} = \nabla_{\mathbf{k}}\times < u_{n\mathbf{k}}|\nabla_{\mathbf{k}}u_{n'\mathbf{k}} >,
\tag{F3}
$$

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