Electric Conductivity: Kubo Formula/Simulation

1989. 11. 11

§. Maxwell's Equations

$$
\begin{cases}
\nabla \times E + \dfrac{1}{c}\dfrac{\partial H}{\partial t} = 0 & (1) \\[2mm]
\nabla \times H - \dfrac{1}{c}\dfrac{\partial E}{\partial t} = \dfrac{4\pi}{c} J & (2) \\[2mm]
\nabla \cdot E = 4\pi \rho & (3) \\[2mm]
\nabla \cdot H = 0 & (4)
\end{cases}
$$

where

$$\partial \rho / \partial t + \nabla \cdot J = 0 \tag{5}$$

(Potentials)

$$
\begin{cases}
E = -\dfrac{1}{c}\dfrac{\partial A}{\partial t} - \nabla \phi & (6) \\[2mm]
H = \nabla \times A & (7)
\end{cases}
$$

(Gauge Transformation)

$$A' = A + \nabla \chi \quad , \quad \phi' = \phi - \frac{1}{c}\frac{\partial}{\partial t}\chi \tag{8}$$

do not alter the field strengths :

$$
\begin{aligned}
E' &= -\frac{1}{c}\frac{\partial A'}{\partial t} - \nabla \phi' \\
&= -\frac{1}{c}\frac{\partial A}{\partial t} \cancel{- \frac{1}{c}\frac{\partial}{\partial t}\nabla \chi} - \nabla \phi \cancel{+ \frac{1}{c}\frac{\partial}{\partial t}\nabla \chi} = E
\end{aligned}
$$

$$
\begin{aligned}
H' &= \nabla \times A' \\
&= \nabla \times A + \underbrace{\nabla \times (\nabla \chi)}_{0} = H
\end{aligned}
$$

(Uniform Electric Field)

$$A = 0, \quad \phi = -Ex \tag{9}$$

$$\phi' = -Ex - \frac{1}{c}\frac{\partial}{\partial t}(\underbrace{-Exct}_{x}) = 0$$

$$A' = \nabla(-Exct) = -Ect$$

$$\begin{cases} A' = -Ect & (10) \\ \phi' = 0 & (11) \end{cases}$$

§. Schrödinger Equation

$$H_{cl} = \frac{1}{2m}(P + \frac{e}{c}A)^2 - e\phi$$

$$H(t) = \frac{P^2}{2m} + \frac{e}{2mc}[PA(r,t) + A(r,t)P] + \frac{e^2}{2mc^2}A^2(r,t) - e\phi(r,t) \tag{12}$$

(Uniform Electric Field)

$$H(t) = \frac{1}{2m}(P - eEt)^2 \tag{13a}$$

$$= \frac{P^2}{2m} - \frac{e}{m}PEt + \frac{e^2}{2m}E^2t^2 \tag{13b}$$

$$H = \frac{P^2}{2m} + eEx$$

§. Current Operator

$$H(t) = \sum_\sigma \int d^3r\, \psi_\sigma^\dagger(r) \left\{ -\frac{\hbar^2}{2m}\nabla^2 + \frac{e}{2mc}\left[\frac{\hbar}{i}\nabla A(r,t) + A(r,t)\frac{\hbar}{i}\nabla\right] + \frac{e^2}{2mc^2}A^2(r,t) - e\phi(r,t) \right\} \psi_\sigma(r)$$

$$\boxed{\begin{aligned} H(t) &= \sum_\sigma \int d^3r\, \psi_\sigma^\dagger(r)\left(-\frac{\hbar^2}{2m}\nabla^2\right)\psi_\sigma(r) - \frac{1}{c}\int d^3r\, A(r,t)\cdot j_p(r) \\ &\quad + \int d^3r \left[-\frac{e}{2mc^2}A^2(r,t) + \phi(r,t)\right]\rho(r) \qquad (14) \\ &\begin{cases} \rho(r) = -e\sum_\sigma \psi_\sigma^\dagger(r)\psi_\sigma(r) & (15) \\ j_p(r) = -\frac{e}{2m}\sum_\sigma \left[\psi_\sigma^\dagger(r)\frac{\hbar}{i}\nabla\psi_\sigma(r) - \left(\frac{\hbar}{i}\nabla\psi_\sigma^\dagger(r)\right)\psi_\sigma(r)\right] & (16) \end{cases} \end{aligned}}$$

(Continuity Equation)

$$i\hbar\frac{\partial}{\partial t}\rho_H(r,t) = \sum_\sigma\int d^3x\, \left[\psi_\sigma^\dagger(r)\psi_\sigma(r),\ \psi_\sigma^\dagger(x)\left(-\frac{\hbar^2}{2m}\nabla_x^2\right)\psi_\sigma(x)\right]$$

$$- \frac{1}{c}\int d^3x\, [\rho(r), j_p(x)]\, A(x,t)$$

$$= \sum_\sigma \int d^3x \left[\psi_\sigma^\dagger(r)\delta(x-r)\left(-\frac{\hbar^2}{2m}\nabla_x^2\right)\psi_\sigma(x) - \psi_\sigma^\dagger(x)\left(-\frac{\hbar^2}{2m}\nabla_x^2\right)\delta(x-r)\psi_\sigma(r) \right]$$

$$+ \frac{e}{2mc}\sum_\sigma\int d^3x\, A(x,t)\, \underbrace{\left[\psi_\sigma^\dagger(r)\psi_\sigma(r),\ \psi_\sigma^\dagger(x)\frac{\hbar}{i}\nabla_x\psi_\sigma(x) - \left(\frac{\hbar}{i}\nabla_x\psi_\sigma^\dagger(x)\right)\psi_\sigma(x)\right]}_{\substack{\psi_\sigma^\dagger(r)\delta(x-r)\left[\frac{\hbar}{i}\nabla_x\psi_\sigma(x)\right] - \psi_\sigma^\dagger(x)\left[\frac{\hbar}{i}\nabla_x\delta(x-r)\right]\psi_\sigma(r) \\ - \psi_\sigma^\dagger(r)\left[\frac{\hbar}{i}\nabla_x\delta(x-r)\right]\psi_\sigma(x) + \left[\frac{\hbar}{i}\nabla_x\psi_\sigma^\dagger(x)\right]\delta(x-r)\psi_\sigma(r)}}$$

$$\therefore i\hbar\frac{\partial}{\partial t}\rho_H(r,t) = \sum_\sigma \left[\psi^\dagger_\sigma(r)\left(-\frac{\hbar^2}{2m}\nabla^2\psi_\sigma(r)\right) + \left(\frac{\hbar^2}{2m}\nabla^2\psi_\sigma(r)\right)\psi_\sigma(r) \right]$$

$$+ \frac{e}{2mc}\sum_\sigma \Big\{ \underbrace{\psi^\dagger_\sigma(r)A(r,t)\left[\frac{\hbar}{i}\nabla\psi_\sigma(r)\right] + \left(\frac{\hbar}{i}\nabla\left[\psi^\dagger_\sigma(r)A(r,t)\right]\right)\psi_\sigma(r)}_{\frac{\hbar}{i}\nabla[\psi^\dagger_\sigma A\psi_\sigma]}$$

$$+ \underbrace{\psi^\dagger_\sigma(r)\left(\frac{\hbar}{i}\nabla\left[A(r,t)\psi_\sigma(r)\right]\right) + \left[\frac{\hbar}{i}\nabla\psi^\dagger_\sigma(r)\right]A(r,t)\psi_\sigma(r)}_{\frac{\hbar}{i}\nabla[\psi^\dagger_\sigma A\psi_\sigma]} \Big\}$$

$$= \nabla\cdot\underbrace{\sum_\sigma\left[\psi^\dagger_\sigma(r)\left(-\frac{\hbar^2}{2m}\nabla\psi_\sigma(r)\right) + \left(\frac{\hbar^2}{2m}\nabla\psi_\sigma(r)\right)\psi_\sigma(r)\right]}_{-i\hbar j_p(r)}$$

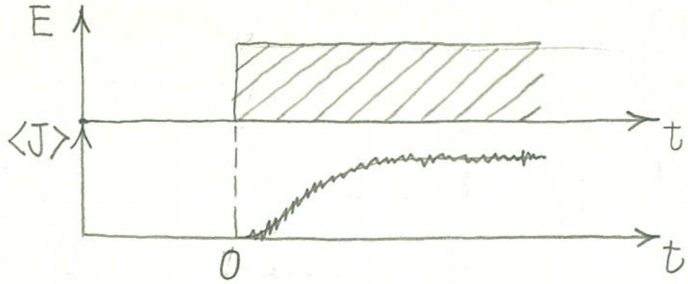
$$+ \frac{e\hbar}{mci}\nabla\cdot\left[A(r,t)\rho(r)\right]$$

multiply $-e$ on both sides

$$\frac{\partial}{\partial t}\rho(r) = -\nabla\cdot j(r) \tag{17}$$

$$j(r) = \underbrace{-\frac{e}{2m}\sum_\sigma\left[\psi^\dagger_\sigma(r)\frac{\hbar}{i}\nabla\psi_\sigma(r) - \left(\frac{\hbar}{i}\nabla\psi^\dagger_\sigma(r)\right)\psi_\sigma(r)\right]}_{j^{(p)}(r)} \underbrace{- \frac{e^2}{mc}\rho(r)A(r,t)}_{j^{(d)}(r)} \tag{18}$$

§. Linear Conductivity



$$\mathcal{H}(t) = H - \frac{1}{\cancel{c}}\int d^3r\, \underbrace{A(r,t)}_{-E\cancel{c}t}\cdot j_x^{(p)}(r)$$

$$\boxed{\begin{aligned} \mathcal{H}(t) &= H + \underbrace{E\,t\,j_x^{(p)}}_{V(t)} && (19)\\ j_x^{(p)} &= -\frac{e}{2m}\sum_\sigma\int d^3r\left[\psi_\sigma^\dagger(r)\frac{\hbar}{i}\nabla_x\psi_\sigma(r) - \left(\frac{\hbar}{i}\nabla_x\psi_\sigma^\dagger(r)\right)\psi_\sigma(r)\right] && (20a)\\ &= -\frac{e}{m}\sum_\sigma\int d^3r\,\psi_\sigma^\dagger(r)\frac{\hbar}{i}\nabla_x\psi_\sigma(r) && (20b)\end{aligned}}$$

$$j_x = j_x^{(p)} - \frac{e^2}{m\cancel{c}}\underbrace{\int d^3r\,\rho(r)}_{N}\ \underbrace{A_x(r,t)}_{-E\cancel{c}t}$$

$$= j_x^{(p)} + \frac{Ne^2Et}{m}$$

$$\therefore\ \frac{\delta\langle j_x(t)\rangle}{\delta E} = \frac{\delta\langle j_x^{(p)}(t)\rangle}{\delta E} + \frac{Ne^2t}{m} \qquad (21)$$

$$\frac{\delta}{\delta E}\langle j_x^{(P)}(t)\rangle$$

$$= \frac{\delta}{\delta E}\langle \Psi_0 | S_-(t_0,t)\, j_{xH}(t)\, S_+(t,t_0) | \Psi_0\rangle$$

Here,

$$\frac{\delta}{\delta E} S_\pm(t,t') = \frac{\delta}{\delta E} T_\pm \exp\left[-\frac{i}{\hbar}\int_{t'}^{t} dt_1\, \underbrace{V_H(t_1)}\right]$$

$$\frac{\delta}{\delta E} V_H(t_1) = t_1 j_{xH}^{(P)}(t_1)$$

$$= -\frac{i}{\hbar}\int_{t'}^{t} dt_1\, T_\pm\left[t_1 j_{xH}^{(P)}(t_1)\, S_\pm(t,t')\right]$$

Noting that $t \gtrless t'$ for $S_\pm(t,t')$,

$$\frac{\delta}{\delta E}\langle j_x^{(P)}(t)\rangle$$

$$= -\frac{i}{\hbar}\int_0^t dt_1\, \langle \Psi_0 | S_-(t_0,t)\, [j_{xH}^{(P)}(t),\, t_1 j_{xH}^{(P)}(t_1)]\, S_+(t,t_0) | \Psi_0\rangle$$

$$\rightarrow -\frac{i}{\hbar}\int_0^t dt_1\, t_1 \,\langle \Psi_0 | [j_{xH}^{(P)}(t),\, j_{xH}^{(P)}(t_1)] | \Psi_0\rangle \qquad (E\rightarrow 0)$$

$$\sigma \equiv \lim_{t\to\infty} \left.\frac{\delta\langle j_x(t)\rangle}{\delta E}\right|_{E\to 0} \tag{21}$$

$$= \lim_{t\to\infty}\left\{-\frac{i}{\hbar}\int_0^t dt\, t_1 \langle \Psi_0 | [j_x(t), j_x(t_1)] | \Psi_0\rangle + \frac{Ne^2 t}{m}\right\} \tag{22}$$

↳ omit (P) since no field exist.

$$\mu \equiv \sigma / N \tag{23}$$

$$= \lim_{t\to\infty}\left\{-\frac{i}{\hbar N}\int_0^t dt_1\, t_1 \langle \Psi_0 | [j_x(t), j_x(t_1)] | \Psi_0\rangle + \frac{e^2 t}{m}\right\} \tag{24}$$

$$\mu = \lim_{t\to\infty}\Big\{ \frac{i}{\hbar N}\int_0^t dt_1 \underbrace{(t-t_1)}_{\tau} \langle\psi_0|\underbrace{[\dot{j}_x(t), \dot{j}_x(t_1)]}_{[\dot{j}_x(t-t_1),\, \dot{j}_x(0)]}|\psi_0\rangle$$

$$- \frac{it}{\hbar N}\int_0^t dt_1 \langle\psi_0|\underbrace{[\dot{j}_x(t), \dot{j}_x(t_1)]}_{[\dot{j}_x(t-t_1),\, \dot{j}_x(0)]}|\psi_0\rangle + \frac{e^2 t}{m}\Big\}$$

$$= \lim_{t\to\infty}\Big\{\frac{i}{\hbar N}\int_0^{t\to\infty} d\tau\,\tau \langle[\dot{j}_x(\tau), \dot{j}_x(0)]\rangle$$

$$- \frac{it}{\hbar N}\int_0^{t\to\infty} d\tau \langle[\dot{j}_x(\tau), \dot{j}_x(0)]\rangle + \frac{e^2 t}{m}\Big\}$$

$$\therefore \mu = \frac{i}{\hbar N}\int_0^\infty dt\, t \langle[\dot{j}_x(t), \dot{j}_x(0)]\rangle$$

$$+ \lim_{t\to\infty} t\Big\{-\frac{i}{\hbar N}\int_0^\infty dt \langle[\dot{j}_x(t), \dot{j}_x(0)]\rangle + \frac{e^2}{m}\Big\} \qquad (1')$$

$$\boxed{\therefore \mu \equiv \lim_{t\to\infty}\frac{1}{N}\frac{\delta\langle j_x(t)\rangle}{\delta E}\Big|_{E\to 0} = \frac{i}{\hbar N}\int_0^\infty dt\, t \langle[\dot{j}_x(t), \dot{j}_x(0)]\rangle \qquad (2')}$$

because

$$\frac{i}{\hbar N}\int_0^\infty dt \langle[\dot{j}_x(t), \dot{j}_x(0)]\rangle = \frac{e^2}{m}. \qquad (3')$$

☺ Define the longitudinal current as

$$j_\ell(\vec{k}) = \hat{k}\cdot\vec{j}(\vec{k}) \qquad (4')$$

so that the continuity equation takes a form

$$\dot{\rho}(\vec{k}) + ik\, j_\ell(\vec{k}) = 0 \qquad (5')$$

Consider a quantity

$$I = \frac{i}{\hbar N}\int_0^\infty dt \langle[\underbrace{\dot{j}_\ell(\vec{k}\to 0,t)}_{\frac{i}{k}\dot{\rho}(\vec{k}\to 0,t)}, j_\ell(-\vec{k}\to 0,0)]\rangle$$

$$= -\frac{1}{\hbar N k}\Big[\langle[\rho(\vec{k},t), j_\ell(-\vec{k},0)]\rangle\Big]_0^{\cancel{\infty}}$$ ⤳ if vanishes quickly

$$= \frac{1}{\hbar N k}\langle[\rho(\vec{k}), j_\ell(-\vec{k})]\rangle$$

Here

∘ $$\rho(\vec{k}) = -e\sum_\sigma\int d^3r\, e^{-i\vec{k}\cdot\vec{r}}\underbrace{\psi_\sigma^+(\vec{r})}_{\frac{1}{\sqrt{V}}\sum_{k_1} a^+_{\vec{k}_1\sigma}e^{-i\vec{k}_1\cdot\vec{r}}}\underbrace{\psi_\sigma(\vec{r})}_{\frac{1}{\sqrt{V}}\sum_{k_2} a_{\vec{k}_2\sigma}e^{i\vec{k}_2\cdot\vec{r}}}$$

$$= -\frac{e}{\cancel{V}}\sum_\sigma\sum_{k_1k_2} a^+_{\vec{k}_1\sigma}a_{\vec{k}_2\sigma}\underbrace{\int d^3r\, e^{i(-\vec{k}-\vec{k}_1+\vec{k}_2)\cdot\vec{r}}}_{\cancel{V}\delta_{\vec{k}_1-\vec{k}_2,-\vec{k}}}$$

$$= -e\sum_{p\sigma} a^+_{\vec{p}-\vec{k}/2\,\sigma}a_{\vec{p}+\vec{k}/2\,\sigma}$$

∘ $$\vec{j}(\vec{k}) = -e\sum_\sigma\int d^3r\, e^{-i\vec{k}\cdot\vec{r}}\Big[\psi_\sigma^+(\vec{r})\frac{\hbar}{i}\nabla\psi_\sigma(\vec{r}) - \Big(\frac{\hbar}{i}\nabla\psi^+_\sigma(\vec{r})\Big)\psi_\sigma(\vec{r})\Big]/2m$$

$$= -\frac{e}{m\cancel{V}}\sum_\sigma\sum_{k_1k_2} a^+_{\vec{k}_1\sigma}a_{\vec{k}_2\sigma}\frac{\hbar(\vec{k}_1+\vec{k}_2)}{2}\underbrace{\int d^3r\, e^{i(-\vec{k}-\vec{k}_1+\vec{k}_2)\cdot\vec{r}}}_{\cancel{V}\delta_{\vec{k}_1-\vec{k}_2,-\vec{k}}}$$

$$= -\frac{e}{m}\sum_{p\sigma}\hbar\vec{p}\, a^+_{\vec{p}-\vec{k}/2\sigma}a_{\vec{p}+\vec{k}/2\sigma}$$

$$\therefore\ j_\ell(\vec{k}) = -\frac{e\hbar}{m}\sum_{\vec{p}\sigma}\hat{k}\cdot\vec{p}\,a^\dagger_{\vec{p}-\vec{k}/2\sigma}a_{\vec{p}+\vec{k}/2\sigma}$$

Then,

$$I = \frac{1}{\cancel{\hbar}Nk}\cdot\frac{e^2\cancel{\hbar}}{m}\sum_{\vec{p}\sigma}\sum_{\vec{p}'\lambda}\hat{k}\cdot\vec{p}'\,\langle[\underbrace{a^\dagger_{\vec{p}-\vec{k}/2\sigma}a_{\vec{p}+\vec{k}/2\sigma},\ a^\dagger_{\vec{p}'+\vec{k}/2\lambda}a_{\vec{p}'-\vec{k}/2\lambda}}_{a^\dagger_{\vec{p}-\vec{k}/2\sigma}\delta_{\vec{p}\vec{p}'}\delta_{\sigma\lambda}a_{\vec{p}'-\vec{k}/2\lambda}\ -\ a^\dagger_{\vec{p}'+\vec{k}/2\lambda}\delta_{\vec{p}\vec{p}'}\delta_{\sigma\lambda}a_{\vec{p}+\vec{k}/2\sigma}}]\rangle$$

$$= \frac{e^2}{mNk}\sum_{\vec{p}\sigma}\hat{k}\cdot\vec{p}\,[\langle a^\dagger_{\underbrace{\vec{p}-\vec{k}/2}_{\vec{p}}\sigma}a_{\vec{p}-\vec{k}/2\sigma}\rangle - \langle a^\dagger_{\underbrace{\vec{p}+\vec{k}/2}_{\vec{p}}\sigma}a_{\vec{p}+\vec{k}/2\sigma}\rangle]$$

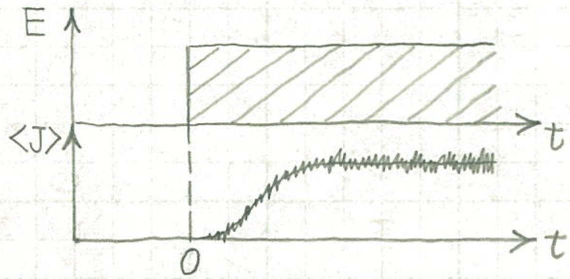
$$= \frac{e^2}{mN\cancel{k}}\sum_{\vec{p}\sigma}\underbrace{\hat{k}\cdot[\cancel{\vec{p}}+\frac{\vec{k}}{2}-\cancel{\vec{p}}+\frac{\vec{k}}{2}]}_{\cancel{k}}\langle a^\dagger_{\vec{p}\sigma}a_{\vec{p}\sigma}\rangle$$

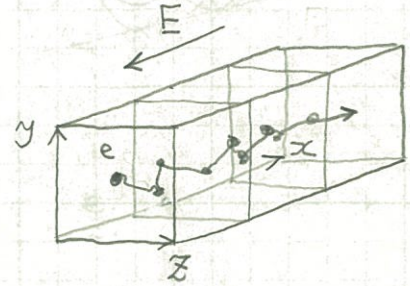
$$= \frac{e^2}{m\cancel{N}}\underbrace{\sum_{\vec{p}\sigma}\langle a^\dagger_{\vec{p}\sigma}a_{\vec{p}\sigma}\rangle}_{\sum_\sigma\int d^3r\langle\psi^\dagger_\sigma(\vec{r})\psi_\sigma(\vec{r})\rangle = \cancel{N}} = \frac{e^2}{m} \quad //$$

§. Simulation for Mobilities

$$\mu \equiv \lim_{t\to\infty} \frac{1}{N} \frac{\langle j_x(t)\rangle}{E} \tag{25}$$

$$\langle j_x(t)\rangle = -\frac{e}{m}\sum_\sigma \int d^3r \, \langle \Phi(t)|\, \hat{\psi}_\sigma^\dagger(r)\, [\tfrac{\hbar}{i}\nabla_x - eEt]\, \hat{\psi}_\sigma(r)\, |\Phi(t)\rangle \tag{26}$$

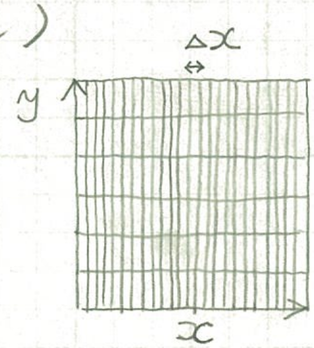


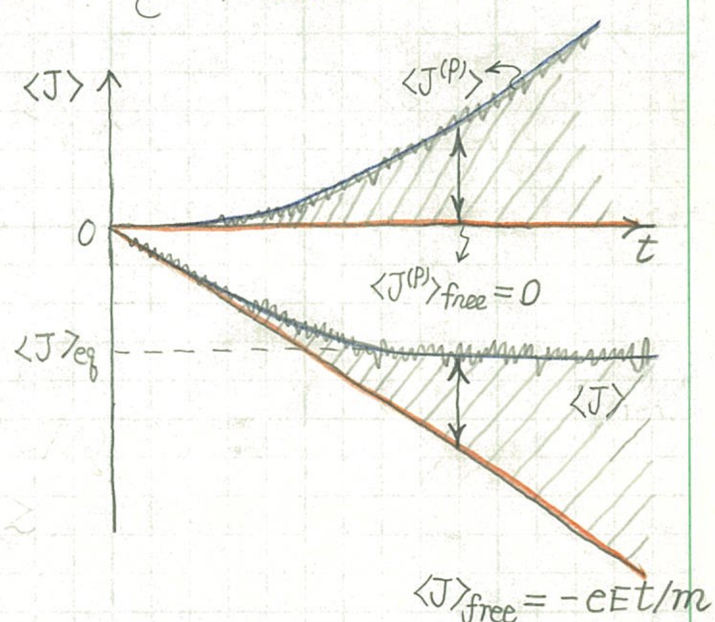


$$e^{-ip^2\Delta t/4m\hbar}\, e^{-iv(r,t)\Delta t/\hbar}\, e^{-ip^2\Delta t/4m\hbar}$$

$$\rightarrow e^{-i(p-eEt)^2\Delta t/4m\hbar}\, e^{-iv(r,t)\Delta t/\hbar}\, e^{-i(p-eEt)^2\Delta t/4m\hbar}$$

(Size of Mesh)





※ Assure that

$$k_{max} = \frac{\pi}{\Delta x} \gtrsim \langle J\rangle_{eq} + \frac{eE\tau_{eq}}{m} \ll \left|\frac{eE\tau_{eq}}{m}\right|$$