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1 Hamiltonian lượng tử hoá lần 2

1.1 Hamiltonian tương tác với ánh sáng

Hamiltonian hệ điện tử trong tinh thể tương tác với trường ngoài(ánh sáng), khi chưa có xét đến tương tác điện tử − điện tử là

$$H = \sum_i = H_{1\mathrm{e}}(\mathbf{r}_i, t) = \sum_i H^0_{1\mathrm{e}}(\mathbf{r}_i) + \sum_i H^{e-L}_{1e}(\mathbf{r}_i, t). \tag{1}$$

Hamiltonian lượng tử hoá lần 2 trong hệ cơ sở trực chuẩn $\left\{|\psi_{\lambda\mathbf{k}}\rangle\right\}$

$$\langle\psi_{\lambda\mathbf{k}}|\psi_{\lambda'\mathbf{k}'}\rangle = \delta_{\lambda,\lambda'}\delta_{\mathbf{k},\mathbf{k}'}, \tag{2}$$

trong đó λ là chỉ số dải với vector sóng $\mathbf{k}$, và Hamiltonian có dạng

$$H = H^0 + H^{e-L}, \tag{3}$$

trong đó

$$H^0 = \sum_{\lambda\lambda'\mathbf{k}\mathbf{k}'} = \langle\psi_{\lambda\mathbf{k}}|\, H^0_{1\mathrm{e}}\, |\psi_{\lambda'\mathbf{k}'}\rangle\, a^\dagger_{\lambda\mathbf{k}} a_{\lambda'\mathbf{k}'}, \tag{4}$$

$$H^{e-L} = \sum_{\lambda\lambda'\mathbf{k}\mathbf{k}'} \langle\psi_{\lambda\mathbf{k}}|\, H^{e-L}_{1e}(\mathbf{r}, t)\, |\psi_{\lambda'\mathbf{k}'}\rangle\, a^\dagger_{\lambda\mathbf{k}} a_{\lambda'\mathbf{k}'}, \tag{5}$$

trong đó các toán tử sinh huỷ tuân theo hệ thức phản giao hoán

$$\{a_{\lambda\mathbf{k}}, a^\dagger_{\lambda\mathbf{k}'}\} = a_{\lambda\mathbf{k}} a^\dagger_{\lambda'\mathbf{k}'} + a^\dagger_{\lambda'\mathbf{k}'} a_{\lambda\mathbf{k}} = \delta_{\lambda,\lambda'}\delta_{\mathbf{k},\mathbf{k}'}, \tag{6}$$

$$\{a_{\lambda\mathbf{k}}, \mathbf{a}_{\lambda'\mathbf{k}'}\} = \{a^\dagger_{\lambda\mathbf{k}}, a^\dagger_{\lambda'\mathbf{k}'}\} = 0. \tag{7}$$

Nếu chọn hệ cơ sở là hàm riêng của $H^0_{1\mathrm{e}}$, tức là

$$H^0\psi_{\lambda\mathbf{k}} = \mathcal{E}_\lambda(\mathbf{k})\psi_{\lambda\mathbf{k}}, \tag{8}$$

thì H^0 trở thành

$$H^0 = \sum_{\lambda\mathbf{k}} \mathcal{E}_\lambda a^\dagger_{\lambda\mathbf{k}} a_{\lambda\mathbf{k}}. \tag{9}$$

$\mathbf{H^{e-L}}$ trong gauge vận tốc

Sử dụng gauge vận tốc, các yếu tố ma trận tương tác giữa điện tử − ánh sáng là

$$\begin{aligned}\langle\psi_{\lambda\mathbf{k}}|\, H^{e-L}_{1\mathrm{e}}(\mathbf{r},t)\,|\psi_{\lambda'\mathbf{k}'}\rangle &= \langle\psi_{\lambda\mathbf{k}}|\,\frac{e}{m}\mathbf{A}(\mathbf{r},t)\cdot\mathbf{p}\,|\psi_{\lambda'\mathbf{k}'}\rangle + \frac{e^2A^2}{2m}\delta_{\lambda,\lambda'}\delta_{\mathbf{k},\mathbf{k}'} \\ &\approx \frac{e}{m}\mathbf{A}(t)\cdot\langle\psi_{\lambda\mathbf{k}}|\,\mathbf{p}\,|\psi_{\lambda'\mathbf{k}'}\rangle + \frac{e^2A^2}{2m}\delta_{\lambda,\lambda'}\delta_{\mathbf{k},\mathbf{k}'},\end{aligned} \tag{10}$$

trong đó yếu tố ma trận xung lượng được khai triển qua hàm Bloch như sau

$$\begin{aligned}\langle\psi_{\lambda\mathbf{k}}|\,\mathbf{p}\,|\psi_{\lambda'\mathbf{k}'}\rangle &= \int\frac{d^3r}{V}u^*_{\lambda\mathbf{k}}e^{-i\mathbf{k}\cdot\mathbf{r}}\mathbf{p}e^{i\mathbf{k}'\cdot\mathbf{r}}u_{\lambda'\mathbf{k}'}(\mathbf{r}) \\ &= \frac{1}{N}\sum_i^N e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_i}\int_{V_{\mathrm{cell}}}\frac{d^3r}{V_{\mathrm{cell}}}u^*_{\lambda\mathbf{k}}(\mathbf{r})e^{-i\mathbf{k}\cdot\mathbf{r}}\mathbf{p}e^{i\mathbf{k}'\cdot\mathbf{r}}u_{\lambda'\mathbf{k}'}(\mathbf{r}),\end{aligned} \tag{11}$$

mà ta có $\sum_i^N e^{i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{R}_i} = N\delta_{\mathbf{k},\mathbf{k}'}$, ta thu được

$$\begin{aligned}\langle\psi_{\lambda\mathbf{k}}|\,\mathbf{p}\,|\psi_{\lambda'\mathbf{k}'}\rangle &= \int_{V_{\mathrm{cell}}}\frac{d^3r}{V_{\mathrm{cell}}}u^*_{\lambda\mathbf{k}}(\mathbf{r})e^{-i\mathbf{k}\cdot\mathbf{r}}\mathbf{p}e^{i\mathbf{k}'\cdot\mathbf{r}}u_{\lambda'\mathbf{k}'}(\mathbf{r}) \\ &= \mathbf{p}_{\lambda\lambda'}(\mathbf{k})\delta_{\mathbf{k},\mathbf{k}'} \equiv \langle u_{\lambda\mathbf{k}}|\,\mathbf{p}(\mathbf{k})\,|u_{\lambda'\mathbf{k}}\rangle\,,\end{aligned} \tag{12}$$

trong đó

$$\mathbf{p}(\mathbf{k}) = e^{-i\mathbf{k}\cdot\mathbf{r}}\mathbf{p}e^{i\mathbf{k}\cdot\mathbf{r}}. \tag{13}$$

Ta biểu diễn Hamiltonian 1 hạt trong không gian k

$$H^0_{1\mathrm{e}}(\mathbf{k}) = e^{-i\mathbf{k}\cdot\mathbf{r}}H^0_{1\mathrm{e}}e^{i\mathbf{k}\cdot\mathbf{r}}, \tag{14}$$

lấy đạo hàm theo k cho phương trình (16), ta có

$$\begin{aligned}\nabla_\mathbf{k}H^0_{1e}(\mathbf{k}) &= -i\mathbf{r}e^{-i\mathbf{k}\cdot\mathbf{r}}H_{1e}e^{i\mathbf{k}\cdot\mathbf{r}} + e^{-i\mathbf{k}\cdot\mathbf{r}}H^0_{1e}i\mathbf{r}e^{i\mathbf{k}\cdot\mathbf{r}} \\ &= ie^{-i\mathbf{k}\cdot\mathbf{r}}\left(H^0_{1e}\mathbf{r} - \mathbf{r}H^0_{1e}\right)e^{i\mathbf{k}\cdot\mathbf{r}} \\ &= ie^{-i\mathbf{k}\cdot\mathbf{r}}[H^0_{1e},\mathbf{r}]e^{i\mathbf{k}\cdot\mathbf{r}} \\ &= i[H^0_{1e}(\mathbf{k}),\mathbf{r}].\end{aligned} \tag{15}$$

Lại có hệ thức giao hoán giữa $[H^0_{1\text{e}}, \mathbf{r}]$

$$
\begin{aligned}
[H^0_{1\text{e}}, \mathbf{r}] &= -\frac{i\hbar}{m}\mathbf{p} \\
\Leftrightarrow e^{-i\mathbf{k}\cdot\mathbf{r}}[H^0_{1\text{e}}, \mathbf{r}]e^{i\mathbf{k}\cdot\mathbf{r}} &= e^{-i\mathbf{k}\cdot\mathbf{r}}\left(-\frac{i\hbar}{m}\mathbf{p}\right)e^{i\mathbf{k}\cdot\mathbf{r}} \\
\Leftrightarrow \nabla_{\mathbf{k}} H^0_{1e}(\mathbf{k}) &= \frac{\hbar}{m}\mathbf{p}(\mathbf{k}) \\
\Leftrightarrow \mathbf{p}(\mathbf{k}) &= \frac{m}{\hbar}\nabla_{\mathbf{k}} H^0_{1e}(\mathbf{k}).
\end{aligned} \tag{16}
$$

Các yếu tố ma trận xung lượng từ phương trình (12) có thể tính được thông qua

$$
\mathbf{p}_{\lambda\lambda'}(\mathbf{k}) = \frac{m}{\hbar}\left\langle u_{\lambda\mathbf{k}}\right| \nabla_{\mathbf{k}} H^0_{1e}(\mathbf{k}) \left|u_{\lambda'\mathbf{k}'}\right\rangle. \tag{17}
$$

Từ phương trình (10), Hamiltonian tương tác điện tử và ánh sáng ở lượng tử hoá lần 2 trong gauge vận tốc có dạng

$$
H^{e-L} = \frac{e}{m}\mathbf{A}(t)\cdot\sum_{\lambda\lambda'\mathbf{k}}\mathbf{p}_{\lambda\lambda'}(\mathbf{k})a^\dagger_{\lambda\mathbf{k}}a_{\lambda'\mathbf{k}} + \frac{e^2A^2}{2m}\sum_{\lambda\mathbf{k}}a^\dagger_{\lambda\mathbf{k}}a_{\lambda\mathbf{k}}. \tag{18}
$$

$\mathbf{H^{e-L}}$ trong gauge độ dài

Trong gauge độ dài, Hamiltonian tương tác điện tử − ánh sáng (5) là

$$
\left\langle\psi_{\lambda\mathbf{k}}\right| H^{e-L}_{1e}(\mathbf{r},t)\left|\psi_{\lambda'\mathbf{k}'}\right\rangle = \left\langle\psi_{\lambda\mathbf{k}}\right| e\mathbf{E}(\mathbf{r},t)\cdot\mathbf{r}\left|\psi_{\lambda'\mathbf{k}'}\right\rangle \simeq e\mathbf{E}(t)\cdot\left\langle\psi_{\lambda\mathbf{k}}\right|\mathbf{r}\left|\psi_{\lambda'\mathbf{k}'}\right\rangle, \tag{19}
$$

trong đó yếu tố ma trận vị trí được cho bởi

$$
\begin{aligned}
\left\langle\psi_{\lambda\mathbf{k}}\right|\mathbf{r}\left|\psi_{\lambda'\mathbf{k}'}\right\rangle &= \int\frac{d^3r}{V}u^*_{\lambda\mathbf{k}}(\mathbf{r})e^{-i\mathbf{k}\cdot\mathbf{r}}\mathbf{r}e^{i\mathbf{k}'\cdot\mathbf{r}}u_{\lambda'\mathbf{k}'}(\mathbf{r}) \\
&= i\nabla_{\mathbf{k}}\left(\int\frac{d^3r}{V}u^*_{\lambda\mathbf{k}}(\mathbf{r})e^{-i\mathbf{k}\cdot\mathbf{r}}e^{i\mathbf{k}'\cdot\mathbf{r}}u_{\lambda'\mathbf{k}'}(\mathbf{r})\right) \\
&\quad - i\int\frac{d^3r}{V}\left(\nabla_{\mathbf{k}}u^*_{\lambda\mathbf{k}}(\mathbf{r})\right)e^{i\mathbf{k}\cdot\mathbf{r}}e^{i\mathbf{k}'\cdot\mathbf{r}}u_{\lambda'\mathbf{k}'}(\mathbf{r}) \\
&= i\nabla_{\mathbf{k}}\left(\frac{1}{N}\sum_i^N e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_i}\int_{V_{\text{cell}}}\frac{d^3r}{V_{\text{cell}}}u^*_{\lambda\mathbf{k}}(\mathbf{r})e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}}u_{\lambda'\mathbf{k}'}(\mathbf{r})\right) \\
&\quad - i\frac{1}{N}\sum_i^N e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_i}\int_{V_{\text{cell}}}\frac{d^3r}{V_{\text{cell}}}(\nabla_{\mathbf{k}}u^*_{\lambda\mathbf{k}}(\mathbf{r}))e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}}u_{\lambda'\mathbf{k}'}(\mathbf{r}).
\end{aligned} \tag{20}
$$

Áp dụng gần đúng sóng dài $k, k' \lll \frac{2\pi}{a}$, ta được

$$\begin{aligned}
\langle\psi_{\lambda\mathbf{k}}|\,\mathbf{r}\,|\psi_{\lambda'\mathbf{k}'}\rangle \simeq\, & i\nabla_{\mathbf{k}}\delta_{\mathbf{k},\mathbf{k}'}\int_{V_{\text{cell}}}\frac{d^3r}{V_{\text{cell}}}\nabla_{\mathbf{k}}u^*_{\lambda\mathbf{k}}(\mathbf{r})u_{\lambda'\mathbf{k}'}(\mathbf{r}) \\
& - i\delta_{\mathbf{k},\mathbf{k}'}\int_{V_{\text{cell}}}\frac{d^3r}{V_{\text{cell}}}(\nabla_{\mathbf{k}}u^*_{\lambda\mathbf{k}}(\mathbf{r}))u_{\lambda'\mathbf{k}'}(\mathbf{r}) \\
=\, & i\nabla_{\mathbf{k}}\delta_{\mathbf{k},\mathbf{k}'}\delta_{\lambda,\lambda'} - i\delta_{\lambda,\lambda'}\langle\nabla_{\mathbf{k}}u_{\lambda\mathbf{k}}|u_{\lambda'\mathbf{k}'}\rangle\,.
\end{aligned} \tag{21}$$

Ta định nghĩa yếu tố ma trận lưỡng cực như sau

$$\boldsymbol{\xi}_{\lambda\lambda'}(\mathbf{k}) = -i\,\langle\nabla_{\mathbf{k}}u_{\lambda\mathbf{k}}|\nabla_{\mathbf{k}}u_{\lambda\mathbf{k}}\rangle\,, \tag{22}$$

như vậy các yếu tố ma trận vị trí ở phương trình (21) được viết lại dưới dạng

$$\langle\psi_{\lambda\mathbf{k}}|\,\mathbf{r}\,|\psi_{\lambda'\mathbf{k}'}\rangle = (\boldsymbol{\xi}_{\lambda\lambda'}(\mathbf{k}) + i\delta_{\lambda\lambda'}\nabla_{\mathbf{k}})\delta_{\mathbf{k},\mathbf{k}'}. \tag{23}$$

Trong trường hợp $\lambda \neq \lambda'$, từ hệ thức giao hoán $[H^0_{1\text{e}}, \mathbf{r}] = -\frac{i\hbar}{m}\mathbf{p}$ và $\langle\psi_{\lambda\mathbf{k}}|\,\mathbf{p}\,|\psi_{\lambda'\mathbf{k}'}\rangle = \mathbf{p}_{\lambda\lambda'}(\mathbf{k})\delta_{\mathbf{k},\mathbf{k}'}$, ta có

$$\begin{aligned}
\mathbf{p} &= \frac{im}{\hbar}[H^0_{1\text{e}}, \mathbf{r}] \\
\Leftrightarrow \langle\psi_{\lambda\mathbf{k}}|\,\mathbf{p}\,|\psi_{\lambda'\mathbf{k}'}\rangle &= \frac{im}{\hbar}\langle\psi_{\lambda\mathbf{k}}|\,[H^0_{1\text{e}}, \mathbf{r}]\,|\psi_{\lambda'\mathbf{k}'}\rangle \\
\Leftrightarrow -\frac{i\hbar}{m}\mathbf{p}_{\lambda\lambda'}(\mathbf{k})\delta_{\mathbf{k},\mathbf{k}'} &= \langle\psi_{\lambda\mathbf{k}}|\,H^0_{1e}\mathbf{r} - \mathbf{r}H^0_{1e}\,|\psi_{\lambda'\mathbf{k}'}\rangle \\
\Leftrightarrow -\frac{i\hbar}{m}\mathbf{p}_{\lambda\lambda'} &= (\mathcal{E}_\lambda(\mathbf{k}) - \mathcal{E}_{\lambda'}(\mathbf{k}))\,\langle\psi_{\lambda\mathbf{k}}|\,\mathbf{r}\,|\psi_{\lambda'\mathbf{k}'}\rangle \\
\Leftrightarrow -\frac{i\hbar}{m}\mathbf{p}_{\lambda\lambda'} &= (\mathcal{E}_\lambda(\mathbf{k}) - \mathcal{E}_{\lambda'}(\mathbf{k}))(\boldsymbol{\xi}_{\lambda\lambda'}(\mathbf{k}) + i\delta_{\lambda\lambda'}\nabla_{\mathbf{k}}) \\
\Leftrightarrow -\frac{i\hbar}{m}\frac{\mathbf{p}_{\lambda\lambda'}}{\mathcal{E}_\lambda(\mathbf{k}) - \mathcal{E}_{\lambda'}(\mathbf{k})} &= \boldsymbol{\xi}_{\lambda\lambda'}(\mathbf{k}).
\end{aligned} \tag{24}$$

Hamiltonian lượng tử hoá lần thứ 2 cho tương tác điện tử − ánh sáng trong gauge độ dài

$$H^{e-L} = e\mathbf{E}(t)\cdot\sum_{\lambda\lambda'\mathbf{k}}\boldsymbol{\xi}_{\lambda\lambda'}(\mathbf{k})a^\dagger_{\lambda\mathbf{k}}a_{\lambda'\mathbf{k}} + ie\mathbf{E}(t)\cdot\sum_{\lambda\mathbf{k}\mathbf{k}'}\nabla_{\mathbf{k}}\delta_{\mathbf{k},\mathbf{k}'}a^\dagger_{\lambda\mathbf{k}}a_{\lambda\mathbf{k}'}, \tag{25}$$

1.2 Toán tử mật độ điện tích

Toán tử mật độ điện tích được định nghĩa là

$$\hat{\rho}_{\lambda'\lambda}(\mathbf{k}) = -\frac{|e|}{V}\sum_{\mathbf{k}}a^\dagger_{\lambda\mathbf{k}}a_{\lambda\mathbf{k}}. \tag{26}$$

ta cần khảo sát sự thay đổi của giá trị trung bình của toán tử mật độ điện tích theo thời gian

$$\langle \rho_{\lambda'\lambda} \rangle = -\frac{|e|}{V} \sum_{\mathbf{k}} \langle a^\dagger_{\lambda\mathbf{k}} a_{\lambda'\mathbf{k}} \rangle. \tag{27}$$

Vậy, ma trận mật độ điện tích rút gọn có thể viết lại dưới dạng

$$\rho_{\lambda'\lambda}(\mathbf{k}) = \langle a^\dagger_{\lambda\mathbf{k}} a_{\lambda'\mathbf{k}} \rangle. \tag{28}$$

Để khảo sát phương trình (27), ta cần khảo sát $a^\dagger_{\lambda\mathbf{k}} a_{\lambda'\mathbf{k}}$ trong bức tranh Heisenberg.

1.3 Phương trình chuyển động

Phương trình chuyển động Heisenberg cho toán tử $a^\dagger_{\lambda\mathbf{k}} a_{\lambda'\mathbf{k}}$

$$\frac{d}{dt} a^\dagger_{\lambda\mathbf{k}} a_{\lambda'\mathbf{k}} = \frac{i}{\hbar} [H, a^\dagger_{\lambda\mathbf{k}} a_{\lambda'\mathbf{k}}] + \cancelto{0}{\frac{\partial}{\partial t} a^\dagger_{\lambda\mathbf{k}} a_{\lambda'\mathbf{k}}}, \tag{29}$$

trong đó

$$\begin{aligned} H &= H^0 + H^{e-L} \\ &= \sum_{\lambda\mathbf{k}} \mathcal{E}_\lambda a^\dagger_{\lambda\mathbf{k}} a_{\lambda\mathbf{k}} + \frac{e}{m} \mathbf{A}(t) \cdot \sum_{\lambda\lambda'\mathbf{k}} \mathbf{p}_{\lambda\lambda'}(\mathbf{k}) a^\dagger_{\lambda\mathbf{k}} a_{\lambda'\mathbf{k}} + \frac{e^2 A^2}{2m} \sum_{\lambda\mathbf{k}} a^\dagger_{\lambda\mathbf{k}} a_{\lambda\mathbf{k}}. \end{aligned} \tag{30}$$

Tính các giao hoán tử

$$\begin{aligned} [H^0, a^\dagger_{\lambda\mathbf{k}} a_{\lambda'\mathbf{k}}] &= \sum_{\nu\mathbf{k}'} \mathcal{E}_\nu(\mathbf{k}') [a^\dagger_{\nu\mathbf{k}'} a_{\nu\mathbf{k}'}, a^\dagger_{\lambda\mathbf{k}} a_{\lambda'\mathbf{k}}] \\ &= \sum_{\nu\mathbf{k}'} \mathcal{E}_\nu(\mathbf{k}') \left(a^\dagger_{\nu\mathbf{k}'} a_{\nu\mathbf{k}'} a^\dagger_{\lambda\mathbf{k}} a_{\lambda'\mathbf{k}} - a^\dagger_{\lambda\mathbf{k}} a_{\lambda'\mathbf{k}} a^\dagger_{\nu\mathbf{k}'} a_{\nu\mathbf{k}'} \right) \\ &= \sum_{\nu\mathbf{k}'} \mathcal{E}_\nu(\mathbf{k}') \Big(a^\dagger_{\nu\mathbf{k}'} (\delta_{\nu\lambda} \delta_{\mathbf{k}',\mathbf{k}} - a^\dagger_{\lambda\mathbf{k}} a_{\nu\mathbf{k}'}) a_{\lambda'\mathbf{k}} \\ &\qquad - a^\dagger_{\lambda\mathbf{k}} (\delta_{\lambda'\nu} \delta_{\mathbf{k},\mathbf{k}'} - a^\dagger_{\nu\mathbf{k}'} a_{\lambda'\mathbf{k}}) a_{\nu\mathbf{k}'} \Big) \\ &= \sum_{\nu\mathbf{k}'} \mathcal{E}_\nu(\mathbf{k}') \Big(a^\dagger_{\nu\mathbf{k}'} \delta_{\nu\lambda} \delta_{\mathbf{k}',\mathbf{k}} a_{\lambda'\mathbf{k}} - \cancel{a^\dagger_{\nu\mathbf{k}'} a^\dagger_{\lambda\mathbf{k}} a_{\nu\mathbf{k}'} a_{\lambda'\mathbf{k}}} \\ &\qquad - a^\dagger_{\lambda\mathbf{k}} \delta_{\lambda'\nu} \delta_{\mathbf{k},\mathbf{k}'} a_{\nu\mathbf{k}'} + \cancel{a^\dagger_{\lambda\mathbf{k}} a^\dagger_{\nu\mathbf{k}'} a_{\lambda'\mathbf{k}} a_{\nu\mathbf{k}'}} \Big) \\ &= \sum_{\nu\mathbf{k}'} \mathcal{E}_\nu(\mathbf{k}') a_{\nu\mathbf{k}'} a_{\lambda'\mathbf{k}} \delta_{\nu\lambda} \delta_{\mathbf{k}',\mathbf{k}} - \sum_{\nu\mathbf{k}'} \mathcal{E}_\nu(\mathbf{k}') a^\dagger_{\lambda\mathbf{k}} a_{\nu\mathbf{k}'} \delta_{\lambda'\nu} \delta_{\mathbf{k}',\mathbf{k}} \\ &= (\mathcal{E}_\lambda(\mathbf{k}) - \mathcal{E}_{\lambda'}(\mathbf{k})) a^\dagger_{\lambda\mathbf{k}} a_{\lambda'\mathbf{k}}. \end{aligned} \tag{31}$$

Trong gauge vận tốc, giao hoán tử của Hamiltonian tương tác điện tử − ánh sáng (18) là

$$
\begin{aligned}
[H^{e-L}, a^\dagger_{\lambda\mathbf{k}} a_{\lambda'\mathbf{k}}] &= \frac{e}{m}\mathbf{A}(t)\cdot\sum_{\mu\nu\mathbf{k}'}\mathbf{p}_{\mu\nu}(\mathbf{k}')[a^\dagger_{\mu\mathbf{k}'}a_{\nu\mathbf{k}'}, a^\dagger_{\lambda\mathbf{k}}a_{\lambda'\mathbf{k}}] \\
&\quad + \frac{e^2A^2}{2m}\sum_{\mu\mathbf{k}'}\cancelto{0}{[a^\dagger_{\mu\mathbf{k}'}a_{\mu\mathbf{k}'}, a^\dagger_{\lambda\mathbf{k}}a_{\lambda\mathbf{k}}]} \\
&= \frac{e}{m}\mathbf{A}(t)\cdot\sum_{\mu\nu\mathbf{k}'}\mathbf{p}_{\mu\nu}(\mathbf{k}')\Big(a^\dagger_{\mu\mathbf{k}'}(\delta_{\nu\lambda}\delta_{\mathbf{k}',\mathbf{k}} - a^\dagger_{\lambda\mathbf{k}}a_{\nu\mathbf{k}'})a_{\lambda'\mathbf{k}} \\
&\quad - a^\dagger_{\lambda\mathbf{k}}(\delta_{\lambda'\mu}\delta_{\mathbf{k},\mathbf{k}'} - a^\dagger_{\mu\mathbf{k}'}a_{\lambda'\mathbf{k}})a_{\nu\mathbf{k}'}\Big) \\
&= \frac{e}{m}\mathbf{A}(t)\cdot\sum_{\mu\nu\mathbf{k}'}\mathbf{p}_{\mu\nu}(\mathbf{k}')\Big(a^\dagger_{\mu\mathbf{k}'}\delta_{\nu\lambda}\delta_{\mathbf{k}',\mathbf{k}}a_{\lambda'\mathbf{k}} - \cancel{a^\dagger_{\mu\mathbf{k}'}a^\dagger_{\lambda\mathbf{k}}a_{\nu\mathbf{k}'}a_{\lambda'\mathbf{k}}} \\
&\quad - a^\dagger_{\lambda\mathbf{k}}\delta_{\lambda'\mu}\delta_{\mathbf{k},\mathbf{k}'}a_{\nu\mathbf{k}'} + \cancel{a^\dagger_{\lambda\mathbf{k}}a^\dagger_{\mu\mathbf{k}'}a_{\lambda'\mathbf{k}}a_{\nu\mathbf{k}'}}\Big) \\
&= \frac{e}{m}\mathbf{A}(t)\cdot\Bigg(\sum_{\mu\nu\mathbf{k}'}\mathbf{p}_{\mu\nu}(\mathbf{k})a^\dagger_{\mu\mathbf{k}'}\delta_{\nu\lambda}\delta_{\mathbf{k}',\mathbf{k}}a_{\lambda'\mathbf{k}} \\
&\quad - \sum_{\mu\nu\mathbf{k}'}\mathbf{p}_{\mu\nu}(\mathbf{k}')a^\dagger_{\lambda\mathbf{k}}\delta_{\lambda'\mu}\delta_{\mathbf{k},\mathbf{k}'}a_{\nu\mathbf{k}'}\Bigg) \\
&= \frac{e}{m}\mathbf{A}(t)\cdot\sum_{\mu}\big(\mathbf{p}_{\mu\lambda}(\mathbf{k})a^\dagger_{\mu\mathbf{k}}a_{\lambda'\mathbf{k}} - \mathbf{p}_{\lambda'\mu}(\mathbf{k})a^\dagger_{\lambda\mathbf{k}'}a_{\mu\mathbf{k}'}\big).
\end{aligned}
\tag{32}
$$

Trong gauge độ dài, giao hoán tử của Hamiltonian tương tác điện tử − ánh sáng (25)

$$
\begin{aligned}
[H^{e-L}, a^{\dagger}_{\lambda\mathbf{k}} a_{\lambda'\mathbf{k}}] &= e\mathbf{E}(t) \cdot \sum_{\mu\nu\mathbf{k}'} \boldsymbol{\xi}_{\mu\nu}(\mathbf{k}')[a^{\dagger}_{\mu\mathbf{k}'} a_{\nu\mathbf{k}'}, a^{\dagger}_{\lambda\mathbf{k}} a_{\lambda'\mathbf{k}}] \\
&\quad + ie\mathbf{E}(t) \cdot \sum_{\mu\mathbf{k}'\mathbf{k}''} \nabla_{\mathbf{k}'} \delta_{\mathbf{k}',\mathbf{k}''} [a^{\dagger}_{\mu\mathbf{k}'} a_{\mu\mathbf{k}''}, a^{\dagger}_{\lambda\mathbf{k}} a_{\lambda'\mathbf{k}}] \\
&= e\mathbf{E}(t) \cdot \sum_{\mu\nu\mathbf{k}'} \boldsymbol{\xi}_{\mu\nu}(\mathbf{k}') \left(a^{\dagger}_{\mu\mathbf{k}'} a_{\nu\mathbf{k}'} a^{\dagger}_{\lambda\mathbf{k}} a_{\lambda'\mathbf{k}} - a^{\dagger}_{\lambda\mathbf{k}} a_{\lambda'\mathbf{k}} a^{\dagger}_{\mu\mathbf{k}'} a_{\nu\mathbf{k}'} \right) \\
&+ie\mathbf{E}(t) \cdot \sum_{\mu\mathbf{k}'\mathbf{k}''} \nabla_{\mathbf{k}'} \delta_{\mathbf{k}',\mathbf{k}''} \left(a^{\dagger}_{\mu\mathbf{k}'} a_{\mu\mathbf{k}''} a^{\dagger}_{\lambda\mathbf{k}} a_{\lambda'\mathbf{k}} - a^{\dagger}_{\lambda\mathbf{k}} a_{\lambda'\mathbf{k}} a^{\dagger}_{\mu\mathbf{k}'} a_{\mu\mathbf{k}''} \right) \\
&= e\mathbf{E}(t) \cdot \sum_{\mu\nu\mathbf{k}'} \boldsymbol{\xi}_{\mu\nu}(\mathbf{k}') \Big(a^{\dagger}_{\mu\mathbf{k}'} (\delta_{\nu\lambda}\delta_{\mathbf{k}',\mathbf{k}} - a^{\dagger}_{\lambda\mathbf{k}} a_{\nu\mathbf{k}'}) a_{\lambda'\mathbf{k}} \\
&\qquad - a^{\dagger}_{\lambda\mathbf{k}} (\delta_{\lambda'\mu}\delta_{\mathbf{k},\mathbf{k}'} - a^{\dagger}_{\mu\mathbf{k}'} a_{\lambda'\mathbf{k}}) a_{\nu\mathbf{k}'} \Big) \\
&+ie\mathbf{E}(t) \cdot \sum_{\mu\mathbf{k}'\mathbf{k}''} \nabla_{\mathbf{k}'} \delta_{\mathbf{k}',\mathbf{k}''} \Big(a^{\dagger}_{\mu\mathbf{k}'} (\delta_{\mu\lambda}\delta_{\mathbf{k}'',\mathbf{k}} - a^{\dagger}_{\lambda\mathbf{k}} a_{\mu\mathbf{k}''}) a_{\lambda'\mathbf{k}} \\
&\qquad - a^{\dagger}_{\lambda\mathbf{k}} (\delta_{\lambda'\mu}\delta_{\mathbf{k},\mathbf{k}'} - a^{\dagger}_{\mu\mathbf{k}'} a_{\lambda'\mathbf{k}}) a_{\mu\mathbf{k}''} \Big) \\
&= e\mathbf{E}(t) \cdot \sum_{\mu\nu\mathbf{k}'} \boldsymbol{\xi}_{\mu\nu}(\mathbf{k}') \Big(a^{\dagger}_{\mu\mathbf{k}'} \delta_{\nu\lambda}\delta_{\mathbf{k}',\mathbf{k}} a_{\lambda'\mathbf{k}} - \cancel{a^{\dagger}_{\mu\mathbf{k}'} a^{\dagger}_{\lambda\mathbf{k}} a_{\nu\mathbf{k}'} a_{\lambda'\mathbf{k}}} \\
&\qquad - a^{\dagger}_{\lambda\mathbf{k}} \delta_{\lambda'\mu}\delta_{\mathbf{k},\mathbf{k}'} a_{\nu\mathbf{k}'} + \cancel{a^{\dagger}_{\lambda\mathbf{k}} a^{\dagger}_{\mu\mathbf{k}'} a_{\lambda'\mathbf{k}} a_{\nu\mathbf{k}'}} \Big) \\
&+ie\mathbf{E}(t) \cdot \sum_{\mu\mathbf{k}'\mathbf{k}''} \nabla_{\mathbf{k}'} \delta_{\mathbf{k}',\mathbf{k}''} \Big(a^{\dagger}_{\mu\mathbf{k}'} \delta_{\mu\lambda}\delta_{\mathbf{k}'',\mathbf{k}} a_{\lambda'\mathbf{k}} - \cancel{a^{\dagger}_{\mu\mathbf{k}'} a^{\dagger}_{\lambda\mathbf{k}} a_{\mu\mathbf{k}''} a_{\lambda'\mathbf{k}}} \\
&\qquad - a^{\dagger}_{\lambda\mathbf{k}} \delta_{\lambda'\mu}\delta_{\mathbf{k},\mathbf{k}'} a_{\mu\mathbf{k}''} + \cancel{a^{\dagger}_{\lambda\mathbf{k}} a^{\dagger}_{\mu\mathbf{k}'} a_{\lambda'\mathbf{k}} a_{\mu\mathbf{k}''}} \Big).
\end{aligned} \tag{33}
$$

Chú ý rằng

$$\nabla_{\mathbf{k}'} \delta_{\mathbf{k}',\mathbf{k}''} = -\nabla_{\mathbf{k}''} \delta_{\mathbf{k}',\mathbf{k}''}, \tag{34}$$

$$\sum_{\mathbf{k}'} (\nabla_{\mathbf{k}'} \delta_{\mathbf{k}',\mathbf{k}}) a^{\dagger}_{\lambda\mathbf{k}'} a_{\lambda'\mathbf{k}} = -\sum_{\mathbf{k}'} \delta_{\mathbf{k}',\mathbf{k}} \nabla_{\mathbf{k}'} a^{\dagger}_{\lambda\mathbf{k}'} a_{\lambda\mathbf{k}} = -(\nabla_{\mathbf{k}} a^{\dagger}_{\lambda\mathbf{k}}) a_{\lambda'\mathbf{k}}, \tag{35}$$

$$\sum_{\mathbf{k}'} (\nabla_{\mathbf{k}'} \delta_{\mathbf{k}',\mathbf{k}}) a^{\dagger}_{\lambda\mathbf{k}'} a_{\lambda'\mathbf{k}'} = -\sum_{\mathbf{k}'} \delta_{\mathbf{k},\mathbf{k}'} \nabla_{\mathbf{k}'} a^{\dagger}_{\lambda\mathbf{k}} a_{\lambda\mathbf{k}'} = -a^{\dagger}_{\lambda\mathbf{k}} (\nabla_{\mathbf{k}} a_{\lambda'\mathbf{k}}), \tag{36}$$

ta được

$$
\begin{aligned}
[H^{e-L}, a^{\dagger}_{\lambda\mathbf{k}} a_{\lambda'\mathbf{k}}] &= e\mathbf{E}(t) \cdot \sum_{\mu} \left(\boldsymbol{\xi}_{\mu\lambda}(\mathbf{k}) a^{\dagger}_{\mu\mathbf{k}} a_{\lambda'\mathbf{k}} - \boldsymbol{\xi}_{\lambda'\mu}(\mathbf{k}) a^{\dagger}_{\lambda\mathbf{k}} a_{\mu\mathbf{k}} \right) \\
&\quad + ie\mathbf{E}(t) \cdot \nabla_{\mathbf{k}} (a^{\dagger}_{\lambda\mathbf{k}} a_{\lambda'\mathbf{k}}).
\end{aligned} \tag{37}
$$

Thay vào phương trình (29) và dùng phương trình (28) ta được phương trình Bloch bán dẫn cho ma trận mật độ rút gọn trong VG

$$\begin{aligned}\frac{d}{dt}a^{\dagger}_{\lambda\mathbf{k}}a_{\lambda'\mathbf{k}} &= -\frac{i}{\hbar}(\mathcal{E}_{\lambda}(\mathbf{k})-\mathcal{E}_{\lambda'}(\mathbf{k}))\rho_{\lambda\lambda'}(\mathbf{k})\\ &\qquad -\frac{ie}{\hbar m}\mathbf{A}(t)\cdot\sum_{\mu}\big(\mathbf{p}_{\mu\lambda}(\mathbf{k})\rho_{\mu\lambda'}(\mathbf{k})-\rho_{\lambda\mu}(\mathbf{k})\mathbf{p}_{\lambda'\mu}(\mathbf{k})\big),\end{aligned} \tag{38}$$

và trong LG

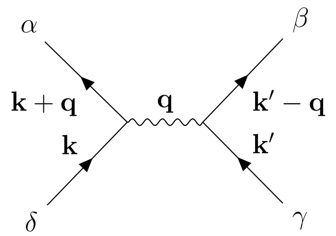
$$\begin{aligned}\frac{d}{dt}a^{\dagger}_{\lambda\mathbf{k}}a_{\lambda'\mathbf{k}} &= -\frac{i}{\hbar}(\mathcal{E}_{\lambda}(\mathbf{k})-\mathcal{E}_{\lambda'}(\mathbf{k}))\rho_{\lambda\lambda'}(\mathbf{k})\\ &\quad -\frac{ie}{\hbar}\mathbf{E}(t)\cdot\sum_{\mu}\big(\boldsymbol{\xi}_{\lambda\mu}(\mathbf{k})\rho_{\mu\lambda'}(\mathbf{k})-\rho_{\lambda\mu}(\mathbf{k})\boldsymbol{\xi}_{\mu\lambda'}(\mathbf{k})\big)+\frac{e}{\hbar}\mathbf{E}(t)\cdot\nabla_{\mathbf{k}}\rho_{\lambda\lambda'}(\mathbf{k}).\end{aligned} \tag{39}$$

1.4 Hamiltonian tương tác Coulomb

Hamiltonian lượng tử hoá lần 2 cho hệ nhiều điện tử tương tác Coulomb là

$$\begin{aligned}H &= H^0 + H^C\\ &= \sum_{\lambda\mathbf{k}}\mathcal{E}_{\lambda}(\mathbf{k})a^{\dagger}_{\lambda\mathbf{k}}a_{\lambda\mathbf{k}}+\frac{1}{2}\sum_{\mathbf{k}\mathbf{k}'\mathbf{q}}\sum_{\alpha\beta\gamma\delta}V^{\alpha\beta\gamma\delta}_{\mathbf{k},\mathbf{k}',\mathbf{q}}a^{\dagger}_{\alpha\mathbf{k}+\mathbf{q}}a^{\dagger}_{\beta\mathbf{k}'-\mathbf{q}}a_{\gamma\mathbf{k}'}a_{\delta\mathbf{k}}.\end{aligned} \tag{40}$$

Các toán tử sinh huỷ tuân theo hệ thức phản giao hoán (6) và (7)



$$\begin{aligned}V^{\alpha\beta\gamma\delta}_{\mathbf{k},\mathbf{k}',\mathbf{q}} &= \big\langle\psi_{\alpha\mathbf{k}+\mathbf{q}}\psi_{\beta}\mathbf{k}'-\mathbf{q}\big|\,V_{\text{e-e}}\,\big|\psi_{\gamma\mathbf{k}'}\psi_{\delta\mathbf{k}}\big\rangle =\\ &= \int\frac{d^3r}{V}\int\frac{d^3r'}{V}e^{-i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')}u^{*}_{\alpha\mathbf{k}+\mathbf{q}}(\mathbf{r})u^{*}_{\beta\mathbf{k}'-\mathbf{q}}(\mathbf{r}')V_{\text{e-e}}(\mathbf{r}-\mathbf{r}')u_{\gamma\mathbf{k}'}(\mathbf{r}')u_{\delta\mathbf{k}}(\mathbf{r}),\end{aligned} \tag{41}$$

trong đó

$$V_{\text{e-e}}(\mathbf{r}-\mathbf{r}') = \frac{e^2}{\epsilon|\mathbf{r}-\mathbf{r}'|}. \tag{42}$$

Biến đổi Fourier(thuận) của thế Coulomb

$$\begin{aligned}V_{\text{e-e}}(\mathbf{q}) &= \int\frac{d^3r}{L^3}V_{\text{e-e}}(\mathbf{r})e^{-i\mathbf{q}\cdot(\mathbf{r})}\\ &= \frac{e^2}{\epsilon V}\int\frac{d^3r}{|\mathbf{r}|}e^{-i\mathbf{q}\cdot\mathbf{r}} = \frac{e^2}{\epsilon V}\int_0^{\infty}dr\int_0^{\pi}d\theta\int_0^{2\pi}d\phi r\sin\theta e^{-iqr\cos\theta}\\ &= \frac{2\pi e^2}{\epsilon V}\int_0^{\infty}rdr\int_0^{2\pi}\sin\theta d\theta e^{iqr\cos\theta} = -i\frac{2\pi e^2}{\epsilon Vq}\int_0^{\infty}dr(e^{iqr}-e^{-iqr})\\ &= -i\frac{2\pi e^2}{\epsilon Vq}\lim_{\gamma\to 0}\int_0^{\infty}dr(e^{iqr}-e^{-iqr})e^{-\gamma r} = \lim_{\gamma\to 0}\frac{4\pi e^2}{\epsilon V}\frac{1}{q^2+\gamma^2} = \frac{4\pi e^2}{\epsilon Vq^2}.\end{aligned} \tag{43}$$

Biến đổi Fourier(ngược) của thế Coulomb

$$V_{\text{e-e}}(\mathbf{r}) = \sum_{\mathbf{q}} V_{\text{e-e}}(\mathbf{q}) e^{i\mathbf{q}\cdot\mathbf{r}}. \tag{44}$$

Thay vào (41), ta có

$$\begin{aligned} V^{\alpha\beta\gamma\delta}_{\mathbf{k},\mathbf{k}',\mathbf{q}} &= \int \frac{d^3r}{V} \int \frac{d^3r'}{V} e^{-i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')} u^*_{\alpha\mathbf{k}+\mathbf{q}}(\mathbf{r}) u^*_{\beta\mathbf{k}'-\mathbf{q}}(\mathbf{r}') \sum_{\mathbf{q}'} V_{\text{e-e}}(\mathbf{q}') e^{i\mathbf{q}'\cdot(\mathbf{r}-\mathbf{r}')} u_{\gamma\mathbf{k}'}(\mathbf{r}') u_{\delta\mathbf{k}}(\mathbf{r}) \\ &= \int \frac{d^3r}{V} \int \frac{d^3r'}{V} \sum_{\mathbf{q}'} V_{\text{e-e}}(\mathbf{q}') e^{i(\mathbf{q}'-\mathbf{q})\cdot(\mathbf{r}-\mathbf{r}')} u^*_{\alpha\mathbf{k}+\mathbf{q}}(\mathbf{r}) u_{\delta\mathbf{k}}(\mathbf{r}) u^*_{\beta\mathbf{k}'-\mathbf{q}}(\mathbf{r}') u_{\gamma\mathbf{k}'}(\mathbf{r}'), \end{aligned} \tag{45}$$

Đặt $\mathbf{r} \to \mathbf{R}_i + \mathbf{r}$, $\mathbf{r}' \to \mathbf{R}_j + \mathbf{r}'$ và sử dụng hệ thức $\sum_i^N e^{i(\mathbf{q}'-\mathbf{q}\cdot\mathbf{R}_i)} = N\delta_{\mathbf{q}',\mathbf{q}}$, và áp dụng gần đúng sóng dài, phương trình trên trở thành

$$\begin{aligned} V^{\alpha\beta\gamma\delta}_{\mathbf{k},\mathbf{k}',\mathbf{q}} &\simeq \frac{1}{N^2} \sum_{i,j} \sum_{\mathbf{q}'} V_{\text{e-e}}(\mathbf{q}') e^{i(\mathbf{q}'-\mathbf{q})\cdot(\mathbf{R}_i-\mathbf{R}_j)} \\ &\quad \times \int_{V_{\text{cell}}} \frac{d^3r}{V} u^*_{\alpha\mathbf{k}+\mathbf{q}}(\mathbf{r}) u_{\delta\mathbf{k}}(\mathbf{r}) \int_{V_{\text{cell}}} \frac{d^3r'}{V} u^*_{\beta\mathbf{k}'-\mathbf{q}}(\mathbf{r}') u_{\gamma\mathbf{k}'}(\mathbf{r}') \\ &\simeq V_{\text{e-e}}(\mathbf{q}) \left\langle u_{\alpha\mathbf{k}+\mathbf{q}} \middle| u_{\delta\mathbf{k}} \right\rangle \left\langle u_{\beta\mathbf{k}'-\mathbf{q}} \middle| u_{\gamma\mathbf{k}'} \right\rangle. \end{aligned} \tag{46}$$

Từ đó ta rút ra phương trình chuyển động Heisenberg với tương tác Coulomb

$$\begin{aligned} \frac{d}{dt} a^\dagger_{\lambda\mathbf{k}} a_{\lambda'\mathbf{k}} &= \frac{i}{\hbar} \langle [H^0 + H^C, a^\dagger_{\lambda\mathbf{k}} a_{\lambda'\mathbf{k}}] \rangle \\ &= \frac{i}{\hbar} \langle \left[\sum_{\nu\mathbf{k}'} \mathcal{E}_\nu(\mathbf{k}') a^\dagger_{\nu\mathbf{k}'} a_{\nu\mathbf{k}'} + \frac{1}{2} \sum_{\mathbf{k}'\mathbf{k}''\mathbf{q}} \sum_{\alpha\beta\gamma\delta} V^{\alpha\beta\gamma\delta}_{\mathbf{k}',\mathbf{k}'',\mathbf{q}} a^\dagger_{\alpha\mathbf{k}'+\mathbf{q}} a^\dagger_{\beta\mathbf{k}''-\mathbf{q}} a_{\gamma\mathbf{k}''} a_{\delta\mathbf{k}'}, a^\dagger_{\lambda\mathbf{k}} a_{\lambda'\mathbf{k}} \right] \rangle \\ &= \frac{i}{\hbar} \sum_{\lambda'\mathbf{k}'} \mathcal{E}_{\lambda'}(\mathbf{k}') \langle \left[a^\dagger_{\lambda'\mathbf{k}'} a_{\lambda'\mathbf{k}'}, a^\dagger_{\lambda\mathbf{k}} a_{\lambda'\mathbf{k}} \right] \rangle \to (\mathcal{E}_\lambda(\mathbf{k}) - \mathcal{E}_{\lambda'}(\mathbf{k})) a^\dagger_{\lambda\mathbf{k}} a_{\lambda'\mathbf{k}} \\ &\qquad + \frac{i}{2\hbar} \sum_{\mathbf{k}'\mathbf{k}''\mathbf{q}} \sum_{\alpha\beta\gamma\delta} V^{\alpha\beta\gamma\delta}_{\mathbf{k}',\mathbf{k}'',\mathbf{q}} \langle \left[a^\dagger_{\alpha\mathbf{k}'+\mathbf{q}} a^\dagger_{\beta\mathbf{k}''-\mathbf{q}} a_{\gamma\mathbf{k}''} a_{\delta\mathbf{k}'}, a^\dagger_{\lambda\mathbf{k}} a_{\lambda'\mathbf{k}} \right] \rangle \\ &= \frac{i}{\hbar} (\mathcal{E}_\lambda(\mathbf{k}) - \mathcal{E}_{\lambda'}(\mathbf{k})) \langle a^\dagger_{\lambda\mathbf{k}} a_{\lambda'\mathbf{k}} \rangle \\ &\qquad + \frac{i}{\hbar} \sum_{\mathbf{k}'\mathbf{q}} \sum_{\alpha\beta\gamma} V^{\alpha\beta\gamma\lambda}_{\mathbf{k},\mathbf{k}',\mathbf{q}} \langle a^\dagger_{\alpha\mathbf{k}+\mathbf{q}} a^\dagger_{\beta\mathbf{k}'-\mathbf{q}} a_{\gamma\mathbf{k}'} a_{\lambda'\mathbf{k}} \rangle \\ &\qquad + \frac{i}{\hbar} \sum_{\mathbf{k}'\mathbf{q}} \sum_{\alpha\gamma\delta} V^{\alpha\lambda'\gamma\delta}_{\mathbf{k}',\mathbf{k}+\mathbf{q},\mathbf{q}} \langle a^\dagger_{\lambda\mathbf{k}} a^\dagger_{\alpha\mathbf{k}'+\mathbf{q}} a_{\gamma\mathbf{k}+\mathbf{q}} a_{\delta'} \rangle, \end{aligned} \tag{47}$$

chú ý

$$
\begin{aligned}
&\frac{i}{2\hbar}\sum_{\mathbf{k}'\mathbf{k}''\mathbf{q}}\sum_{\alpha\beta\gamma\delta} V^{\alpha\beta\gamma\delta}_{\mathbf{k}',\mathbf{k}'',\mathbf{q}}\left[a^\dagger_{\alpha\mathbf{k}'+\mathbf{q}}a^\dagger_{\beta\mathbf{k}''-\mathbf{q}}a_{\gamma\mathbf{k}''}a_{\delta\mathbf{k}'}, a^\dagger_{\lambda\mathbf{k}}a_{\lambda'\mathbf{k}}\right] \\
&= \frac{i}{2\hbar}\sum_{\mathbf{k}'\mathbf{k}''\mathbf{q}}\sum_{\alpha\beta\gamma\delta} V^{\alpha\beta\gamma\delta}_{\mathbf{k}',\mathbf{k}'',\mathbf{q}}\left(a^\dagger_{\alpha\mathbf{k}'+\mathbf{q}}a^\dagger_{\beta\mathbf{k}''-\mathbf{q}}a_{\gamma\mathbf{k}''}a_{\delta\mathbf{k}'}a^\dagger_{\lambda\mathbf{k}}a_{\lambda'\mathbf{k}} - a^\dagger_{\lambda\mathbf{k}}a_{\lambda'\mathbf{k}}a^\dagger_{\alpha\mathbf{k}'+\mathbf{q}}a^\dagger_{\beta\mathbf{k}''-\mathbf{q}}a_{\gamma\mathbf{k}''}a_{\delta\mathbf{k}'}\right) \\
&= \frac{i}{2\hbar}\sum_{\mathbf{k}'\mathbf{k}''\mathbf{q}}\sum_{\alpha\beta\gamma\delta} V^{\alpha\beta\gamma\delta}_{\mathbf{k}',\mathbf{k}'',\mathbf{q}}\Big(a^\dagger_{\alpha\mathbf{k}'+\mathbf{q}}a^\dagger_{\beta\mathbf{k}''-\mathbf{q}}a_{\gamma\mathbf{k}''}(\delta_{\delta\lambda}\delta_{\mathbf{k}',\mathbf{k}} - a^\dagger_{\lambda\mathbf{k}}a_{\delta\mathbf{k}'})a_{\lambda'\mathbf{k}} \\
&\quad - a^\dagger_{\lambda\mathbf{k}}(\delta_{\lambda'\alpha}\delta_{\mathbf{k},\mathbf{k}'+\mathbf{q}} - a^\dagger_{\alpha\mathbf{k}'+\mathbf{q}}a_{\lambda'\mathbf{k}})a^\dagger_{\beta\mathbf{k}''-\mathbf{q}}a_{\gamma\mathbf{k}''}a_{\delta\mathbf{k}'}\Big) \\
&= \frac{i}{2\hbar}\sum_{\mathbf{k}'\mathbf{k}''\mathbf{q}}\sum_{\alpha\beta\gamma\delta} V^{\alpha\beta\gamma\delta}_{\mathbf{k}',\mathbf{k}'',\mathbf{q}}\Big(a^\dagger_{\alpha\mathbf{k}'+\mathbf{q}}a^\dagger_{\beta\mathbf{k}''-\mathbf{q}}a_{\gamma\mathbf{k}''}\delta_{\delta\lambda}\delta_{\mathbf{k}',\mathbf{k}}a_{\lambda'\mathbf{k}} - a^\dagger_{\alpha\mathbf{k}'+\mathbf{q}}a^\dagger_{\beta\mathbf{k}''-\mathbf{q}}a_{\gamma\mathbf{k}''}a^\dagger_{\lambda\mathbf{k}}a_{\delta\mathbf{k}'}a_{\lambda'\mathbf{k}} \\
&\quad - a^\dagger_{\lambda\mathbf{k}}\delta_{\lambda'\alpha}\delta_{\mathbf{k},\mathbf{k}'+\mathbf{q}}a^\dagger_{\beta\mathbf{k}''-\mathbf{q}}a_{\gamma\mathbf{k}''}a_{\delta\mathbf{k}'} + a^\dagger_{\lambda\mathbf{k}}a^\dagger_{\alpha\mathbf{k}'+\mathbf{q}}a_{\lambda'\mathbf{k}}a^\dagger_{\beta\mathbf{k}''-\mathbf{q}}a_{\gamma\mathbf{k}''}a_{\delta\mathbf{k}'}\Big) \\
&= \frac{i}{2\hbar}\sum_{\mathbf{k}'\mathbf{k}''\mathbf{q}}\sum_{\alpha\beta\gamma\delta} V^{\alpha\beta\gamma\delta}_{\mathbf{k}',\mathbf{k}'',\mathbf{q}}\Big(a^\dagger_{\alpha\mathbf{k}'+\mathbf{q}}a^\dagger_{\beta\mathbf{k}''-\mathbf{q}}a_{\gamma\mathbf{k}''}\delta_{\delta\lambda}\delta_{\mathbf{k}',\mathbf{k}}a_{\lambda'\mathbf{k}} - a^\dagger_{\alpha\mathbf{k}'+\mathbf{q}}a^\dagger_{\beta\mathbf{k}''-\mathbf{q}}(\delta_{\gamma\lambda}\delta_{\mathbf{k}'',\mathbf{k}} - a^\dagger_{\lambda\mathbf{k}}a_{\gamma\mathbf{k}''})a_{\delta\mathbf{k}'}a_{\lambda'\mathbf{k}} \\
&\quad - a^\dagger_{\lambda\mathbf{k}}\delta_{\lambda'\alpha}\delta_{\mathbf{k},\mathbf{k}'+\mathbf{q}}a^\dagger_{\beta\mathbf{k}''-\mathbf{q}}a_{\gamma\mathbf{k}''}a_{\delta\mathbf{k}'} + a^\dagger_{\lambda\mathbf{k}}a^\dagger_{\alpha\mathbf{k}'+\mathbf{q}}(\delta_{\lambda'\beta}\delta_{\mathbf{k},\mathbf{k}''-\mathbf{q}} - a^\dagger_{\beta\mathbf{k}''-\mathbf{q}}a_{\lambda'\mathbf{k}})a_{\gamma\mathbf{k}''}a_{\delta\mathbf{k}'}\Big) \\
&= \frac{i}{2\hbar}\sum_{\mathbf{k}'\mathbf{k}''\mathbf{q}}\sum_{\alpha\beta\gamma\delta} V^{\alpha\beta\gamma\delta}_{\mathbf{k}',\mathbf{k}'',\mathbf{q}}\Big(a^\dagger_{\alpha\mathbf{k}'+\mathbf{q}}a^\dagger_{\beta\mathbf{k}''-\mathbf{q}}a_{\gamma\mathbf{k}''}\delta_{\delta\lambda}\delta_{\mathbf{k}',\mathbf{k}}a_{\lambda'\mathbf{k}} - a^\dagger_{\alpha\mathbf{k}'+\mathbf{q}}a^\dagger_{\beta\mathbf{k}''-\mathbf{q}}\delta_{\gamma\lambda}\delta_{\mathbf{k}'',\mathbf{k}}a_{\delta\mathbf{k}'}a_{\lambda'\mathbf{k}} \\
&\quad + \cancel{a^\dagger_{\alpha\mathbf{k}'+\mathbf{q}}a^\dagger_{\beta\mathbf{k}''-\mathbf{q}}a^\dagger_{\lambda\mathbf{k}}a_{\gamma\mathbf{k}''}a_{\delta\mathbf{k}'}a_{\lambda'\mathbf{k}}} - a^\dagger_{\lambda\mathbf{k}}\delta_{\lambda'\alpha}\delta_{\mathbf{k},\mathbf{k}'+\mathbf{q}}a^\dagger_{\beta\mathbf{k}''-\mathbf{q}}a_{\gamma\mathbf{k}''}a_{\delta\mathbf{k}'} \\
&\quad + a^\dagger_{\lambda\mathbf{k}}a^\dagger_{\alpha\mathbf{k}'+\mathbf{q}}\delta_{\lambda'\beta}\delta_{\mathbf{k},\mathbf{k}''-\mathbf{q}}a_{\gamma\mathbf{k}''}a_{\delta\mathbf{k}'} - \cancel{a^\dagger_{\lambda\mathbf{k}}a^\dagger_{\alpha\mathbf{k}'+\mathbf{q}}a^\dagger_{\beta\mathbf{k}''-\mathbf{q}}a_{\lambda'\mathbf{k}}a_{\gamma\mathbf{k}''}a_{\delta\mathbf{k}'}}\Big) \\
&= \frac{i}{2\hbar}\sum_{\mathbf{k}''\mathbf{q}}\sum_{\alpha\beta\gamma} V^{\alpha\beta\gamma\lambda}_{\mathbf{k},\mathbf{k}'',\mathbf{q}}a^\dagger_{\alpha\mathbf{k}+\mathbf{q}}a^\dagger_{\beta\mathbf{k}''-\mathbf{q}}a_{\gamma\mathbf{k}''}a_{\lambda'\mathbf{k}} \underbrace{- \frac{i}{2\hbar}\sum_{\mathbf{k}'\mathbf{q}}\sum_{\alpha\beta\delta} V^{\alpha\beta\lambda\delta}_{\mathbf{k}',\mathbf{k},\mathbf{q}}\overbrace{a^\dagger_{\alpha\mathbf{k}'+\mathbf{q}}a^\dagger_{\beta\mathbf{k}-\mathbf{q}}}^{=-a^\dagger_{\beta\mathbf{k}-\mathbf{q}}a^\dagger_{\alpha\mathbf{k}'+\mathbf{q}}}a_{\delta\mathbf{k}'}a_{\lambda'\mathbf{k}}}_{\mathbf{q}\to-\mathbf{q},\alpha\leftrightarrow\beta,\delta\to\gamma,V_{-\mathbf{q}}=V_{\mathbf{q}}} \\
&\quad \underbrace{- \frac{i}{2\hbar}\sum_{\mathbf{k}''\mathbf{q}}\sum_{\beta\gamma\delta} V^{\lambda'\beta\gamma\delta}_{\mathbf{k}-\mathbf{q},\mathbf{k}'',\mathbf{q}}a^\dagger_{\lambda\mathbf{k}}a^\dagger_{\beta\mathbf{k}''-\mathbf{q}}\overbrace{a_{\gamma\mathbf{k}''}a_{\delta\mathbf{k}-\mathbf{q}}}^{=-a_{\delta\mathbf{k}-\mathbf{q}}a_{\gamma\mathbf{k}''}}}_{\mathbf{q}\to-\mathbf{q},\delta\leftrightarrow\gamma,\beta\to\alpha,V_{-\mathbf{q}}=V_{\mathbf{q}}} + \frac{i}{2\hbar}\sum_{\mathbf{k}'\mathbf{q}}\sum_{\alpha\gamma\delta} V^{\alpha\lambda'\gamma\delta}_{\mathbf{k}',\mathbf{k}+\mathbf{q},\mathbf{q}}a^\dagger_{\lambda\mathbf{k}}a^\dagger_{\alpha\mathbf{k}'+\mathbf{q}}a_{\gamma\mathbf{k}+\mathbf{q}}a_{\delta\mathbf{k}'} \\
&= \frac{i}{2\hbar}\sum_{\mathbf{k}''\mathbf{q}}\sum_{\alpha\beta\gamma} V^{\alpha\beta\gamma\lambda}_{\mathbf{k},\mathbf{k}'',\mathbf{q}}a^\dagger_{\alpha\mathbf{k}+\mathbf{q}}a^\dagger_{\beta\mathbf{k}''-\mathbf{q}}a_{\gamma\mathbf{k}''}a_{\lambda'\mathbf{k}} + \frac{i}{2\hbar}\sum_{\mathbf{k}'\mathbf{q}}\sum_{\alpha\beta\gamma} V^{\alpha\beta\lambda\gamma}_{\mathbf{k}',\mathbf{k},\mathbf{q}}a^\dagger_{\alpha\mathbf{k}+\mathbf{q}}a^\dagger_{\beta\mathbf{k}'-\mathbf{q}}a_{\gamma\mathbf{k}'}a_{\lambda'\mathbf{k}} \\
&+ \quad \frac{i}{2\hbar}\sum_{\mathbf{k}''\mathbf{q}}\sum_{\alpha\gamma\delta} V^{\lambda'\alpha\gamma\delta}_{\mathbf{k}',\mathbf{k}+\mathbf{q},\mathbf{q}}a^\dagger_{\lambda\mathbf{k}}a^\dagger_{\alpha\mathbf{k}''+\mathbf{q}}a_{\gamma\mathbf{k}''}a_{\delta\mathbf{k}+\mathbf{q}} + \frac{i}{2\hbar}\sum_{\mathbf{k}'\mathbf{q}}\sum_{\alpha\gamma\delta} V^{\alpha\lambda'\gamma\delta}_{\mathbf{k}',\mathbf{k}+\mathbf{q},\mathbf{q}}a^\dagger_{\lambda\mathbf{k}}a^\dagger_{\alpha\mathbf{k}'+\mathbf{q}}a_{\gamma\mathbf{k}'}a_{\delta\mathbf{k}+\mathbf{q}}.
\end{aligned}
$$

Phương trình (47) là phương trình không đóng. Vì thế, ta cần áp dụng gần đúng giá trị trung bình của 4 toán tử trong phương trình (47) bằng tích của 2 giá trị trung bình của 2 toán tử(gần đúng Hartree-Fock), sao cho có được cặp toán tử liên quan

$$\begin{aligned}
\langle a^\dagger_{\alpha\mathbf{k}+\mathbf{q}} a^\dagger_{\beta\mathbf{k}'-\mathbf{q}} a_{\gamma\mathbf{k}'} a_{\lambda'\mathbf{k}}\rangle &\simeq -\langle a^\dagger_{\alpha\mathbf{k}+\mathbf{q}} a_{\gamma\mathbf{k}+\mathbf{q}}\rangle \langle a^\dagger_{\beta\mathbf{k}} a_{\lambda'\mathbf{k}}\rangle \delta_{\mathbf{k}'+\mathbf{k}+\mathbf{q}}, \\
\langle a^\dagger_{\lambda\mathbf{k}} a^\dagger_{\alpha\mathbf{k}'+\mathbf{q}} a_{\gamma\mathbf{k}+\mathbf{q}} a_{\delta'}\rangle &\simeq \langle a^\dagger_{\alpha\mathbf{k}+\mathbf{q}} a_{\gamma\mathbf{k}+\mathbf{q}}\rangle \langle a^\dagger_{\lambda\mathbf{k}} a_{\delta\mathbf{k}}\rangle \delta_{\mathbf{k},\mathbf{k}'}.
\end{aligned} \tag{48}$$

Thay phương trình trên vào (47), ta được

$$\begin{aligned}
\frac{d}{dt}\langle a^\dagger_{\lambda\mathbf{k}} a_{\lambda'\mathbf{k}}\rangle &= \frac{i}{\hbar}(\mathcal{E}_\lambda(\mathbf{k}) - \mathcal{E}_{\lambda'}(\mathbf{k}))\langle a^\dagger_{\lambda\mathbf{k}} a_{\lambda'\mathbf{k}}\rangle \\
&\quad \underbrace{-\frac{i}{\hbar}\sum_{\mathbf{q}}\sum_{\alpha\beta\gamma} V^{\alpha\beta\gamma\lambda}_{\mathbf{k},\mathbf{k}+\mathbf{q},\mathbf{q}} \langle a^\dagger_{\alpha\mathbf{k}+\mathbf{q}} a_{\gamma\mathbf{k}+\mathbf{q}}\rangle \langle a^\dagger_{\beta\mathbf{k}} a_{\lambda'\mathbf{k}}\rangle}_{\beta\to\gamma,\gamma\to\mu} \\
&\quad \underbrace{+\frac{i}{\hbar}\sum_{\mathbf{q}}\sum_{\alpha\gamma\delta} V^{\alpha\lambda'\gamma\delta}_{\mathbf{k},\mathbf{k}+\mathbf{q},\mathbf{q}} \langle a^\dagger_{\alpha\mathbf{k}+\mathbf{q}} a_{\gamma\mathbf{k}+\mathbf{q}}\rangle \langle a^\dagger_{\lambda\mathbf{k}} a_{\delta\mathbf{k}}\rangle}_{\gamma\to\beta,\delta\to\mu} \\
&= \frac{i}{\hbar}(\mathcal{E}_\lambda(\mathbf{k}) - \mathcal{E}_{\lambda'}(\mathbf{k}))\langle a^\dagger_{\lambda\mathbf{k}} a_{\lambda'\mathbf{k}}\rangle \\
&\quad - \frac{i}{\hbar}\sum_{\mathbf{q}}\sum_{\alpha\mu\beta} V^{\alpha\mu\beta\lambda}_{\mathbf{k},\mathbf{k}+\mathbf{q},\mathbf{q}} \langle a^\dagger_{\alpha\mathbf{k}+\mathbf{q}} a_{\beta\mathbf{k}+\mathbf{q}}\rangle \langle a^\dagger_{\mu\mathbf{k}} a_{\lambda'\mathbf{k}}\rangle \\
&\quad + \frac{i}{\hbar}\sum_{\mathbf{q}}\sum_{\alpha\beta\mu} V^{\alpha\lambda'\beta\mu}_{\mathbf{k},\mathbf{k}+\mathbf{q},\mathbf{q}} \langle a^\dagger_{\alpha\mathbf{k}+\mathbf{q}} a_{\beta\mathbf{k}+\mathbf{q}}\rangle \langle a^\dagger_{\lambda\mathbf{k}} a_{\mu\mathbf{k}}\rangle \\
&= \frac{i}{\hbar}(\mathcal{E}_\lambda(\mathbf{k}) - \mathcal{E}_{\lambda'}(\mathbf{k}))\langle a^\dagger_{\lambda\mathbf{k}} a_{\lambda'\mathbf{k}}\rangle \\
&\quad - \frac{i}{\hbar}\sum_{\mu}\left[\Sigma_{\mu\lambda}(\mathbf{k})\langle a^\dagger_{\mu\mathbf{k}} a_{\lambda'\mathbf{k}}\rangle - \Sigma_{\lambda'\mu}(\mathbf{k})\langle a^\dagger_{\lambda\mathbf{k}} a_{\mu\mathbf{k}}\rangle\right],
\end{aligned} \tag{49}$$

trong đó

$$\begin{aligned}
\Sigma_{\mu\lambda}(\mathbf{k}) &= \sum_{\alpha\beta\mathbf{q}} V^{\alpha\mu\beta\lambda}_{\mathbf{k},\mathbf{k}+\mathbf{q},\mathbf{q}} \langle a^\dagger_{\alpha\mathbf{k}+\mathbf{q}} a_{\beta\mathbf{k}+\mathbf{q}}\rangle, \\
\Sigma_{\lambda'\mu}(\mathbf{k}) &= \sum_{\alpha\beta\mathbf{q}} V^{\alpha\lambda'\beta\mu}_{\mathbf{k},\mathbf{k}+\mathbf{q},\mathbf{q}} \langle a^\dagger_{\alpha\mathbf{k}+\mathbf{q}} a_{\beta\mathbf{k}+\mathbf{q}}\rangle.
\end{aligned} \tag{50}$$

Sử dụng định nghĩa (28), ta có được phương trình chuyển động trong gần đúng Hartree-Fock có tương tác Coulomb

$$\begin{aligned}
\frac{d}{dt}\rho_{\lambda\lambda'}(\mathbf{k}) &= -\frac{i}{\hbar}(\mathcal{E}_\lambda(\mathbf{k}) - \mathcal{E}_{\lambda'}(\mathbf{k}))\rho_{\lambda\lambda'}(\mathbf{k}) \\
&\quad + \frac{i}{\hbar}\sum_{\mu}\left[\Sigma_{\lambda\mu}(\mathbf{k})\rho_{\mu\lambda'}(\mathbf{k}) - \rho_{\lambda\mu}\Sigma_{\mu\lambda'}(\mathbf{k})\right],
\end{aligned} \tag{51}$$

trong đó

$$
\begin{aligned}
\Sigma_{\mu\lambda}(\mathbf{k}) &= \sum_{\alpha\beta\mathbf{q}} V^{\alpha\mu\beta\lambda}_{\mathbf{k},\mathbf{k}+\mathbf{q},\mathbf{q}} \rho^{\beta\alpha}_{\mathbf{k}+\mathbf{q}}, \\
\Sigma_{\lambda'\mu}(\mathbf{k}) &= \sum_{\alpha\beta\mathbf{q}} V^{\alpha\lambda'\beta\mu}_{\mathbf{k},\mathbf{k}+\mathbf{q},\mathbf{q}} \rho^{\beta\alpha}_{\mathbf{k}+\mathbf{q}},
\end{aligned}
\tag{52}
$$

là năng lượng riêng trao đổi.

Kết hợp phương trình (51) vào phương trình (39) ta được phương trình Bloch bán dẫn có tương tác ánh sáng và tương tác Coulomb trong gauge độ dài là

$$
\begin{aligned}
\frac{d}{dt}\rho_{\lambda\lambda'}(\mathbf{k}) = &-\frac{i}{\hbar}(\mathcal{E}_\lambda(\mathbf{k}) - \mathcal{E}_{\lambda'}(\mathbf{k}))\rho_{\lambda\lambda'}(\mathbf{k}) \\
&+ \frac{i}{\hbar}\sum_{\mu}\left[\Sigma_{\lambda\mu}(\mathbf{k})\rho_{\mu\lambda'}(\mathbf{k}) - \rho_{\lambda\mu}\Sigma_{\mu\lambda'}(\mathbf{k})\right] \\
&- \frac{ie}{\hbar}\mathbf{E}(t)\cdot\sum_{\mu}\big(\boldsymbol{\xi}_{\lambda\mu}(\mathbf{k})\rho_{\mu\lambda'}(\mathbf{k}) - \rho_{\lambda\mu}(\mathbf{k})\boldsymbol{\xi}_{\mu\lambda'}(\mathbf{k})\big) + \frac{e}{\hbar}\mathbf{E}(t)\cdot\nabla_{\mathbf{k}}\rho_{\lambda\lambda'}(\mathbf{k}).
\end{aligned}
\tag{53}
$$

đổi các chỉ số $\lambda \to v, \lambda' \to c$

$$
\begin{aligned}
\frac{d}{dt}\rho_{vc}(\mathbf{k}) = &\frac{i}{\hbar}\big(\mathcal{E}_c(\mathbf{k}) - \mathcal{E}_v(\mathbf{k})\big)\rho_{vc}(\mathbf{k}) \\
&+ \frac{i}{\hbar}\sum_{\mu}[\Sigma_{v\mu}(\mathbf{k})\rho_{\mu c}(\mathbf{k}) - \rho_{v\mu}\Sigma_{\mu c}(\mathbf{k})] \\
&- \frac{ie}{\hbar}\mathbf{E}(t)\cdot\sum_{\mu}\big(\boldsymbol{\xi}_{v\mu}(\mathbf{k})\rho_{\mu c}(\mathbf{k}) - \rho_{v\mu}(\mathbf{k})\boldsymbol{\xi}_{\mu c}(\mathbf{k})\big) \\
= &\frac{i}{\hbar}\big(\mathcal{E}_c(\mathbf{k}) - \mathcal{E}_v(\mathbf{k})\big)\rho_{vc}(\mathbf{k}) \\
&+ \frac{i}{\hbar}[\Sigma_{vv}(\mathbf{k})\rho_{vc}(\mathbf{k}) - \cancelto{1}{\rho_{vv}(\mathbf{k})}\Sigma_{vc}(\mathbf{k}) + \Sigma_{vc}(\mathbf{k})\cancelto{0}{\rho_{cc}(\mathbf{k})} - \rho_{vc}(\mathbf{k})\Sigma_{cc}(\mathbf{k})] \\
&- \frac{ie}{\hbar}\mathbf{E}(t)\cdot\big(\boldsymbol{\xi}_{vv}(\mathbf{k})\rho_{vc}(\mathbf{k}) - \rho_{vv}(\mathbf{k})\boldsymbol{\xi}_{vc}(\mathbf{k}) + \boldsymbol{\xi}_{vc}(\mathbf{k})\rho_{cc}(\mathbf{k}) - \rho_{vc}(\mathbf{k})\boldsymbol{\xi}_{cc}(\mathbf{k})\big) \\
= &\frac{i}{\hbar}\big(\mathcal{E}_c(\mathbf{k}) - \mathcal{E}_v(\mathbf{k})\big)\rho_{vc}(\mathbf{k}) + \frac{ie}{\hbar}\mathbf{E}(t)\cdot\boldsymbol{\xi}_{vc}(\mathbf{k}) - \frac{i}{\hbar}\Sigma_{vc}(\mathbf{k}) \\
= &\frac{i}{\hbar}\big(\mathcal{E}_c(\mathbf{k}) - \mathcal{E}_v(\mathbf{k})\big)\rho_{vc}(\mathbf{k}) + \frac{ie}{\hbar}\mathbf{E}(t)\cdot\boldsymbol{\xi}_{vc}(\mathbf{k}) - \frac{i}{\hbar}\sum_{\alpha\beta\mathbf{q}} V^{\alpha v\beta c}_{\mathbf{k},\mathbf{k}+\mathbf{q},\mathbf{q}}\rho^{\beta\alpha}_{\mathbf{k}+\mathbf{q}}
\end{aligned}
\tag{54}
$$

$$
\begin{aligned}
\frac{d}{dt}\rho_{vc}(\mathbf{k}) = &\frac{i}{\hbar}\big(\mathcal{E}_c(\mathbf{k}) - \mathcal{E}_v(\mathbf{k})\big)\rho_{vc}(\mathbf{k}) + \frac{ie}{\hbar}\mathbf{E}(t)\cdot\boldsymbol{\xi}_{vc}(\mathbf{k}) \\
&- \frac{i}{\hbar}\sum_{c'v'\mathbf{k}'} V_{c'vv'c}(\mathbf{k},\mathbf{k}',\mathbf{k}'-\mathbf{k})\rho_{v'c'}(\mathbf{k}')
\end{aligned}
\tag{55}
$$

trong đó

$$
V_{\lambda_1\lambda_2\lambda_3\lambda_4}(\mathbf{k},\mathbf{k}',\mathbf{k}'-\mathbf{k}) = \frac{e^2}{2\varepsilon\varepsilon_0 L^2}\frac{1}{|\mathbf{k}'-\mathbf{k}|}\sum_j C^{\lambda_1 *}_j(\mathbf{k}')C^{\lambda_4}_j(\mathbf{k})\sum_{j'} C^{\lambda_2 *}_{j'}(\mathbf{k})C^{\lambda_3}_{j'}(\mathbf{k}')
\tag{56}
$$

Trong gauge vận tốc ta có

$$
\begin{aligned}
\frac{d}{dt}\rho_{\lambda\lambda'}(\mathbf{k}) = &-\frac{i}{\hbar}(\mathcal{E}_\lambda(\mathbf{k}) - \mathcal{E}_{\lambda'}(\mathbf{k}))\rho_{\lambda\lambda'}(\mathbf{k}) \\
&+ \frac{i}{\hbar}\sum_\mu \left[\Sigma_{\lambda\mu}(\mathbf{k})\rho_{\mu\lambda'}(\mathbf{k}) - \rho_{\lambda\mu}\Sigma_{\mu\lambda'}(\mathbf{k})\right] \\
&- \frac{ie}{\hbar m}\mathbf{A}(t)\cdot\sum_\mu \big(\mathbf{p}_{\mu\lambda}(\mathbf{k})\rho_{\mu\lambda'}(\mathbf{k}) - \rho_{\lambda\mu}(\mathbf{k})\mathbf{p}_{\lambda'\mu}(\mathbf{k})\big).
\end{aligned}
\tag{57}
$$

2 Hamiltonian tight-binding 3 bands

2.1 Tương tác Coulomb

$$
H_F = -\frac{i}{\hbar}\sum_{c,v,\mathbf{k}'} V_{\lambda_1\lambda_2\lambda_3\lambda_4}(\mathbf{k},\mathbf{k}',\mathbf{k}'-\mathbf{k})\rho_{\lambda_1\lambda_3}(\mathbf{k}') \tag{58}
$$

trong đó

$$
V_{\lambda_1\lambda_2\lambda_3\lambda_4}(\mathbf{k},\mathbf{k}',\mathbf{k}'-\mathbf{k}) = \frac{e^2}{2\varepsilon\varepsilon_0 L^2}\frac{1}{|\mathbf{k}'-\mathbf{k}|}\sum_j C_j^{\lambda_1 *}(\mathbf{k}')C_j^{\lambda_4}(\mathbf{k})\sum_{j'} C_{j'}^{\lambda_2 *}(\mathbf{k})C_{j'}^{\lambda_3}(\mathbf{k}') \tag{59}
$$

Optical polarization

$$
\mathbf{P}(t) = \frac{e}{L^2}\sum_{c,v,\mathbf{k}} \boldsymbol{\xi}_{cv}(\mathbf{k})\rho_{vc}(\mathbf{k}), \tag{60}
$$

$$
\frac{d}{dt}\rho_{vc}(\mathbf{k}) = \frac{i}{\hbar}(\mathcal{E}_c(\mathbf{k}) - \mathcal{E}_v(\mathbf{k}) + \frac{i\hbar}{T_2})\rho_{vc}(\mathbf{k}) + \frac{i}{\hbar}e\mathbf{E}(t)\cdot\boldsymbol{\xi}_{vc}(\mathbf{k}) \tag{61}
$$