How to see that these concepts survive interactions?

Bloch's theorem is valid only for non-interacting electrons. Once interaction is switched on, bands are not well defined, and therefore Bloch theorem is not valid.

Thouless introduced a trick with the twisted boundary condit. [Q. Niu, D.J. Thouless, Y-Shi Wu, PRB 31, 3372 (1985)]

Let the many body wave function $\Phi(\vec{r}_1,\vec{r}_2,\ldots\vec{r}_N)$ have the following boundary conditions

$$\Phi\left(\vec{r}_1+\begin{pmatrix}L_x\\0\\0\end{pmatrix},\vec{r}_2,\ldots\right)=e^{i\theta_x L_x}\,\Phi(\vec{r}_1,\vec{r}_2,\ldots)$$

$$\Phi\left(\vec{r}_1+\begin{pmatrix}0\\L_y\\0\end{pmatrix},\vec{r}_2\ldots\right)=e^{i\theta_y L_y}\,\Phi(\vec{r}_1,\vec{r}_2,\ldots)$$

If the system size is large, the precise form of the boundary condition should not matter, as long as it satisfies basic laws. Such B.C. are used to derive Berry phase formula for the interacting system.

To derive it, we will use Kubo formula for electric conductivity. We will compute Hall effect σ_{xy}, which is a current response $\langle j_x\rangle$ due to magnetic field in z-direction.

The action in the presence of the B-field is $S=S_0-\int \vec{j}_y\cdot\vec{A}\,dt$.

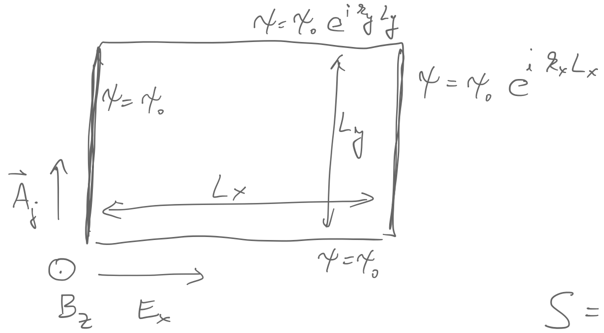
The derivation for polarization is analogous, except that the coupling for polarization is $S=S_0+\int\frac{\partial H}{\partial x}\dot{x}\,dt$

Reminder: $H=\int d^3r\,\psi^\dagger(\vec{r})\Big[\underbrace{\tfrac{1}{2m}\big(-i\hbar\tfrac{\partial}{\partial\vec{r}}-e\vec{A}\big)^2}_{-\frac{\hbar^2}{2m}\nabla^2+\frac{ie\hbar}{2m}\left(\frac{\partial}{\partial\vec{r}}\vec{A}+\vec{A}\frac{\partial}{\partial\vec{r}}\right)+\cancel{\frac{e^2}{2m}A^2}}+V_{ext}(\vec{r})\Big]\psi(\vec{r})+V_{int}[\psi^\dagger,\psi]$

$$H=\underbrace{\int d^3r\,\psi^\dagger(\vec{r})\Big[-\tfrac{\hbar^2}{2m}\nabla^2+V_{ext}(\vec{r})\Big]\psi(\vec{r})+V_{int}[\psi^\dagger\psi]}_{H_0}+\underbrace{\frac{ie\hbar}{2m}\int\vec{A}(\vec{r})\Big[\psi^\dagger(\vec{r})\frac{\partial}{\partial\vec{r}}\psi(\vec{r})-\underbrace{\Big(\frac{\partial}{\partial\vec{r}}\psi^\dagger\Big)}_{\text{by parts}}\psi(\vec{r})\Big]}_{-\int\vec{A}(\vec{r})\cdot\vec{j}(\vec{r})\,d^3r}$$

because $\vec{j}=\frac{e\hbar}{2mi}\left[\psi^\dagger\vec{\nabla}\psi-(\nabla\psi^\dagger)\psi\right]$

Hence: $S=S_0-\int\vec{A}\cdot\vec{j}\,dt$



$$\vec{B}=\vec{\nabla}\times\vec{A}=\begin{pmatrix}\frac{\partial}{\partial x}\\ \frac{\partial}{\partial y}\\ \frac{\partial}{\partial z}\end{pmatrix}\times\underbrace{\begin{pmatrix}0\\ Bx\\ 0\end{pmatrix}}=\begin{pmatrix}0\\0\\B\end{pmatrix}$$

This choice is called Landau gage

and $\vec{E}=-\frac{\partial\vec{A}}{\partial t}$

$E_y=-i\omega A_y$

$$S=S_0-\int\vec{A}\cdot\vec{j}\,d^4$$

$$\langle j_x(x)\rangle=\frac{1}{Z}\int\mathcal{D}[\psi^\dagger\psi]\,e^{-S_0+\int\vec{A}\cdot\vec{j}\,d^{4\prime}}j_x(x)\approx\frac{1}{Z_0}\int\mathcal{D}[\psi^\dagger\psi]\,e^{-S_0}\left(j_x(x)+\int\vec{A}(x')\vec{j}(x')\,j_x(x)\,d^4x'\right)=\int d^4x' A_y(x')\langle j_y(x')j_x(x)\rangle$$

note $\langle j_x\rangle_0=0$

$$\sum_{\vec{q},i\omega}\underbrace{\langle j_x(\vec{q},\omega)\rangle}_{\sigma^{xy}_q E_y(q,\omega)}e^{i\omega\tau-i\vec{q}\vec{r}}=\sum_{\vec{q},i\omega}\underbrace{A_y(\vec{q},\omega)}_{\frac{E_y(q,\omega)}{\omega}}\int e^{i\omega\tau'-i\vec{q}\vec{r}'}\langle j_y(\vec{r}',\tau')j_x(\vec{r},\tau)\rangle\,d^3r'd\tau'$$

Tricky issue:

real axis: $A_y(\omega)=\frac{E_y(\omega)}{-i\omega}$

imag. axis: $A_y(i\omega)=\frac{E_y(i\omega)}{-i(i\omega)}$

$A_y(i\omega)=\frac{E_y(i\omega)}{\omega}$

$$\sigma^{xy}_q(i\omega)\,e^{i\omega\tau-i\vec{q}\vec{r}}=\frac{1}{\omega}\int e^{i\omega\tau'-i\vec{q}\vec{r}'}\langle j_y(\vec{r}',\tau')j_x(\vec{r},\tau)\rangle\,d^3r'd\tau'$$

$$\sigma^{xy}_q(i\omega)=\frac{1}{\omega}\int e^{i\omega\tau-i\vec{q}\vec{r}}\langle j_y(\vec{r},\tau)j_x(0,0)\rangle\,d^3r\,d\tau$$

; $\vec{J}=e\vec{v}$ where

$\vec{v}=\frac{1}{m}(\vec{p}-e\vec{A})$

$q\to 0$

$$\sigma^{xy}(i\omega)=\frac{e^2}{\omega}\int e^{i\omega\tau}\frac{1}{Z}\mathrm{Tr}\Big(e^{-\beta H}e^{H\tau}\underbrace{\int j_y(\vec{r})\,d^3r}_{J_y}\,e^{-H\tau}\underbrace{j_x(0)}_{\frac{1}{V}J_x}\Big)d\tau$$

$$\sigma^{xy}(i\omega)=\frac{e^2}{\omega V}\sum_{\substack{m\\M}}\underbrace{\langle m|v_y(\vec{r})|M\rangle}_{(v_y)_{mM}}\underbrace{\langle M|v_x(0)|m\rangle}_{(v_x)_{Mm}}\frac{e^{-\beta E_m}}{Z}\underbrace{\int_0^\beta e^{\tau(E_m-E_M+i\omega)}d\tau}_{\frac{e^{\beta E_m-E_M}-1}{i\omega+E_m-E_M}}$$

$$\sigma^{xy}(i\omega)=\frac{e^2}{\omega V}\sum_{mM}\frac{(v_y)_{mM}(v_x)_{Mm}}{i\omega+E_m-E_M}\left(\frac{e^{-\beta E_M}}{Z}-\frac{e^{-\beta E_m}}{Z}\right)$$

first $T\to 0$

$$\sigma^{xy}(i\omega)=\frac{e^2}{\omega V}\sum_M\left[\frac{(v_x)_{0M}(v_y)_{M0}}{\underbrace{i\omega+E_M-E_0}_{\frac{1}{E_M-E_0}\left(1+\frac{i\omega}{E_M-E_0}\right)}}-\frac{(v_y)_{0M}(v_x)_{M0}}{\underbrace{i\omega+E_0-E_M}_{-\frac{1}{E_M-E_0}\left(1-\frac{i\omega}{E_M-E_0}\right)}}\right]$$

(for $M=0$ vanishes, hence $M>0$)

next $\omega\to 0$

$$\sigma^{xy}=\frac{e^2}{\omega V}\sum_{M>0}\left[\underbrace{\frac{(v_x)_{0M}(v_y)_{M0}+(v_y)_{0M}(v_x)_{M0}}{(E_M-E_0)}}+i\omega\frac{(v_x)_{0M}(v_y)_{M0}-(v_y)_{0M}(v_x)_{M0}}{(E_M-E_0)^2}\right]$$

From gauge invariance we can prove that it vanishes (Otherwise diverges)

$$\sigma^{xy}=\frac{ie^2}{V}\sum_{M>0}\frac{(v_x)_{0M}(v_y)_{M0}-(v_y)_{0M}(v_x)_{M0}}{(E_M-E_0)^2}$$

$$\hat{v}_x = \frac{1}{m}\left(-i\frac{\partial}{\partial x}\right)$$

$$\hat{v}_y = \frac{1}{m}\left(-i\frac{\partial}{\partial y} - eBx\right)$$

at $T=0$ we have the ground state $|0\rangle \equiv |\phi_0\rangle$ and expectation values:

$$(v_x)_{00} = \langle\phi_0|\hat{v}_x|\phi_0\rangle \quad \text{and} \quad (v_y)_{00} = \langle\phi_0|\hat{v}_y|\phi_0\rangle$$

Next we make a unitary transformation $|\phi\rangle = e^{-i\sum_i \vec{\varkappa}\cdot\vec{r}_i}|\phi_0\rangle$ which twists the boundary condition. We see $\phi(r_1+L_x,\dots) = e^{-i\varkappa_x L_x}\phi_0(r_1+L_x,\dots)$ and we require $\varkappa_x L_x \in [-\pi,\pi]$, hence the change of momentum is really small for large crystal, i.e., $\varkappa_x \sim \frac{\pi}{L_x}$. If we have insulator (no gap closing while adding the twist) we expect equivalently good solution).

ϕ is a function of many variables $\phi(r_1, r_2, \dots r_N)$ but let's concentrate on r_1 only:

$$\phi(r_1+L_x) = e^{-i\varkappa_x L_x} e^{-i\varkappa_x r_1}\phi_0(r_1+L_x) = e^{-i\varkappa_x L_x + ik_x L_x} e^{-\varkappa_x r_1}\phi_0(r_1) = e^{i(k_x-\varkappa_x)L_x}\phi(r_1)$$

Hence, we see a slight change of phase through the crystal.

What is momentum in this new state compared to $|\phi_0\rangle$?

$$(v_x)_{00} = \langle\phi| e^{-i\sum\vec{\varkappa}\vec{r}_i} v_x e^{i\sum\vec{\varkappa}\vec{r}_i}|\phi\rangle \text{ hence}$$

$$(v_x)_{00} = \langle\phi| e^{-i\sum\vec{\varkappa}\vec{r}_i}\frac{1}{m}\left(-ii\varkappa_x - i\frac{\partial}{\partial x}\right)e^{i\sum\vec{\varkappa}\vec{r}_i}|\phi\rangle = \langle\phi_0|\frac{1}{m}\left(-i\frac{\partial}{\partial x}+\varkappa_x\right)|\phi_0\rangle$$

$$(v_y)_{00} = \langle\phi| e^{-i\sum\vec{\varkappa}\vec{r}_i}\frac{1}{m}\left(-i\frac{\partial}{\partial y}+\varkappa_y - eBx\right)e^{i\sum_i\vec{\varkappa}\vec{r}_i}|\phi\rangle = \langle\phi_0|\frac{1}{m}\left(-i\frac{\partial}{\partial y} - eBx + \varkappa_y\right)|\phi_0\rangle$$

This transformation is thus equivalent to transforming operators

$$\left.\begin{aligned} -i\frac{\partial}{\partial x} &\to -i\frac{\partial}{\partial x}+\varkappa_x \\ -i\frac{\partial}{\partial y} &\to -i\frac{\partial}{\partial y}+\varkappa_y \end{aligned}\right\} \text{ hence the Hamiltonian is } \tilde{H} =$$

The corresponding transformed Hamiltonian is thus:

$$\tilde{H} = \sum_i \frac{\left(-i\frac{\partial}{\partial x_i}+\varkappa_x\right)^2}{2m_i} + \frac{\left(-i\frac{\partial}{\partial y_i}+\varkappa_y - eBx_i\right)^2}{2m_i} + V_{int}$$

and therefore: $\quad \dfrac{\partial\tilde{H}}{\partial\varkappa_x} = \sum_i \dfrac{\left(-i\frac{\partial}{\partial x_i}+\varkappa_x\right)}{m_i} = v_x \quad$ and $\quad \dfrac{\partial\tilde{H}}{\partial\varkappa_y} = \sum_i \dfrac{\left(-i\frac{\partial}{\partial y_i}+\varkappa_y - eBx_i\right)}{m_i} = v_y$

Finally we can write conductivity for the state with twisted B.C.:

$$\sigma^{xy} = \frac{ie^2}{V}\sum_{n>0}\frac{(v_x)_{0n}(v_y)_{n0}-(v_y)_{0n}(v_x)_{n0}}{(E_n-E_0)^2}$$

$$\Rightarrow \frac{ie^2}{V}\sum_{n>0}\frac{\langle\phi_0|\frac{\partial\tilde H}{\partial\theta_x}|\phi_n\rangle\langle\phi_n|\frac{\partial\tilde H}{\partial\theta_y}|\phi_0\rangle-\langle\phi_0|\frac{\partial\tilde H}{\partial\theta_y}|\phi_n\rangle\langle\phi_n|\frac{\partial\tilde H}{\partial\theta_x}|\phi_0\rangle}{(E_n-E_0)^2}$$

Next we try to simplify the products!

$$\frac{\partial}{\partial\theta_x}\langle\phi_0|\tilde H|\phi_n\rangle = \langle\frac{\partial\phi_0}{\partial\theta_x}|\tilde H|\phi_n\rangle+\langle\phi_0|\tilde H|\frac{\partial\phi_n}{\partial\theta_x}\rangle+\langle\phi_0|\frac{\partial\tilde H}{\partial\theta_x}|\phi_n\rangle$$

$$\frac{\partial}{\partial\theta_x}E_0\delta_{n0}=0=E_n\langle\frac{\partial\phi_0}{\partial\theta_x}|\phi_n\rangle+\underbrace{E_0\langle\phi_0|\frac{\partial\phi_n}{\partial\theta_x}\rangle}+\langle\phi_0|\frac{\partial\tilde H}{\partial\theta_x}|\phi_n\rangle$$

but $\langle\phi_0|\frac{\partial\phi_n}{\partial\theta_x}\rangle=\underbrace{\frac{\partial}{\partial\theta_x}\langle\phi_0|\phi_n\rangle}_{=0}-\langle\frac{\partial\phi_0}{\partial\theta_x}|\phi_n\rangle$

Finally we simplified to:

$n\neq0$: $\langle\phi_0|\frac{\partial\tilde H}{\partial\theta_x}|\phi_n\rangle=-(E_n-E_0)\langle\frac{\partial\phi_0}{\partial\theta_x}|\phi_n\rangle$

Similarly we can get (just conjugating and replacing $\theta_x\to\theta_y$)

$$\langle\phi_n|\frac{\partial\tilde H}{\partial\theta_y}|\phi_0\rangle=-(E_n-E_0)\langle\phi_n|\frac{\partial\phi_0}{\partial\theta_y}\rangle$$

We plug this back to σ^{xy} to get

$$\sigma^{xy}=\frac{ie^2}{V}\sum_{n>0}\frac{(E_n-E_0)^2\left[\langle\frac{\partial\phi_0}{\partial\theta_x}|\phi_n\rangle\langle\phi_n|\frac{\partial\phi_0}{\partial\theta_y}\rangle-\langle\frac{\partial\phi_0}{\partial\theta_y}|\phi_n\rangle\langle\phi_n|\frac{\partial\phi_0}{\partial\theta_x}\rangle\right]}{(E_n-E_0)^2}$$

$$\sigma^{xy}=\frac{ie^2}{V}\quad\langle\frac{\partial\phi_0}{\partial\theta_x}|\Big(\sum_n|\phi_n\rangle\langle\phi_n|\Big)|\frac{\partial\phi_0}{\partial\theta_y}\rangle-\langle\frac{\partial\phi_0}{\partial\theta_y}|\Big(\sum_n|\phi_n\rangle\langle\phi_n|\Big)\frac{\partial\phi_0}{\partial\theta_x}\rangle\Big]$$

$$\sigma^{xy}=\frac{ie^2}{V}\left[\langle\frac{\partial\phi_0}{\partial\theta_x}|\frac{\partial\phi_0}{\partial\theta_y}\rangle-\langle\frac{\partial\phi_0}{\partial\theta_y}|\frac{\partial\phi_0}{\partial\theta_x}\rangle\right]$$

The result should be insensitive to this twist in the B.C. as long as there is a gap in the spectrum for any choice of θ_x,θ_y. We will average over the twist $\in[0,2\pi]$:

$\theta_x L_x=\tilde\theta_x\in[0,2\pi]$ and $\theta_y L_y=\tilde\theta_y\in[0,2\pi]$

$$\sigma^{xy}=\frac{ie^2}{V}\frac{L_xL_y}{(2\pi)^2}\int_0^{2\pi}d\tilde\theta_x\int_0^{2\pi}d\tilde\theta_y\;\left[\underbrace{\langle\frac{\partial\phi_0}{\partial\tilde\theta_x}|\frac{\partial\phi_0}{\partial\tilde\theta_y}\rangle-\langle\frac{\partial\phi_0}{\partial\tilde\theta_y}|\frac{\partial\phi_0}{\partial\tilde\theta_x}\rangle}\right]$$

Chern theorem has something to do with it!

We recall the Chern theorem:

$$-2\iint \mathrm{Im}\left\langle \frac{\partial M}{\partial \lambda_\mu} \middle| \frac{\partial M}{\partial \lambda_\nu} \right\rangle d\lambda_\mu\, d\lambda_\nu = 2\pi C$$

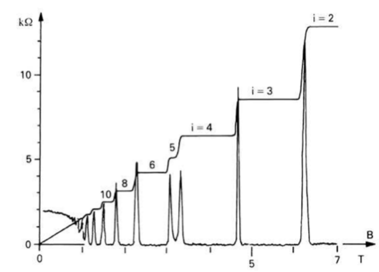
Which here mean that when we change the twist $\tilde{\theta}_x$ or $\tilde{\theta}_y$ for 2π, we should get the same state, hence the twist of $2\pi C$ (for arbitrary c) should give the same answer.

We hence recognize:

$$\sigma^{xy} = \frac{ie^2}{V}\frac{L_x L_y}{(2\pi)^2}\int_0^{2\pi} d\tilde{\theta}_x \int_0^{2\pi} d\tilde{\theta}_y \underbrace{\left[\left\langle \frac{\partial \Phi_0}{\partial \tilde{\theta}_x} \middle| \frac{\partial \Phi_0}{\partial \tilde{\theta}_y}\right\rangle - \left\langle \frac{\partial \Phi_0}{\partial \tilde{\theta}_y} \middle| \frac{\partial \Phi_0}{\partial \tilde{\theta}_x}\right\rangle\right]}_{2i\,\mathrm{Im}\left\langle \frac{\partial \Phi_0}{\partial \theta_x} \middle| \frac{\partial \Phi_0}{\partial \theta_y}\right\rangle} = e^2 \frac{L_x L_y}{V}\frac{2\pi}{(2\pi)^2} C = \frac{e^2}{2\pi}\cdot C$$

for 2D system $\frac{L_x L_y}{V} = 1$

This is Thouless's proof of 2D quantization of the integer quantum Hall effect.



He also prove fractional quantum Hall effect.

Key point: The ground state $|\Phi_0\rangle$ is degenerate p-times.

Then we need an extra sum over degenerate ground states:

$$\sigma^{xy} = \frac{ie^2}{V}\sum_{0\in p}\left[\left\langle \frac{\partial \Phi_0}{\partial \theta_x} \middle| \frac{\partial \Phi_0}{\partial \theta_y}\right\rangle - \left\langle \frac{\partial \Phi_0}{\partial \theta_y} \middle| \frac{\partial \Phi_0}{\partial \theta_x}\right\rangle\right]$$

degenerate ground states.

Assumption: There is no coupling between these states, so the system is in one of those states, and we can not reach different $|\Phi_0\rangle$ by single particle (low energy) excitations.

Key point! When we twist the B.C. we are allowed to switch from one state of the set to another, hence in the worse case scenario it might be necessary to twist the phase up to $2\pi \cdot p \cdot C$ to get to the same state!

degeneracy

Thouless therefore argued that the correct averaging for degenerate set is

$$\sigma^{xy} = \frac{ie^2}{V}\frac{L_x L_y}{(2\pi)^2}\frac{1}{p}\int_0^{2\pi p} d\tilde{\theta}_x \int_0^{2\pi} d\tilde{\theta}_y \left[\left\langle \frac{\partial \Phi_0}{\partial \tilde{\theta}_x}\middle|\frac{\partial \Phi_0}{\partial \tilde{\theta}_y}\right\rangle - \left\langle \frac{\partial \Phi_0}{\partial \tilde{\theta}_y}\middle|\frac{\partial \Phi_0}{\partial \tilde{\theta}_x}\right\rangle\right]$$

We will get one of the p states when phase is changed for 2π, and we need $2\pi p$ phase to get back to original state.

The space to integrate for Chern theorem, which should be modified to:

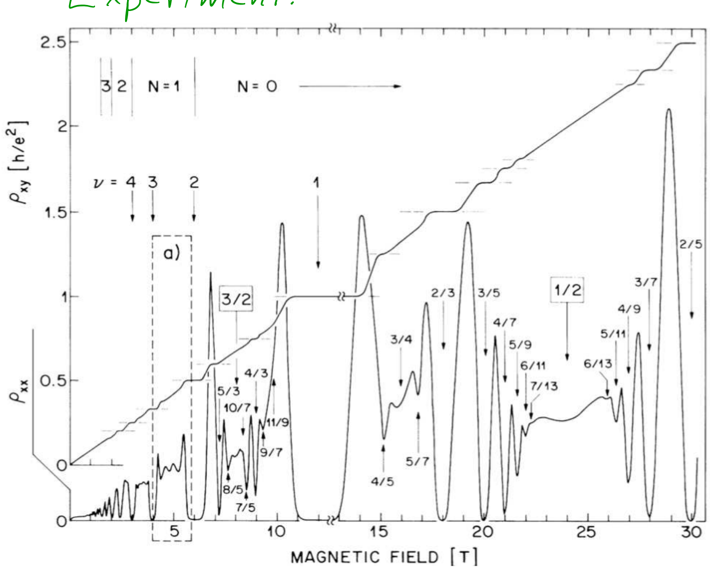
$$-2\int_0^{2\pi p}\int_0^{2\pi} \mathrm{Im}\left\langle \frac{\partial M}{\partial \lambda_\mu}\middle|\frac{\partial M}{\partial \lambda_\nu}\right\rangle d\lambda_\mu \, d\lambda_\nu = 2\pi C$$

Finally the result is:

$$\sigma^{xy} = \frac{e^2}{2\pi p} \cdot C$$

Laughlin wrote down a concrete wave function, which gives such conductivity (Both Laughlin and Thouless got Nobel prize.)

Experiment:



Note that if we started with $S = S_0 + \int \frac{\partial H}{\partial x}\dot{x}\, dt$ we could derive polarization. By playing with the twist B.C. we would then get:

$$\langle \Delta P^{\alpha}_{cm}\rangle = \frac{V_{cell}}{(2\pi)^3}\int_0^1 d\lambda \int_{BZ} d^3\theta \left\{\left\langle \frac{\partial \Phi_0}{\partial \lambda}\middle|\frac{\partial \Phi_0}{\partial \vec{\theta}}\right\rangle - \left\langle \frac{\partial \Phi_0}{\partial \vec{\theta}}\middle|\frac{\partial \Phi_0}{\partial \lambda}\right\rangle\right\} \qquad \alpha = x, y, z$$

After using Stokes theorem, as in non-interacting case, we would get

$$\langle \Delta P^{\alpha}_{cm}\rangle = \frac{2V_{cell}}{(2\pi)^3}\int_{BZ} d^3\theta \, \mathrm{Im}\left\{\langle \Phi_\theta(\lambda=1)|\frac{\partial}{\partial \theta_\alpha}|\Phi_\theta(\lambda=1)\rangle - \langle \Phi_\theta(\lambda=0)|\frac{\partial}{\partial \theta_\alpha}|\Phi_\theta(\lambda=0)\rangle\right\}$$

many body state with twisted B.c.