Lectures on Berry phase related phyiscs

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June 19, 2018

Contents of lectures

Topics

- Berry phase and physical properties
- Berry phase and physical properties 2
- Berry phase and physical properties 3
- Berry curvature and anomalous Hall conductivity
- Topological invariant: Chern number and Z_2
- Computing Chern number and Z_2 as local quantity

Electric polarization expressed by wave function

$$P = \frac{e}{V}\sum_{n=1}^{occ}\langle\psi_n|\boldsymbol{r}|\psi_n\rangle$$

$$H|\psi_n\rangle = E_n|\psi_n\rangle$$

$$\begin{aligned}
\frac{dP}{dt} &= \frac{e}{V}\sum_{n=1}^{occ}\frac{d}{dt}\langle\psi_n|\boldsymbol{r}|\psi_n\rangle \\
&= \frac{e}{V}\sum_{n=1}^{occ}\left(\langle\dot{\psi}_n|\boldsymbol{r}|\psi_n\rangle + \langle\psi_n|\boldsymbol{r}|\dot{\psi}_n\rangle\right) \\
&= \frac{e}{V}\sum_{n=1}^{occ}\sum_{m=1}^{\infty}(\langle\dot{\psi}_n|\psi_m\rangle\langle\psi_m|\boldsymbol{r}|\psi_n\rangle \\
&+ \langle\psi_n|\boldsymbol{r}|\psi_m\rangle\langle\psi_m|\dot{\psi}_n\rangle)
\end{aligned}$$

Electric currents and polarization II

Electric polarization expressed by wave function

$$\begin{aligned}\frac{d\boldsymbol{P}}{dt} &= \frac{e}{V}\sum_{n=1}^{occ}\sum_{m=1}^{\infty}\left(\langle\dot{\psi}_n|\psi_m\rangle\langle\psi_m|\boldsymbol{r}|\psi_n\rangle\right. \\ &+ \left.\langle\psi_n|\boldsymbol{r}|\psi_m\rangle\langle\psi_m|\dot{\psi}_n\rangle\right)\end{aligned}$$

Velocity operator

$$\begin{aligned}\langle\psi_m|\boldsymbol{v}|\psi_n\rangle &= i\hbar\langle\psi_m|[\boldsymbol{r}, H]|\psi_n\rangle = i\hbar(E_n - E_m)\langle\psi_m|\boldsymbol{r}|\psi_n\rangle \\ \langle\psi_m|\boldsymbol{r}|\psi_n\rangle &= \frac{\langle\psi_m|\boldsymbol{v}|\psi_n\rangle}{i\hbar(E_n - E_m)} \\ \langle\psi_n|\boldsymbol{r}|\psi_m\rangle &= (\langle\psi_m|\boldsymbol{r}|\psi_n\rangle)^*\end{aligned}$$

Electric currents and polarization III

Electric polarization expressed by wave function

$$\frac{dP}{dt} = \frac{-ie}{V\hbar}\sum_{n=1}^{occ}\sum_{m\neq n}\left(\frac{\langle\dot{\psi}_n|\psi_m\rangle\langle\psi_m|v|\psi_n\rangle}{(E_n - E_m)} - c.c\right)$$

Bloch wavefunction and its periodic part

$$\begin{aligned}
|\psi_n^{\boldsymbol{k}}\rangle &= e^{i\boldsymbol{k}\cdot\boldsymbol{r}}|u_n^{\boldsymbol{k}}\rangle \\
H|\psi_n^{\boldsymbol{k}}\rangle &= E_n^{\boldsymbol{k}}|\psi_n^{\boldsymbol{k}}\rangle \\
e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}He^{i\boldsymbol{k}\cdot\boldsymbol{r}}|u_n^{\boldsymbol{k}}\rangle &= E_n^{\boldsymbol{k}}|u_n^{\boldsymbol{k}}\rangle \\
\tilde{H}|u_n^{\boldsymbol{k}}\rangle &= E_n^{\boldsymbol{k}}|u_n^{\boldsymbol{k}}\rangle \\
\langle\psi_m^{\boldsymbol{k}}|v|\psi_n^{\boldsymbol{k}}\rangle &= \langle u_m^{\boldsymbol{k}}|\tilde{v}|u_n^{\boldsymbol{k}}\rangle
\end{aligned}$$

Electric currents and polarization IV

Heisenberg Equation of Motion

$$
\begin{aligned}
i\hbar\frac{d\boldsymbol{r}}{dt} &= [\boldsymbol{r}, H] \\
i\hbar\boldsymbol{v} &= [\boldsymbol{r}, H]
\end{aligned}
$$

Bloch wavefunction and its periodic part

$$
\begin{aligned}
\tilde{H} &= e^{-i\boldsymbol{k}\cdot\boldsymbol{r}} H e^{i\boldsymbol{k}\cdot\boldsymbol{r}} \\
e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}[\boldsymbol{r}, H]e^{i\boldsymbol{k}\cdot\boldsymbol{r}} &= e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}\left(i\hbar\frac{d\boldsymbol{r}}{dt}\right)e^{i\boldsymbol{k}\cdot\boldsymbol{r}} = i\hbar\tilde{\boldsymbol{v}} \\
\text{if } [\nabla_{\boldsymbol{k}}, H] = 0, & \\
\nabla_{\boldsymbol{k}}\tilde{H} &= -i\boldsymbol{r}e^{-i\boldsymbol{k}\cdot\boldsymbol{r}} H e^{i\boldsymbol{k}\cdot\boldsymbol{r}} + e^{-i\boldsymbol{k}\cdot\boldsymbol{r}} H e^{i\boldsymbol{k}\cdot\boldsymbol{r}} i\boldsymbol{r} \\
\nabla_{\boldsymbol{k}}\tilde{H} &= -i[\boldsymbol{r}, \tilde{H}] = \hbar\tilde{\boldsymbol{v}} \\
\langle\psi_m^{\boldsymbol{k}}|\boldsymbol{v}|\psi_n^{\boldsymbol{k}}\rangle &= \langle u_m^{\boldsymbol{k}}|\tilde{\boldsymbol{v}}|u_n^{\boldsymbol{k}}\rangle = \langle u_m^{\boldsymbol{k}}|\frac{\nabla_{\boldsymbol{k}}\tilde{H}}{\hbar}|u_n^{\boldsymbol{k}}\rangle
\end{aligned}
$$

Electric currents and polarization V

Electric polarization expressed by wave function

$$
\begin{aligned}
\frac{dP}{dt} &= \frac{-ie}{8\pi^3\hbar}\int_{BZ} d\boldsymbol{k} \sum_{n=1}^{occ}\sum_{m\neq n}\left(\frac{\langle\dot{\psi}_n^{\boldsymbol{k}}|\psi_m^{\boldsymbol{k}}\rangle\langle\psi_m^{\boldsymbol{k}}|v|\psi_n^{\boldsymbol{k}}\rangle}{(E_n^{\boldsymbol{k}}-E_m^{\boldsymbol{k}})} - c.c\right)\\
&= \frac{-ie}{8\pi^3\hbar}\int_{BZ} d\boldsymbol{k} \sum_{n=1}^{occ}\sum_{m\neq n}\left(\frac{\langle\dot{u}_n^{\boldsymbol{k}}|u_m^{\boldsymbol{k}}\rangle\langle u_m^{\boldsymbol{k}}|\tilde{v}|u_n^{\boldsymbol{k}}\rangle}{(E_n^{\boldsymbol{k}}-E_m^{\boldsymbol{k}})} - c.c\right)\\
&= \frac{-ie}{8\pi^3}\int_{BZ} d\boldsymbol{k} \sum_{n=1}^{occ}\sum_{m\neq n}\left(\frac{\langle\dot{u}_n^{\boldsymbol{k}}|u_m^{\boldsymbol{k}}\rangle\langle u_m^{\boldsymbol{k}}|\nabla_{\boldsymbol{k}}\tilde{H}|u_n^{\boldsymbol{k}}\rangle}{(E_n^{\boldsymbol{k}}-E_m^{\boldsymbol{k}})} - c.c\right)\\
&= \frac{-ie}{8\pi^3}\int_{BZ} d\boldsymbol{k} \sum_{n=1}^{occ}\left(\langle\dot{u}_n^{\boldsymbol{k}}|\nabla_{\boldsymbol{k}}u_n^{\boldsymbol{k}}\rangle - \langle\nabla_{\boldsymbol{k}}u_n^{\boldsymbol{k}}|\dot{u}_n^{\boldsymbol{k}}\rangle\right)
\end{aligned}
$$

Electric currents and polarization VI

First-order perturbation theory

$$
\begin{aligned}
\delta\tilde{H} &= \tilde{H}(k+\Delta k) - \tilde{H}(k) \\
|u_n^{\boldsymbol{k}+\boldsymbol{\Delta k}}\rangle &= |u_n^{\boldsymbol{k}}\rangle \\
&+ \sum_{m\neq n} |u_m^{\boldsymbol{k}}\rangle \frac{\langle u_m^{\boldsymbol{k}}|\delta\tilde{H}|u_n^{\boldsymbol{k}}\rangle}{E_n^{\boldsymbol{k}} - E_m^{\boldsymbol{k}}} + O(\delta\tilde{H}^2) \\
|\nabla_{\boldsymbol{k}} u_n^{\boldsymbol{k}}\rangle &\simeq \sum_{m\neq n} |u_m^{\boldsymbol{k}}\rangle \frac{\langle u_m^{\boldsymbol{k}}|\nabla_{\boldsymbol{k}}\tilde{H}|u_n^{\boldsymbol{k}}\rangle}{E_n^{\boldsymbol{k}} - E_m^{\boldsymbol{k}}}
\end{aligned}
$$

Ordinary derivative to partial derivative

$$
\frac{d}{dt}|u_{k_\alpha,t}\rangle = \partial_{k_\alpha}|u_{k_\alpha,t}\rangle \frac{dk_\alpha}{dt} + \partial_t|u_{k_\alpha,t}\rangle = \partial_t|u_{k_\alpha,t}\rangle
$$

Electric currents and polarization VII

Electric polarization expressed by wave function

$$\int_0^{\Delta t} dt \frac{d\boldsymbol{P}}{dt} = \boldsymbol{P}(\Delta t) - \boldsymbol{P}(0)$$

$$= \frac{-ie}{8\pi^3} \int_0^{\Delta t} dt \int_{BZ} d\boldsymbol{k} \sum_{n=1}^{occ} \left(\langle \dot{u}_n^{\boldsymbol{k}} | \nabla_{\boldsymbol{k}} u_n^{\boldsymbol{k}} \rangle - \langle \nabla_{\boldsymbol{k}} u_n^{\boldsymbol{k}} | \dot{u}_n^{\boldsymbol{k}} \rangle \right)$$

$$= \frac{-ie}{8\pi^3} \int_0^{\Delta t} dt \int_{BZ} d\boldsymbol{k} \sum_{n=1}^{occ} \left(\partial_t \langle u_n^{\boldsymbol{k}} | \nabla_{\boldsymbol{k}} u_n^{\boldsymbol{k}} \rangle - \nabla_{\boldsymbol{k}} \langle u_n^{\boldsymbol{k}} | \dot{u}_n^{\boldsymbol{k}} \rangle \right)$$

For k_α direction,

$$P_\alpha(\Delta t) - P_\alpha(0)$$

$$= \frac{ie}{8\pi^3} \int dk_\beta dk_\gamma \times$$

$$\int_0^{\Delta t} dt \int_0^{G_\alpha} dk_\alpha \sum_{n=1}^{occ} \left(\partial_{k_\alpha} \langle u_n^{\boldsymbol{k}} | \partial_t u_n^{\boldsymbol{k}} \rangle - \partial_t \langle u_n^{\boldsymbol{k}} | \partial_{k_\alpha} u_n^{\boldsymbol{k}} \rangle \right)$$

Electric polarization expressed by wave function

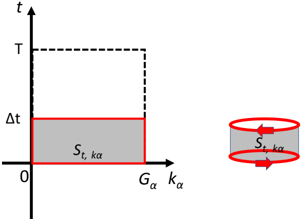
$$\boldsymbol{\nabla}_{k_\alpha,t} \equiv (\partial_{k_\alpha}, \partial_t, \partial), \quad \boldsymbol{A}^n = (A^n_{k_\alpha}, A^n_t, 0)$$
$$d\boldsymbol{S} = (0, 0, dtdk_\alpha), \quad A^n_\mu = \langle u^{\boldsymbol{k}}_n | \partial_\mu u^{\boldsymbol{k}}_n \rangle$$

$$\begin{aligned} & P_\alpha(\Delta t) - P_\alpha(0) \\ = \ & \frac{ie}{8\pi^3} \int dk_\beta dk_\gamma \sum_{n=1}^{occ} \int_{S_{t,k_\alpha}} (\boldsymbol{\nabla}_{k_\alpha,t} \times \boldsymbol{A}^n) \cdot d\boldsymbol{S}_{t,\alpha} \\ = \ & \frac{ie}{8\pi^3} \int dk_\beta dk_\gamma \sum_{n=1}^{occ} \oint_{\partial S_{t,k_\alpha}} \boldsymbol{A}^n \cdot d\boldsymbol{l} \end{aligned}$$

Electric currents and polarization IX

Electric polarization expressed by wave function

$$
\begin{aligned}
&\sum_{n=1}^{occ} \oint_{\partial S_{t,k\alpha}} \boldsymbol{A}^n \cdot d\boldsymbol{l} = \\
&\sum_{n=1}^{occ} \int_0^{G_\alpha} dk_\alpha \left(\langle u_n^{\boldsymbol{k}}(0) | \partial_{k_\alpha} u_n^{\boldsymbol{k}}(0) \rangle - \langle u_n^{\boldsymbol{k}}(\Delta t) | \partial_{k_\alpha} u_n^{\boldsymbol{k}}(\Delta t) \rangle \right) \\
+ \; &\int_0^{\Delta t} dt \left(\langle u_n^{G_\alpha} | \partial_t u_n^{G_\alpha} \rangle - \langle u_n^0 | \partial_t u_n^0 \rangle \right)
\end{aligned}
$$



Electric currents and polarization X

Electric polarization expressed by wave function

$$\sum_{n=1}^{occ} \oint_{\partial S_{t,k\alpha}} \boldsymbol{A}^n \cdot d\boldsymbol{l} =$$

$$-\sum_{n=1}^{occ} \int_0^{G_\alpha} dk_\alpha \left(\langle u_n^{\boldsymbol{k}}(\Delta t) | \partial_{k_\alpha} u_n^{\boldsymbol{k}}(\Delta t) \rangle - \langle u_n^{\boldsymbol{k}}(0) | \partial_{k_\alpha} u_n^{\boldsymbol{k}}(0) \rangle \right)$$

$$P_\alpha(t) = \frac{-ie}{8\pi^3} \int dk_\beta dk_\gamma \sum_{n=1}^{occ} \int_0^{G_\alpha} dk_\alpha \langle u_n^{\boldsymbol{k}}(t) | \partial_{k_\alpha} | u_n^{\boldsymbol{k}}(t) \rangle$$

$$= \frac{e}{8\pi^3} \int dk_\beta dk_\gamma \sum_{n=1}^{occ} \mathrm{Im} \int_0^{G_\alpha} dk_\alpha \langle u_n^{\boldsymbol{k}}(t) | \partial_{k_\alpha} | u_n^{\boldsymbol{k}}(t) \rangle$$

Example: Orthorhombic unitcell

Case: $(k_\beta, k_\gamma) = (0,0)$ sampling , $G_\beta = \frac{2\pi}{b}$, $G_\gamma = \frac{2\pi}{c}$

$$
\begin{aligned}
P_\alpha(t) &= \frac{e}{8\pi^3}\int dk_\beta dk_\gamma \sum_{n=1}^{occ} \mathrm{Im}\int_0^{G_\alpha} dk_\alpha \langle u_n^{\boldsymbol{k}}(t)|\partial_{k_\alpha}|u_n^{\boldsymbol{k}}(t)\rangle \\
&= \frac{e}{8\pi^3}\int dk_\beta dk_\gamma \phi(t) \\
&= \frac{e}{8\pi^3}\frac{2\pi}{b}\frac{2\pi}{c}\phi(t) = \frac{e}{2\pi bc}\phi(t) = \frac{ea}{2\pi abc}\phi(t) \\
&= \frac{ea}{2\pi\Omega_{cell}}\phi(t) = \frac{ea}{\Omega_{cell}}\left(\frac{\phi(t)}{2\pi}\right)
\end{aligned}
$$

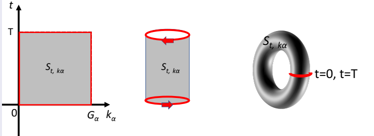
Electric currents and polarization XII

What is a Chern number in $k_\alpha - t$ space?

- Electron moves $a = \langle x(T)\rangle - \langle x(0)\rangle$, i.e., $v_\alpha T = a$.
- Chern number C is given by $2\pi C$ as an integrated Berry curvature over any 2D manifold.

Example: one electron in a unit cell ($C = 1$)

$$
\begin{aligned}
& P_\alpha(T) - P_\alpha(0) \\
= \; & \frac{ie}{8\pi^3}\int dk_\beta dk_\gamma \int_{S_{t,k\alpha}} (\boldsymbol{\nabla}_{k_\alpha,t} \times \boldsymbol{A}) \cdot d\boldsymbol{S}_{t,\alpha} \\
= \; & \frac{ea}{\Omega_{cell}}\left(\frac{\phi(T) - \phi(0)}{2\pi}\right) = \frac{ea}{\Omega_{cell}}
\end{aligned}
$$



Computing Electric Polarization I

Numerical calculation of Berry Phase

$$
\begin{aligned}
P_\alpha(t) &= \frac{e}{8\pi^3}\int dk_\beta dk_\gamma \sum_{n=1}^{occ} \mathrm{Im}\int_0^{G_\alpha} dk_\alpha \langle u_n^{\boldsymbol{k}}(t)|\partial_{k_\alpha}|u_n^{\boldsymbol{k}}(t)\rangle \\
&= \frac{e}{8\pi^3}\int dk_\beta dk_\gamma \phi(t) \\
\phi(t) &= \sum_{n=1}^{occ} \mathrm{Im}\int_0^{G_\alpha} dk_\alpha \langle u_n^{\boldsymbol{k}}(t)|\partial_{k_\alpha}|u_n^{\boldsymbol{k}}(t)\rangle
\end{aligned}
$$

Numerical calculation of Berry Phase

$$\phi(t) = \sum_{n=1}^{occ} \mathrm{Im} \int_0^{G_\alpha} dk_\alpha \langle u_n^{\boldsymbol{k}}(t) | \partial_{k_\alpha} | u_n^{\boldsymbol{k}}(t) \rangle$$

We difine overlap matrix $S(\boldsymbol{k}, \boldsymbol{k}')$, where
$S_{nm}(\boldsymbol{k}, \boldsymbol{k}') \equiv \langle u_n^{\boldsymbol{k}}(t) | u_n^{\boldsymbol{k}}(t) \rangle$.
We use well-known matrix identity, det exp $A =$ exp tr A, when $A = \log S \leftrightarrow \exp A = S$. log det$S =$ tr log$S$.

$$\begin{aligned} \phi(t) &= \mathrm{Im} \int_0^{G_\alpha} dk_\alpha \mathrm{tr} \partial_{k'_\alpha} \langle u_n^{\boldsymbol{k}}(t) | u_m^{\boldsymbol{k}'}(t) \rangle |_{\boldsymbol{k}'=\boldsymbol{k}} \\ &= \mathrm{Im} \int_0^{G_\alpha} dk_\alpha \mathrm{tr} \partial_{k'_\alpha} S(\boldsymbol{k}, \boldsymbol{k}') |_{\boldsymbol{k}=\boldsymbol{k}'} \end{aligned}$$

Computing Electric Polarization III

Numerical calculation of Berry Phase

- $A = \log S \leftrightarrow \exp A = S$
- $\det \exp A = \exp \operatorname{tr} A$, $\log \det S = \operatorname{tr} \log S$
- $S_{nm}(\boldsymbol{k}, \boldsymbol{k}')|_{\boldsymbol{k}=\boldsymbol{k}'} = \delta_{mn}$

$$
\begin{aligned}
\phi(t) &= \operatorname{Im} \int_0^{G_\alpha} dk_\alpha \operatorname{tr} \partial_{k'_\alpha} S(\boldsymbol{k}, \boldsymbol{k}')|_{\boldsymbol{k}=\boldsymbol{k}'} \\
&= \operatorname{Im} \int_0^{G_\alpha} dk_\alpha \operatorname{tr} \left[\frac{\partial_{k'_\alpha} S(\boldsymbol{k}, \boldsymbol{k}')}{S(\boldsymbol{k}, \boldsymbol{k}')} \right]_{|_{\boldsymbol{k}=\boldsymbol{k}'}} \\
&= \operatorname{Im} \int_0^{G_\alpha} dk_\alpha \operatorname{tr} \partial_{k'_\alpha} \log\, S(\boldsymbol{k}, \boldsymbol{k}')|_{\boldsymbol{k}=\boldsymbol{k}'} \\
&= \operatorname{Im} \int_0^{G_\alpha} dk_\alpha \partial_{k'_\alpha} \log\, \det S(\boldsymbol{k}, \boldsymbol{k}')|_{\boldsymbol{k}=\boldsymbol{k}'}
\end{aligned}
$$

Computing Electric Polarization IV

Numerical calculation of Berry Phase

$$\phi(t) \;=\; \mathrm{Im} \int_0^{G_\alpha} dk_\alpha \partial_{k'_\alpha} \log\, \det S(\boldsymbol{k}, \boldsymbol{k}')|_{\boldsymbol{k}=\boldsymbol{k}'}$$

If we use k-point sampling mesh J along k_α direction, $k_{\alpha,s} = sG_\alpha/J$ and $\Delta k_\alpha = G_\alpha/\mathrm{J}$.

$$\phi(t) = \mathrm{Im} \lim_{\Delta k_\alpha \to 0} \sum_{s=0}^{J-1} \Delta k_\alpha \times$$

$$\frac{\log\det S_{nm}(k_{\alpha,s}, k_{\alpha,s} + \Delta k_\alpha) - \log\det S_{nm}(k_{\alpha,s}, k_{\alpha,s})}{\Delta k_\alpha}$$

$$\phi(t) = \mathrm{Im} \lim_{\Delta k_\alpha \to 0} \sum_{s=0}^{J-1} \log\det S_{nm}(k_{\alpha,s} k_{\alpha,s} + \Delta k_\alpha)$$

Numerical calculation of Berry Phase

$$P_\alpha(t) = \frac{e}{8\pi^3} \int dk_\beta dk_\gamma$$
$$\mathrm{Im} \lim_{\Delta k_\alpha \to 0} \sum_{s=0}^{J-1} \log \det S_{nm}(k_{\alpha,s} k_{\alpha,s} + \Delta k_\alpha)$$

Expectation value of position operator in PBC

Ill-defined position operator in PBC

$$\begin{aligned} \psi_k(x+L) &= \psi(x) \\ \hat{A}\psi_k(x) &= \phi(x) = \phi(x+L) \\ \hat{x}\psi_k(x) &= x\psi_k(x) \neq (x+L)\psi_k(x+L) \end{aligned}$$

Resta's definition of position operator in PBC

$$\begin{aligned} \langle \hat{x} \rangle &= \frac{L}{2\pi} \mathrm{Im} \log \int dx \psi_k(x)^* e^{i\frac{2\pi}{L}\hat{x}} \psi_k(x) \\ &= \int dx \psi_k(x+L)^* e^{i\frac{2\pi}{L}\hat{x}} \psi_k(x+L) \\ &= \frac{L}{2\pi} \mathrm{Im} \log \langle \psi_k | e^{i\frac{2\pi}{L}\hat{x}} | \psi_k \rangle \end{aligned}$$

Expectation value of position operator in PBC II

Resta's definition of position operator in PBC and electric current for thermodynamic limit

$$
\begin{aligned}
\frac{d\langle \hat{x} \rangle}{dt} &= \frac{d}{dt}\frac{L}{2\pi}\mathrm{Im}\log\langle \psi_k | e^{i\frac{2\pi}{L}\hat{x}} | \psi_k \rangle \\
&= \frac{L}{2\pi}\mathrm{Im}\frac{\langle \dot{\psi}_k | e^{i\frac{2\pi}{L}\hat{x}} | \psi_k \rangle + \langle \psi_k | e^{i\frac{2\pi}{L}\hat{x}} | \dot{\psi}_k \rangle}{\langle \psi_k | e^{i\frac{2\pi}{L}\hat{x}} | \psi_k \rangle} \\
&\simeq \langle \dot{\psi}_k | \hat{x} | \psi_k \rangle + \langle \psi_k | \hat{x} | \dot{\psi}_k \rangle
\end{aligned}
$$

(for $L = Na$, $N \to \infty$.)