Title: 14/15 PSI - Condensed Matter-Lecture 12

Date: Nov 25, 2014 10:45 AM

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Abstract:

Polarization ambiguity

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- Berry phase has the same ambiguity.

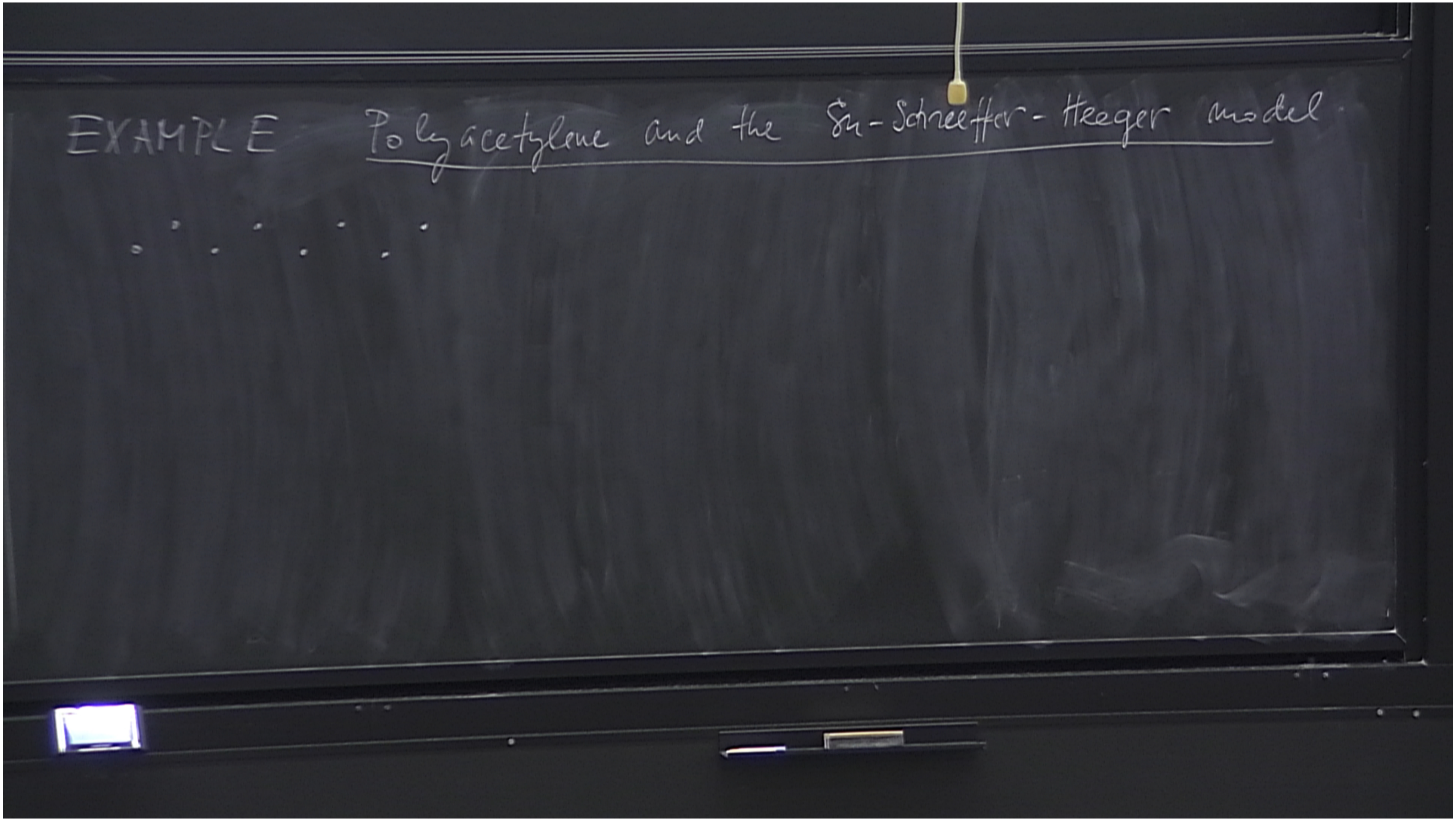
Under gauge transf

$|u(k)\rangle \to e^{i\phi(k)}|u(k)\rangle$ with

$\phi(\frac{\pi}{a}) - \phi(-\frac{\pi}{a}) = 2\pi n$ we have

$P \to P + ne.$

EXAMPLE Polyacetylene and the Su-Schrieffer-Heeger model


EXAMPLE Polyacetylene and the Su-Schrieffer-Heeger model

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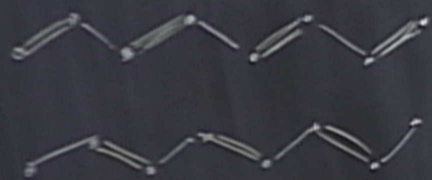
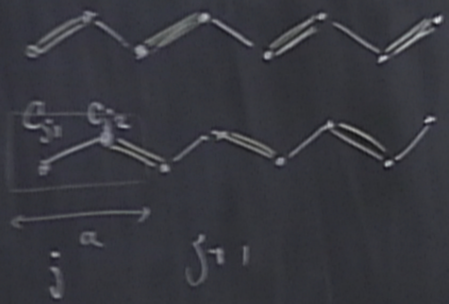
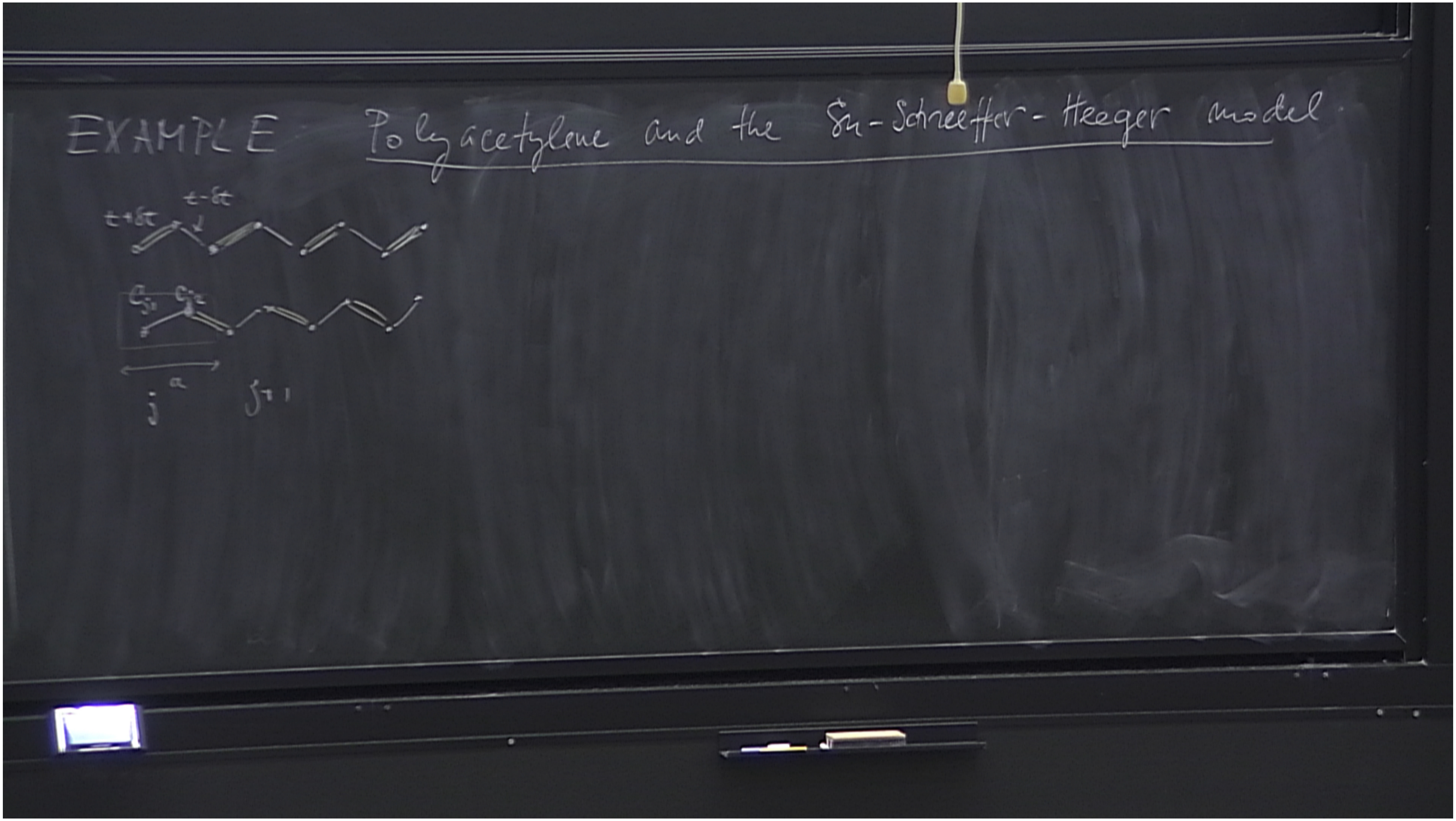
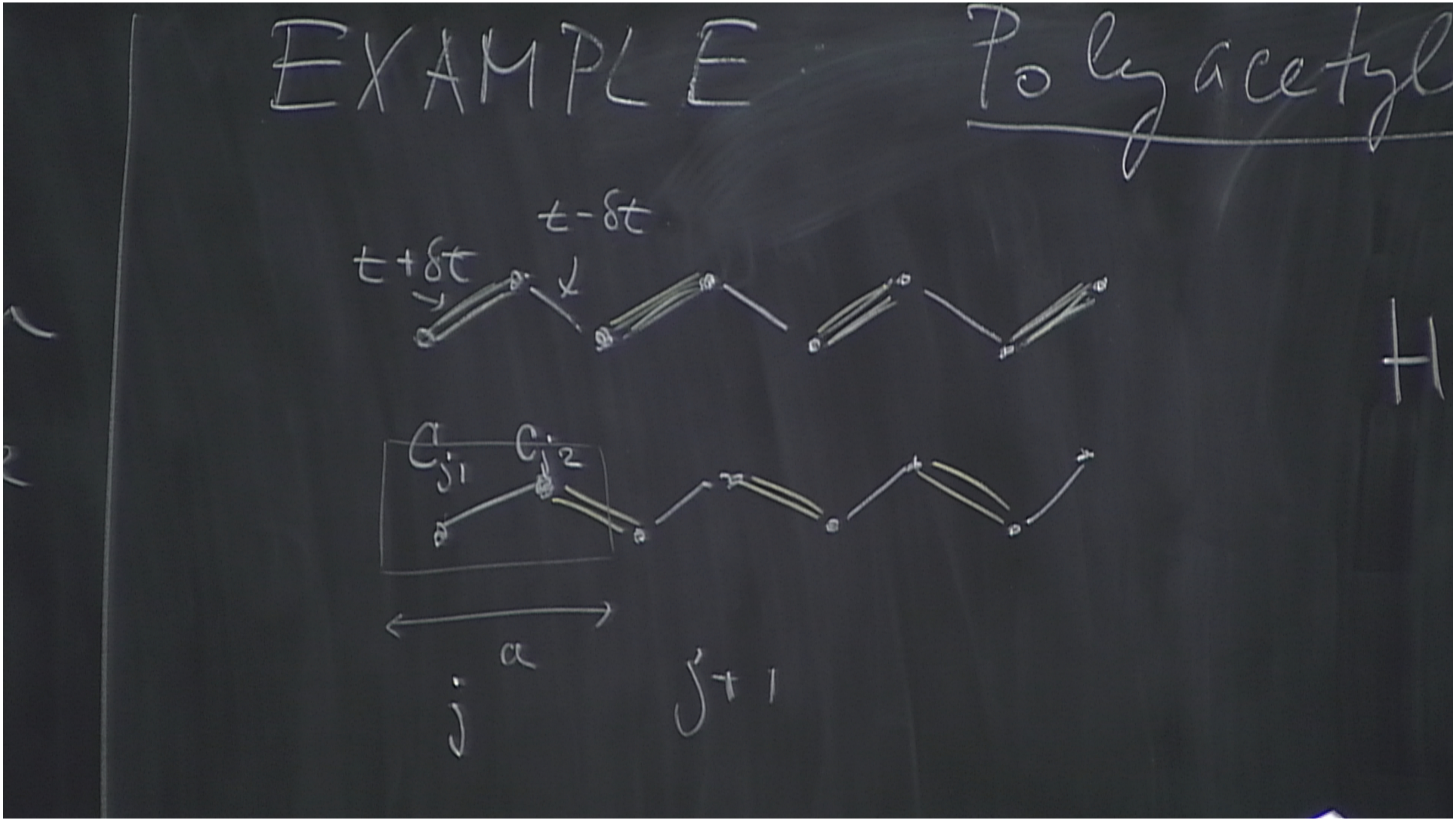
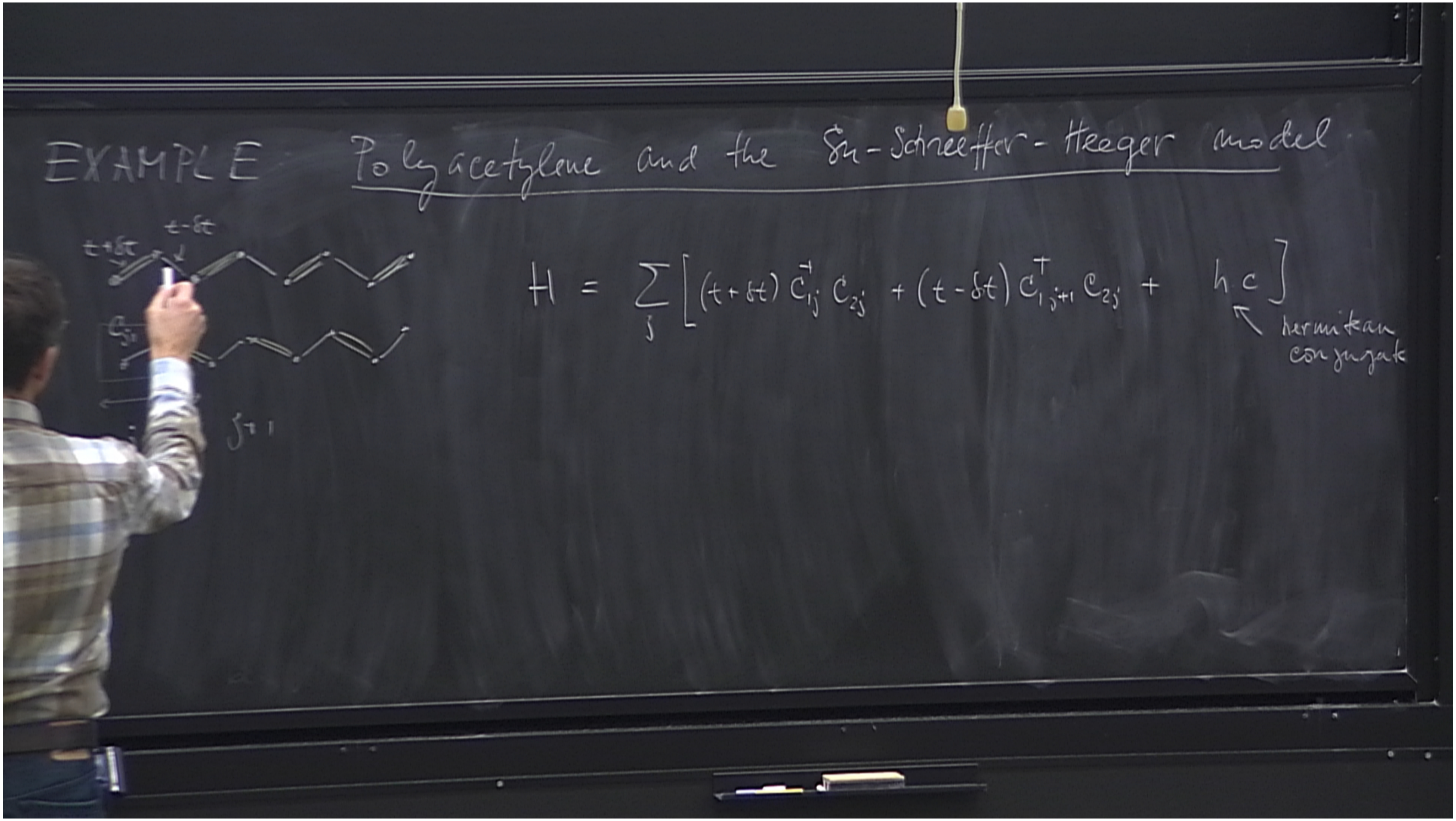


EXAMPLE: Polyacetylene and the Su-Schrieffer-Heeger model

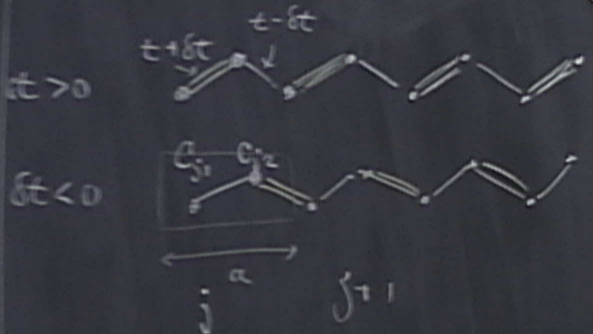



EXAMPLE
Polyacetylene and the Su-Schrieffer-Heeger model.
t+δt
t-δt
c_{j1}
c_{j2}
a
j
j+1


EXAMPLE Polyacetyl
t - δt
t + δt
C j1
C j2
a
j
j+1


EXAMPLE
Polyacetylene and the Su-Schrieffer-Heeger model
t+δt
t−δt
j+1
$H = \sum_j \left[(t+\delta t)\, c^\dagger_{1j} c_{2j} + (t-\delta t)\, c^\dagger_{1,j+1} c_{2j} + h.c. \right]$
hermitian conjugate

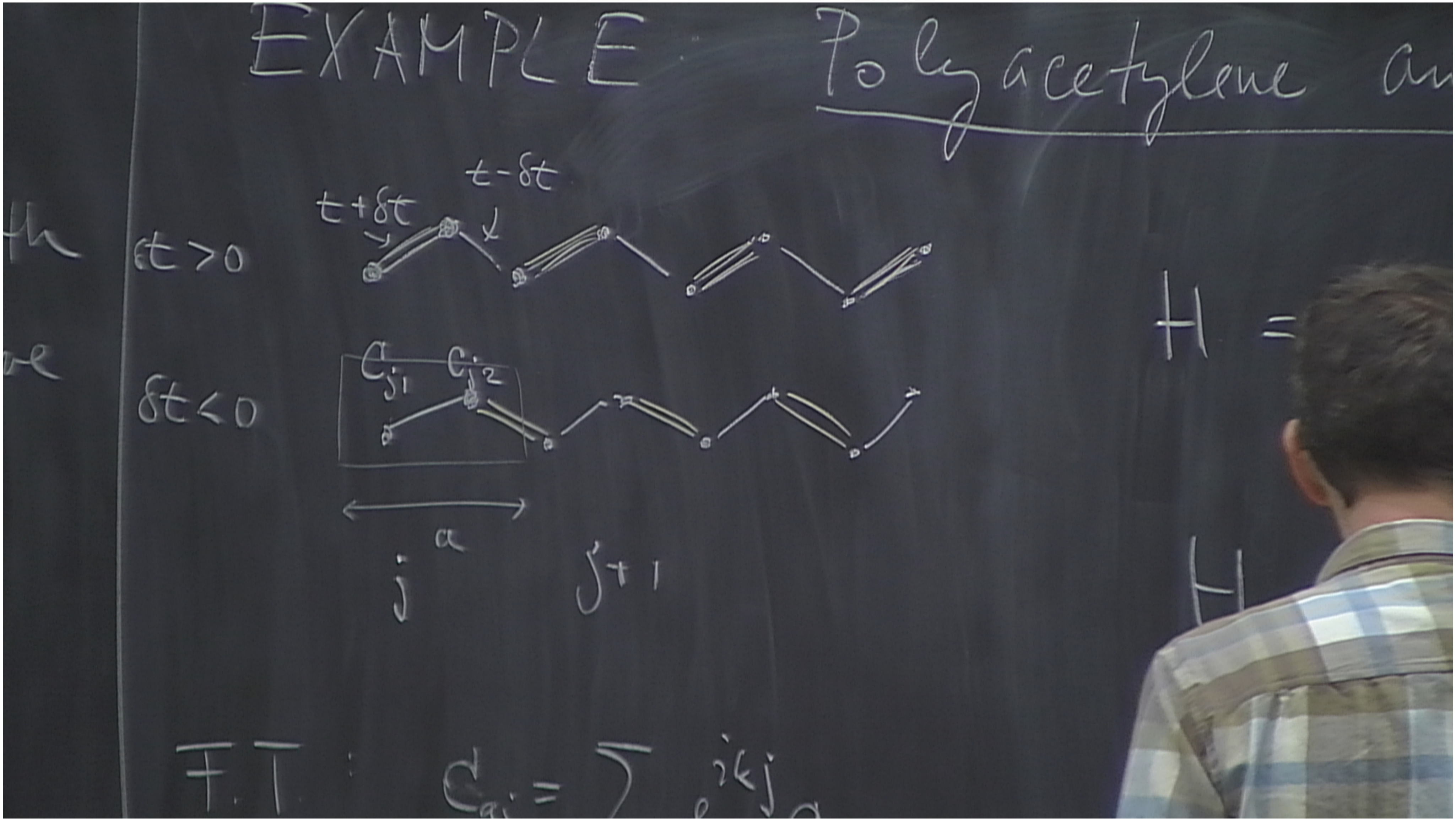
EXAMPLE: Polyacetylene and the Su-Schreeffer-Heeger model

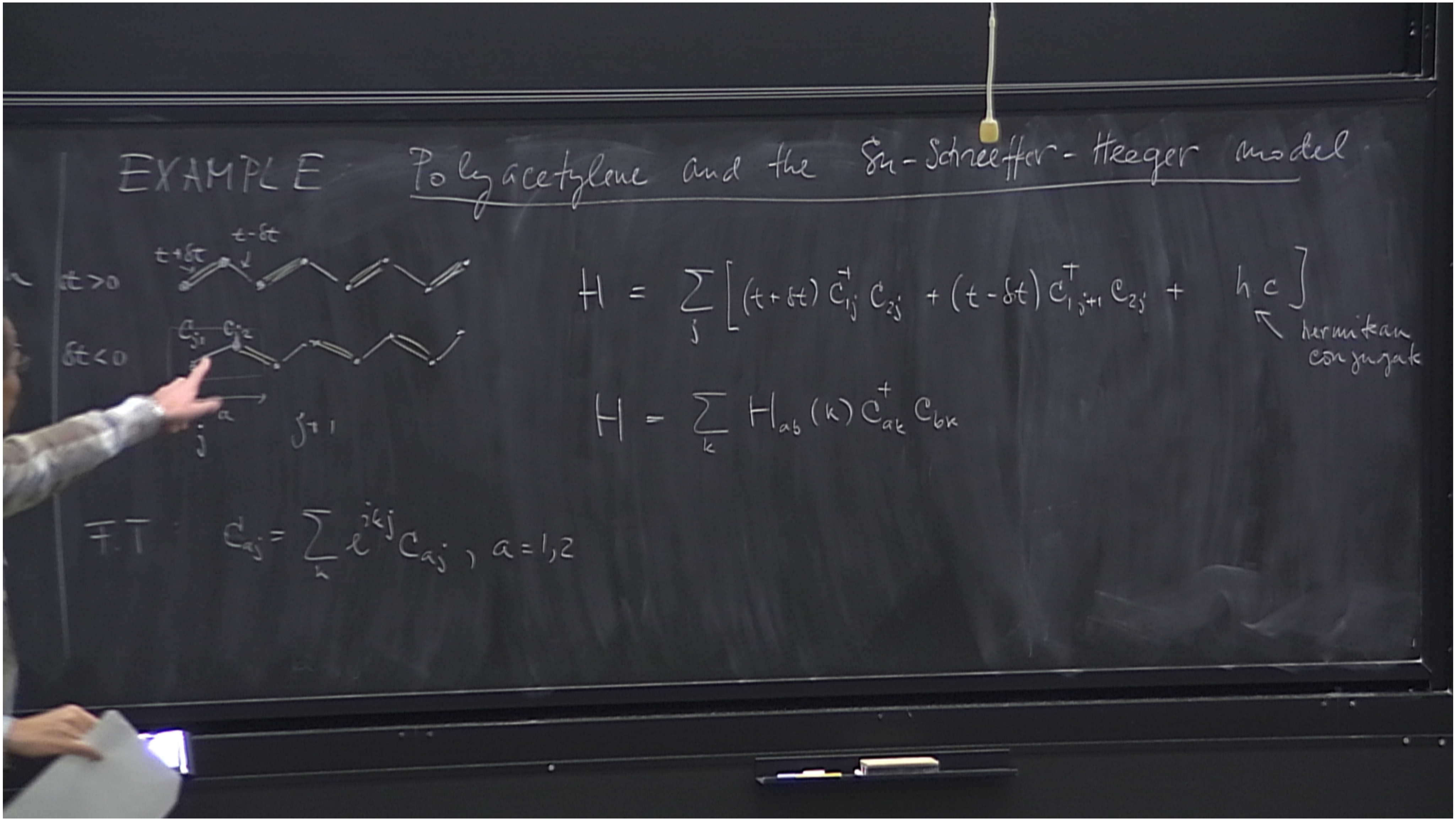


$$H = \sum_j \left[(t+\delta t)\, c^\dagger_{1j}\, c_{2j} + (t-\delta t)\, c^\dagger_{1,j+1}\, c_{2j} + h\,c \right]$$

hermitian conjugate

F.T: $c_{aj} = \sum_k e^{ikj} c_{aj}\ ,\ a=1,2$

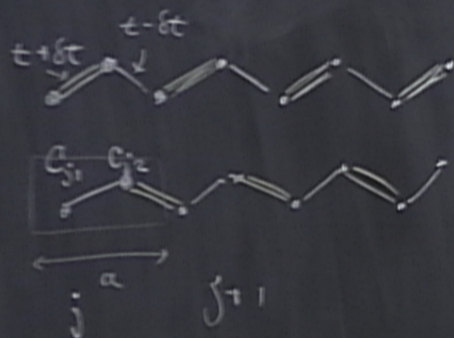

EXAMPLE
Polyacetylene
t - δt
t + δt
δt > 0
δt < 0
a
j
j+1
H =
F.T.


EXAMPLE Polyacetylene and the Su-Schrieffer-Heeger model
$t+\delta t$ $t-\delta t$
$\delta t>0$
$\delta t<0$
c_{j1} c_{j2}
a
j $j+1$
$H = \sum_j \left[(t+\delta t)\, c^\dagger_{1j} c_{2j} + (t-\delta t)\, c^\dagger_{1,j+1} c_{2j} + h.c. \right]$
hermitian conjugate
$H = \sum_k H_{ab}(k)\, c^\dagger_{ak} c_{bk}$
F.T: $c_{aj} = \sum_k e^{ikj} c_{aj}$, $a=1,2$

EXAMPLE: Polyacetylene and the Su-Schrieffer-Heeger model

$\delta t > 0$

$\delta t < 0$



$$H = \sum_j \left[(t+\delta t)\, c^\dagger_{1j} c_{2j} + (t-\delta t)\, c^\dagger_{1,j+1} c_{2j} + h.c. \right]$$

hermitian conjugate

$$H = \sum_k \underbrace{H_{ab}(k)}_{2\times 2 \text{ matrix}} c^\dagger_{ak} c_{bk}$$

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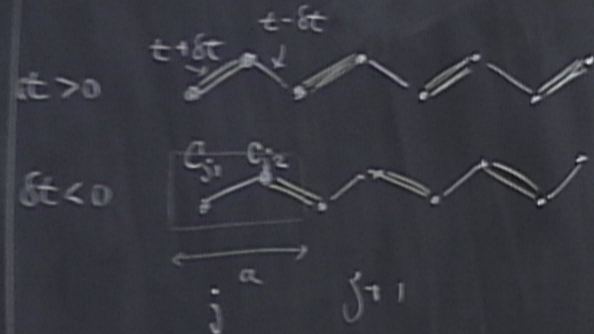
EXAMPLE: Polyacetylene and the Su-Schrieffer-Heeger model



$$H = \sum_j \left[(t+\delta t)\, c^\dagger_{1j} c_{2j} + (t-\delta t)\, c^\dagger_{1,j+1} c_{2j} + h.c. \right]$$

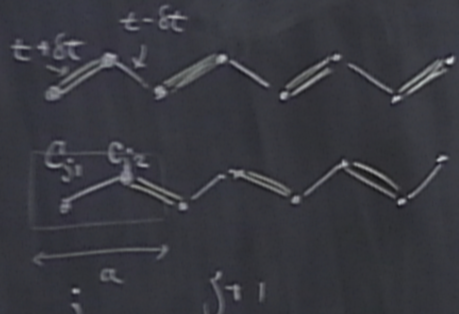
hermitian conjugate

$$H = \sum_k \underbrace{H_{ab}(k)}_{2\times 2 \text{ matrix}} c^\dagger_{ak} c_{bk}$$

$$H(\vec{k}) = \vec{d}(\vec{k}) \cdot \vec{\sigma}$$

F.T: $c_{aj} = \sum_k e^{ikj} c_{aj}, \quad a = 1,2$

EXAMPLE Polyacetylene and the Su-Schreeffer-Heeger model



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hermitian conjugate

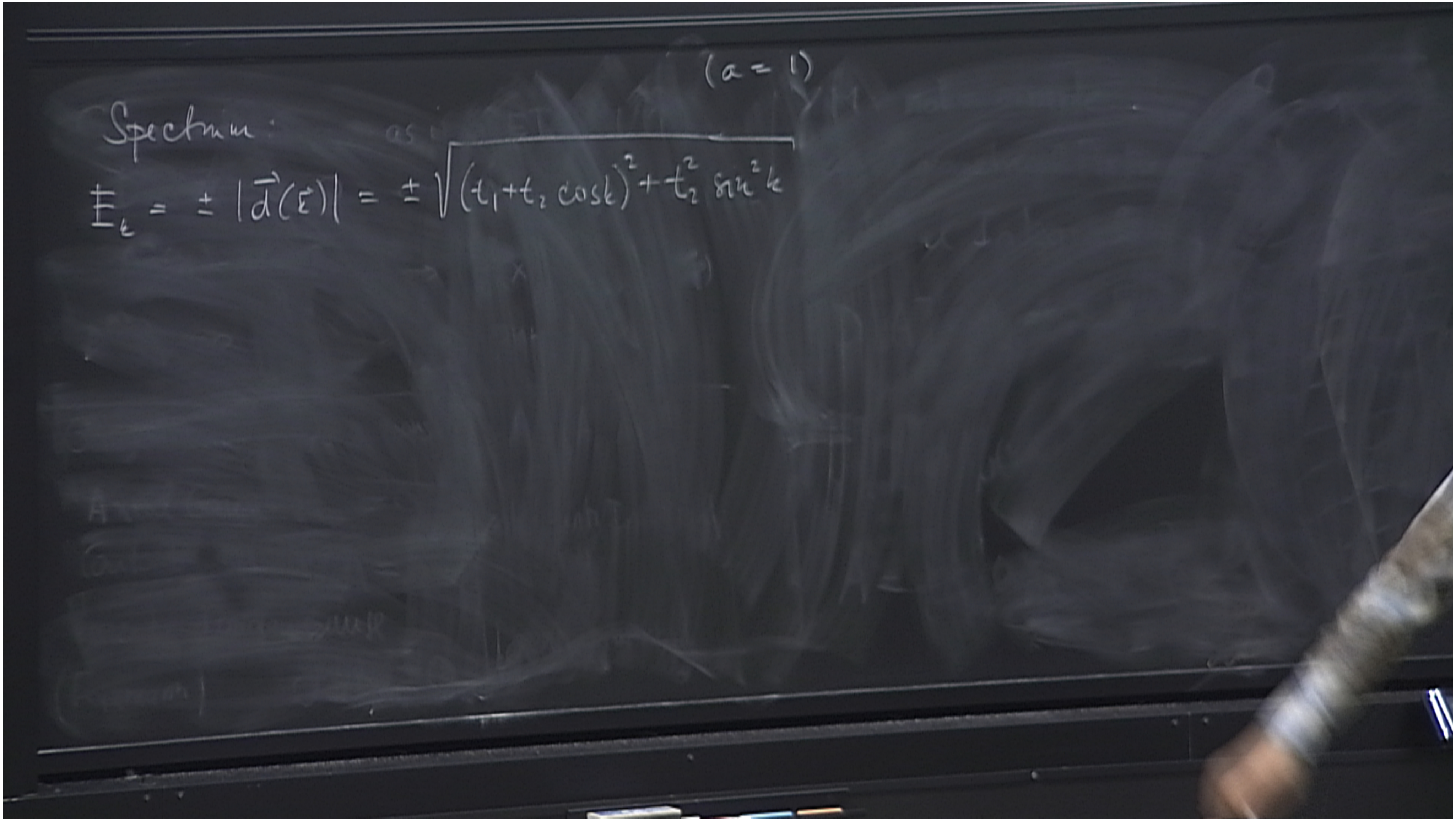
$$H = \sum_k \underbrace{H_{ab}(k)}_{2\times 2 \text{ matrix}} c^\dagger_{ak} c_{bk}$$

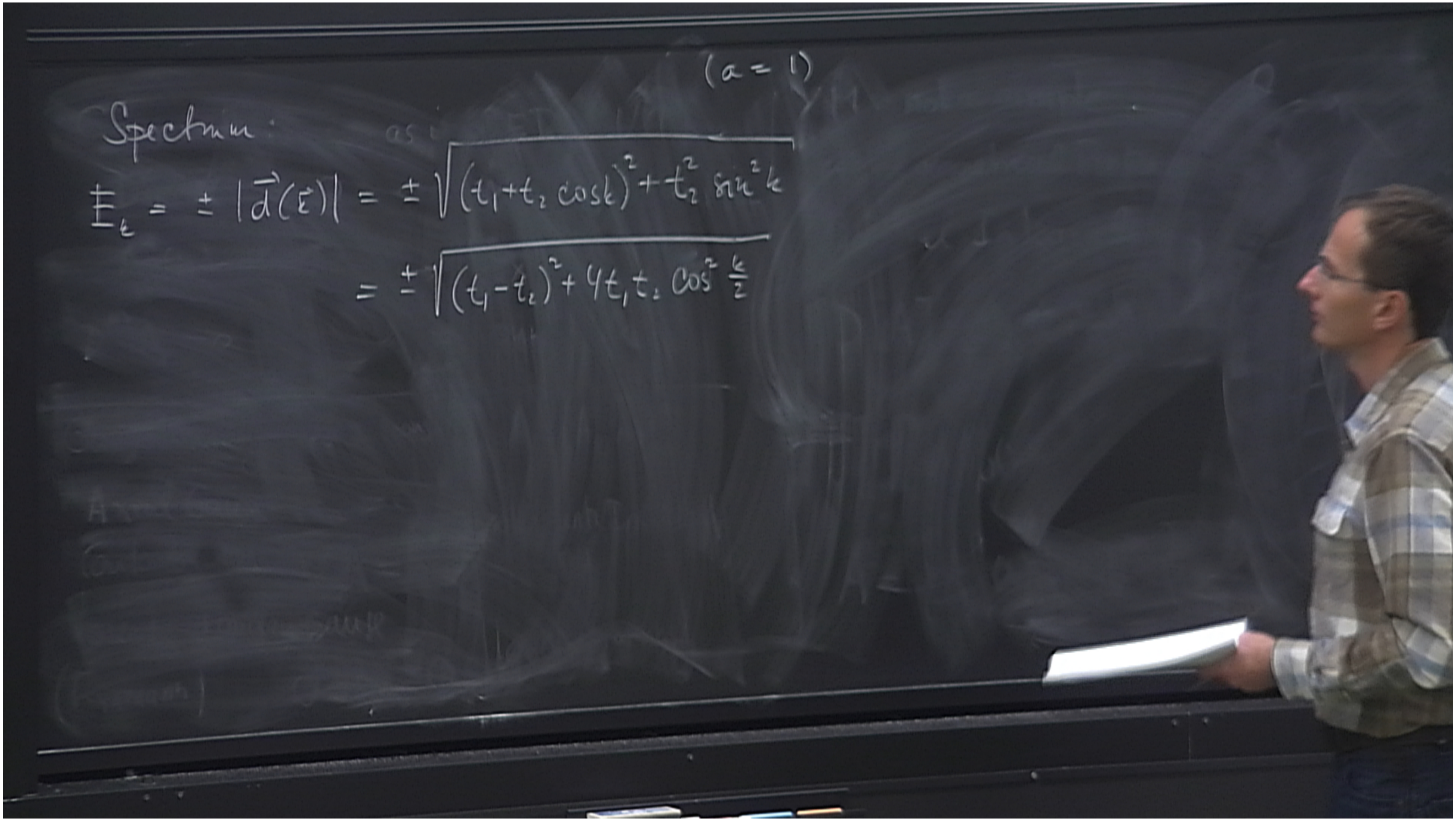
$$H(k) = \vec{d}(k)\cdot\vec{\sigma}$$

F.T : $c_{aj} = \sum_k e^{ikj} c_{aj}$, $a = 1,2$

$$d_x(k) = t_1 + t_2 \cos ka$$
$$d_y(k) = t_2 \sin ka$$
$$d_z(k) = 0$$

$$t_1 = t + \delta t$$
$$t_2 = t - \delta t$$


(a = 1)
Spectrum:
$E_k = \pm |\vec{d}(k)| = \pm \sqrt{(t_1 + t_2 \cos k)^2 + t_2^2 \sin^2 k}$


$(a=1)$
Spectrum:
$E_k = \pm |\vec{d}(k)| = \pm\sqrt{(t_1+t_2\cos k)^2 + t_2^2 \sin^2 k}$
$= \pm\sqrt{(t_1-t_2)^2 + 4t_1t_2\cos^2\frac{k}{2}}$

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Spectrum:

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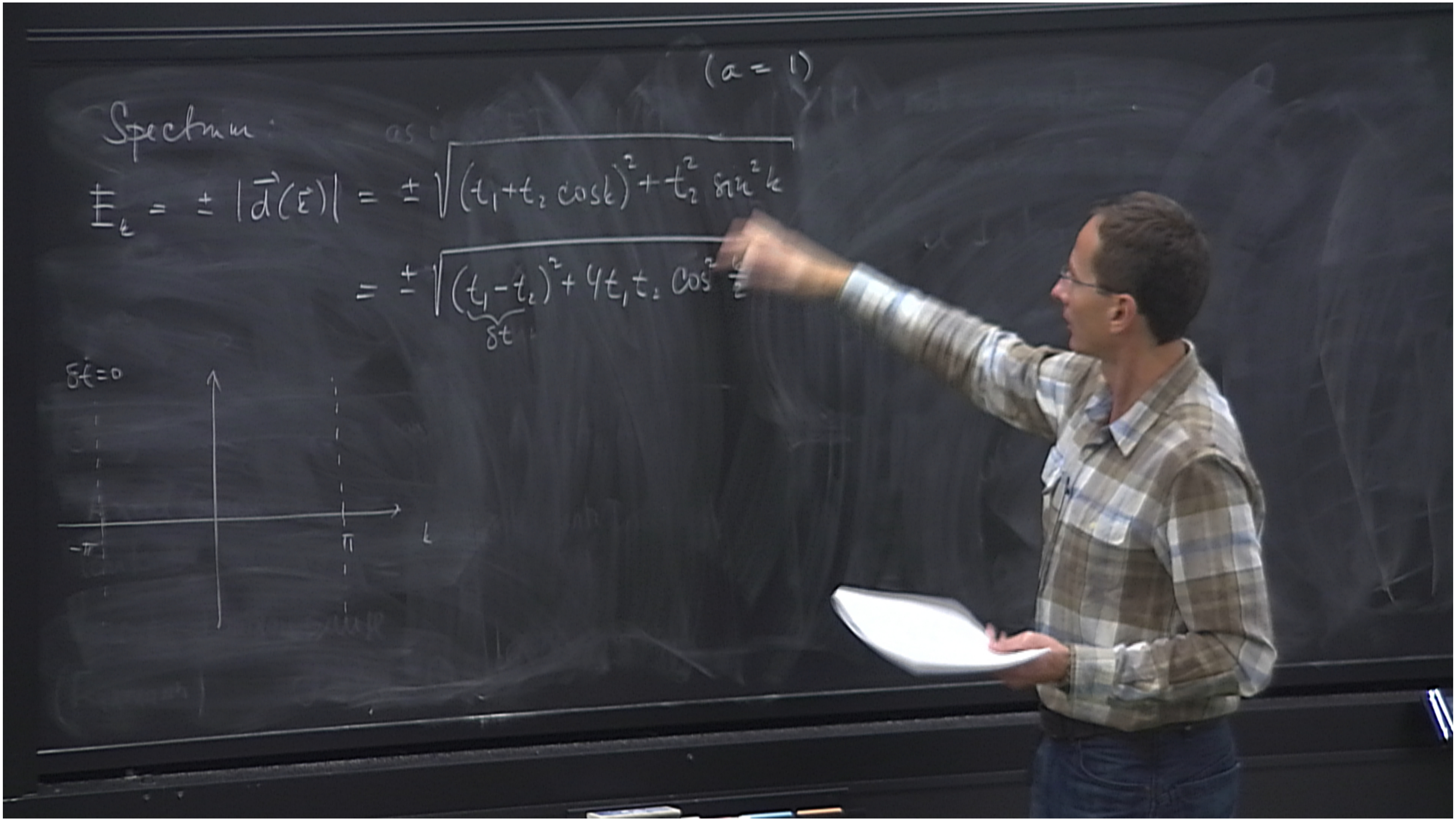
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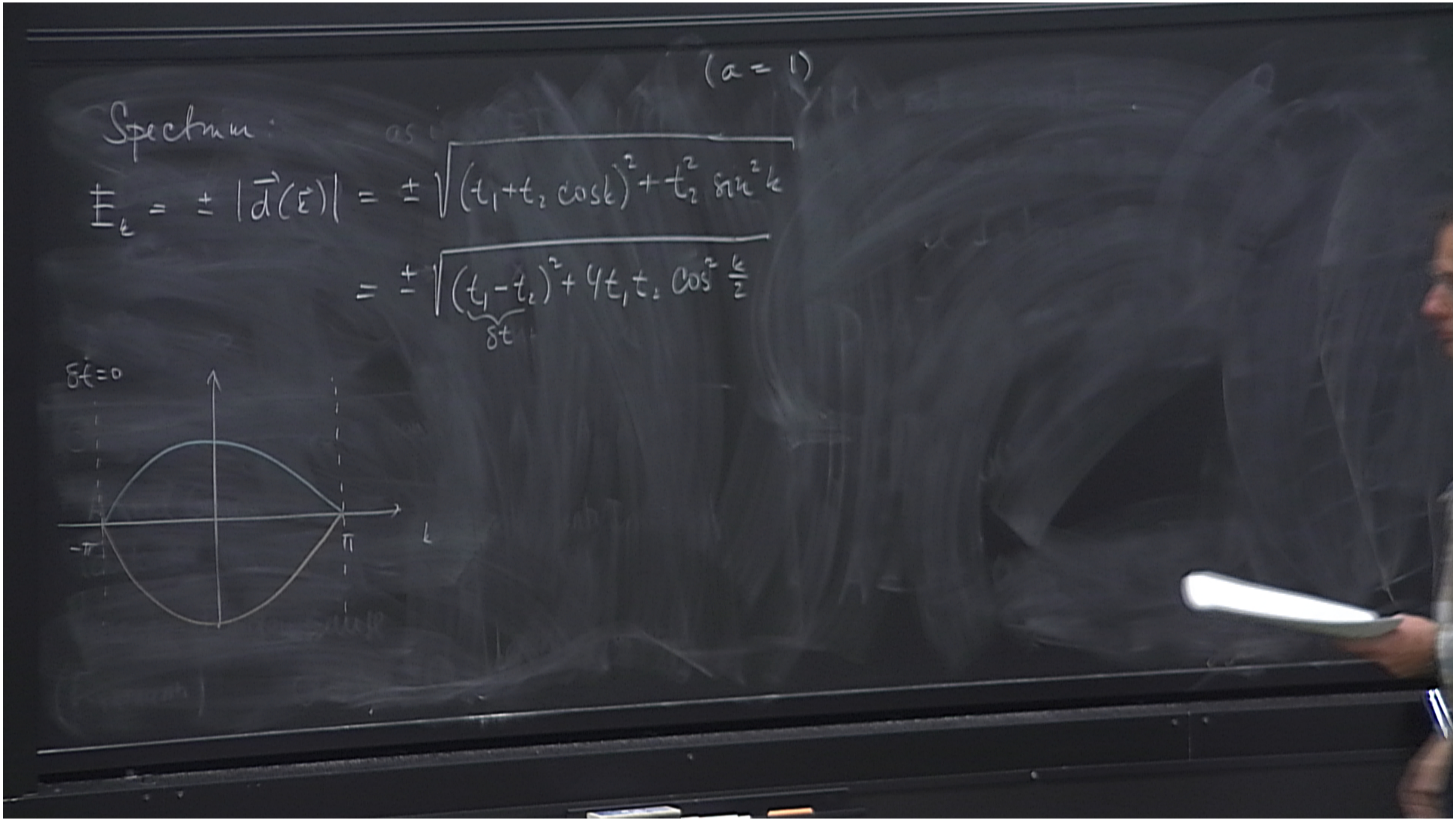
$= \pm \sqrt{(\underbrace{t_1 - t_2}_{\delta t})^2 + 4 t_1 t_2 \cos^2}$
$\delta t = 0$
$-\pi$
π
k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π
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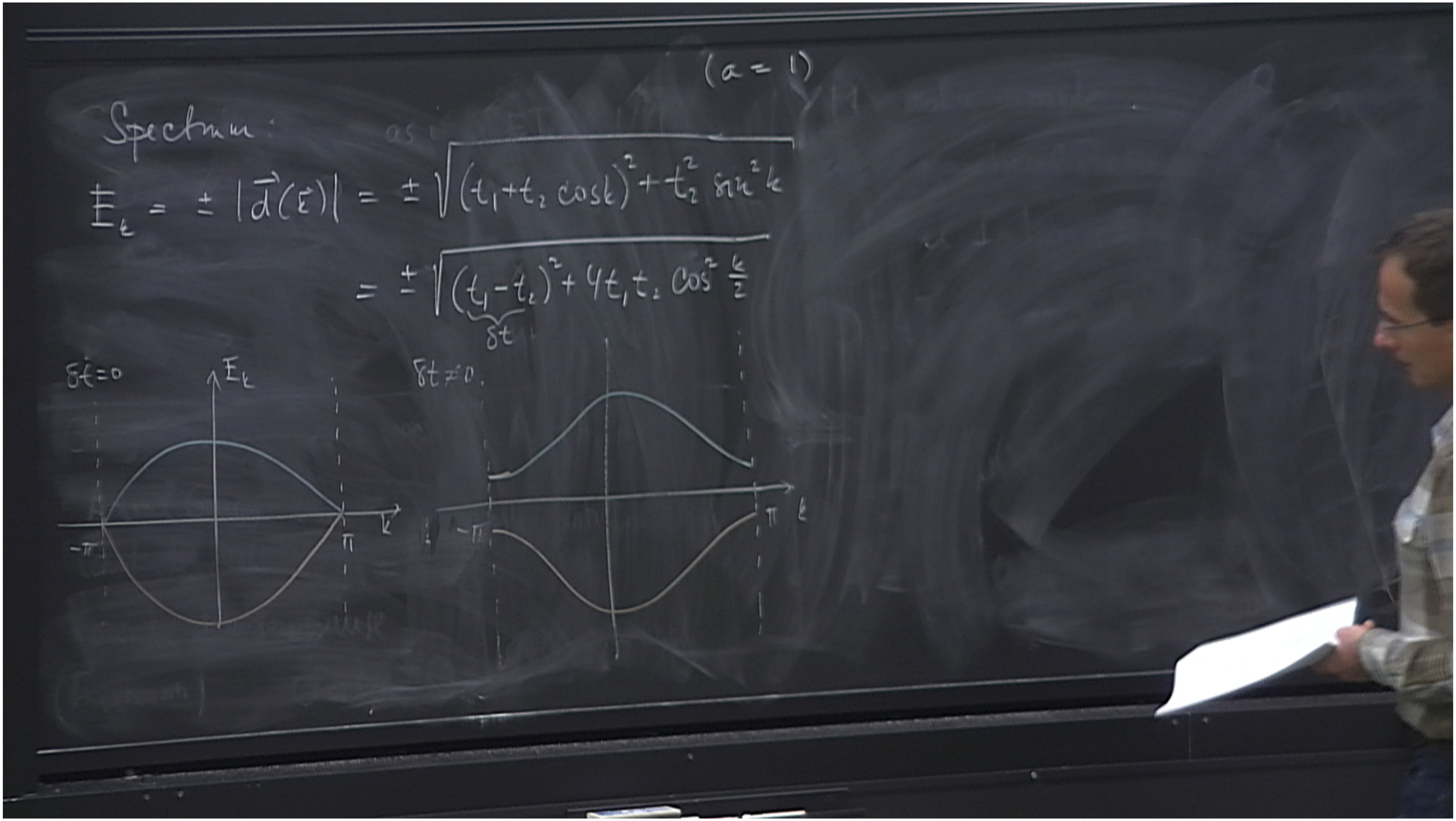
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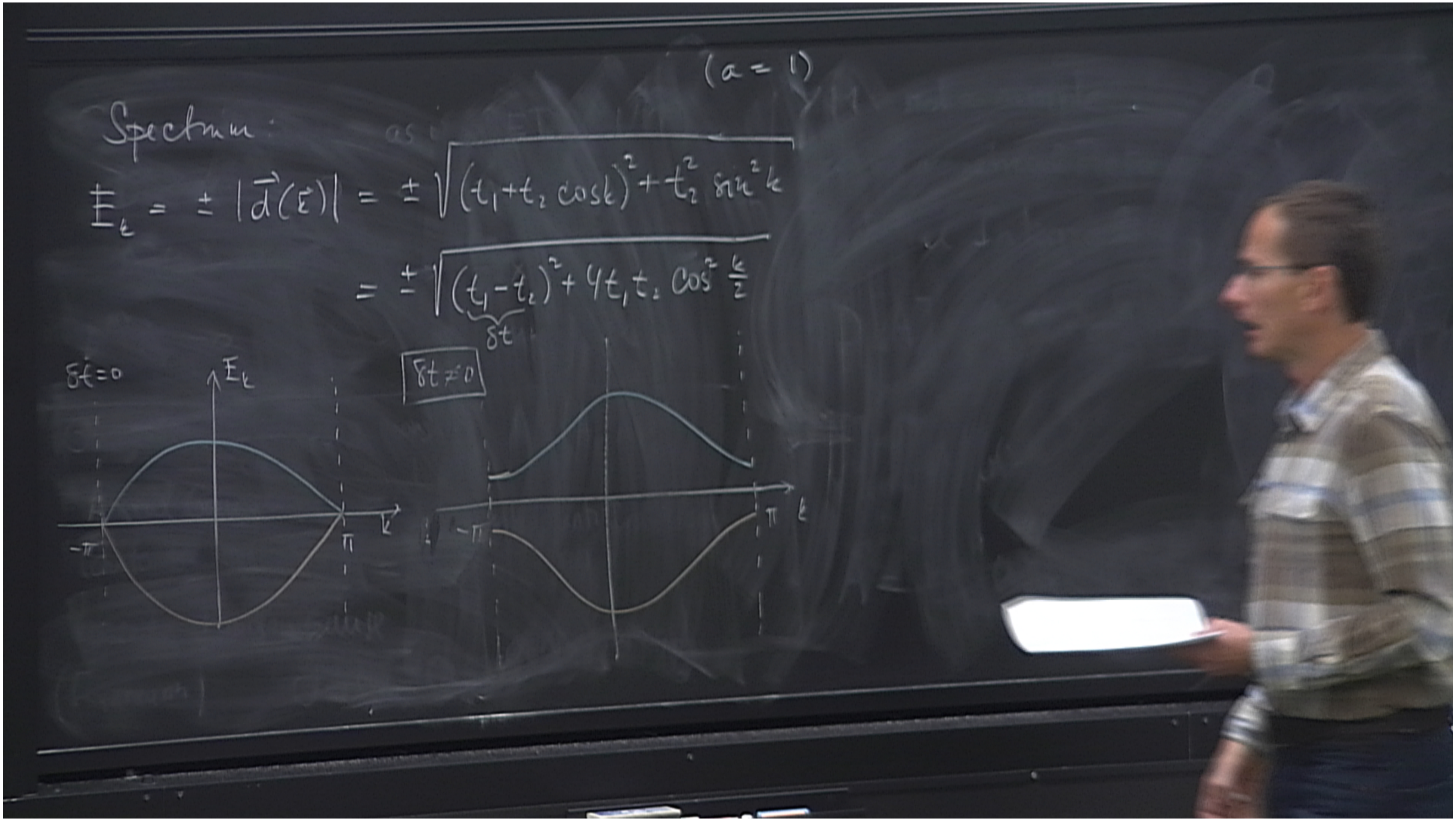
Spectrum:
E_k = ± |d(k)| = ± √((t_1 + t_2 cos k)^2 + t_2^2 sin^2 k)
= ± √((t_1 − t_2)^2 + 4 t_1 t_2 cos^2 (k/2))
δt
δt = 0
E_k
−π
π
k
δt ≠ 0.
−π
π
k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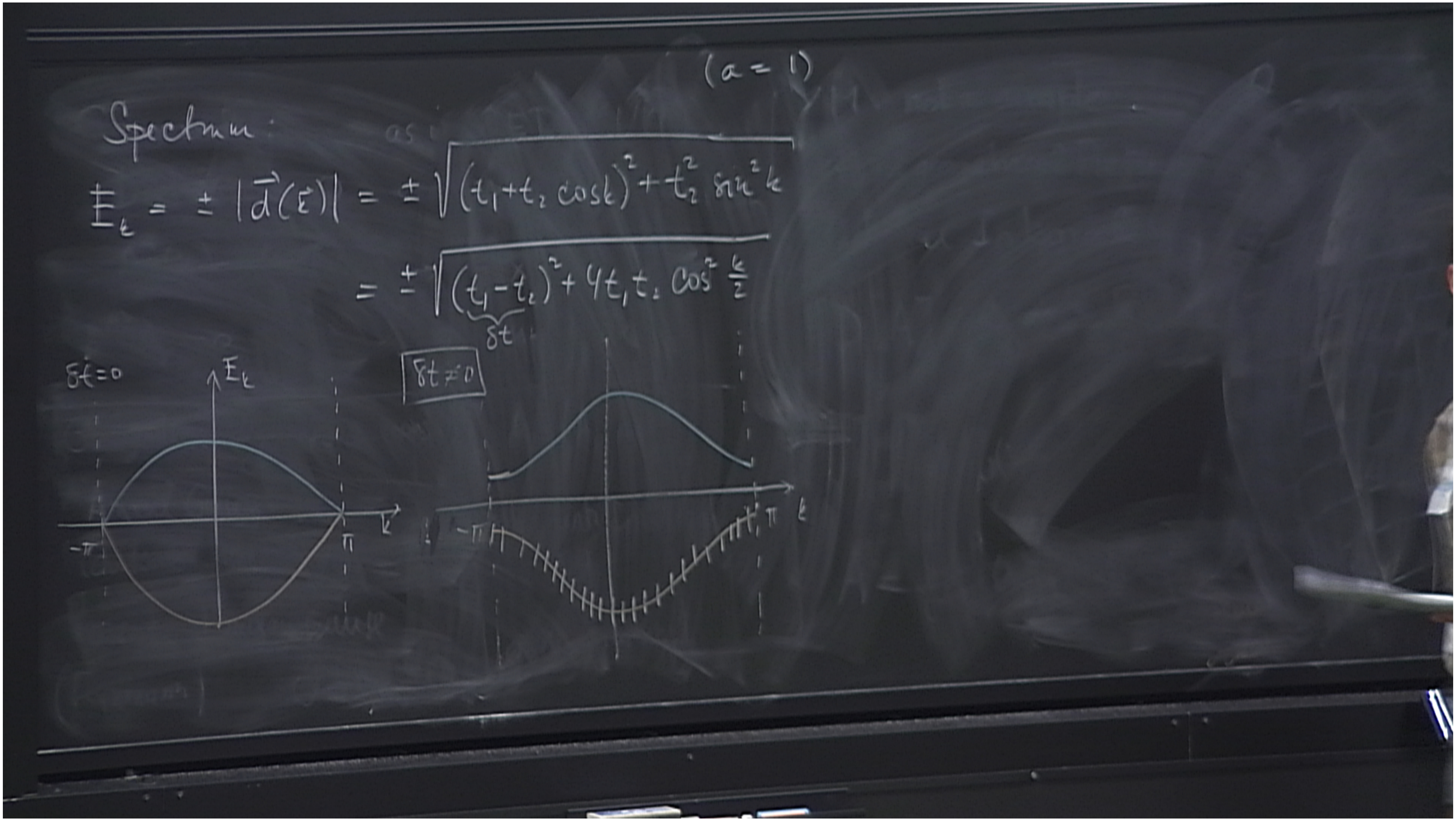
$\delta t = 0$
E_k
$-\pi$
π
k
$\boxed{\delta t \neq 0}$
$-\pi$
π
k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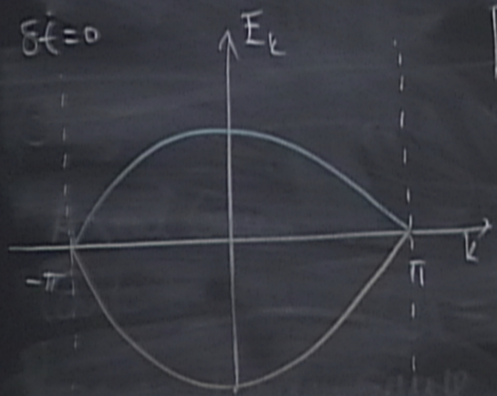

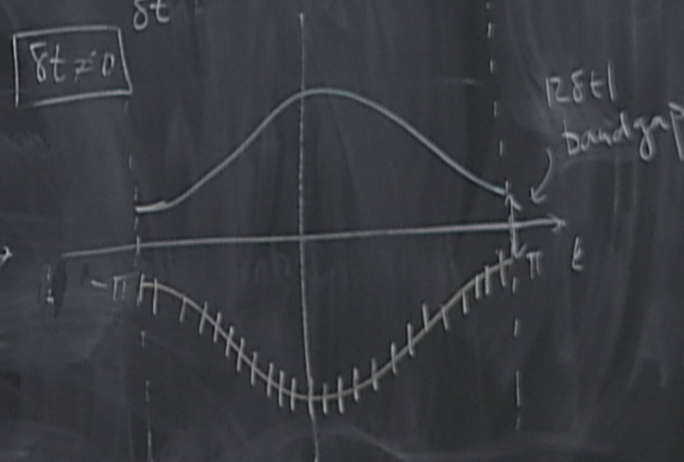

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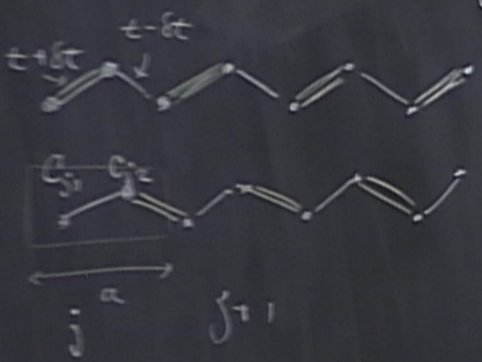

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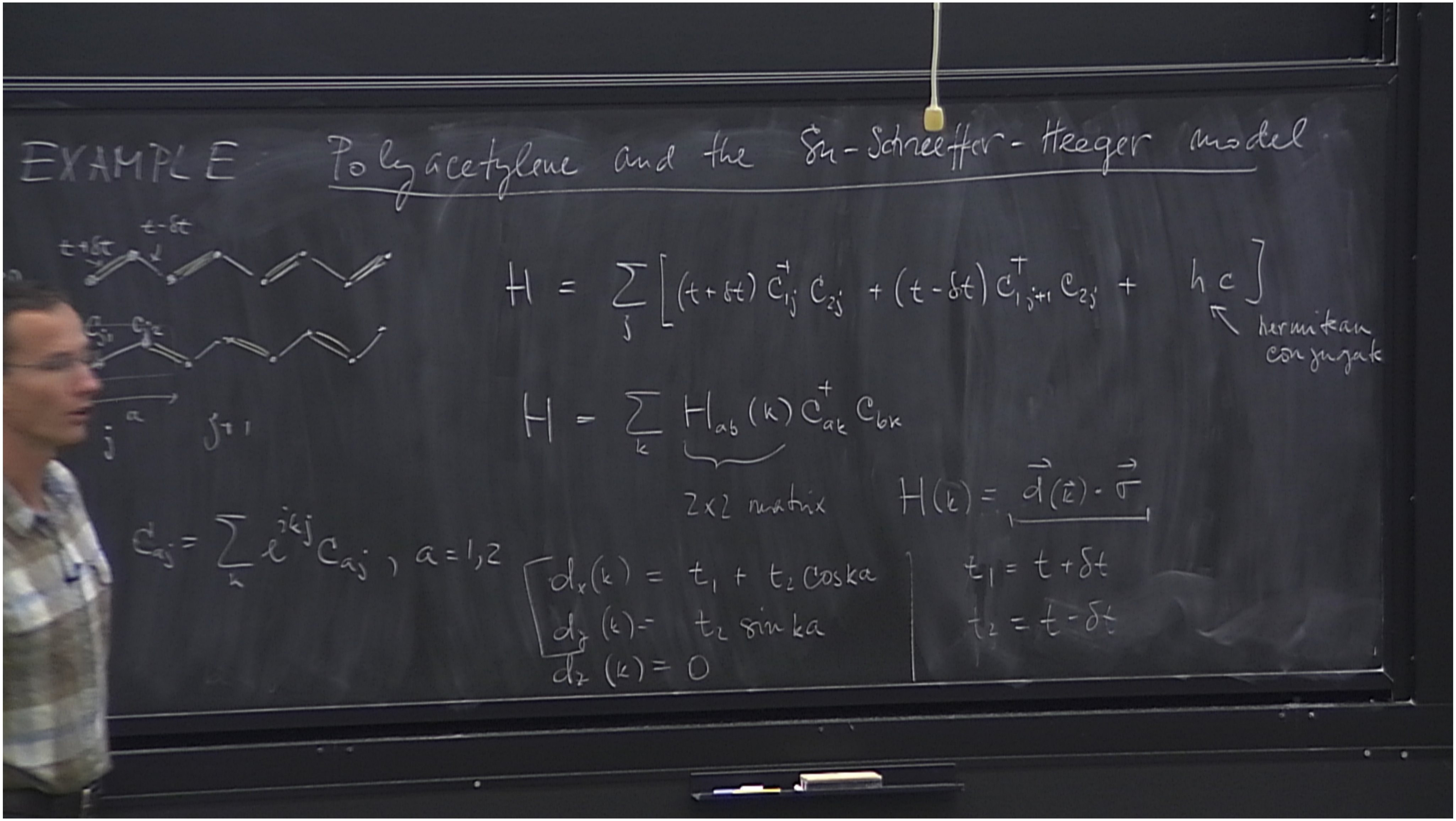
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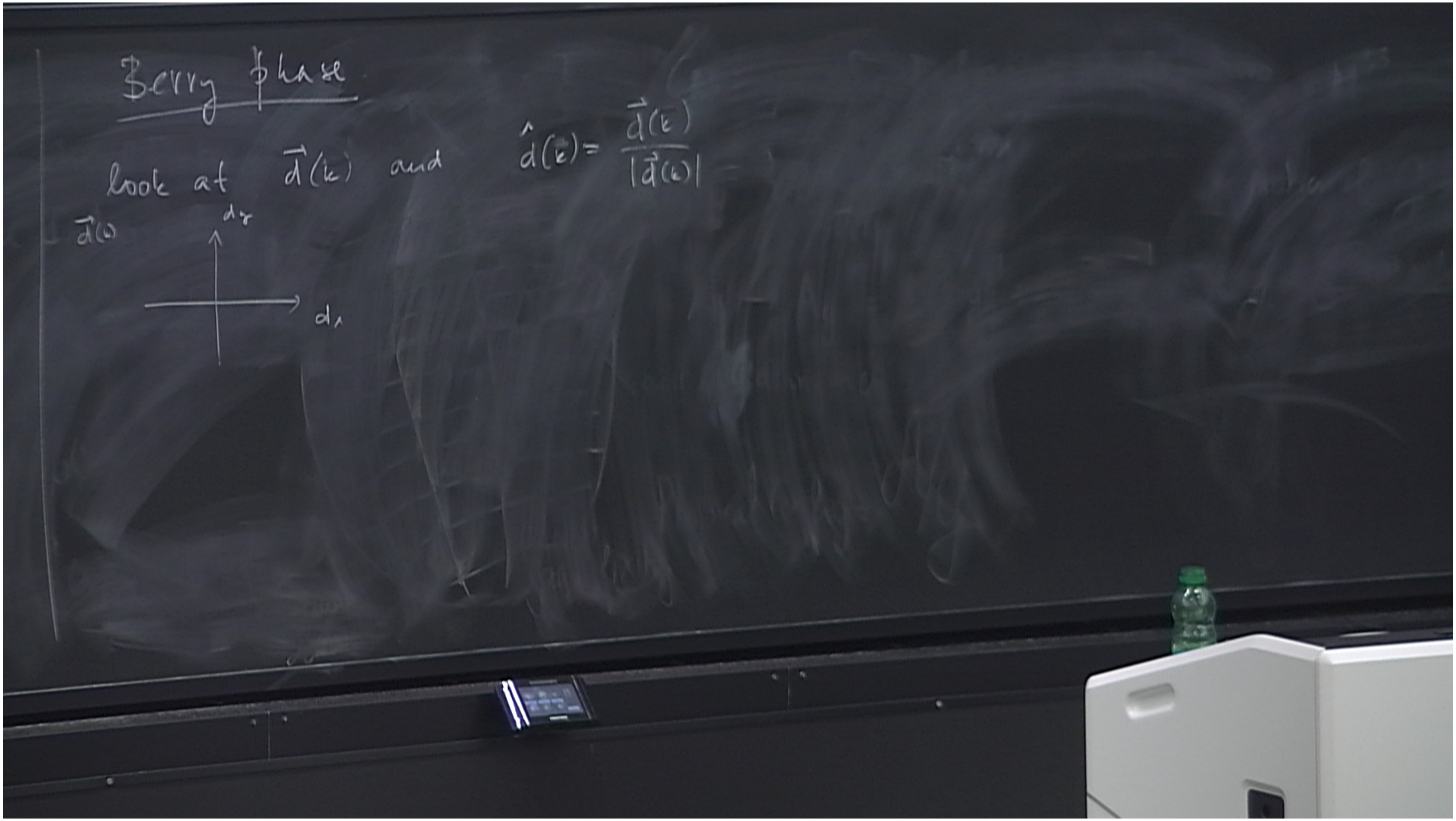
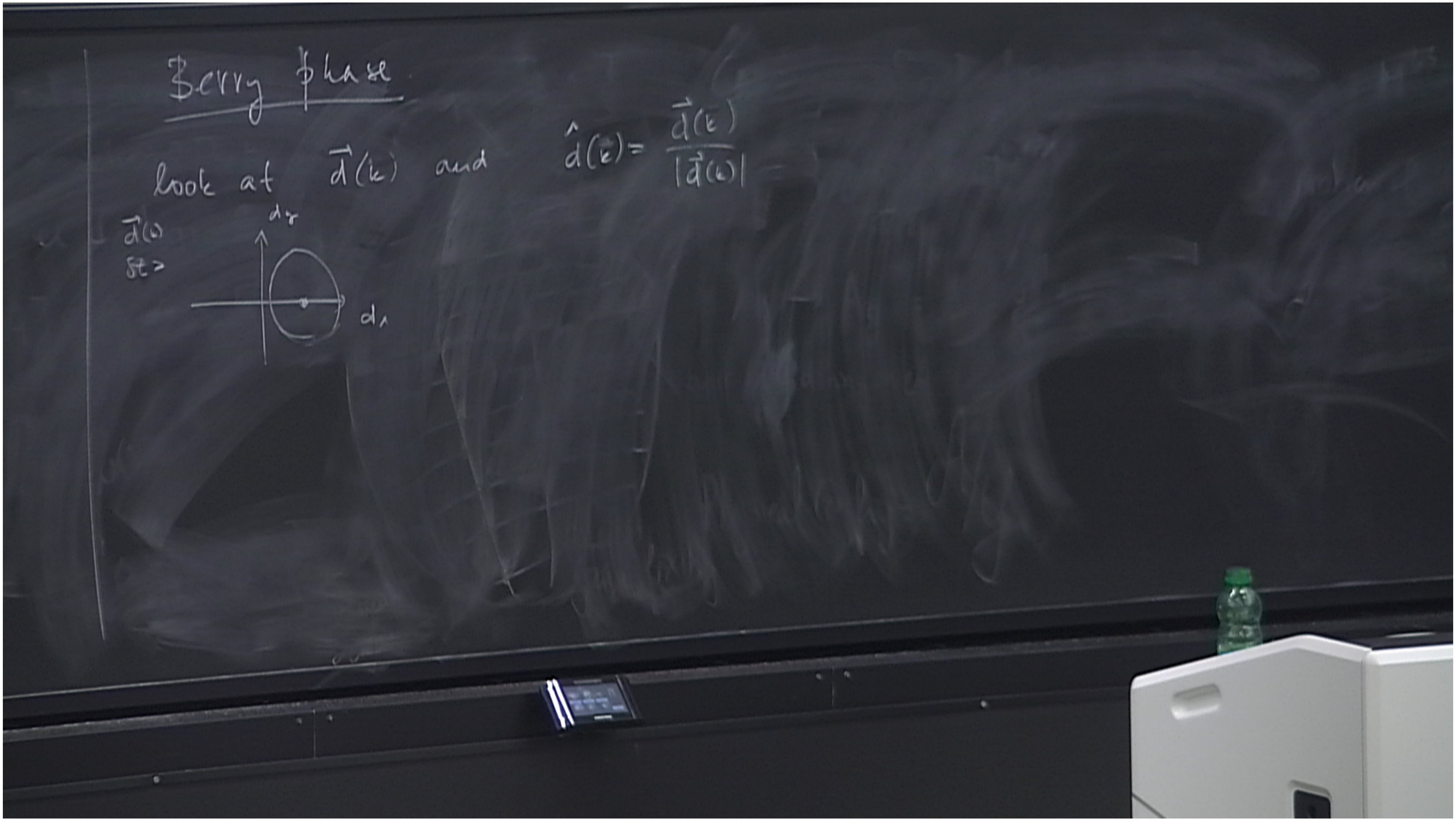

Berry phase
look at $\vec{d}(k)$ and $\hat{d}(\vec{k}) = \frac{\vec{d}(k)}{|\vec{d}(k)|}$
$\vec{d}(k)$
d_y
d_x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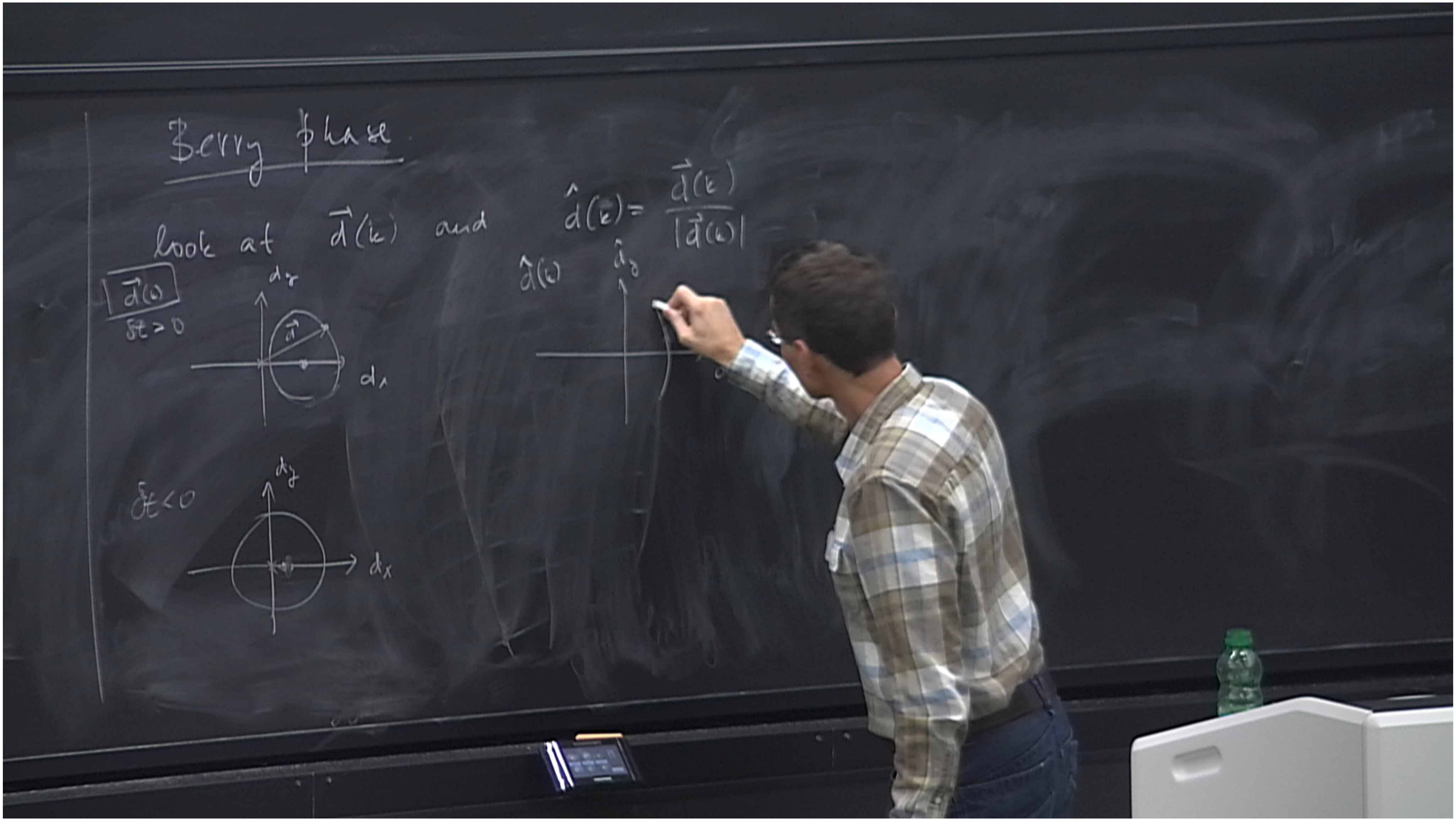
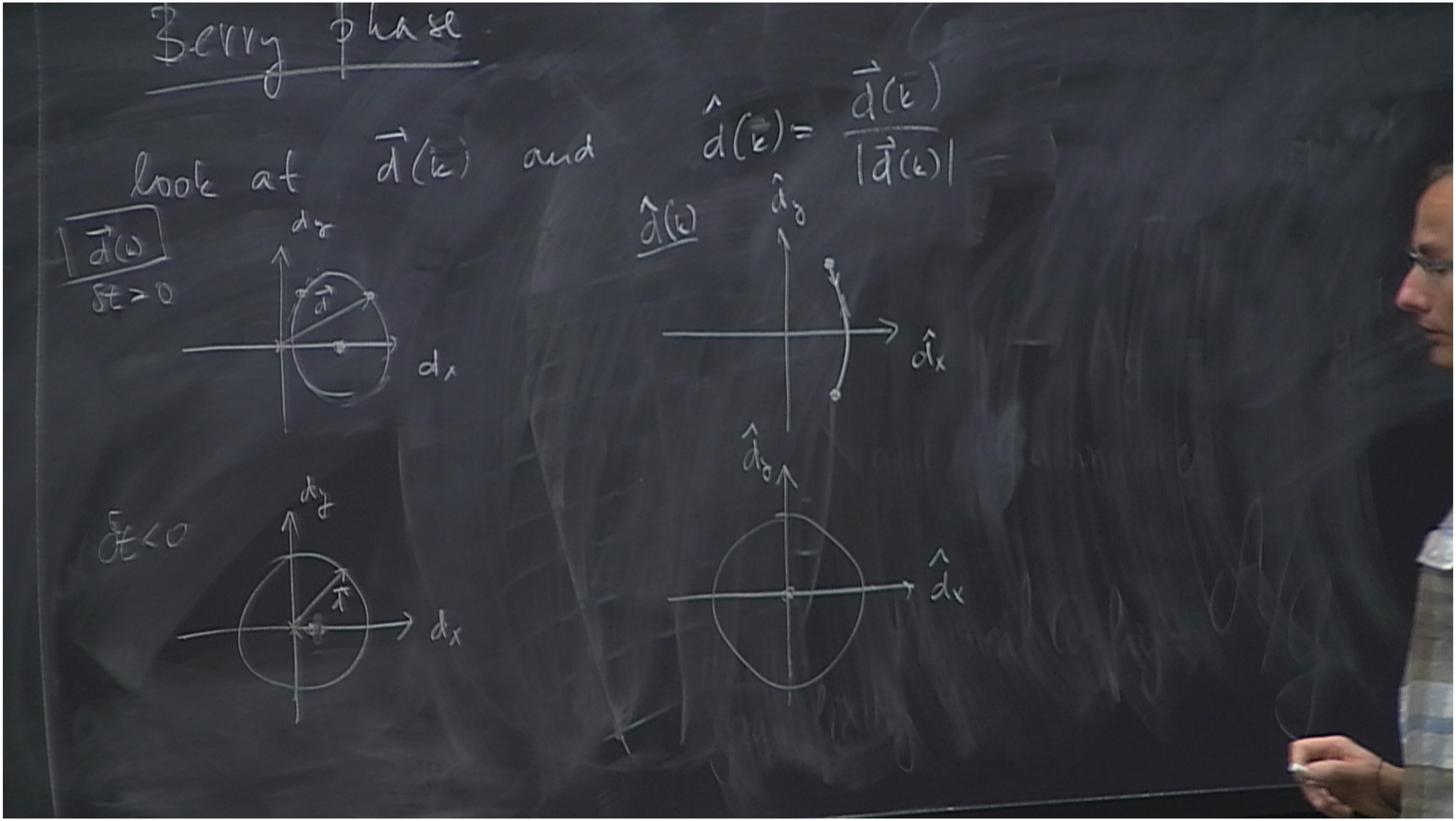
$\vec{d}(k)$
st >
d_y
d_x



Berry phase
look at $\vec{d}(k)$ and $\hat{d}(k) = \frac{\vec{d}(k)}{|\vec{d}(k)|}$
$\vec{d}(k)$
$\delta t > 0$
d_y
d_x
$\delta t < 0$
$\hat{d}(k)$
$\hat{d}_y$


Berry phase
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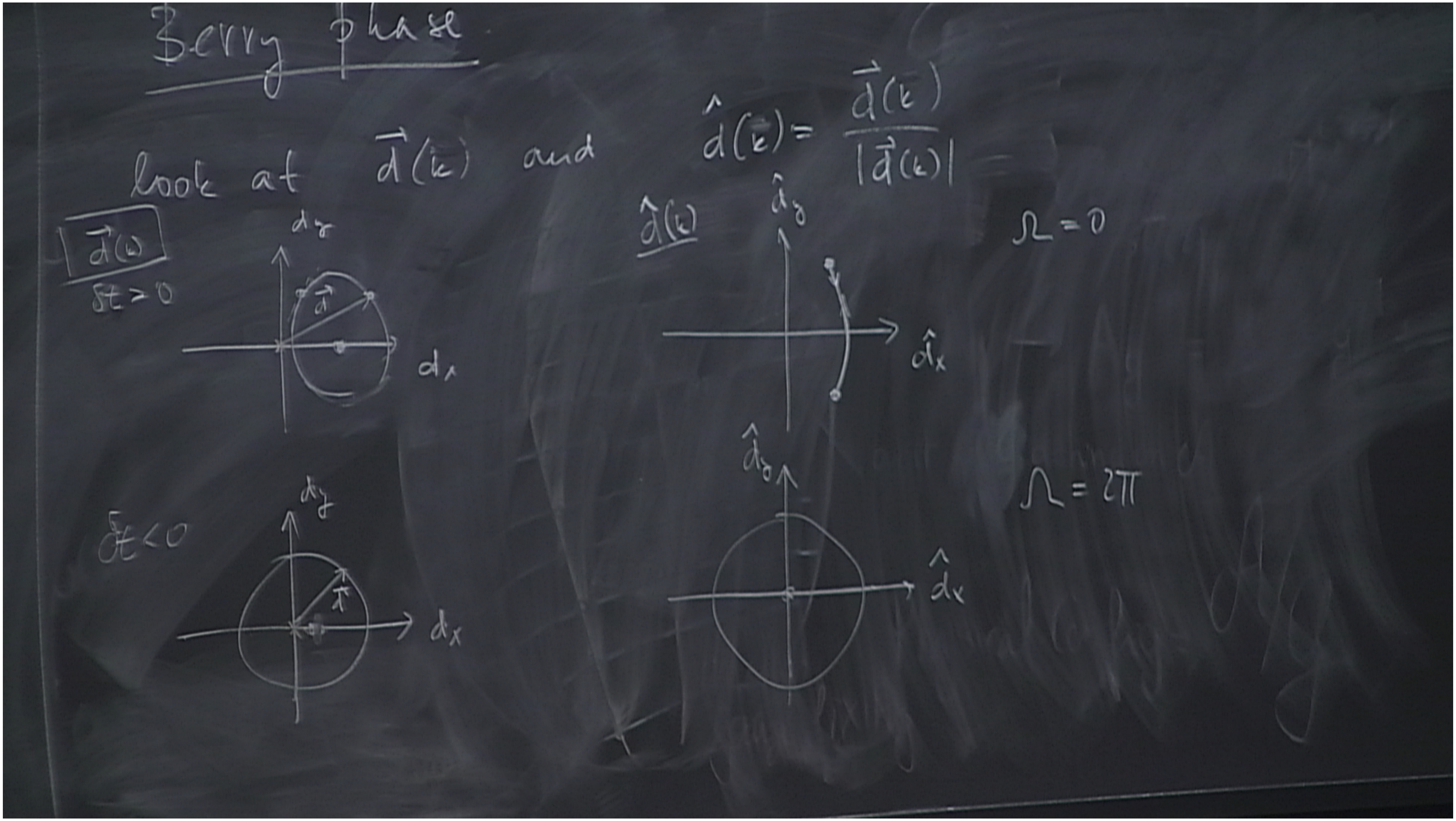
$\boxed{\vec{d}(k)}$
$\delta t > 0$
d_y
$\vec{d}$
d_x
$\delta t < 0$
d_y
d_x
$\hat{d}(k)$
$\hat{d}_y$
$\hat{d}_x$
$\hat{d}_y$
$\hat{d}_x$


Berry phase
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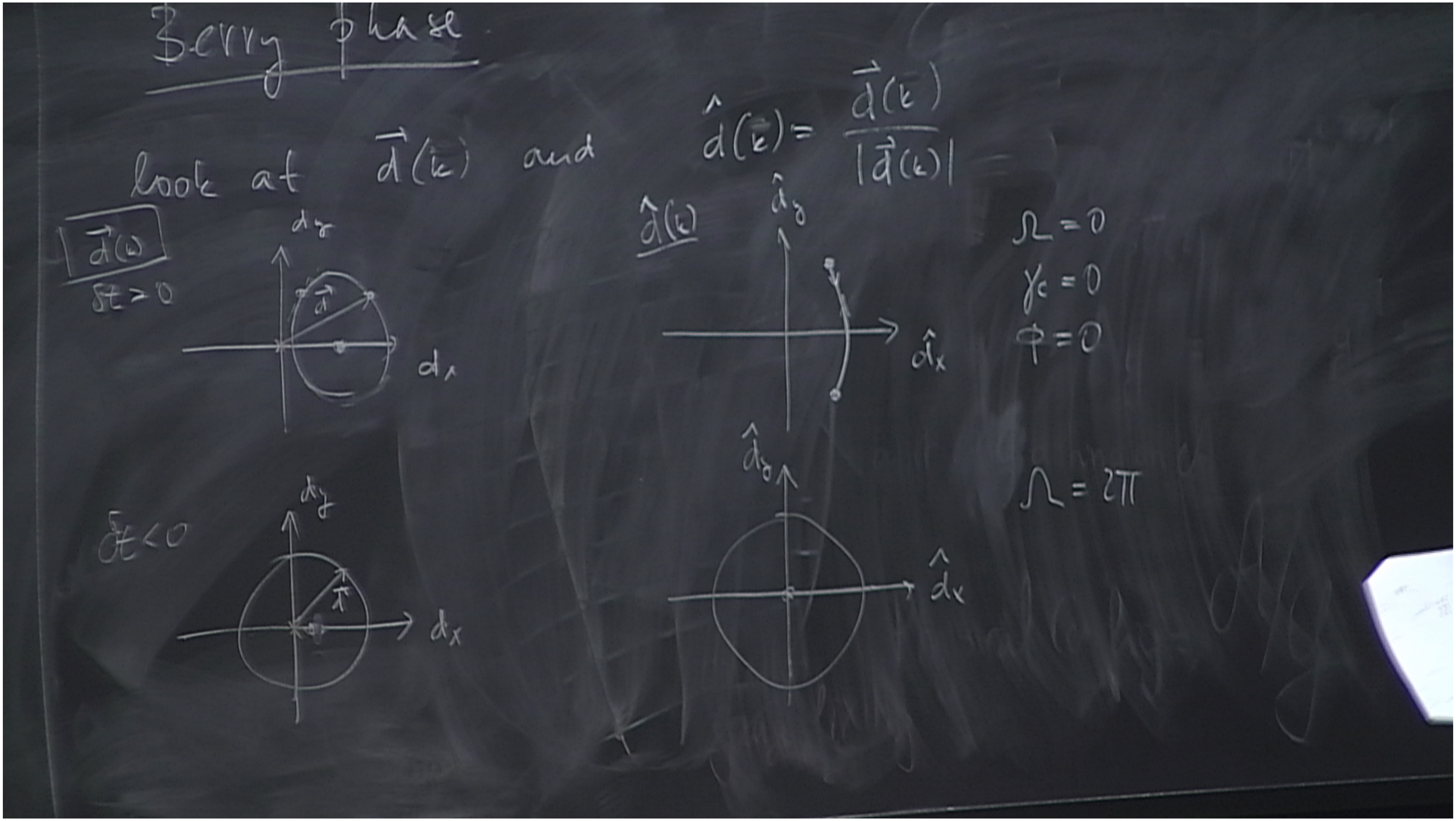
$\vec{d}(k)$
$\delta t > 0$
d_y
d_x
$\delta t < 0$
$\hat{d}(k)$
$\hat{d}_y$
$\hat{d}_x$
$\Omega = 0$
$\Omega = 2\pi$


Berry phase
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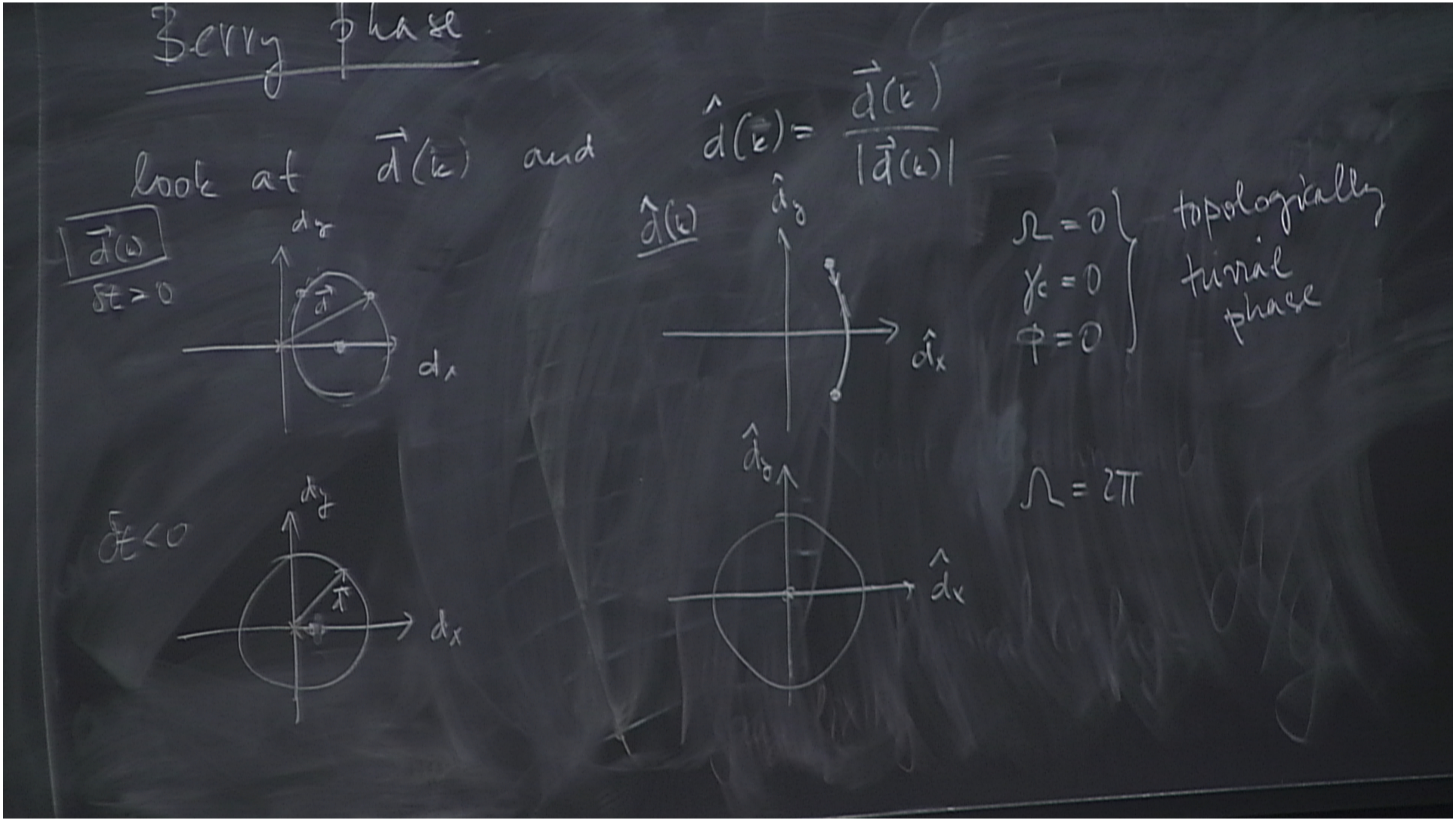
$\vec{d}(k)$
$\delta t > 0$
d_y
d_x
$\delta t < 0$
$\hat{d}(k)$
$\hat{d}_y$
$\hat{d}_x$
$\Omega = 0$
$\gamma_c = 0$
$\phi = 0$
$\Omega = 2\pi$


Berry phase
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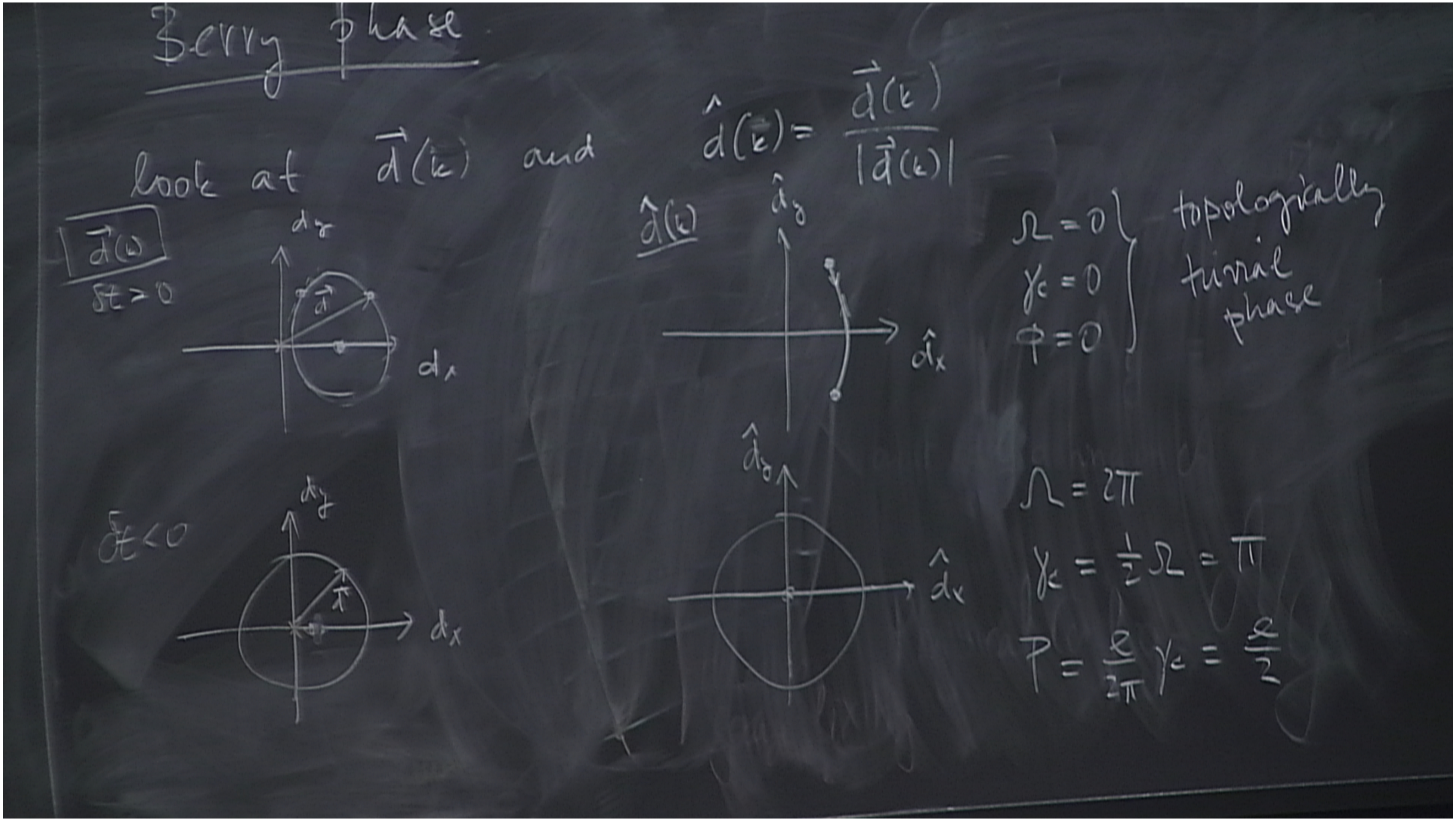
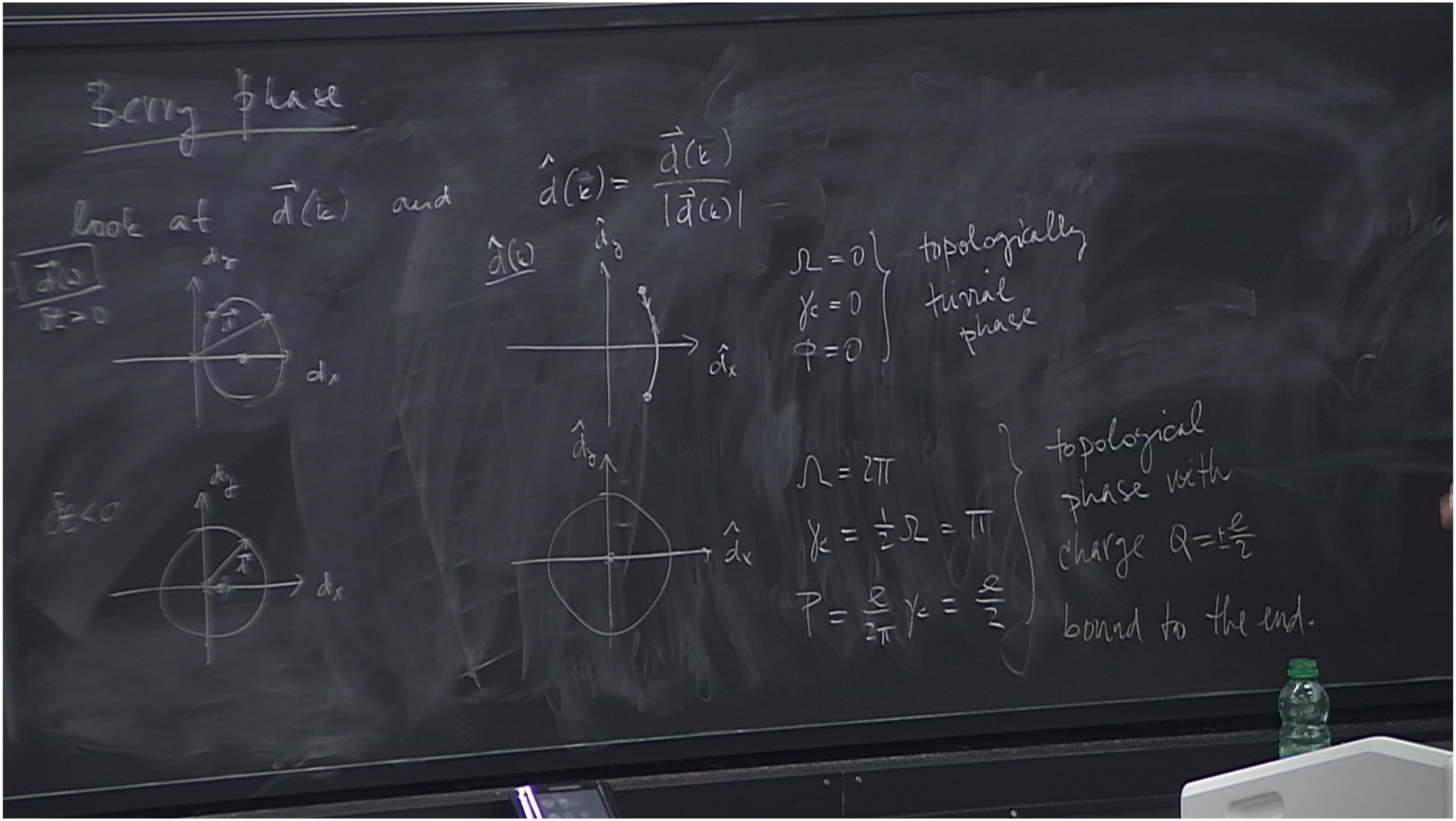
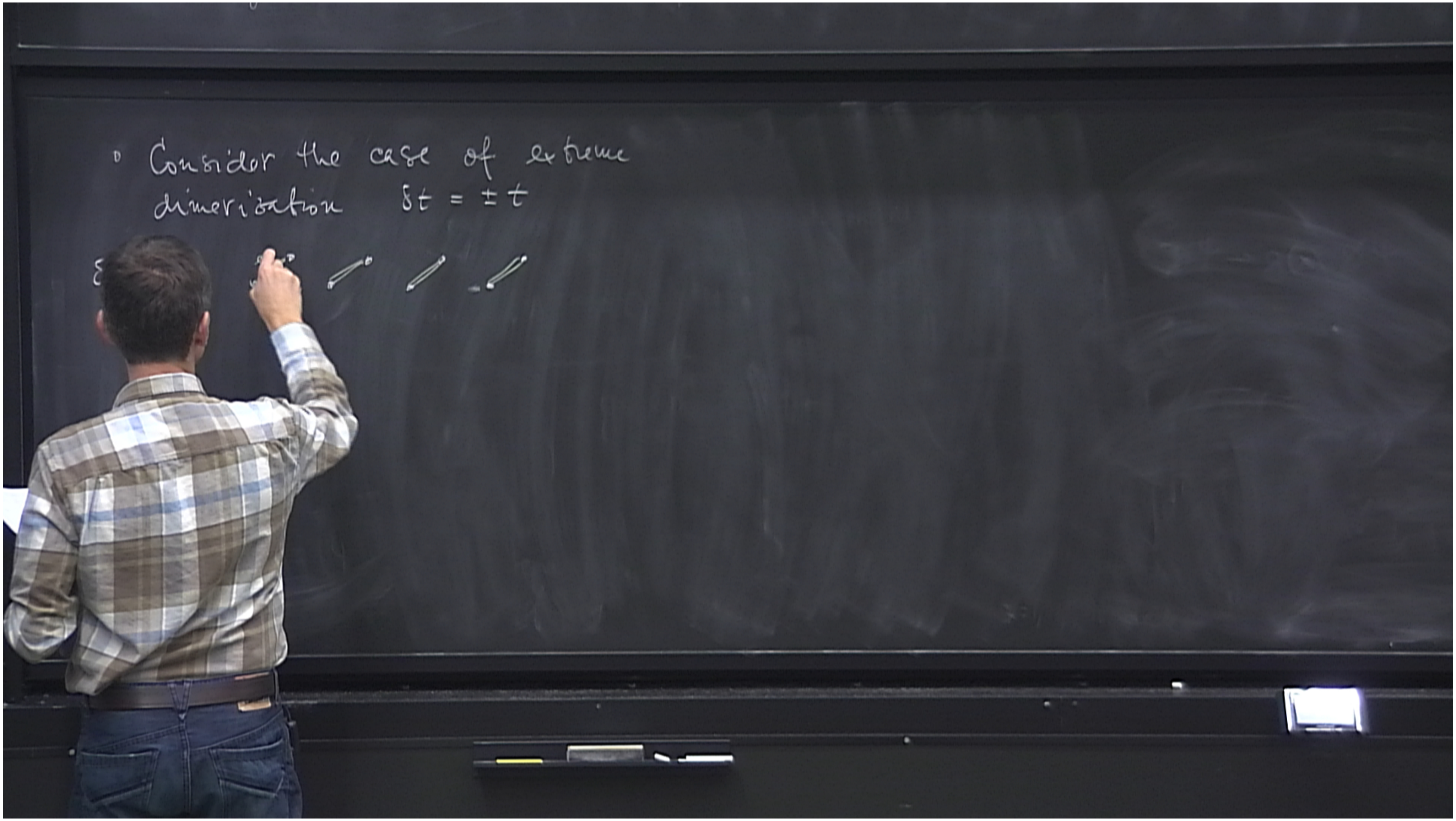
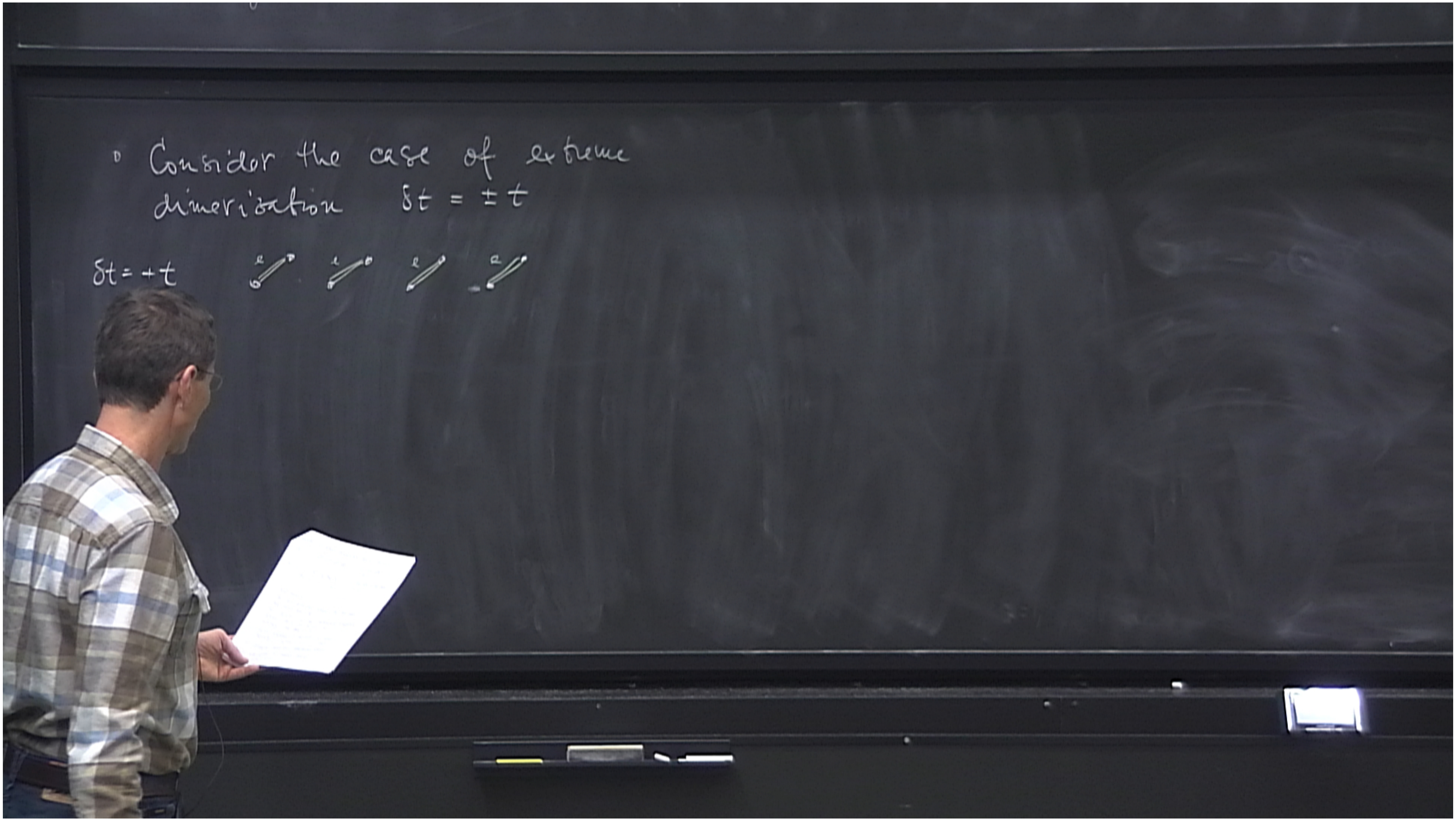
$\vec{d}(k)$
$\delta t > 0$
d_y
d_x
$\hat{d}(k)$
$\hat{d}_y$
$\hat{d}_x$
$\Omega = 0$
$\gamma_c = 0$
$\varphi = 0$
topologically trivial phase
$\delta t < 0$
$\Omega = 2\pi$

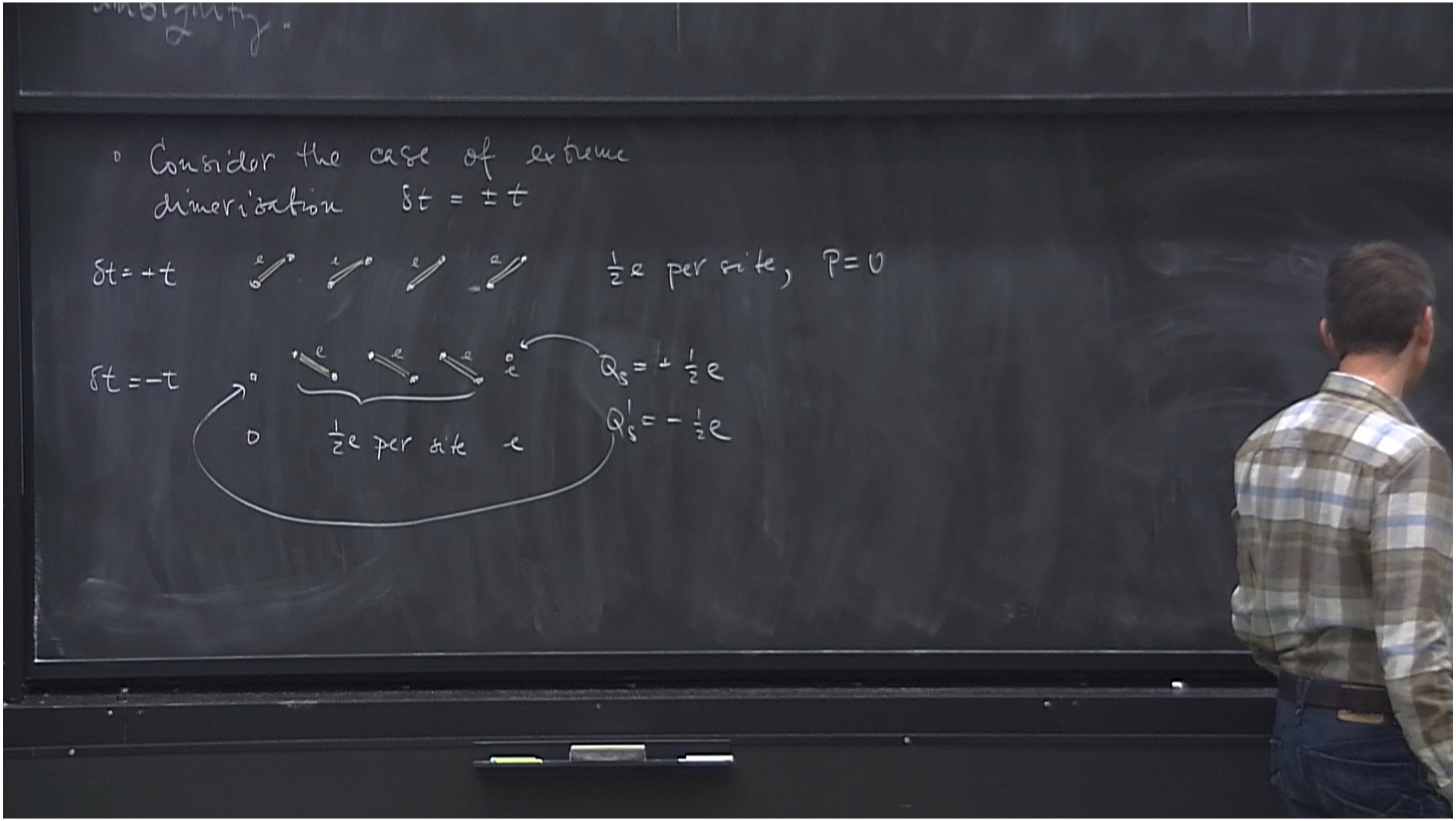

Berry phase
look at $\vec{d}(k)$ and $\hat{d}(k) = \frac{\vec{d}(k)}{|\vec{d}(k)|}$
$\boxed{\vec{d}(k)}$
$\delta t > 0$
d_y
$\vec{d}$
d_x
$\hat{d}(k)$
$\hat{d}_y$
$\hat{d}_x$
$\Omega = 0$
$\gamma_c = 0$
$\phi = 0$
topologically trivial phase
$\delta t < 0$
d_y
d_x
$\hat{d}_y$
$\hat{d}_x$
$\Omega = 2\pi$
$\gamma_c = \frac{1}{2}\Omega = \pi$
$P = \frac{e}{2\pi}\gamma_c = \frac{e}{2}$

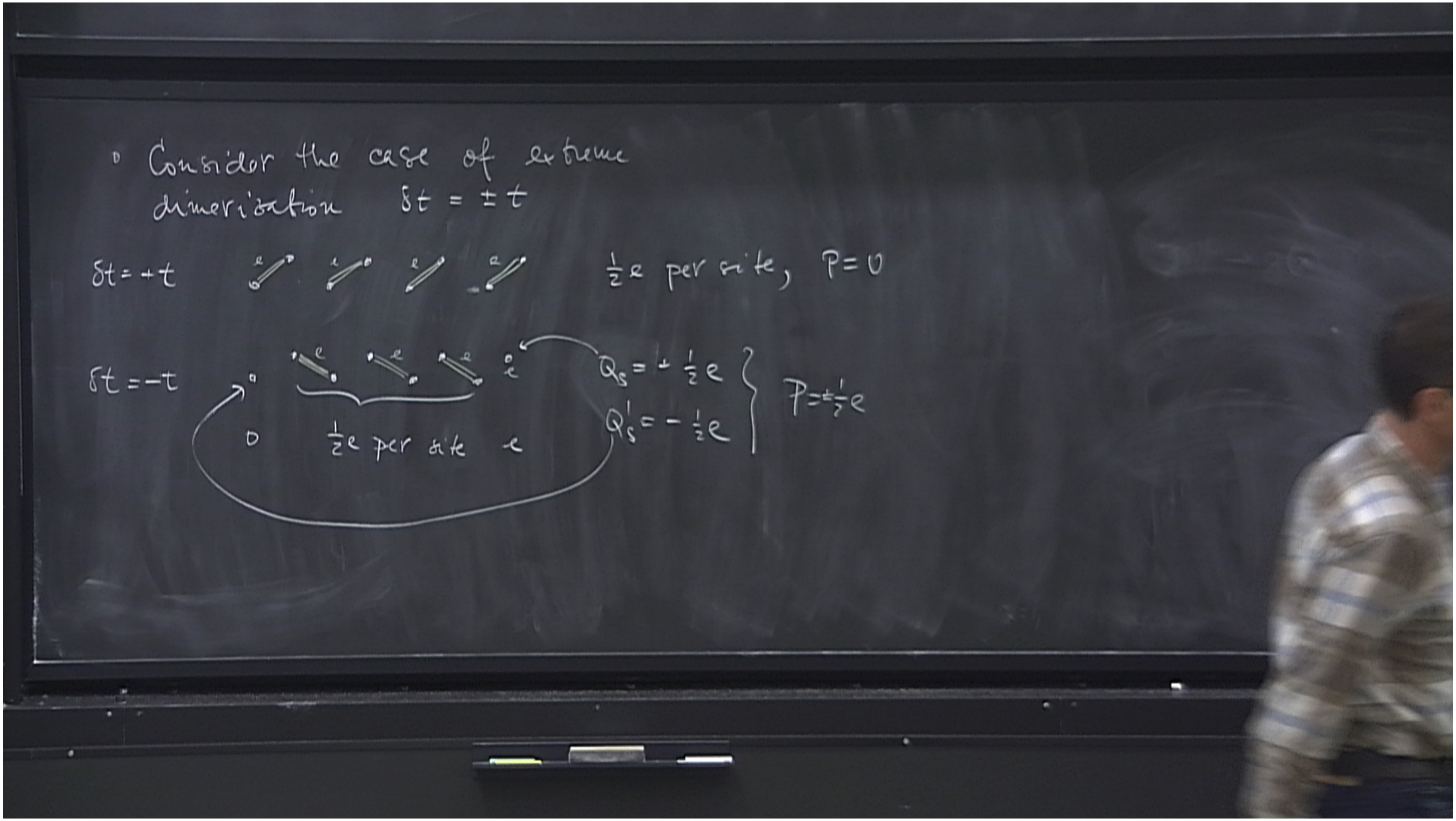

Berry phase
look at $\vec{d}(k)$ and
$\hat{d}(k) = \frac{\vec{d}(k)}{|\vec{d}(k)|}$
$\vec{d}(k)$
$\delta t > 0$
d_y
d_x
$\delta t < 0$
$\hat{d}(k)$
$\hat{d}_y$
$\hat{d}_x$
$\Omega = 0$
$\gamma_c = 0$
$\varphi = 0$
topologically trivial phase
$\Omega = 2\pi$
$\gamma_c = \frac{1}{2}\Omega = \pi$
$P = \frac{e}{2\pi}\gamma_c = \frac{e}{2}$
topological phase with charge $Q = \pm\frac{e}{2}$ bound to the end.

- Consider the case of extreme dimerization $\delta t = \pm t$


Consider the case of extreme
dimerization $\delta t = \pm t$


Consider the case of extreme
dimerization $\delta t = \pm t$
$\delta t = +t$


ambiguity.
Consider the case of extreme dimerization δt = ±t
δt = +t
½e per site, P = 0
δt = −t
Q_s = +½e
Q'_s = −½e
½e per site


Consider the case of extreme dimerization δt = ±t
δt = +t
e e e e
½e per site, P = 0
δt = −t
e e e e
Q_s = + ½e
Q'_s = − ½e
P = ±½e
½e per site
e

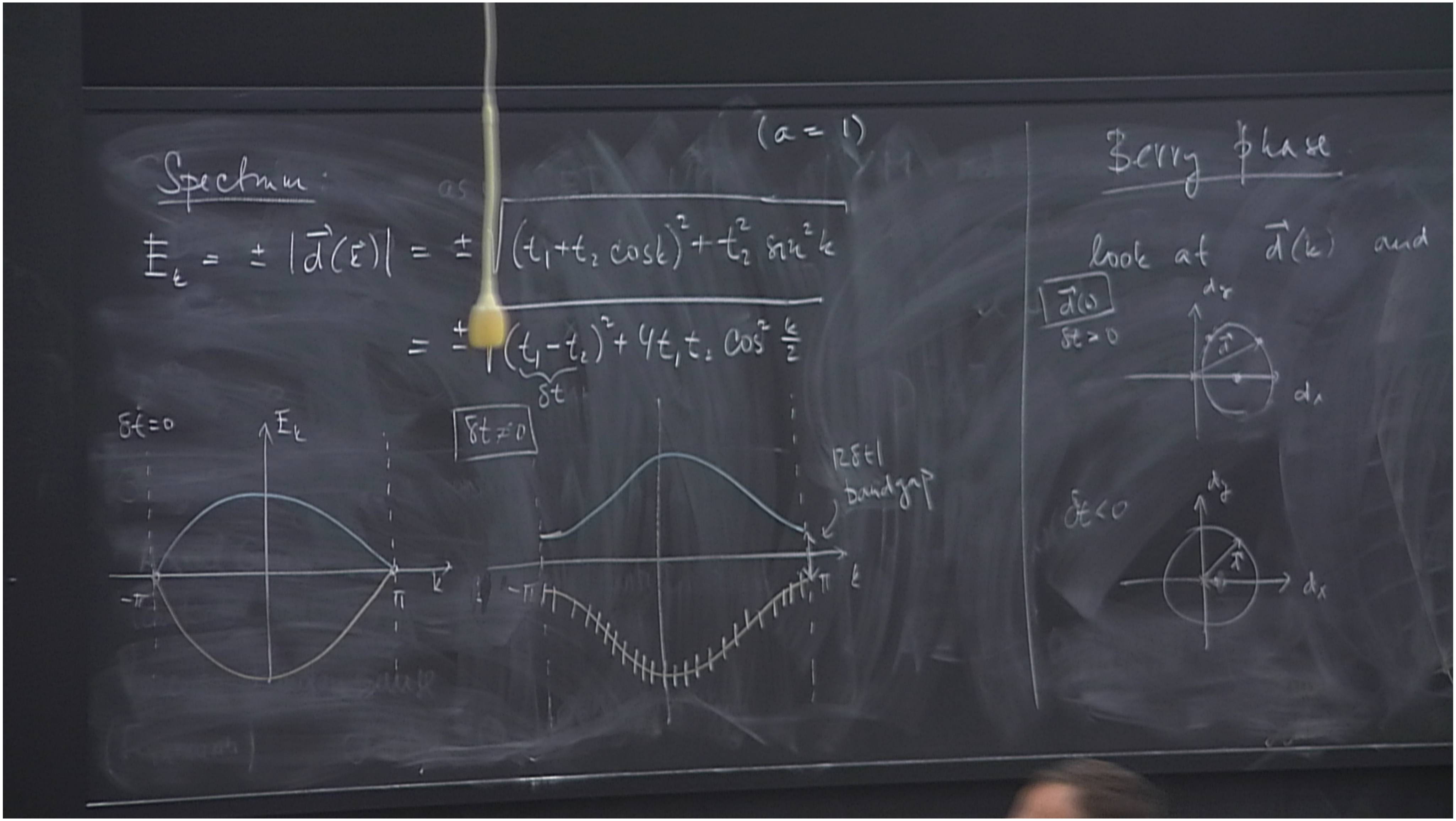
- Consider the case of extreme dimerization $\delta t = \pm t$

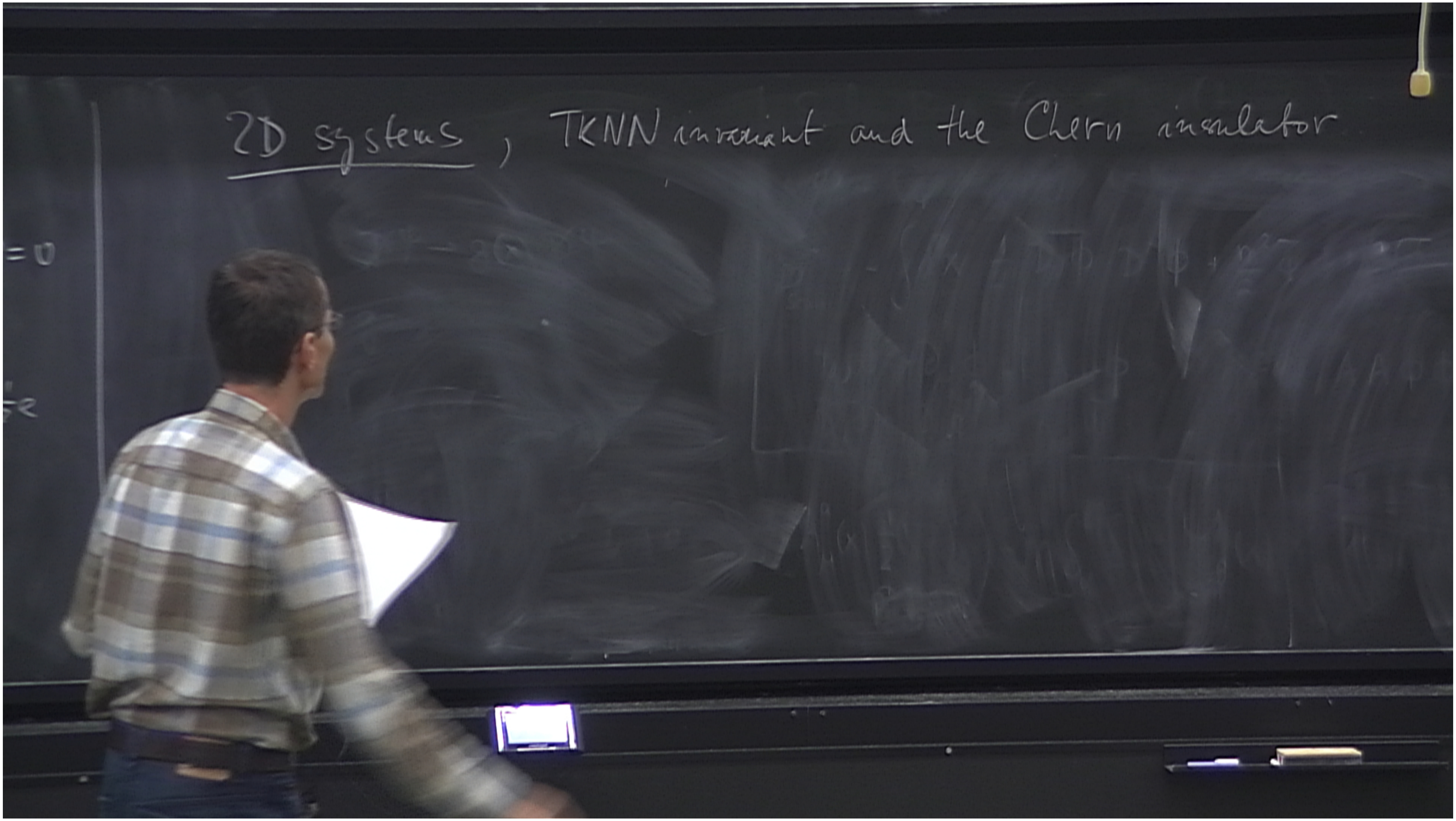
$\delta t = +t$ e e e e $\frac{1}{2}e$ per site, $P = 0$

$\delta t = -t$ e e e e $Q_s = +\frac{1}{2}e$, $Q_s' = -\frac{1}{2}e$ $P = \pm\frac{1}{2}e$

$\frac{1}{2}e$ per site   e

$\delta t \neq -t$


(a = 1)
Spectrum:
$E_k = \pm |\vec{d}(k)| = \pm \sqrt{(t_1 + t_2 \cos k)^2 + t_2^2 \sin^2 k}$
$= \pm \sqrt{(t_1 - t_2)^2 + 4 t_1 t_2 \cos^2 \frac{k}{2}}$
δt
δt=0
E_k
−π
π
k
δt≠0
\|2δt\|
bandgap
Berry phase
look at $\vec{d}(k)$ and
$\vec{d}(k)$
δt>0
d_y
d_x
δt<0


2D systems, TKNN invariant and the Chern insulator

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[Thouless, Kohmoto, Nightingale & den Nijs, PRL 49, 405 (1982)]

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$$\sigma_{xy} = \frac{e^2}{h} n$$

where $n \in \mathbb{Z}$ is the Chern number

$$n = \frac{1}{2\pi} \int_{BZ} d^2k \, \mathcal{F}_{xy}(\vec{k}) \, ,$$

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$= 0$

ke

2D systems, TKNN invariant and the Chern insulator

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"In a 2D band insulator, Hall conductivity ($\sigma_{xx} = 0$)

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Berry

$$\mathcal{F}_{xy}(\vec{k}) = \left(\vec{\nabla}_k \times \vec{\mathcal{A}}(\vec{k}) \right)_{xy}$$

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$\sigma_{xx} = 0$

insulator, Hall conductivity

n

the Chern number

$(\vec{k})$, and $\frac{e^2}{h}$ is

the quantum of conductance.

$$\mathcal{F}_{xy}(\vec{k}) = \left(\vec{\nabla}_k \times \vec{\mathcal{A}}(\vec{k})\right)_{xy}$$

Berry curvature

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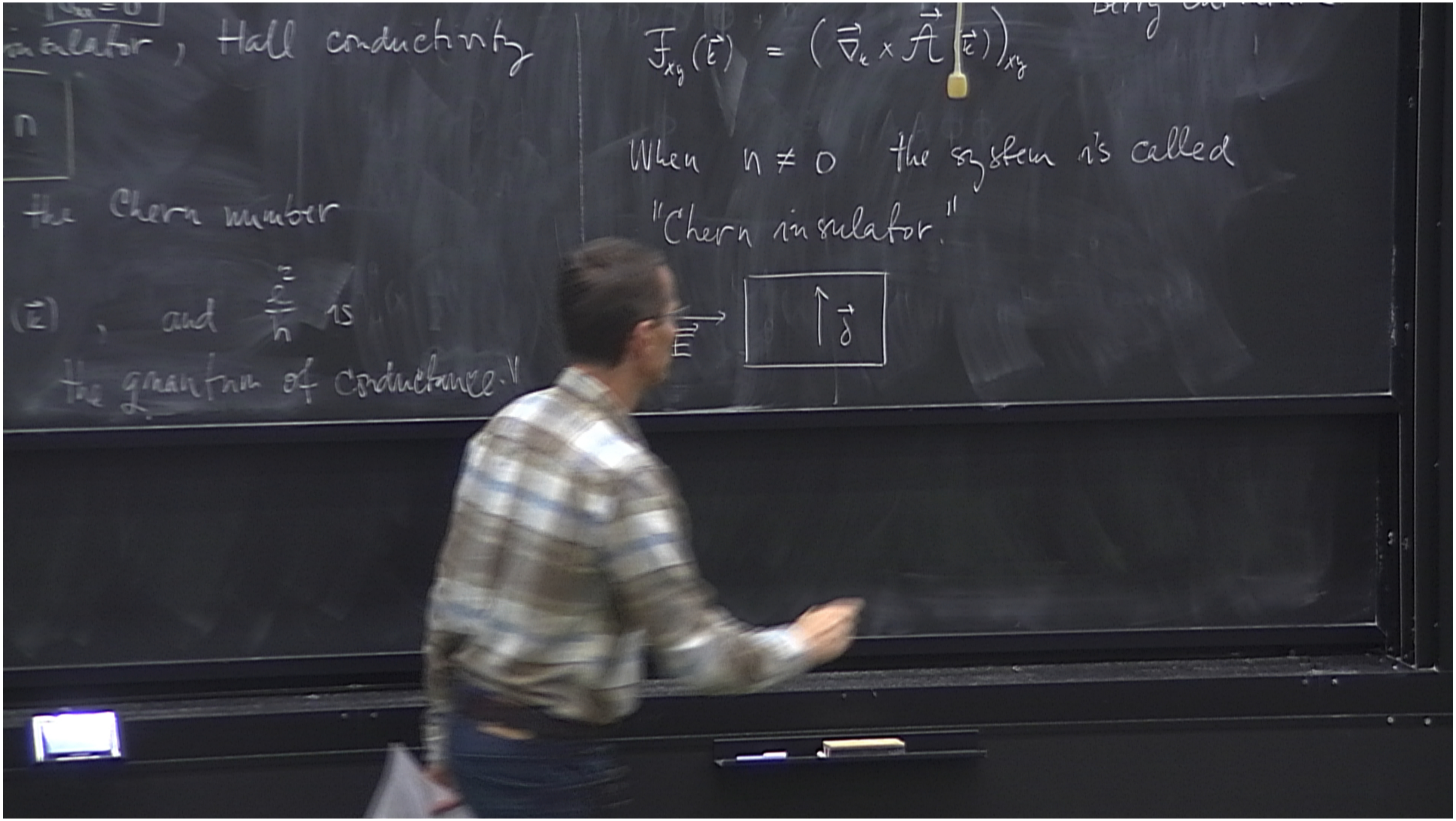
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the Chern number
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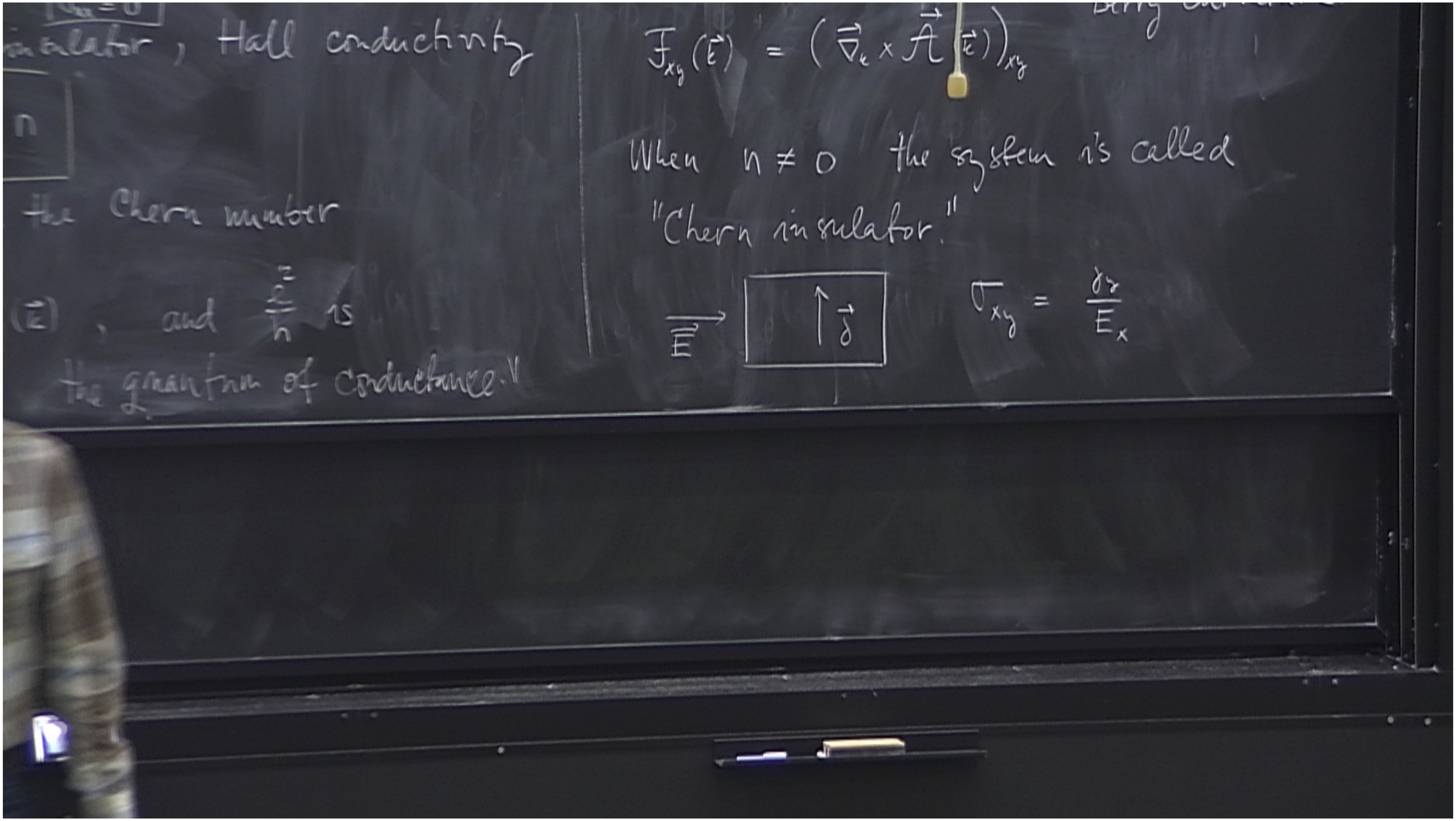
the quantum of conductance.
$\vec{E}$
$\vec{j}$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$\vec{E}$ $\vec{j}$ $\vec{j}$

$$\sigma_{xy} = \frac{j_y}{E_x}$$

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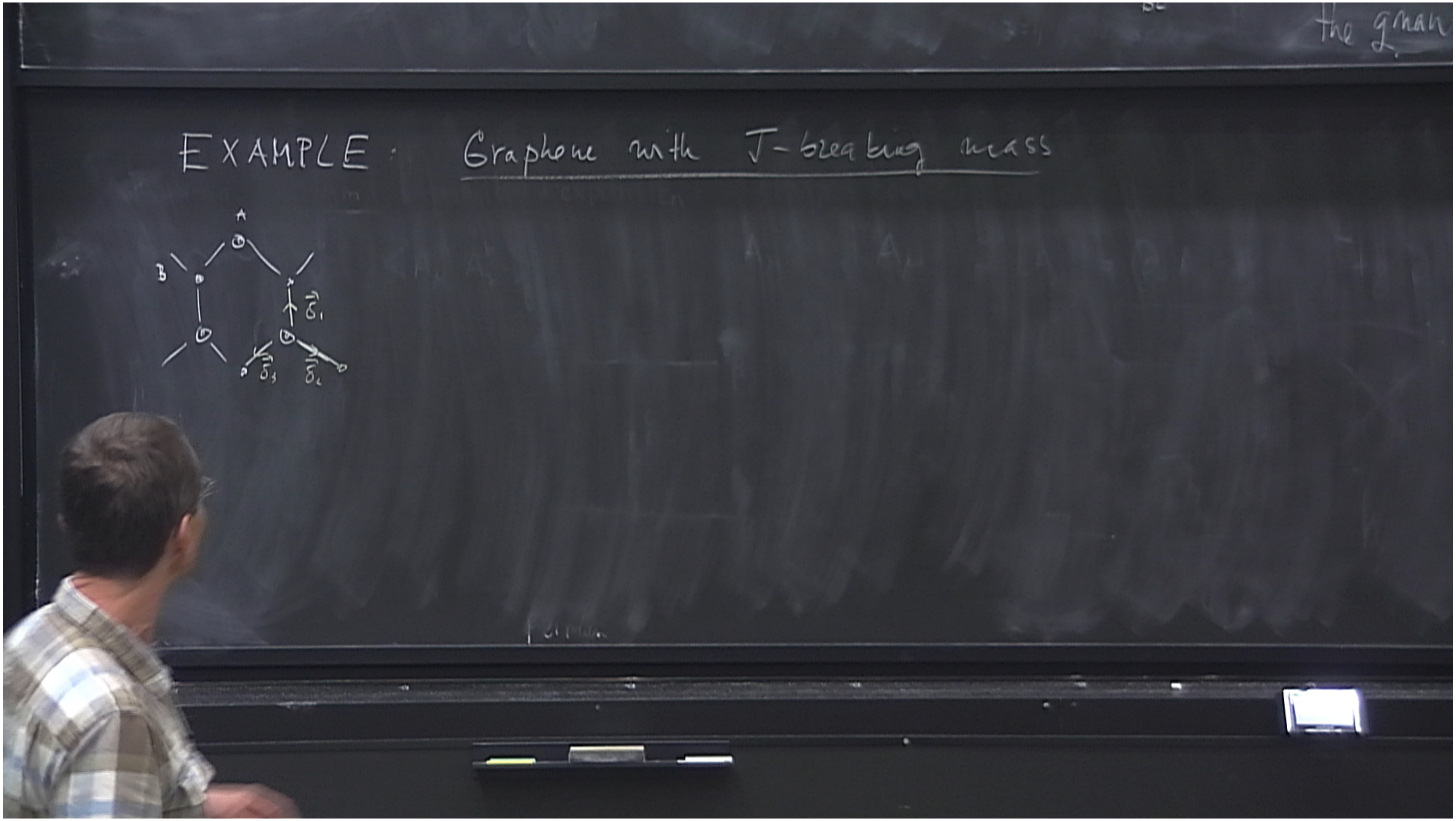
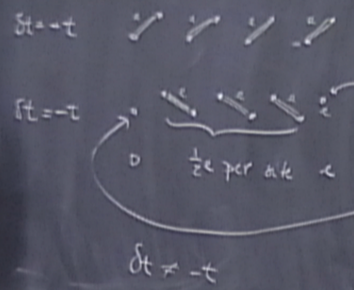

EXAMPLE: Graphene with T-breaking mass
B
$\vec{\delta}_1$
$\vec{\delta}_3$
$\vec{\delta}_2$



$\delta t = -t$ — $\frac{1}{2}e$ per site, $P = 0$

$\delta t = -t$ — $\frac{1}{2}e$ per site — $Q = +\frac{1}{2}e$, $Q = -\frac{1}{2}e$ } $P = \pm\frac{1}{2}e$

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$\boxed{\sigma_{xx} = 0}$

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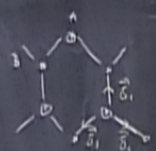
$\vec{E}$ $\boxed{\vec{J}\ \uparrow\vec{J}}$

$$\sigma_{xy} = \frac{J_y}{E_x}$$

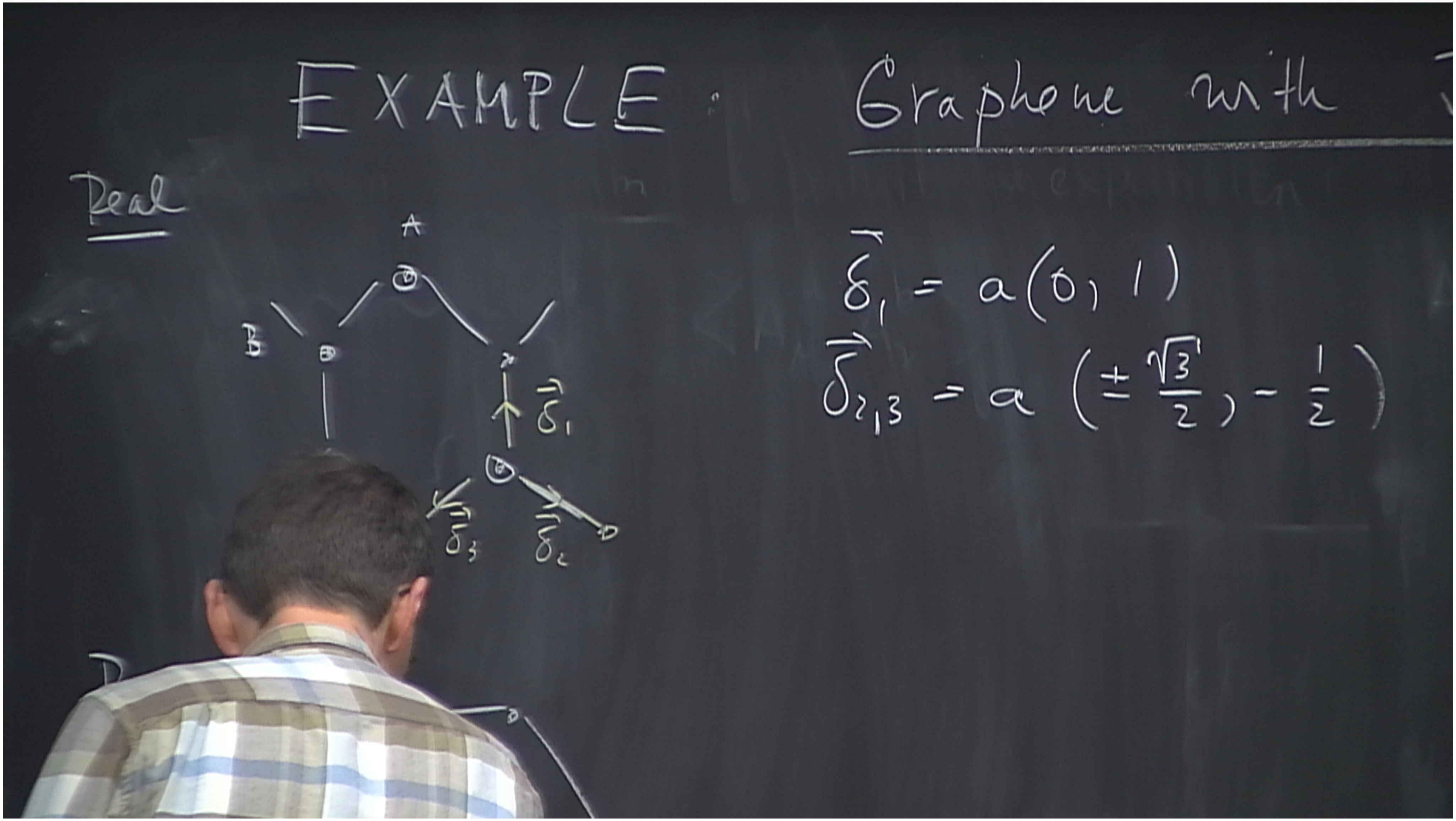
$$\sigma_{xx} = \frac{J_x}{E_x}$$

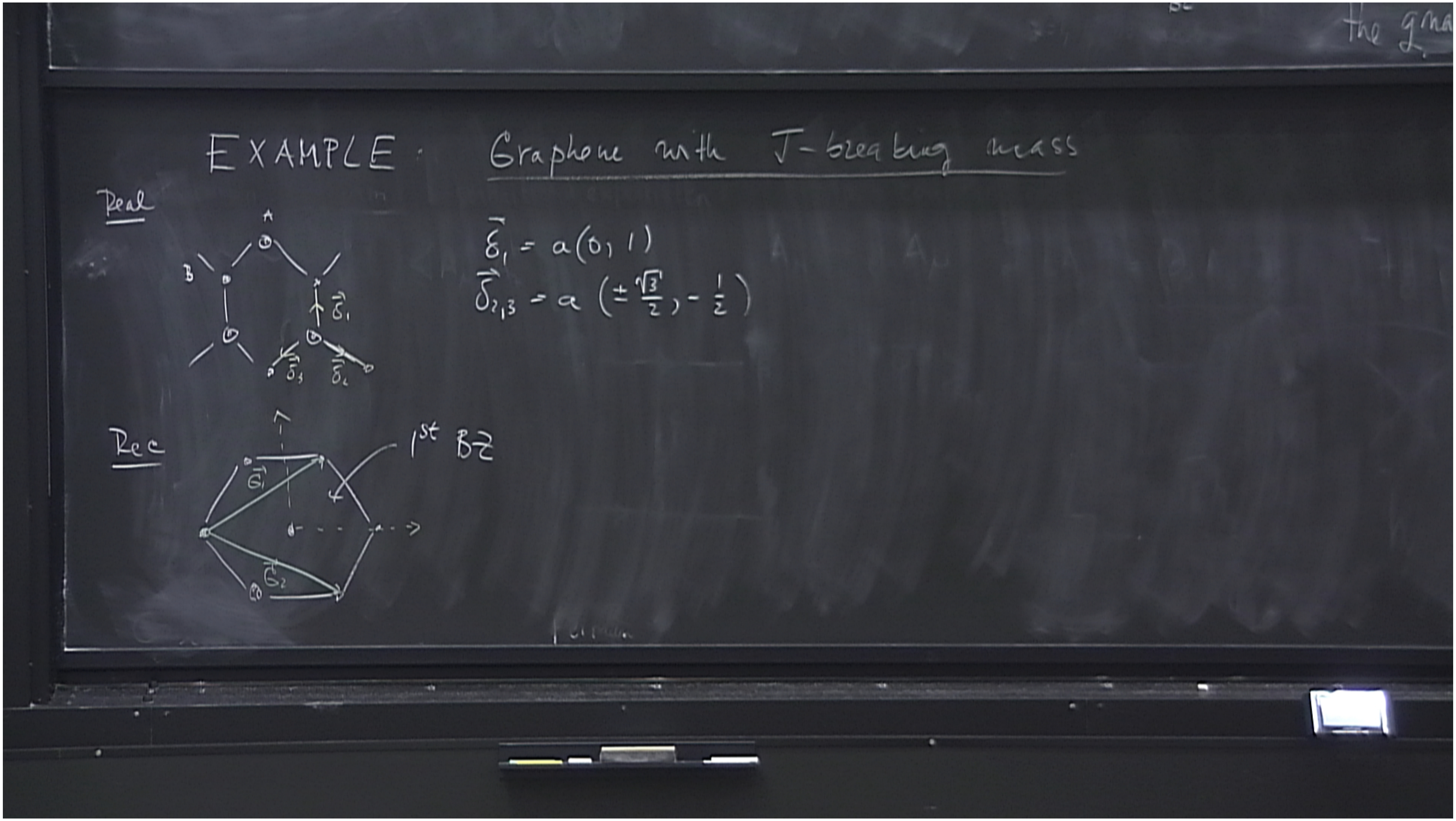
EXAMPLE Graphene with T-breaking mass

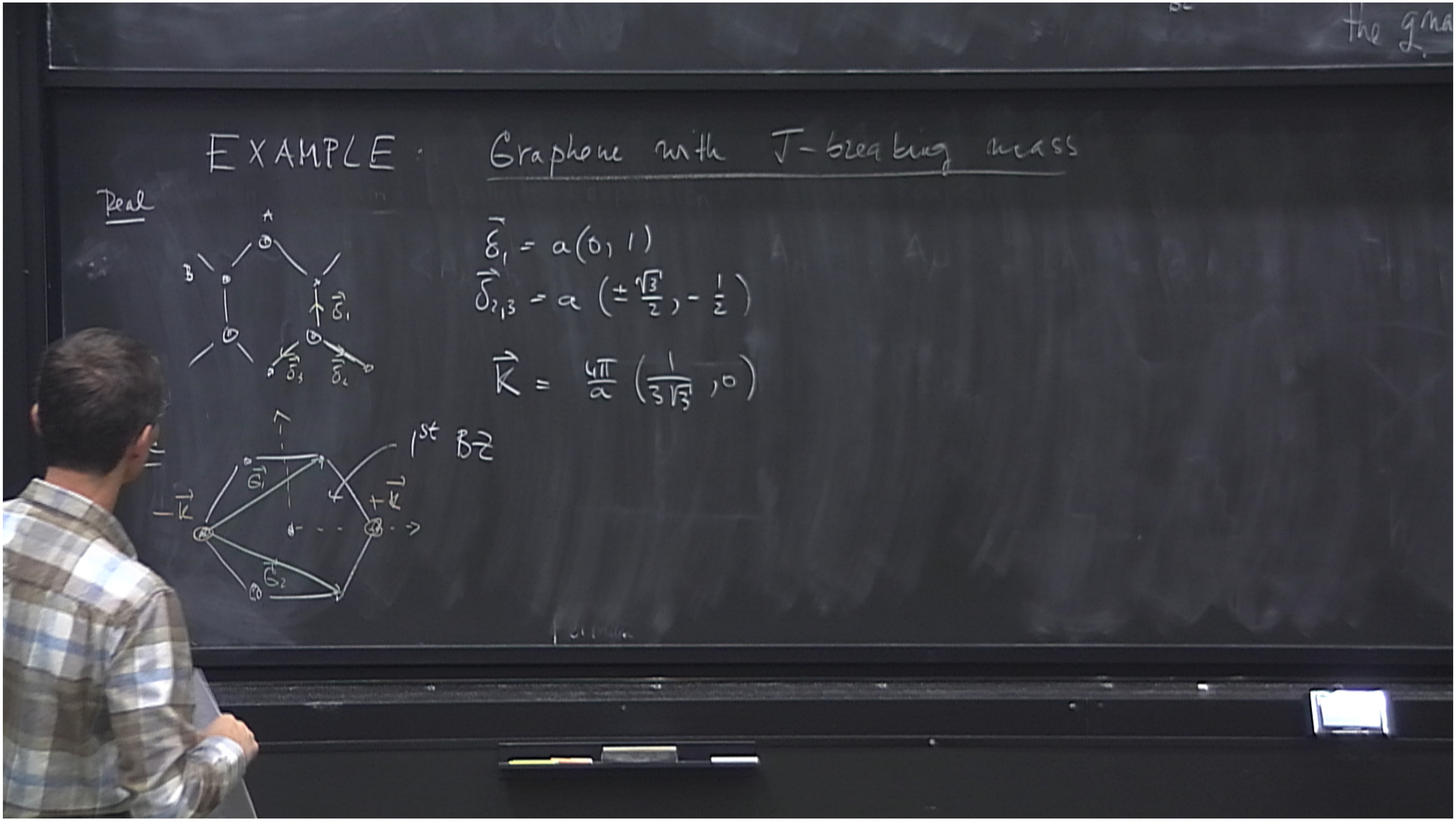


$\vec{\delta}_1 = a(0, 1)$

$\vec{\delta}_{2,3} = a\left(\pm\frac{\sqrt{3}}{2}, -\frac{1}{2}\right)$

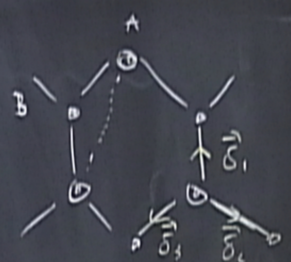

EXAMPLE: Graphene with
Real
A
B
$\vec{\delta}_1$
$\vec{\delta}_3$
$\vec{\delta}_2$
$\vec{\delta}_1 = a(0, 1)$
$\vec{\delta}_{2,3} = a\left(\pm\frac{\sqrt{3}}{2}, -\frac{1}{2}\right)$


EXAMPLE: Graphene with T-breaking mass
Real
B
$\vec{\delta}_1$
$\vec{\delta}_3$
$\vec{\delta}_2$
$\vec{\delta}_1 = a(0, 1)$
$\vec{\delta}_{2,3} = a\left(\pm\frac{\sqrt{3}}{2}, -\frac{1}{2}\right)$
Rec
1^{st} BZ
$\vec{G}_1$
$\vec{G}_2$


EXAMPLE: Graphene with T-breaking mass
Real
A
B
$\vec{\delta}_1$
$\vec{\delta}_2$
$\vec{\delta}_3$
$\vec{\delta}_1 = a(0, 1)$
$\vec{\delta}_{2,3} = a\left(\pm\frac{\sqrt{3}}{2}, -\frac{1}{2}\right)$
$\vec{K} = \frac{4\pi}{a}\left(\frac{1}{3\sqrt{3}}, 0\right)$
1st BZ
$\vec{G}_1$
$\vec{G}_2$
$-\vec{K}$
$+\vec{K}$

EXAMPLE: Graphene with T-breaking mass

Real



$$\vec{\delta}_1 = a(0, 1)$$

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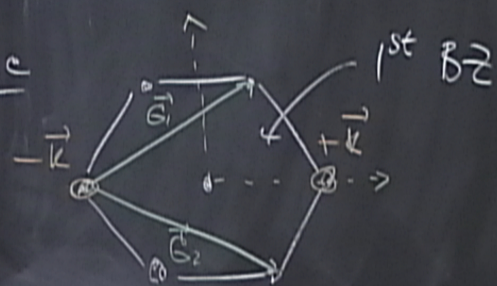
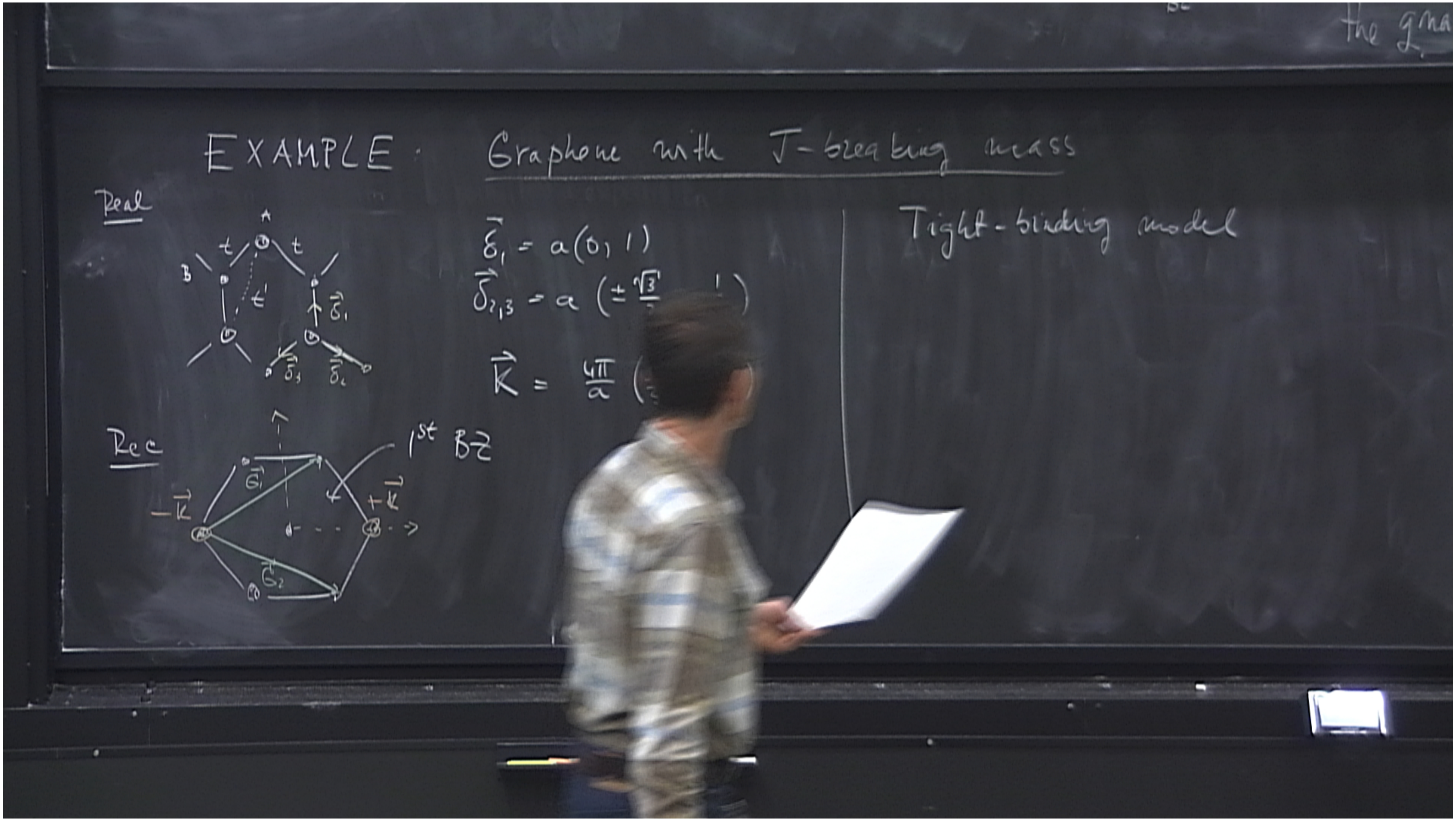
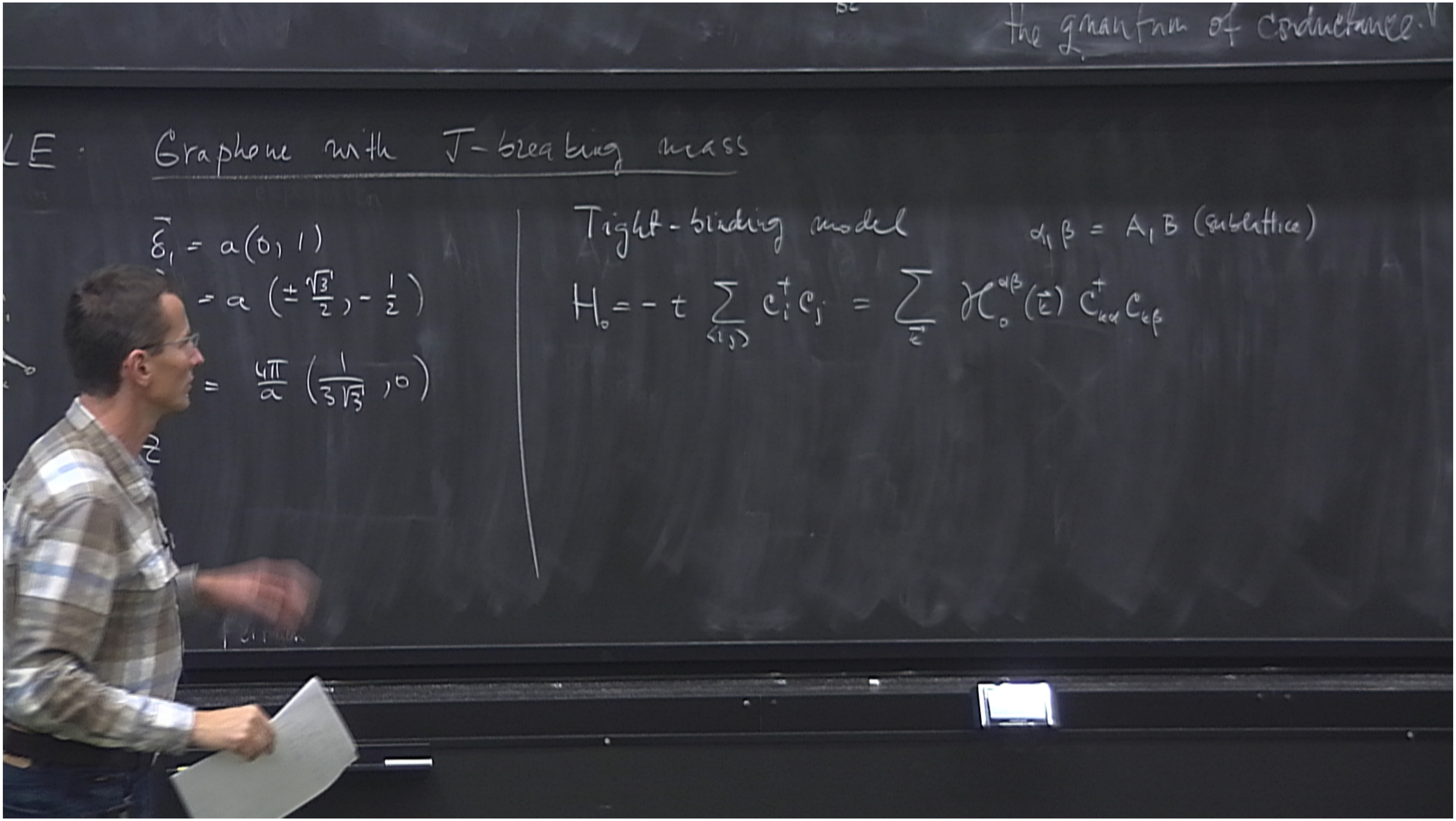
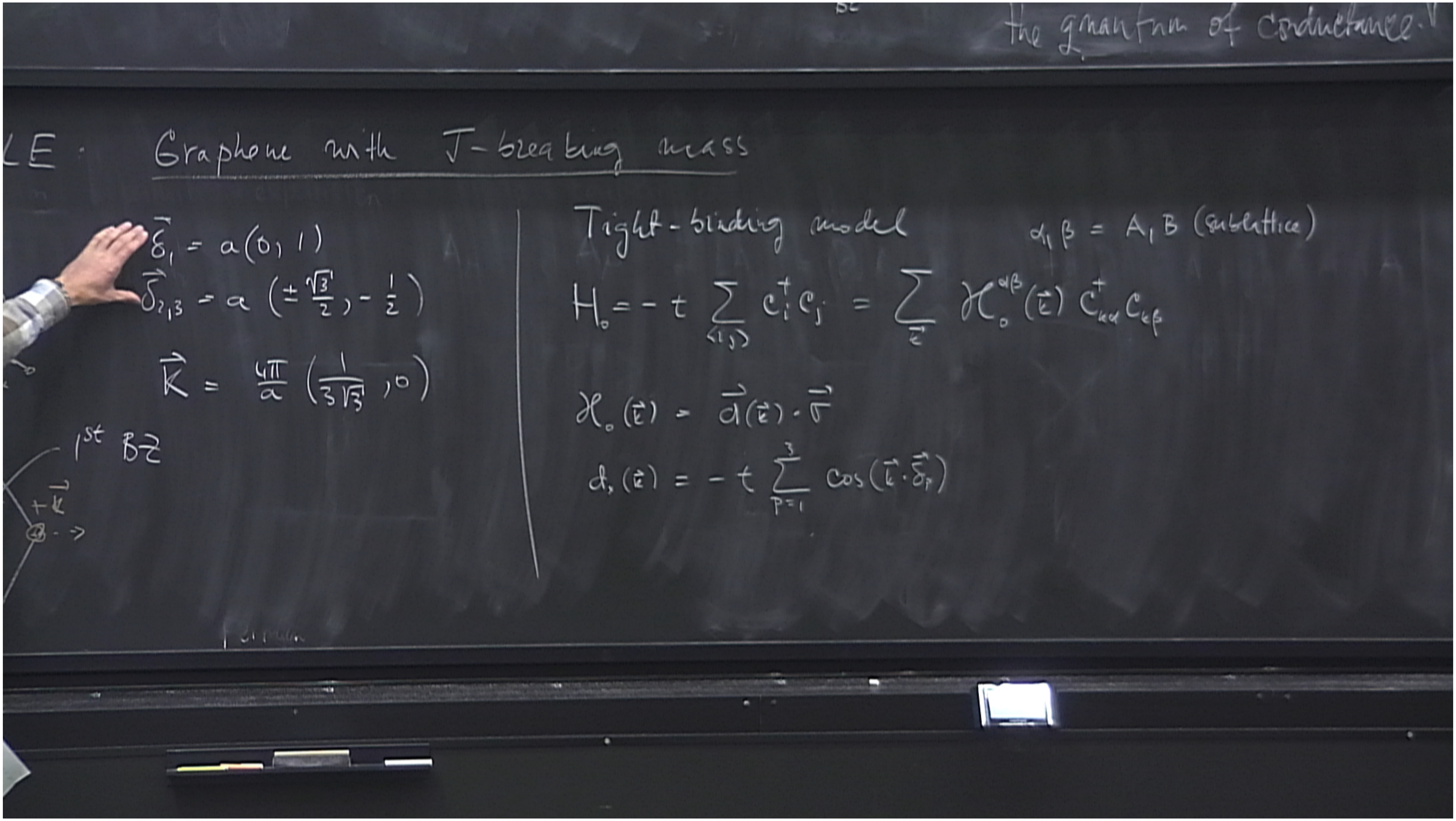



EXAMPLE: Graphene with T-breaking mass
Real
Rec
1st BZ
δ1 = a(0, 1)
Tight-binding model


the quantum of conductance.
Graphene with T-breaking mass
$\vec{\delta}_1 = a(0, 1)$
$= a\left(\pm\frac{\sqrt{3}}{2}, -\frac{1}{2}\right)$
$= \frac{4\pi}{a}\left(\frac{1}{3\sqrt{3}}, 0\right)$
Tight-binding model
$\alpha, \beta = A, B$ (sublattice)
$H_0 = -t \sum_{\langle ij \rangle} c_i^\dagger c_j = \sum_{\vec{k}} \mathcal{H}_0^{\alpha\beta}(\vec{k})\, c_{k\alpha}^\dagger c_{k\beta}$


the quantum of conductance
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1^{st} BZ
$+\vec{K}$
Tight-binding model
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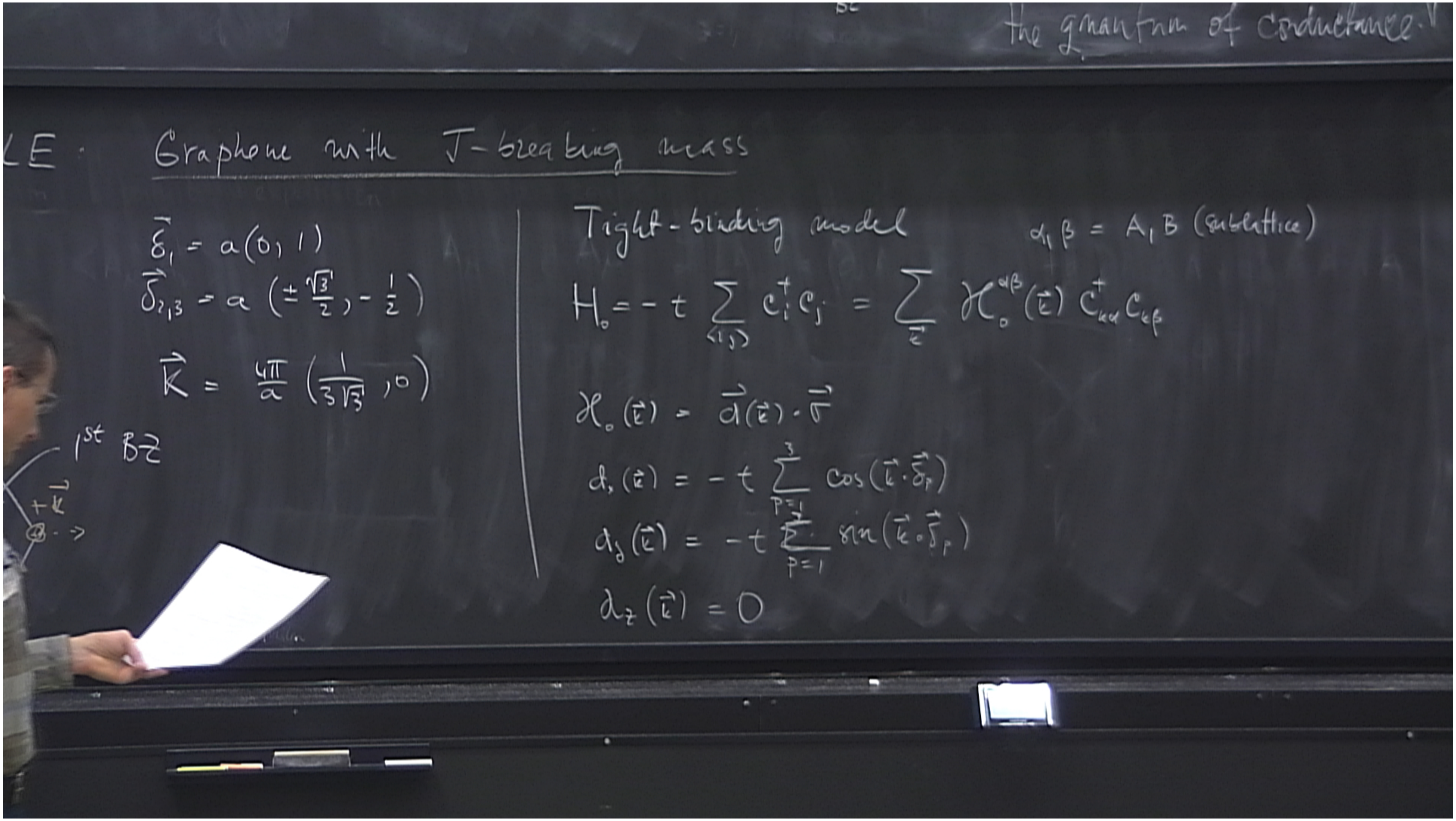
$H_0 = -t \sum_{\langle i,j \rangle} c_i^\dagger c_j = \sum_{\vec{k}} \mathcal{H}_0^{\alpha\beta}(\vec{k})\, c_{k\alpha}^\dagger c_{k\beta}$
$\mathcal{H}_0(\vec{k}) = \vec{d}(\vec{k}) \cdot \vec{\sigma}$
$d_x(\vec{k}) = -t \sum_{p=1}^{3} \cos(\vec{k}\cdot\vec{\delta}_p)$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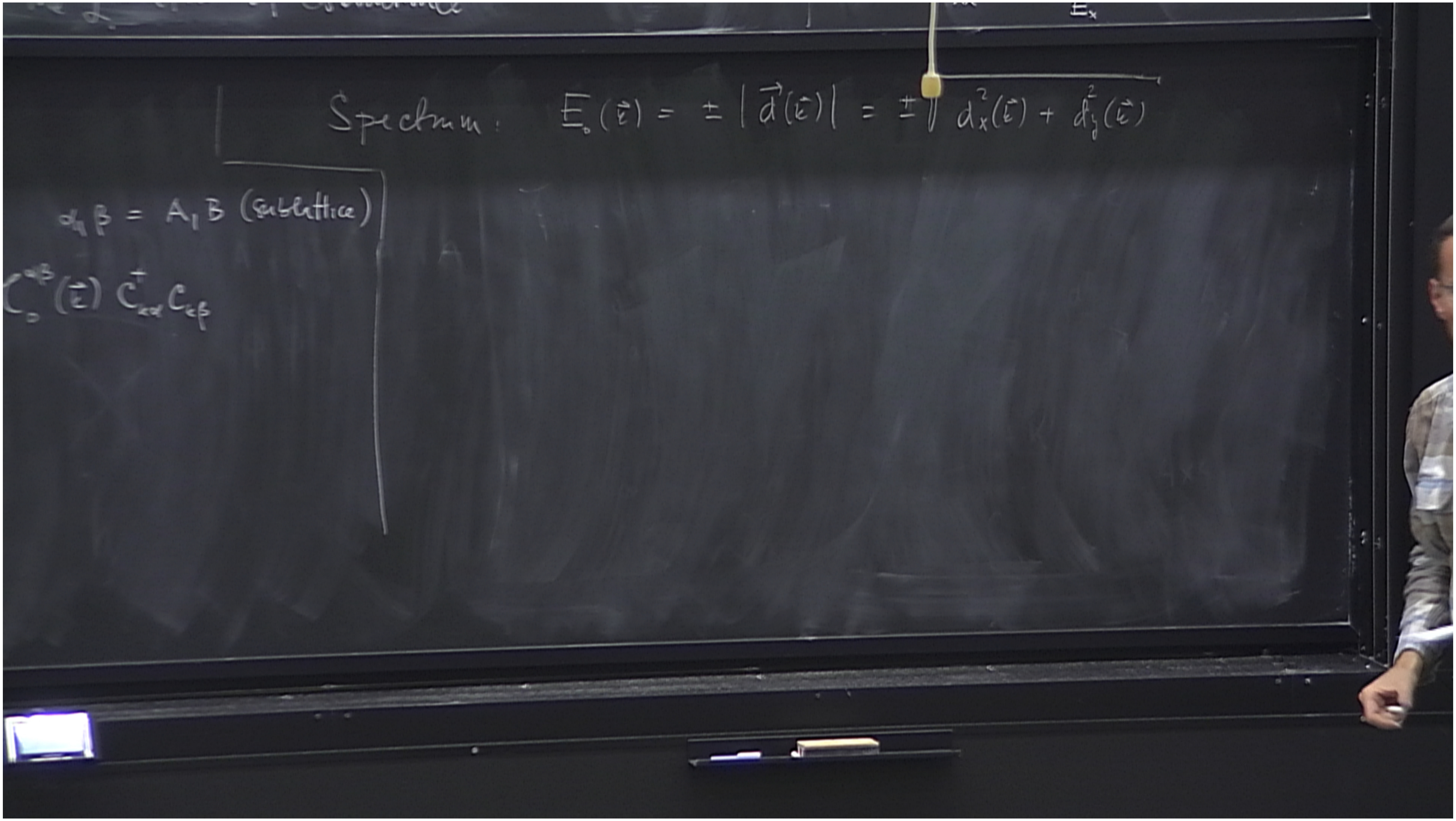
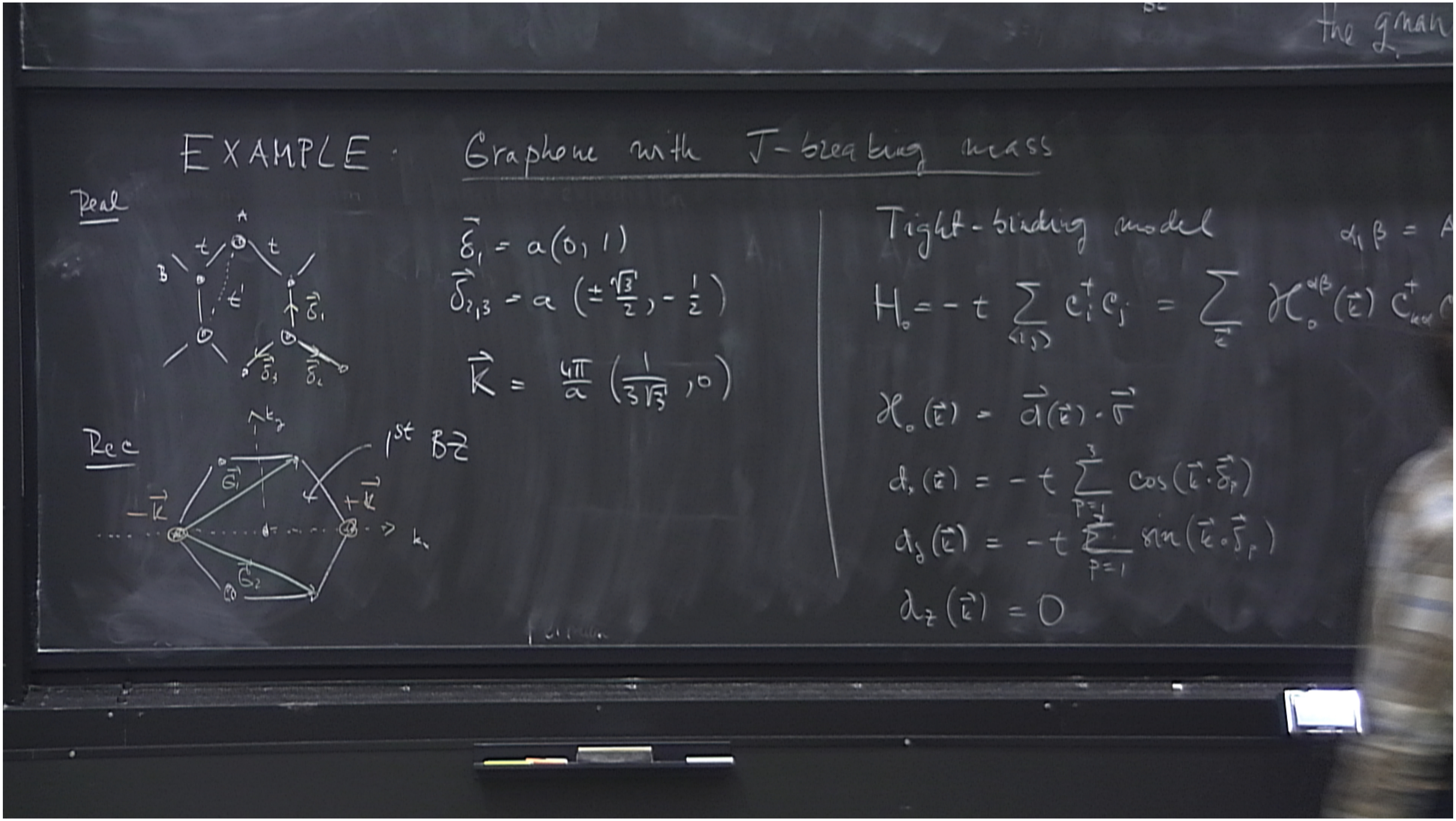
$d_y(\vec{k}) = -t \sum_{p=1} \sin(\vec{k} \cdot \vec{\delta}_p)$
$d_z(\vec{k}) = 0$


Spectrum: $E_\pm(\vec{k}) = \pm|\vec{d}(\vec{k})| = \pm\sqrt{d_x^2(\vec{k}) + d_y^2(\vec{k})}$
$\alpha, \beta = A, B$ (sublattice)
$C_0^{\alpha\beta}(\vec{k})\, c^\dagger_{k\alpha} c_{k\beta}$


EXAMPLE: Graphene with T-breaking mass
Real
t
t
B
t'
$\vec{\delta}_1$
$\vec{\delta}_3$
$\vec{\delta}_2$
Rec
k_y
1st BZ
$\vec{G}_1$
$\vec{G}_2$
$-\vec{K}$
$+\vec{K}$
k_x
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$H_0 = -t \sum_{\langle i,j \rangle} c_i^\dagger c_j = \sum_{\vec{k}} \mathcal{H}_0^{\alpha\beta}(\vec{k})\, c_{k\alpha}^\dagger$
$\mathcal{H}_0(\vec{k}) = \vec{d}(\vec{k}) \cdot \vec{\sigma}$
$d_x(\vec{k}) = -t \sum_{p=1}^{3} \cos(\vec{k}\cdot\vec{\delta}_p)$
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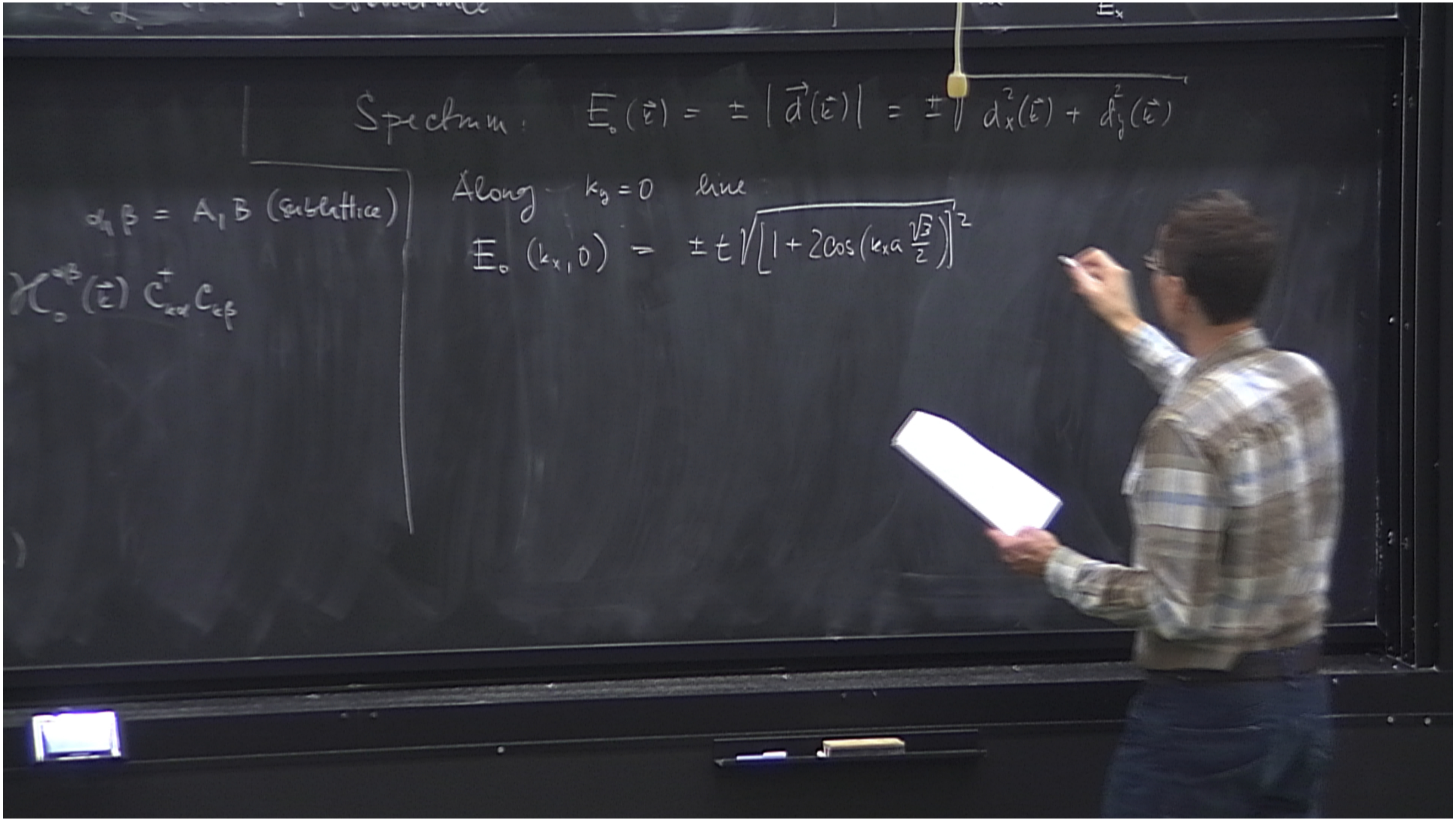
Spectrum: $E_0(\vec{k}) = \pm|\vec{d}(\vec{k})| = \pm\sqrt{d_x^2(\vec{k}) + d_y^2(\vec{k})}$
Along $k_y = 0$ line
$E_0(k_x, 0) = \pm t\sqrt{\left[1 + 2\cos\left(k_x a \frac{\sqrt{3}}{2}\right)\right]^2}$
$\alpha, \beta = A, B$ (sublattice)
$\mathcal{H}_0^{\alpha\beta}(\vec{k})\, C^{\dagger}_{k\alpha} C_{k\beta}$

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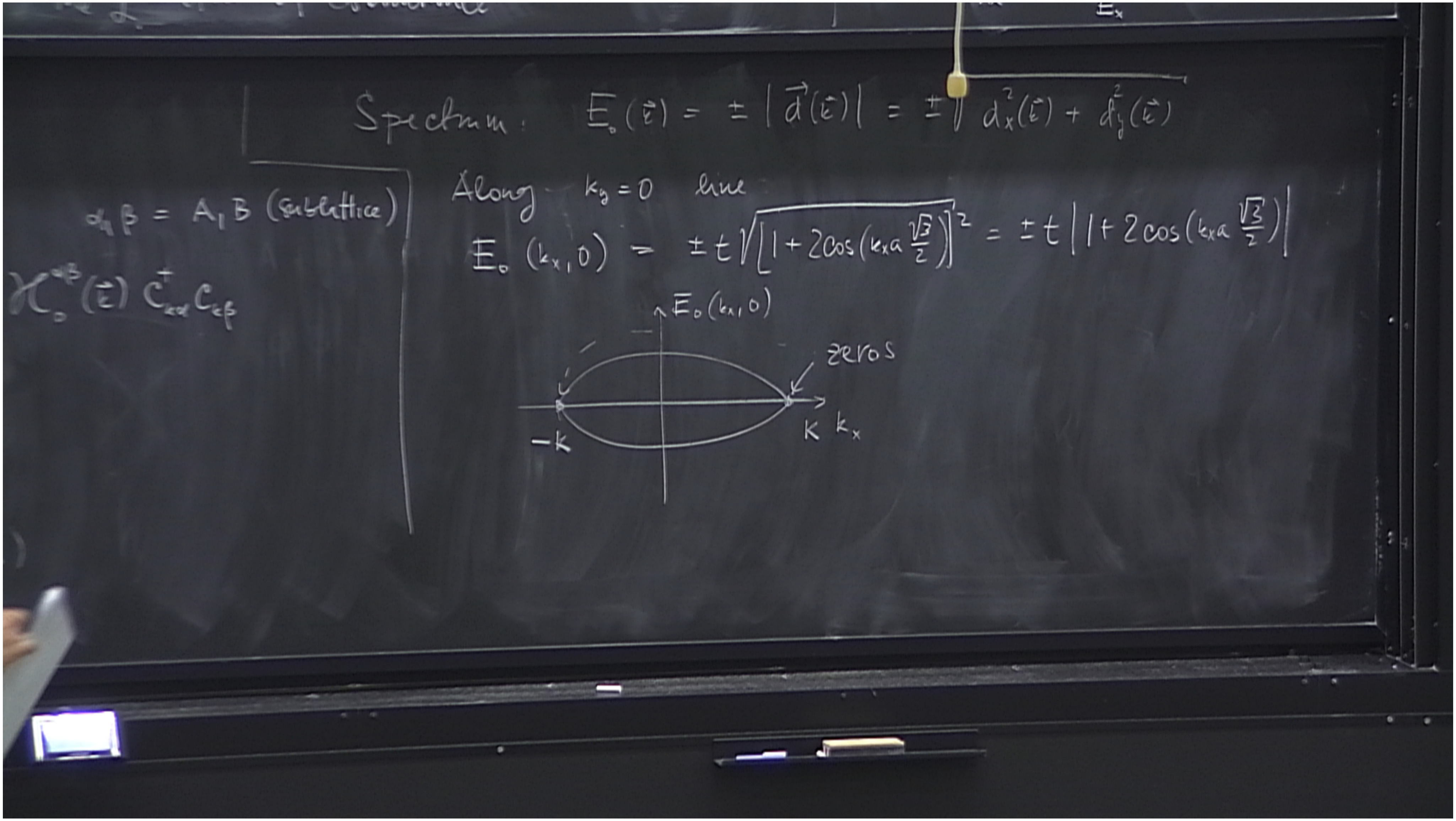
$\alpha, \beta = A, B$ (sublattice)

$\mathcal{H}_0^{\alpha\beta}(\vec{k})\, c^\dagger_{k\alpha} c_{k\beta}$

Along $k_y = 0$ line

$$E_0(k_x, 0) = \pm t \sqrt{\left[1 + 2\cos\left(k_x a \tfrac{\sqrt{3}}{2}\right)\right]^2} = \pm t \left| 1 + 2\cos\left(k_x a \tfrac{\sqrt{3}}{2}\right) \right|$$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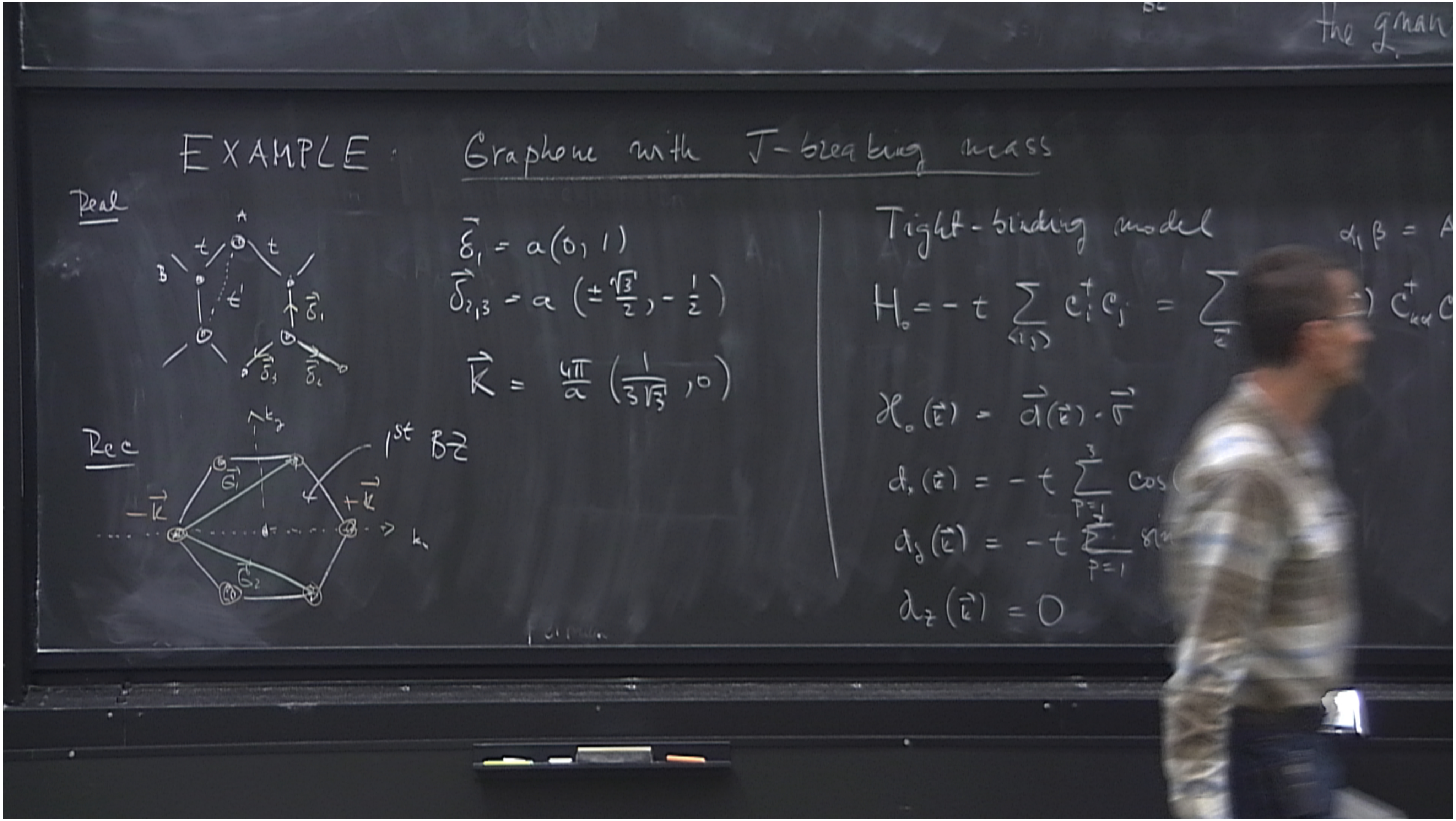
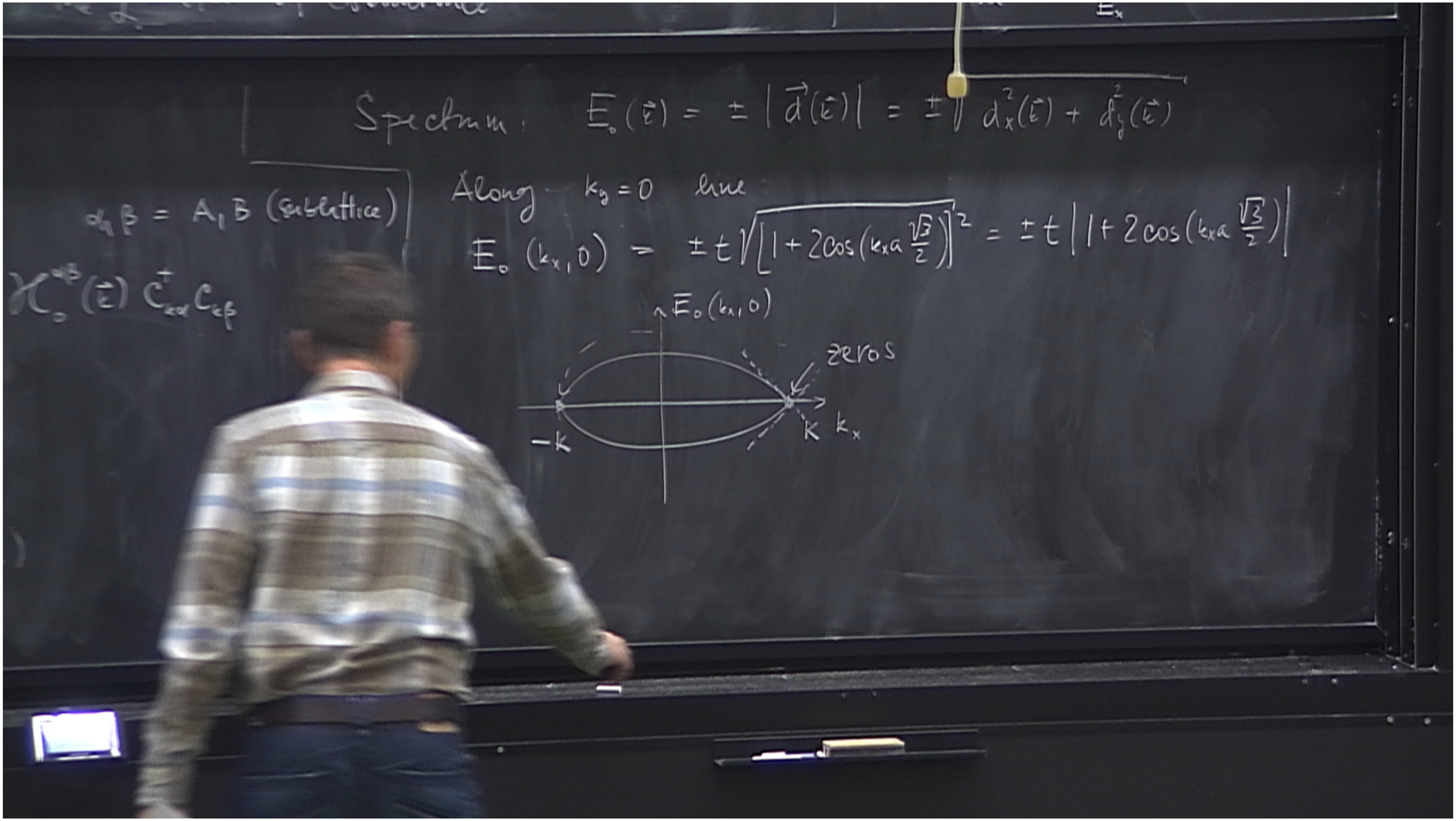
$E_0(k_x, 0)$
zeros
$-K$
K
k_x



EXAMPLE: Graphene with T-breaking mass
Real
Rec
1st BZ
Tight-binding model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Along $k_y = 0$ line
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$\mathcal{H}_0^{\alpha\beta}(\vec{k})\, C^\dagger_{k\alpha} C_{k\beta}$
$E_0(k_x, 0)$
zeros
$-K$
K
k_x

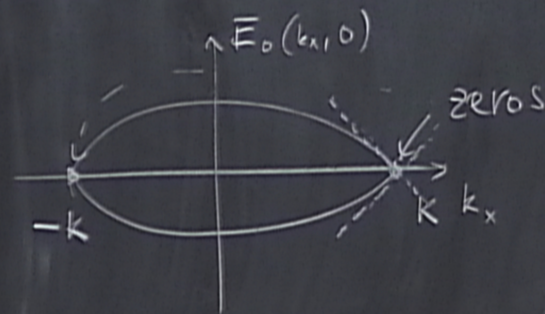
$\alpha, \beta = A, B$ (sublattice)

$\mathcal{H}_0^{\alpha\beta}(\vec{k})\, c^{\dagger}_{k\alpha} c_{k\beta}$

Spectrum: $E_0(\vec{k}) = \pm |\vec{d}(\vec{k})| = \pm\sqrt{d_x^2(\vec{k}) + d_y^2(\vec{k})}$

Along $k_y = 0$ line

$$E_0(k_x, 0) = \pm t\sqrt{\left[1 + 2\cos\left(k_x a \tfrac{\sqrt{3}}{2}\right)\right]^2} = \pm t\left|1 + 2\cos\left(k_x a \tfrac{\sqrt{3}}{2}\right)\right|$$



- point zeros in the BZ at $\vec{k} = \pm\vec{K}$
- dispersion is linear near these points

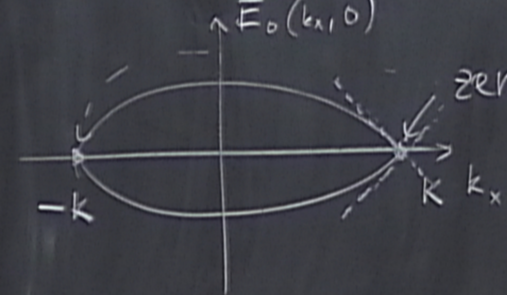
$\alpha, \beta = A, B$ (sublattice)

$\mathcal{H}_0^{\alpha\beta}(\vec{k})\, c^\dagger_{k\alpha} c_{k\beta}$

Spectrum: $E_0(\vec{k}) = \pm |\vec{d}(\vec{k})| = \pm\sqrt{d_x^2(\vec{k}) + d_y^2(\vec{k})}$

Along $k_y = 0$ line

$$E_0(k_x, 0) = \pm t\sqrt{\left[1 + 2\cos\left(k_x a \tfrac{\sqrt{3}}{2}\right)\right]^2} = \pm t\left|1 + 2\cos\left(k_x a \tfrac{\sqrt{3}}{2}\right)\right|$$



- point zeros in the BZ at $\vec{k} = \pm\vec{K}$
- dispersion is linear near these points

• $t \simeq 2.3\,eV$

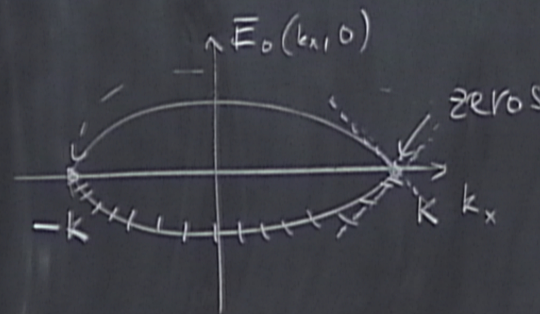
Spectrum: $E_0(\vec{k}) = \pm |\vec{d}(\vec{k})| = \pm\sqrt{d_x^2(\vec{k}) + d_y^2(\vec{k})}$

$\alpha, \beta = A, B$ (sublattice)

$\mathcal{H}_0^{\alpha\beta}(\vec{k})\, c^{\dagger}_{k\alpha} c_{k\beta}$

Along $k_y = 0$ line

$$E_0(k_x, 0) = \pm t\sqrt{\left[1 + 2\cos\left(k_x a \frac{\sqrt{3}}{2}\right)\right]^2} = \pm t\left|1 + 2\cos\left(k_x a \frac{\sqrt{3}}{2}\right)\right|$$



- point zeros in the BZ at $\vec{k} = \pm\vec{K}$
- dispersion is linear near these points

• $t \simeq 2.3\,eV$

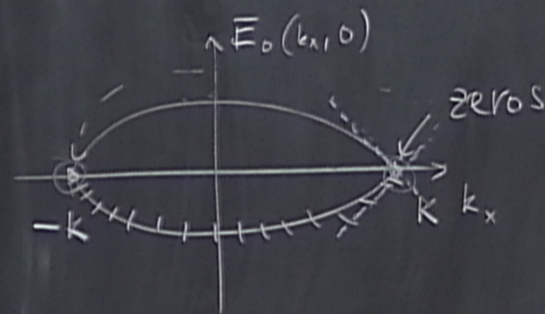
Spectrum: $E_0(\vec{k}) = \pm|\vec{d}(\vec{k})| = \pm\sqrt{d_x^2(\vec{k}) + d_y^2(\vec{k})}$

$\alpha, \beta = A, B$ (sublattice)

$\mathcal{H}_0^{\alpha\beta}(\vec{k})\, c^\dagger_{k\alpha} c_{k\beta}$

Along $k_y = 0$ line

$$E_0(k_x, 0) = \pm t\sqrt{\left[1 + 2\cos\left(k_x a \frac{\sqrt{3}}{2}\right)\right]^2} = \pm t\left|1 + 2\cos\left(k_x a \frac{\sqrt{3}}{2}\right)\right|$$



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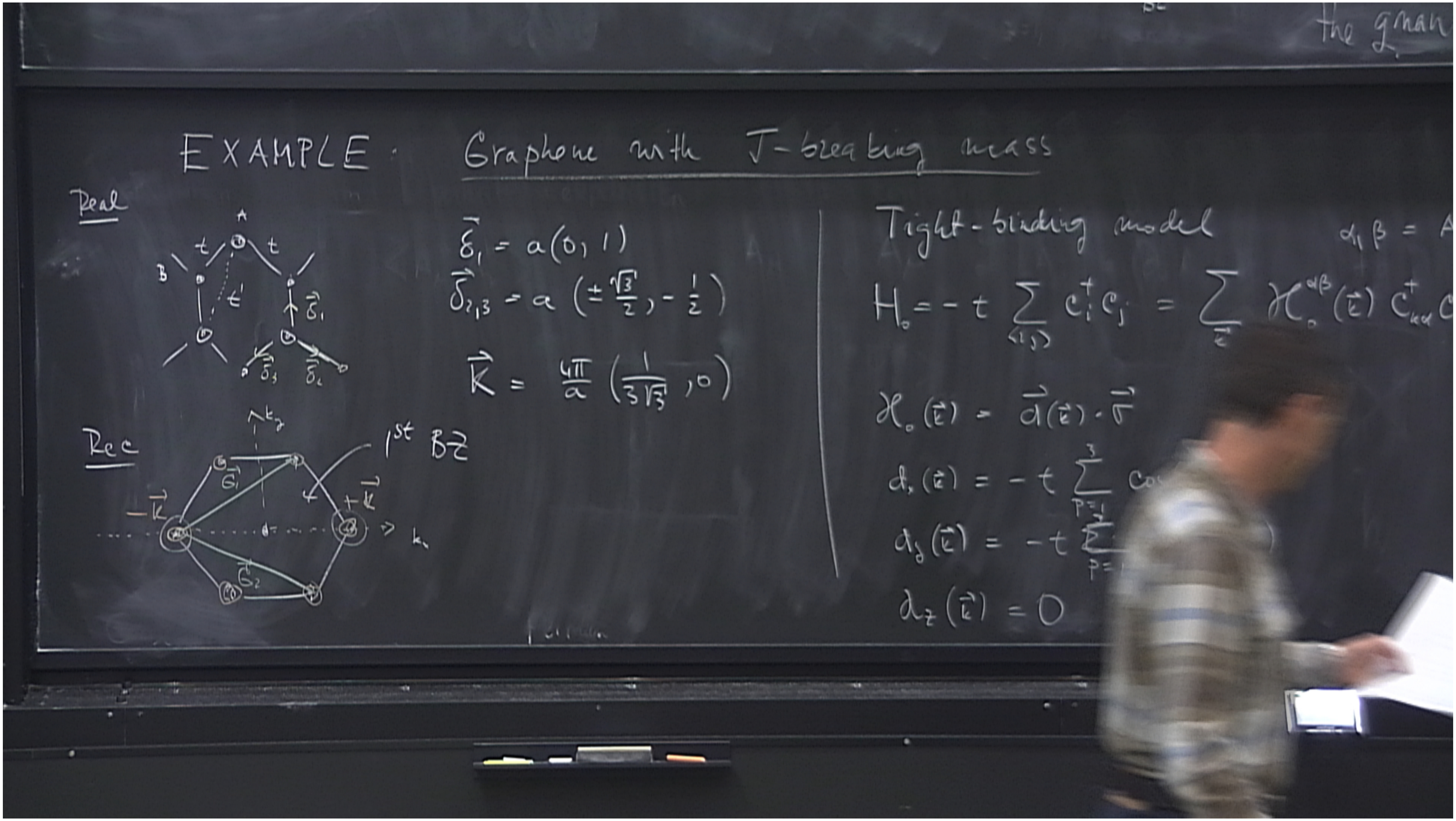
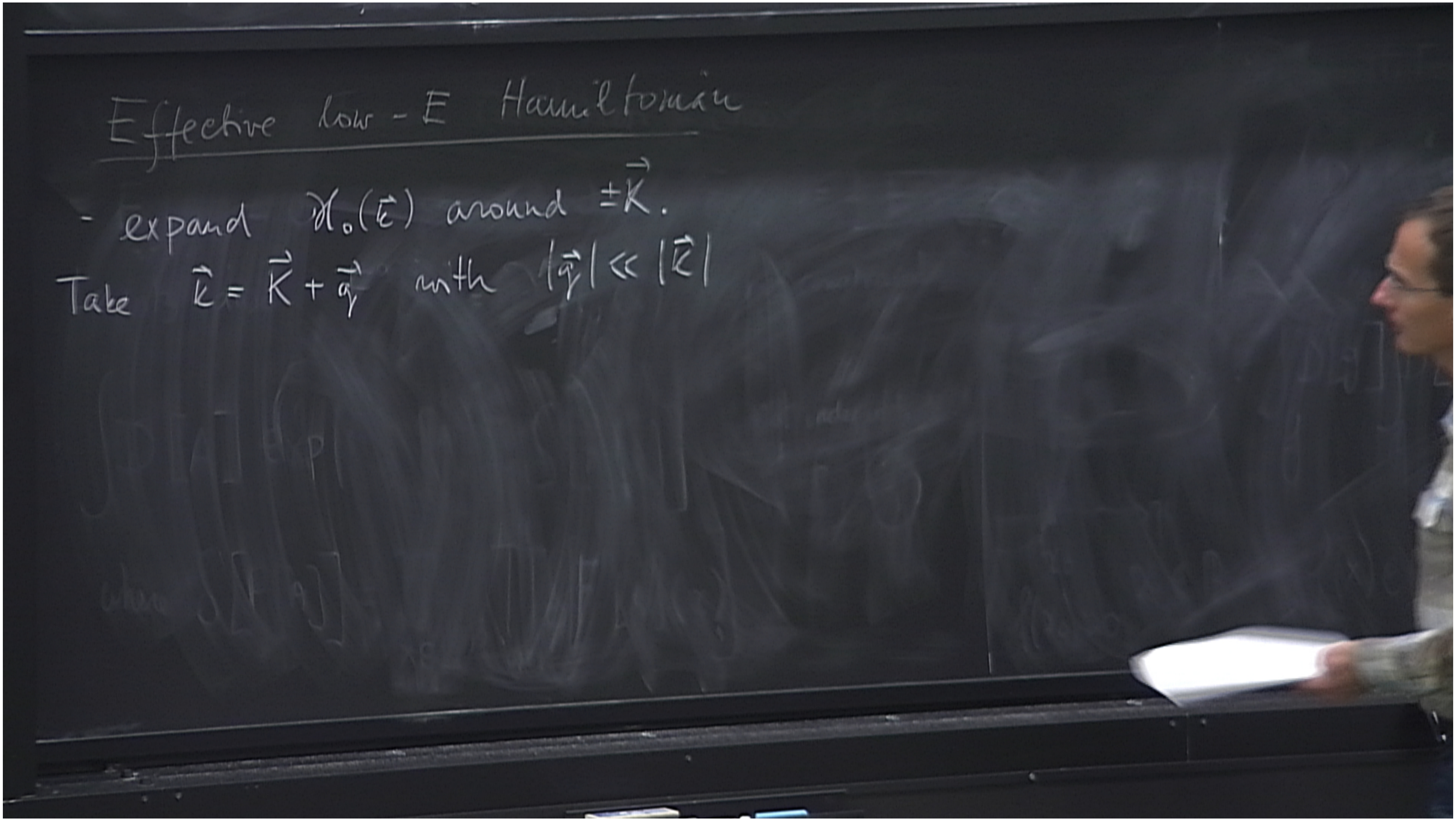
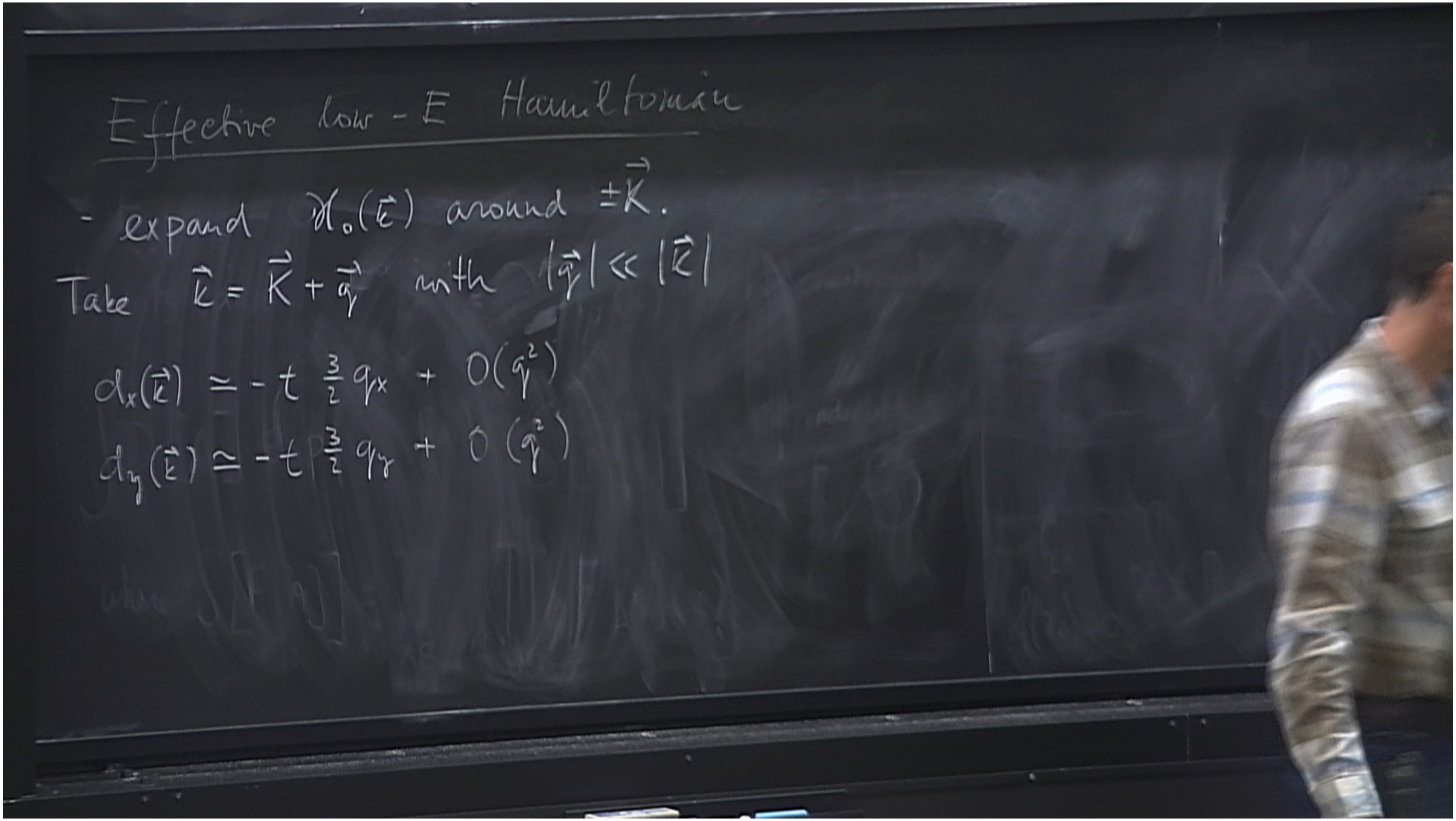

EXAMPLE: Graphene with T-breaking mass
Real
Rec
1st BZ
Tight-binding model


Effective low-E Hamiltonian
- expand $\mathcal{H}_0(\vec{k})$ around $\pm\vec{K}$.
Take $\vec{k} = \vec{K} + \vec{q}$ with $|\vec{q}| \ll |\vec{k}|$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Take $\vec{k} = \vec{K} + \vec{q}$ with $|\vec{q}| \ll |\vec{k}|$
$d_x(\vec{k}) \simeq -t\,\frac{3}{2} q_x + O(q^2)$
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Effective low-E Hamiltonian

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near $-\vec{K}$

$$d_x(\vec{k}) \simeq \pm t \, \tfrac{3}{2} q_x + O(q^2) \qquad (\text{near } +\vec{K})$$

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Effective low-E Hamiltonian

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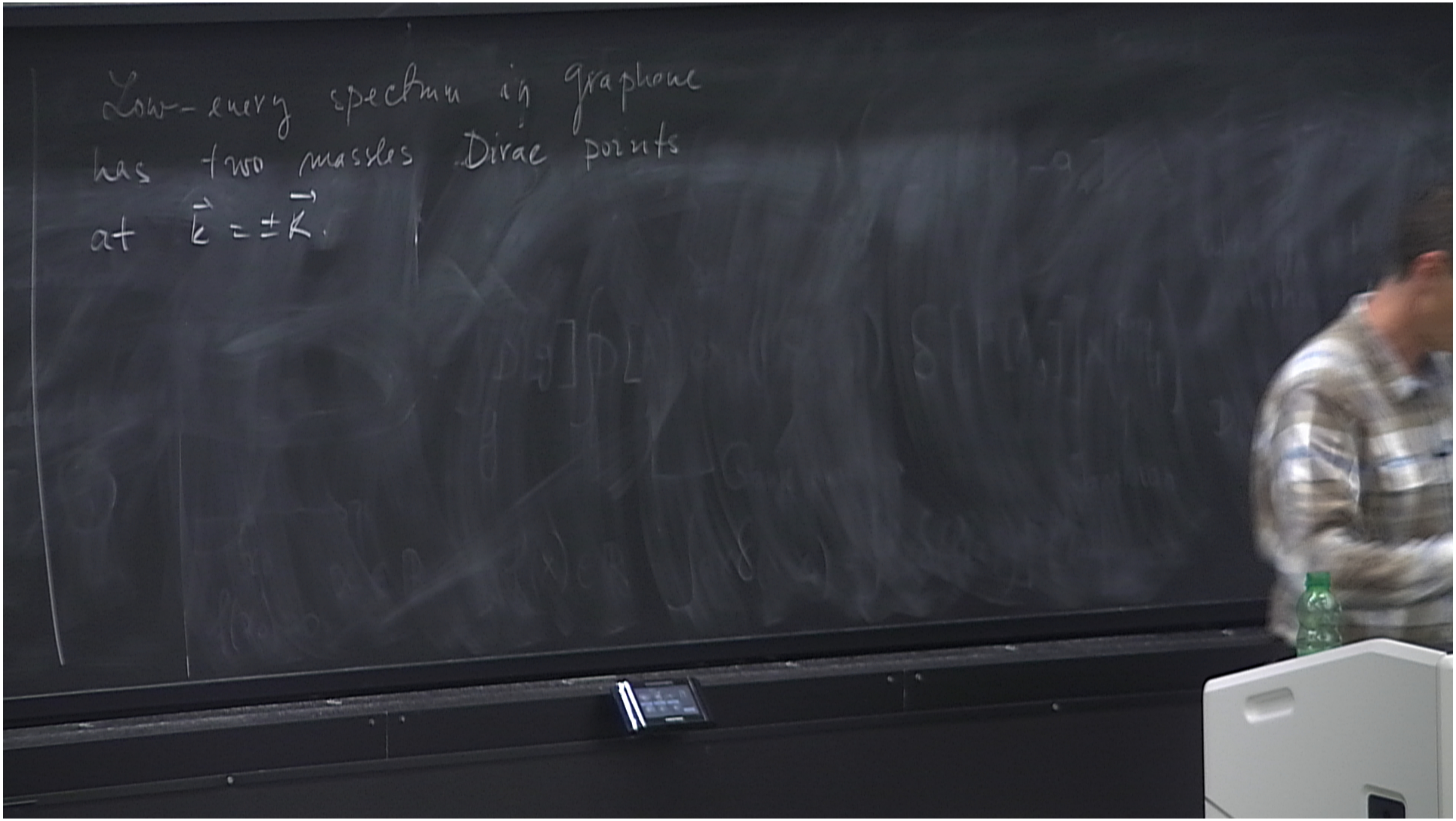
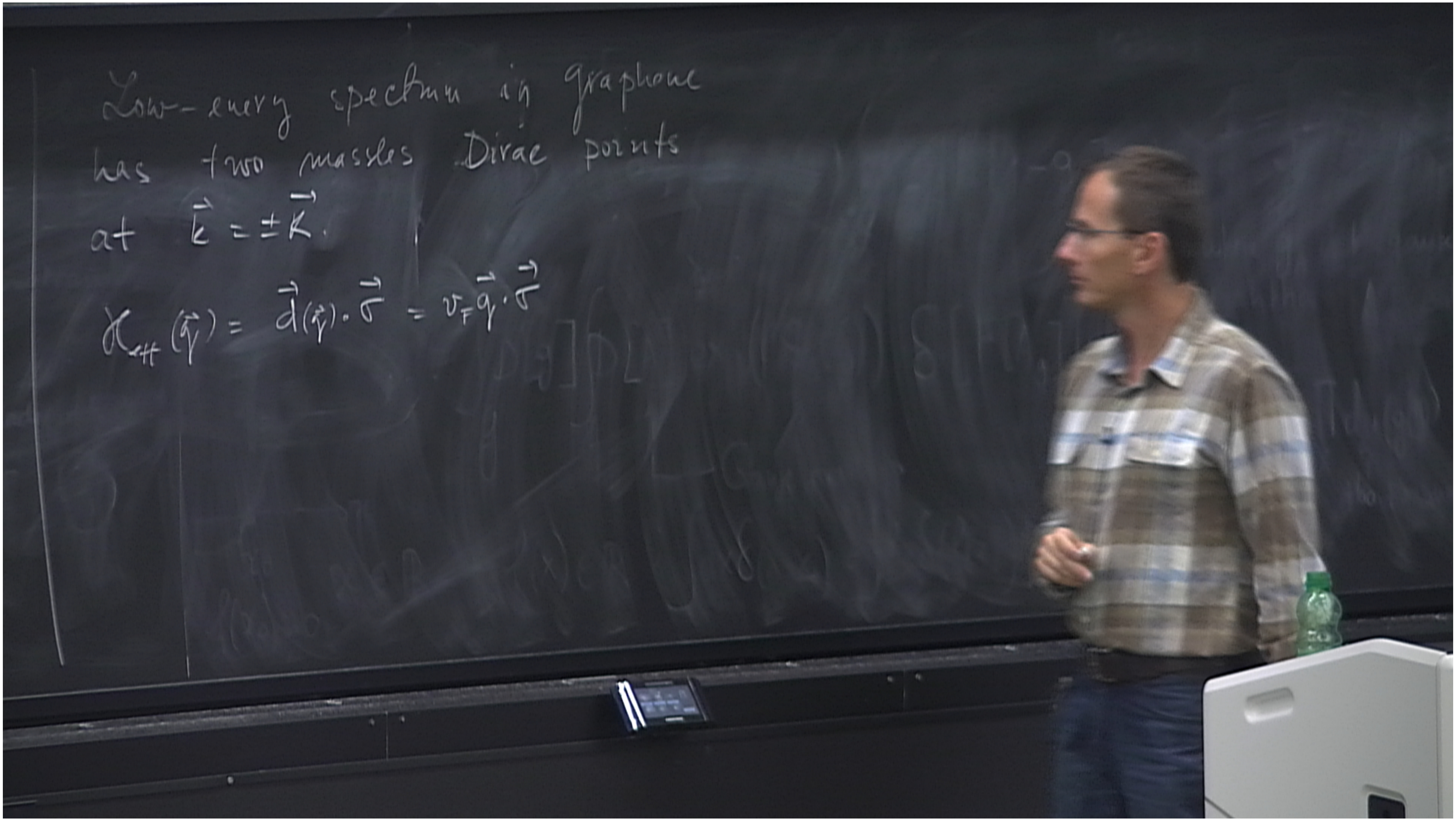
$$\mathcal{H}^{\pm K}_{eff}(\vec{q}) = v_F\left(\pm q_x \sigma_x + q_y \sigma_y\right), \quad v_F = -\tfrac{3}{2} t a$$


Low-energy spectrum in graphene
has two massless Dirac points
at $\vec{k} = \pm\vec{K}$.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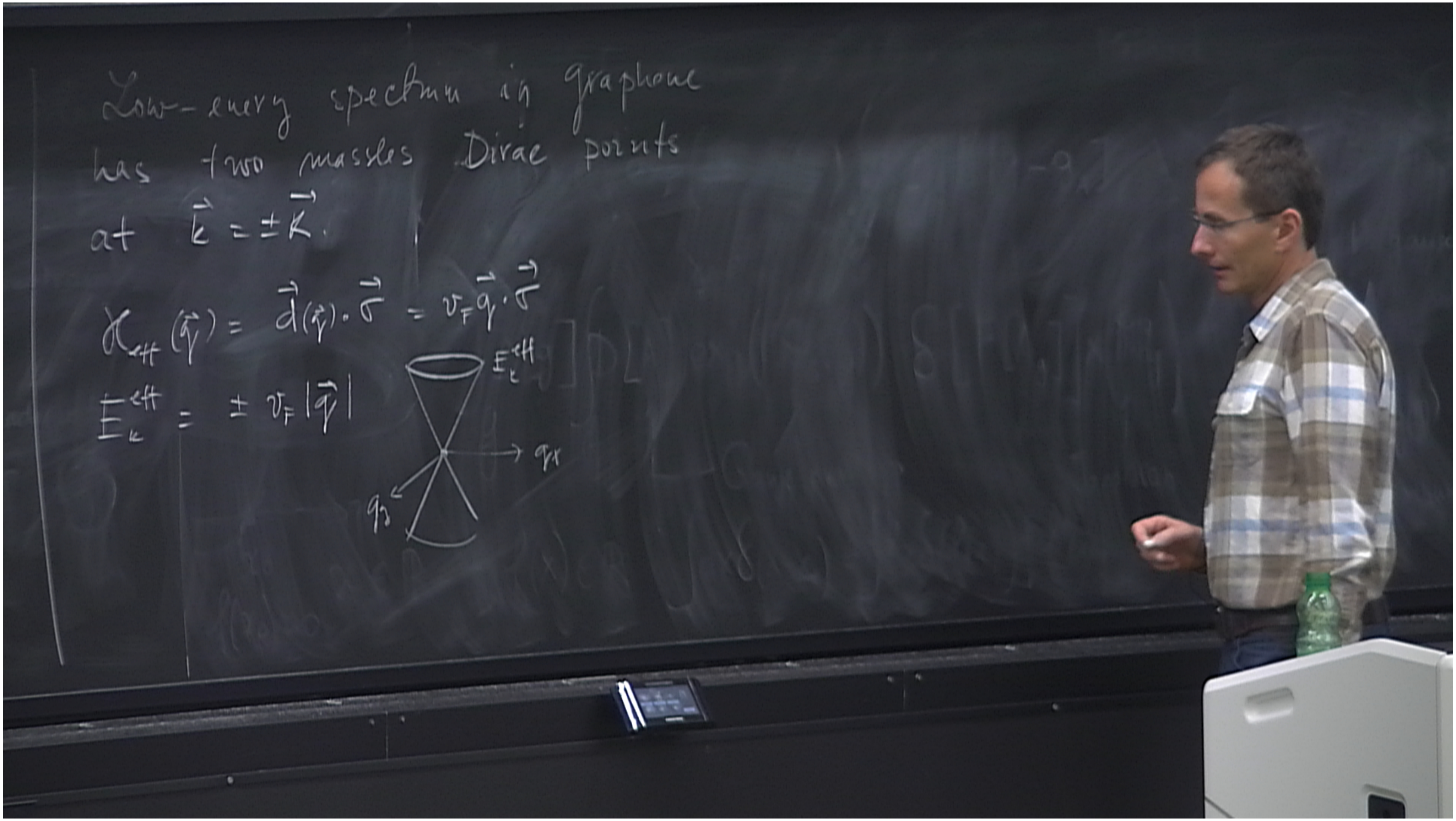
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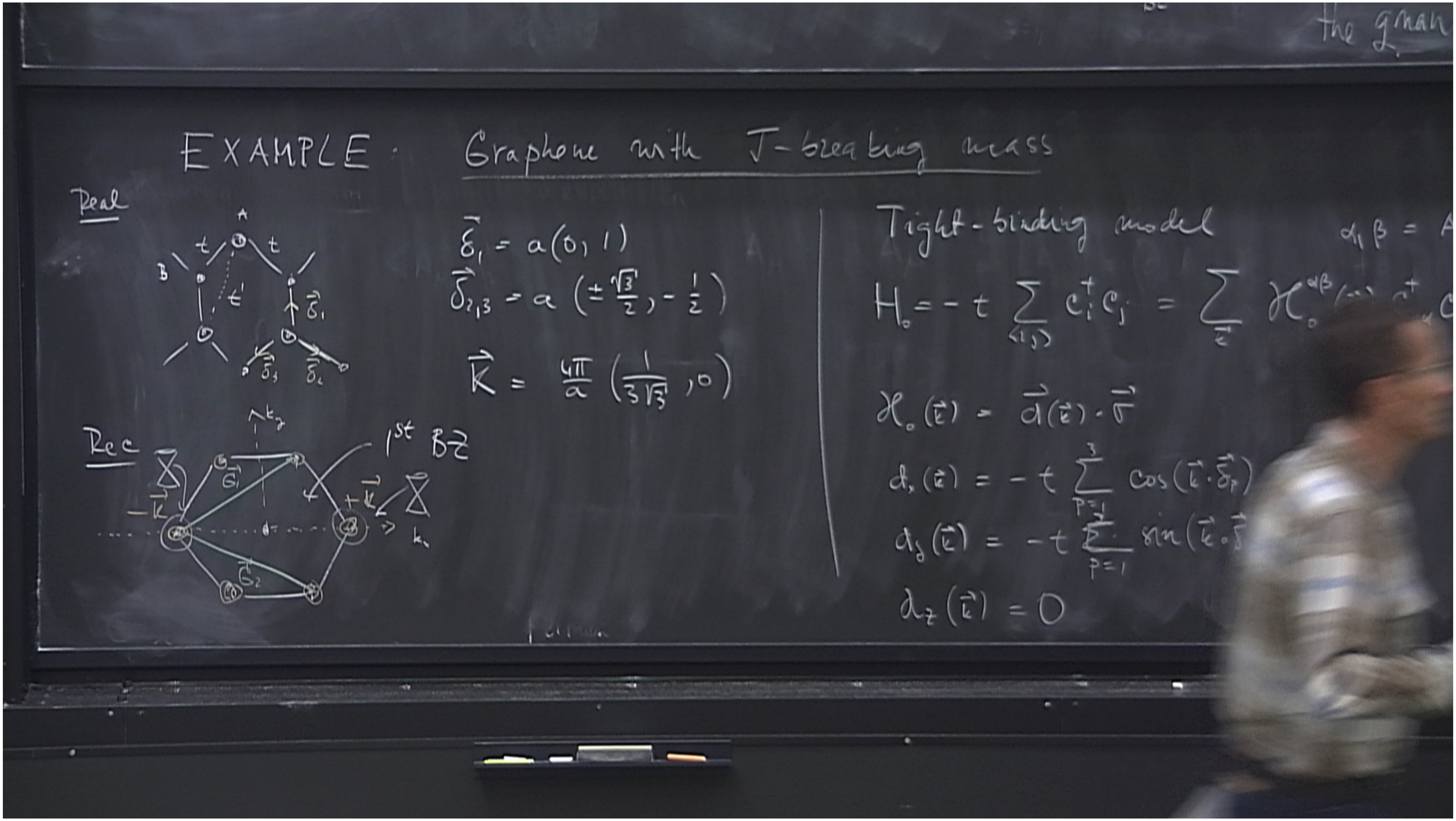
$E_k^{eff} = \pm v_F|\vec{q}|$
E_k^{eff}
q_x
q_y


EXAMPLE: Graphene with T-breaking mass
Real
Rec
1st BZ
$\vec{\delta}_1 = a(0,1)$
$\vec{\delta}_{2,3} = a\left(\pm\frac{\sqrt{3}}{2}, -\frac{1}{2}\right)$
$\vec{K} = \frac{4\pi}{a}\left(\frac{1}{3\sqrt{3}}, 0\right)$
Tight-binding model
$H_0 = -t\sum_{\langle i,j\rangle} c_i^\dagger c_j = \sum_{\vec{k}} \mathcal{H}_0^{\alpha\beta}$
$\mathcal{H}_0(\vec{k}) = \vec{d}(\vec{k})\cdot\vec{\sigma}$
$d_x(\vec{k}) = -t\sum_{p=1}^{3}\cos(\vec{k}\cdot\vec{\delta}_p)$
$d_y(\vec{k}) = -t\sum_{p=1}^{3}\sin(\vec{k}\cdot\vec{\delta}$
$d_z(\vec{k}) = 0$

Effective low-E Hamiltonian

- expand $\mathcal{H}_0(\vec{k})$ around $\pm\vec{K}$.

Take $\vec{k} = \vec{K} + \vec{q}$ with $|\vec{q}| \ll |\vec{k}|$

near $-\vec{K}$

$$d_x(\vec{k}) \simeq \pm t\,\frac{3}{2} q_x + O(q^2) \qquad (\text{near } +\vec{K})$$

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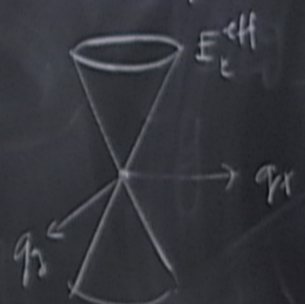
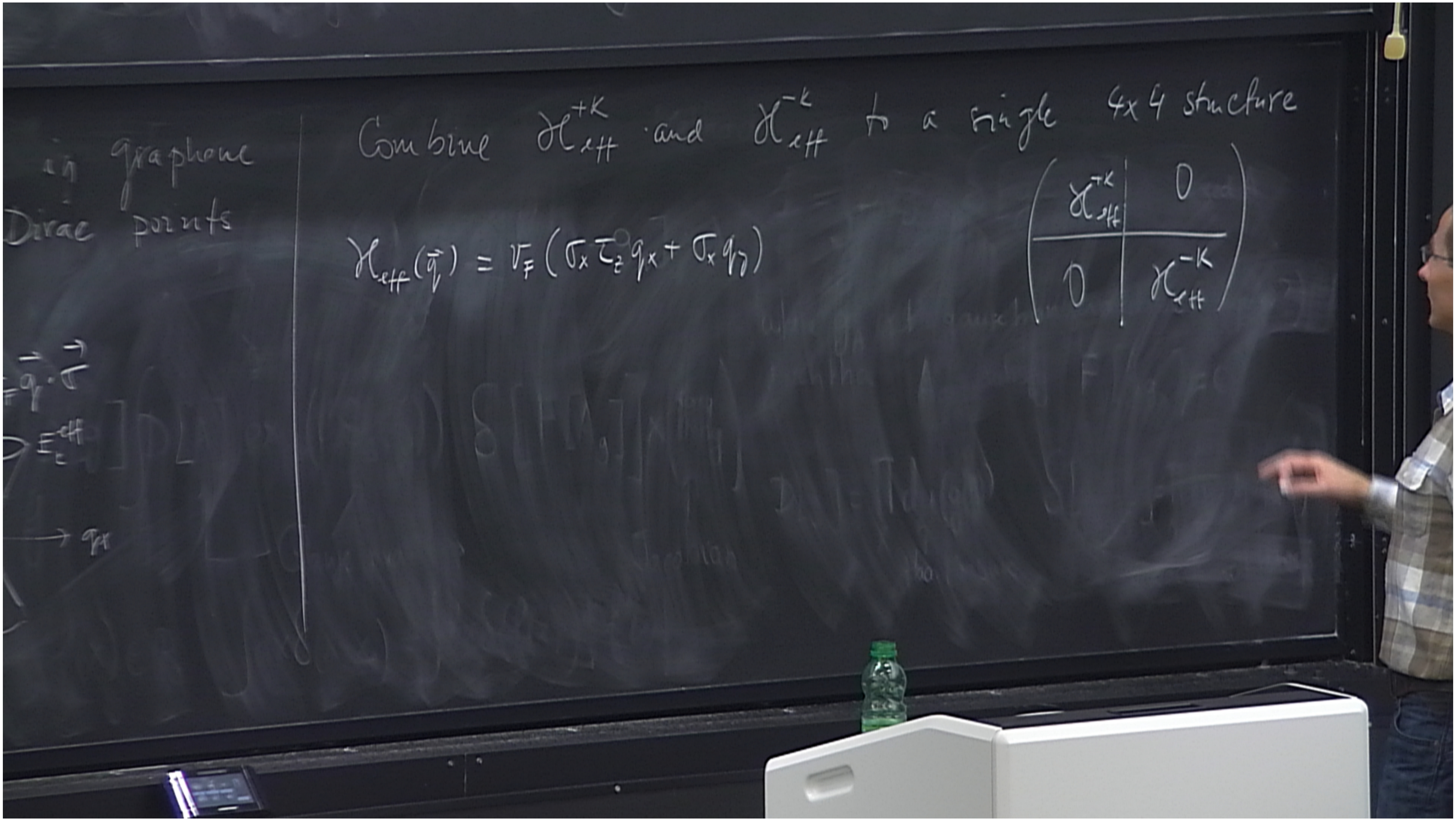
$$\boxed{\mathcal{H}^{\pm K}_{eff}(\vec{q}) = v_F(\pm q_x\sigma_x + q_y\sigma_y)}\,, \quad v_F = -\frac{3}{2}ta$$

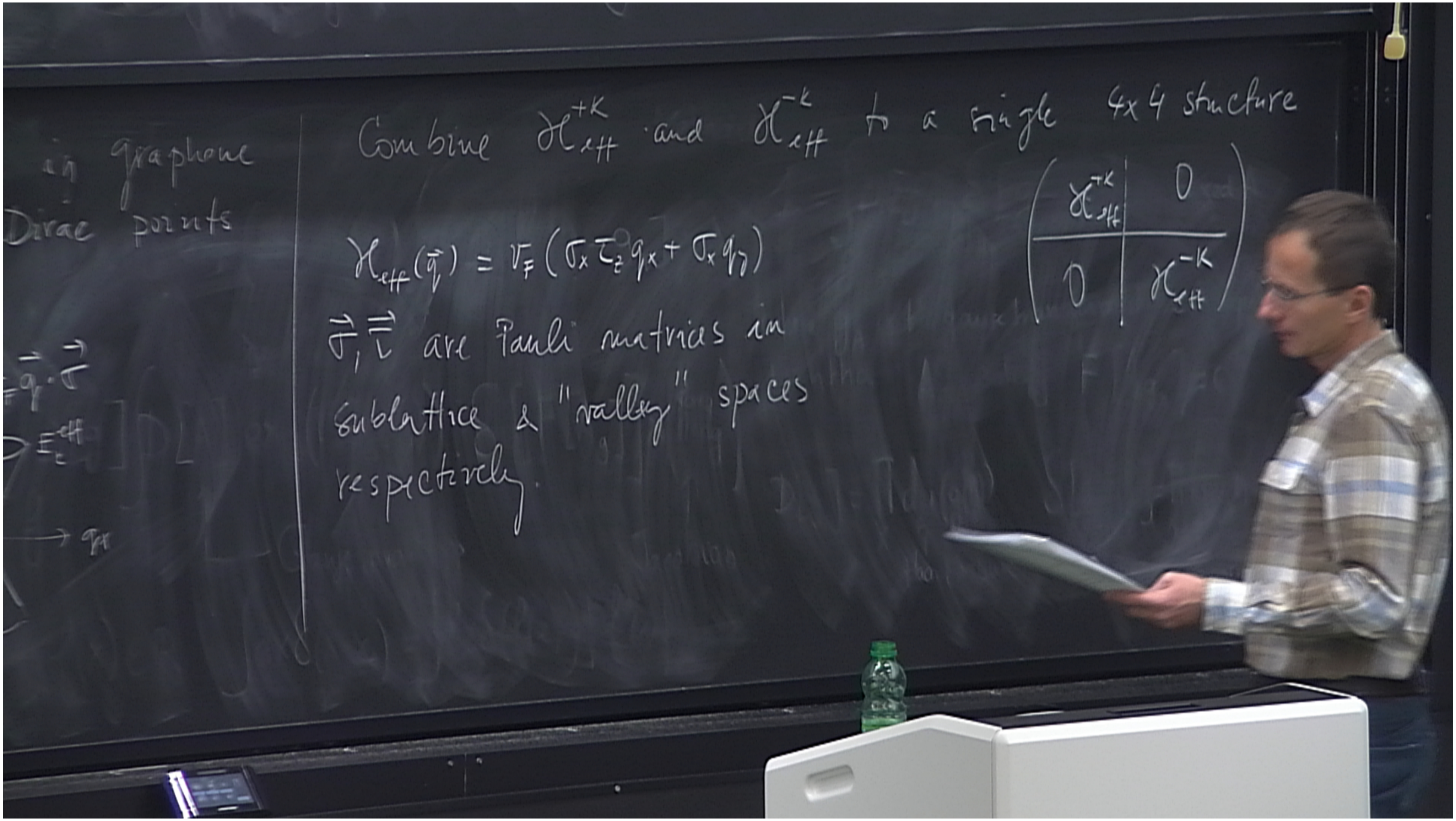
Low-energy spectrum in graph
has two massless Dirac poi
at $\vec{k} = \pm\vec{K}$.

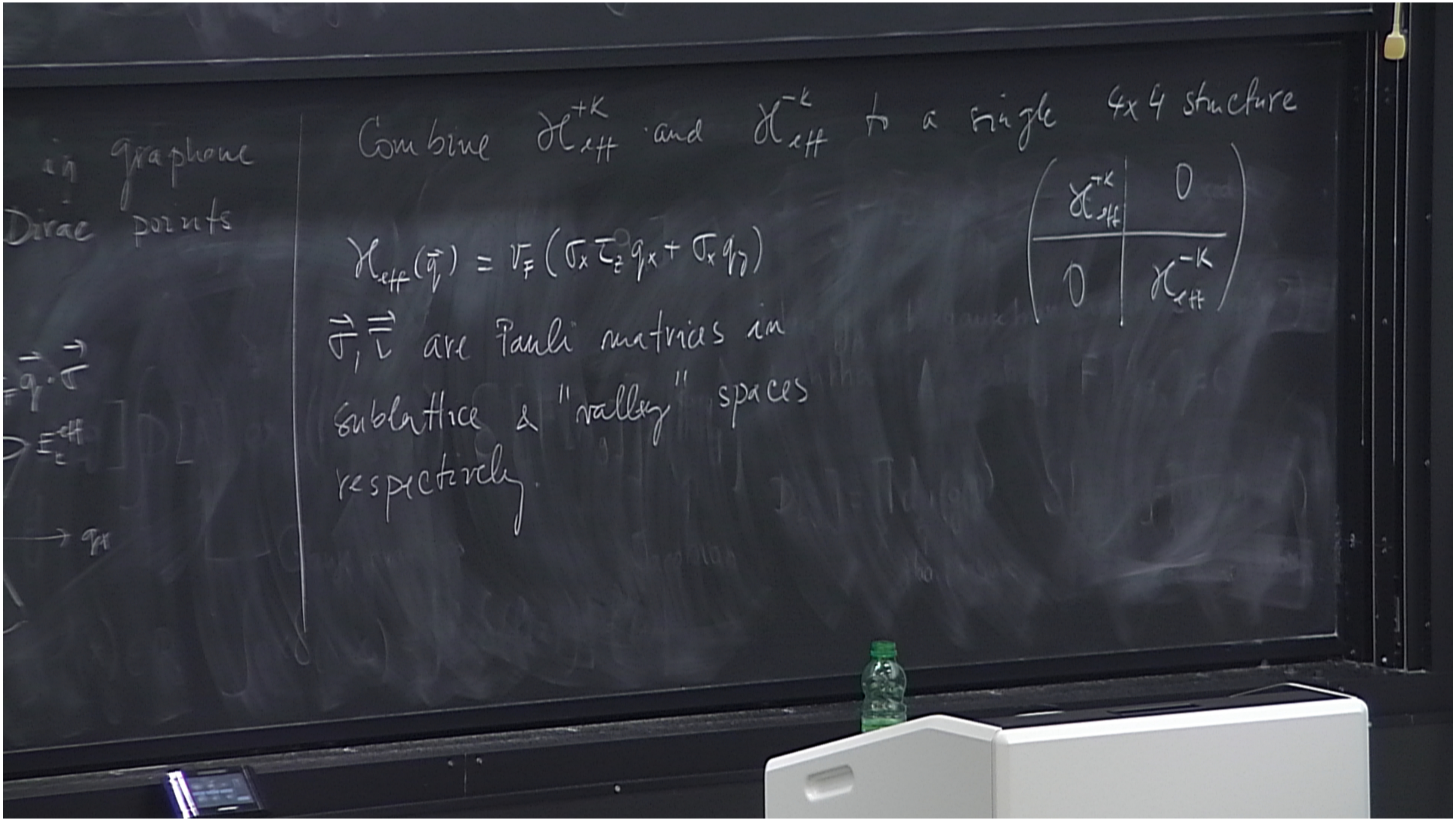
$$\mathcal{H}_{eff}(\vec{q}) = \vec{d}(\vec{q})\cdot\vec{\sigma} = v_F\vec{q}\cdot\vec{\sigma}$$

$$E^{eff}_k = \pm v_F|\vec{q}|$$




in graphene
Dirac points
Combine $\mathcal{H}^{+K}_{eff}$ and $\mathcal{H}^{-K}_{eff}$ to a single 4x4 structure
$\mathcal{H}_{eff}(\vec{q}) = v_F(\sigma_x \tau_z q_x + \sigma_x q_y)$
$\left(\begin{array}{c|c} \mathcal{H}^{+K}_{eff} & 0 \\ \hline 0 & \mathcal{H}^{-K}_{eff} \end{array}\right)$


Combine $\mathcal{H}_{eff}^{+K}$ and $\mathcal{H}_{eff}^{-K}$ to a single 4x4 structure
$\begin{pmatrix} \mathcal{H}_{eff}^{+K} & 0 \\ 0 & \mathcal{H}_{eff}^{-K} \end{pmatrix}$
$\mathcal{H}_{eff}(\vec{q}) = v_F(\sigma_x \tau_z q_x + \sigma_x q_y)$
$\vec{\sigma}, \vec{\tau}$ are Pauli matrices in
sublattice & "valley" spaces
respectively.
in graphene
Dirac points



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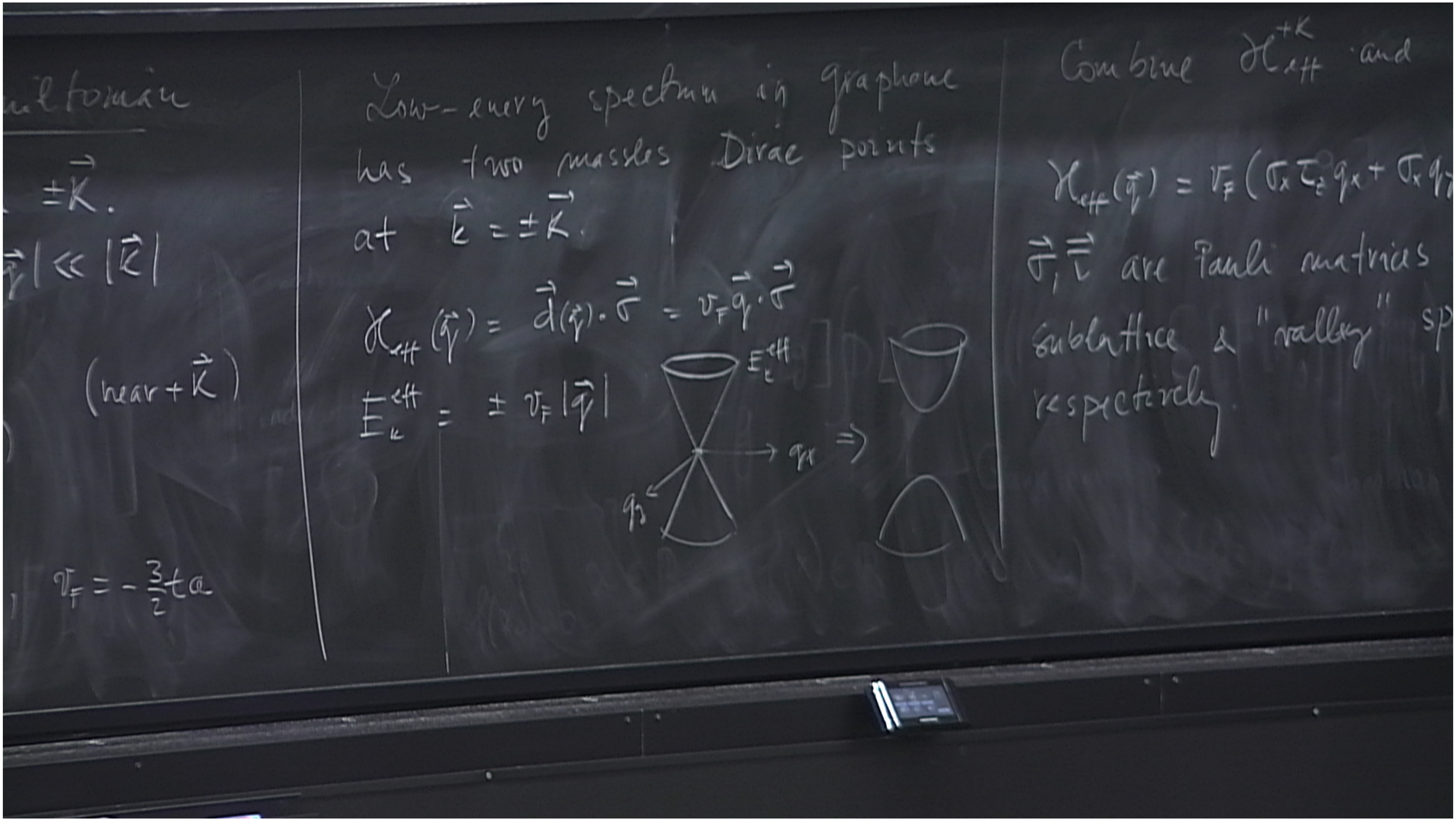
$\lambda_z(\vec{k}) = 0$

Dirac points at $\pm\vec{K}$ are protected by symmetries.



iltonian
$\pm\vec{K}$.
$|\vec{q}| \ll |\vec{K}|$
(near $+\vec{K}$)
$v_F = -\frac{3}{2}ta$
Low-energy spectrum in graphene
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E_k^{eff}
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Combine $\mathcal{H}_{eff}^{+K}$ and
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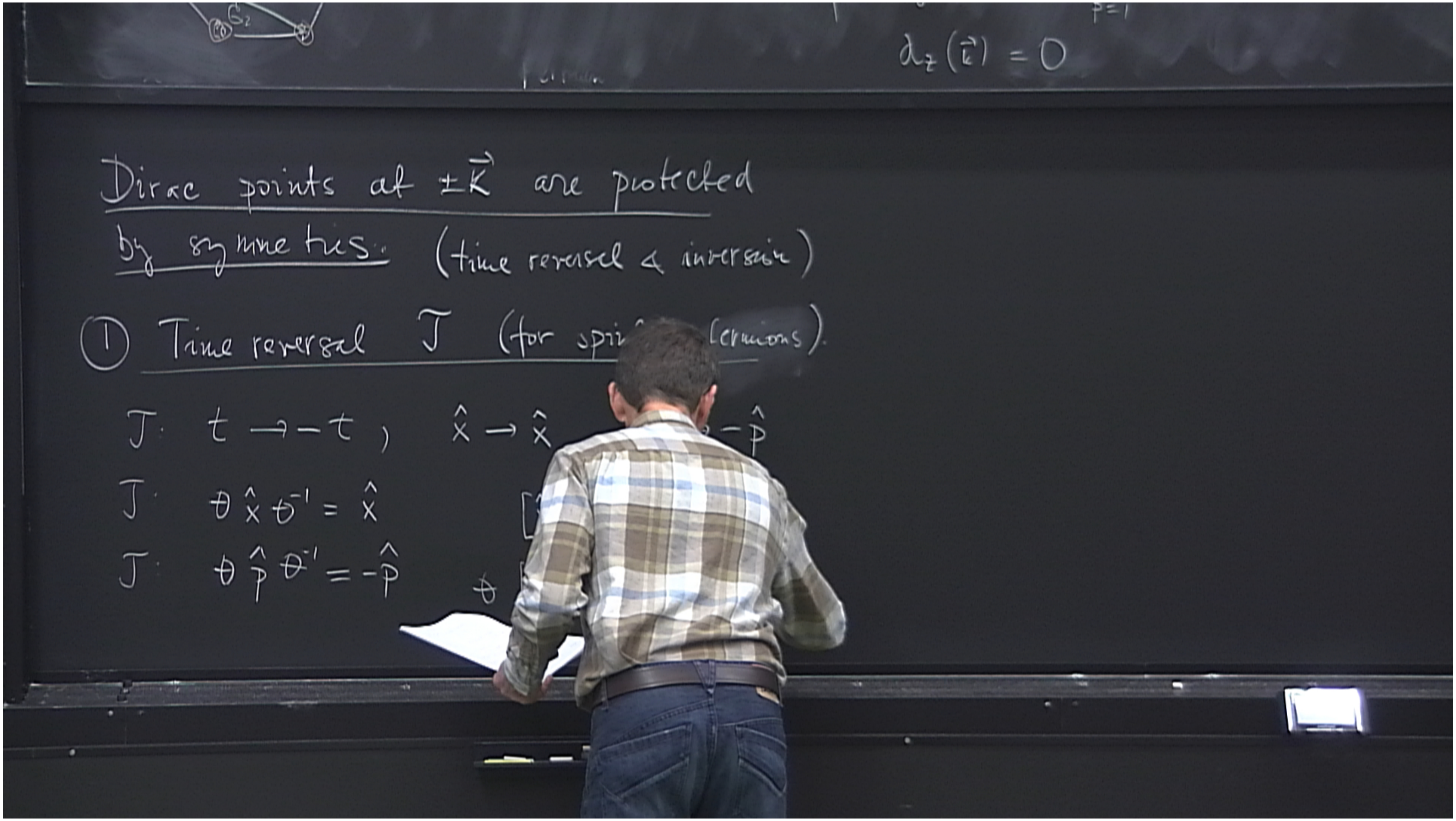
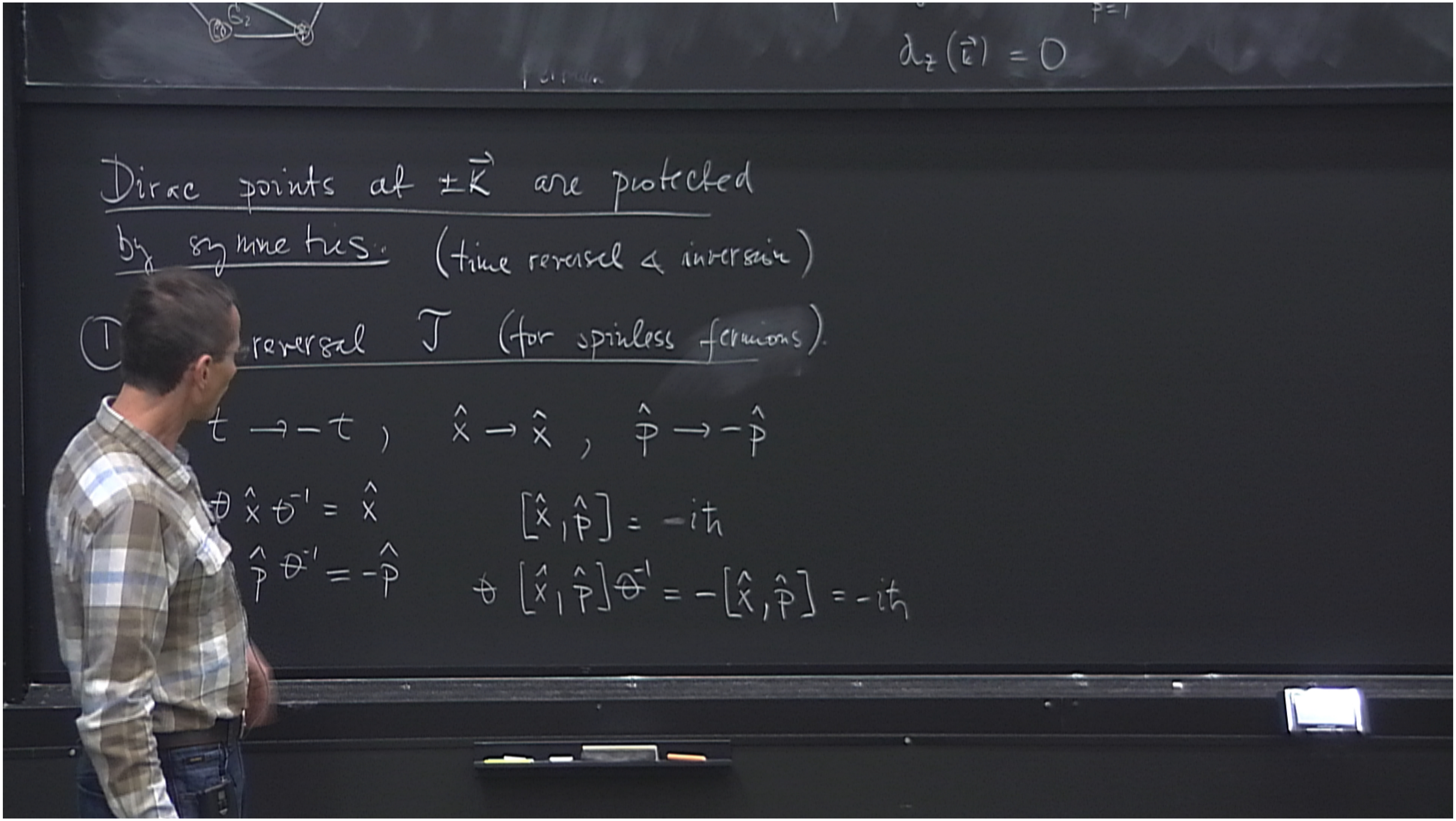
$\lambda_z(\vec{k}) = 0$

Dirac points at $\pm\vec{K}$ are protected by symmetries. (time reversal & inversion)


$\lambda_z(\vec{k}) = 0$
Dirac points at $\pm\vec{K}$ are protected
by symmetries. (time reversal & inversion)
① Time reversal $\mathcal{T}$
$\mathcal{T}$: $t \to -t$, $\hat{x} \to \hat{x}$
$\mathcal{T}$: $\theta \hat{x} \theta^{-1} = \hat{x}$
$\mathcal{T}$: $\theta \hat{p} \theta^{-1} = -\hat{p}$



$\lambda_z(\vec{k}) = 0$
Dirac points at $\pm\vec{K}$ are protected by symmetries. (time reversal & inversion)
① reversal T (for spinless fermions).
$t \to -t$, $\hat{x} \to \hat{x}$, $\hat{p} \to -\hat{p}$
$\Theta \hat{x} \Theta^{-1} = \hat{x}$
$[\hat{x}, \hat{p}] = -i\hbar$
$\hat{p} \Theta^{-1} = -\hat{p}$
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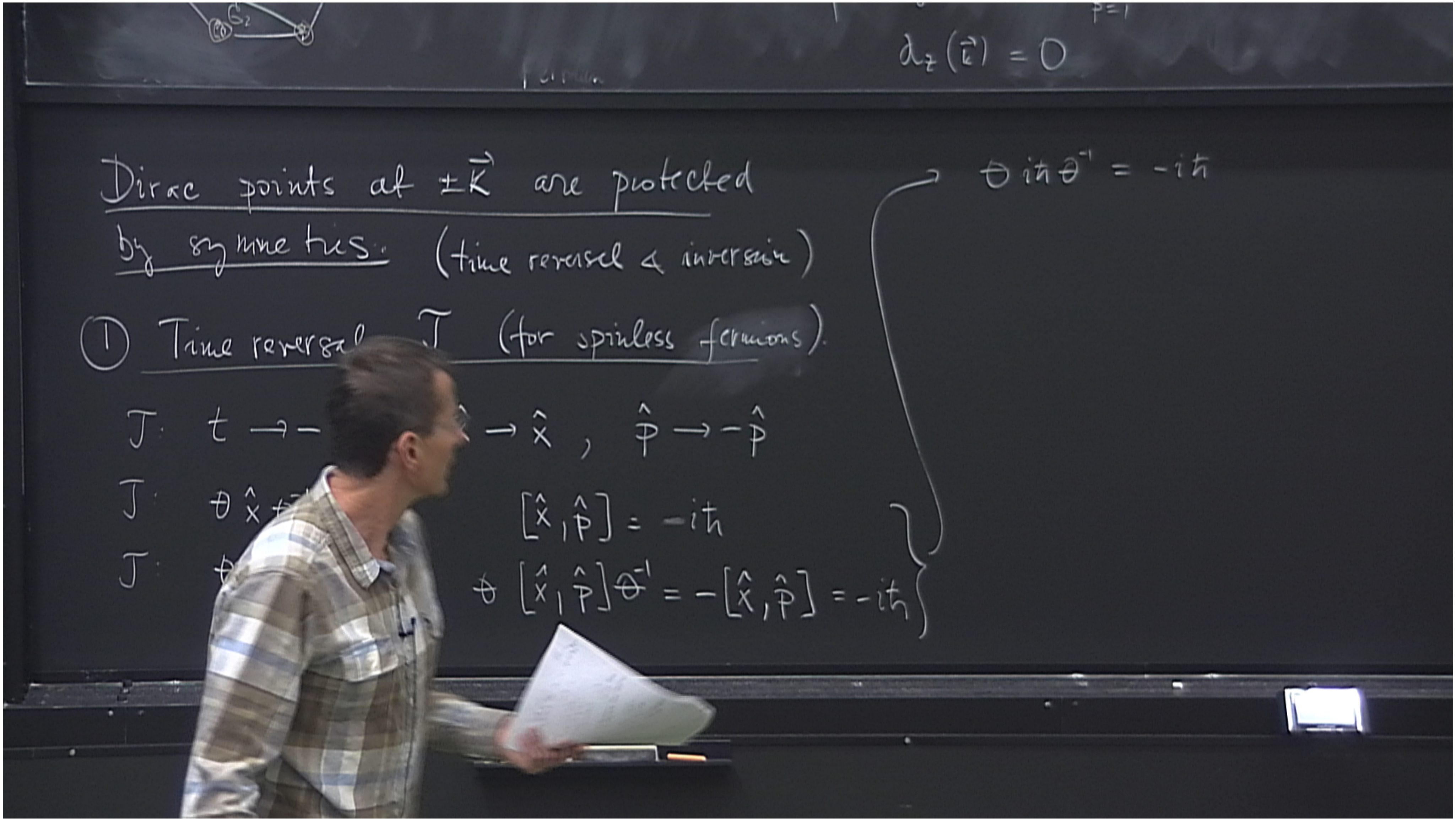
$d_z(\vec{k}) = 0$
Dirac points at $\pm\vec{K}$ are protected
by symmetries. (time reversal & inversion)
① Time reversal T (for spinless fermions).
T: $t \to -$ … $\to \hat{x}$, $\hat{p} \to -\hat{p}$
T: $\theta\,\hat{x}$ …
$[\hat{x},\hat{p}] = -i\hbar$
T: …
$\theta\,[\hat{x},\hat{p}]\,\theta^{-1} = -[\hat{x},\hat{p}] = -i\hbar$
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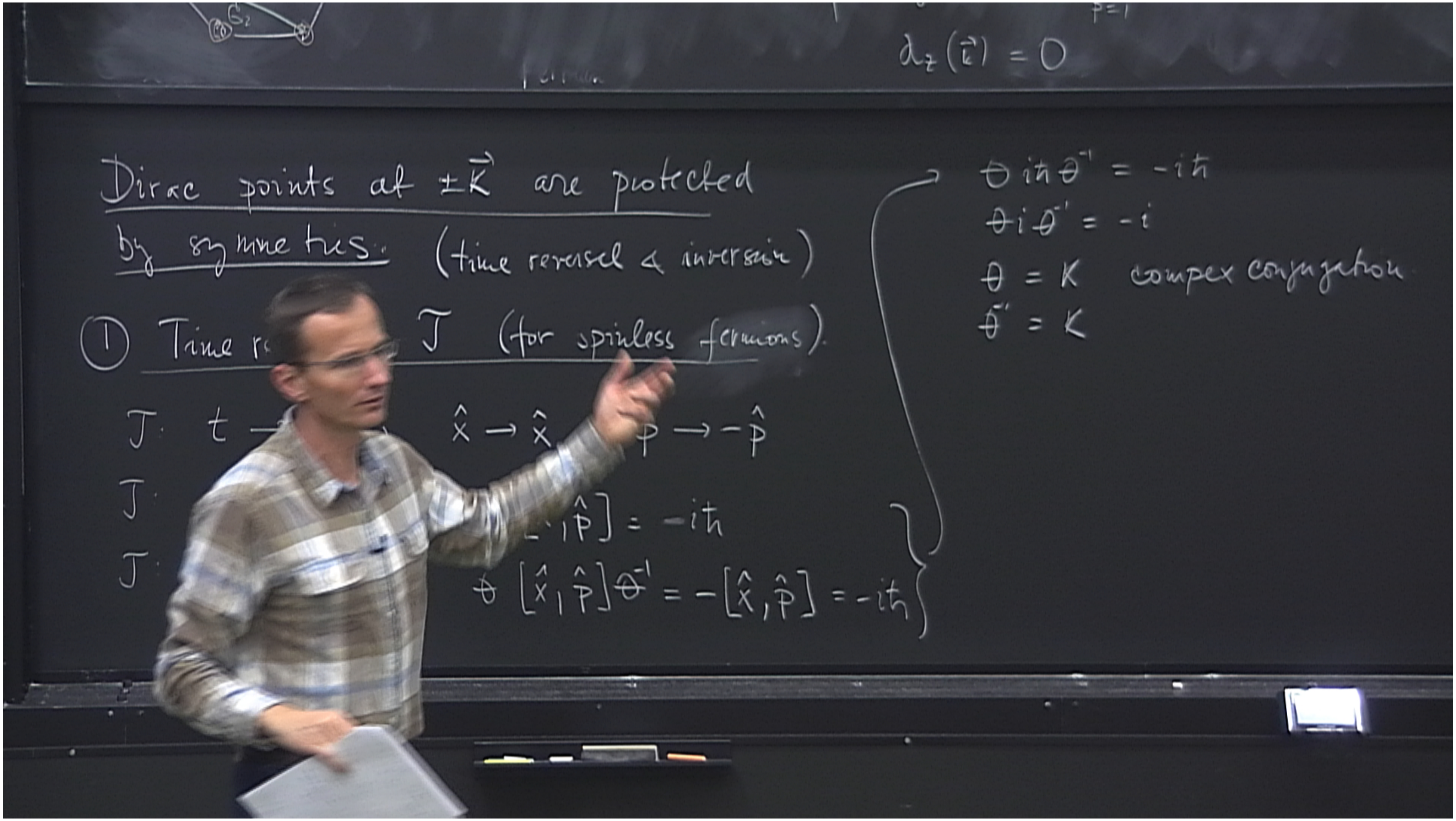
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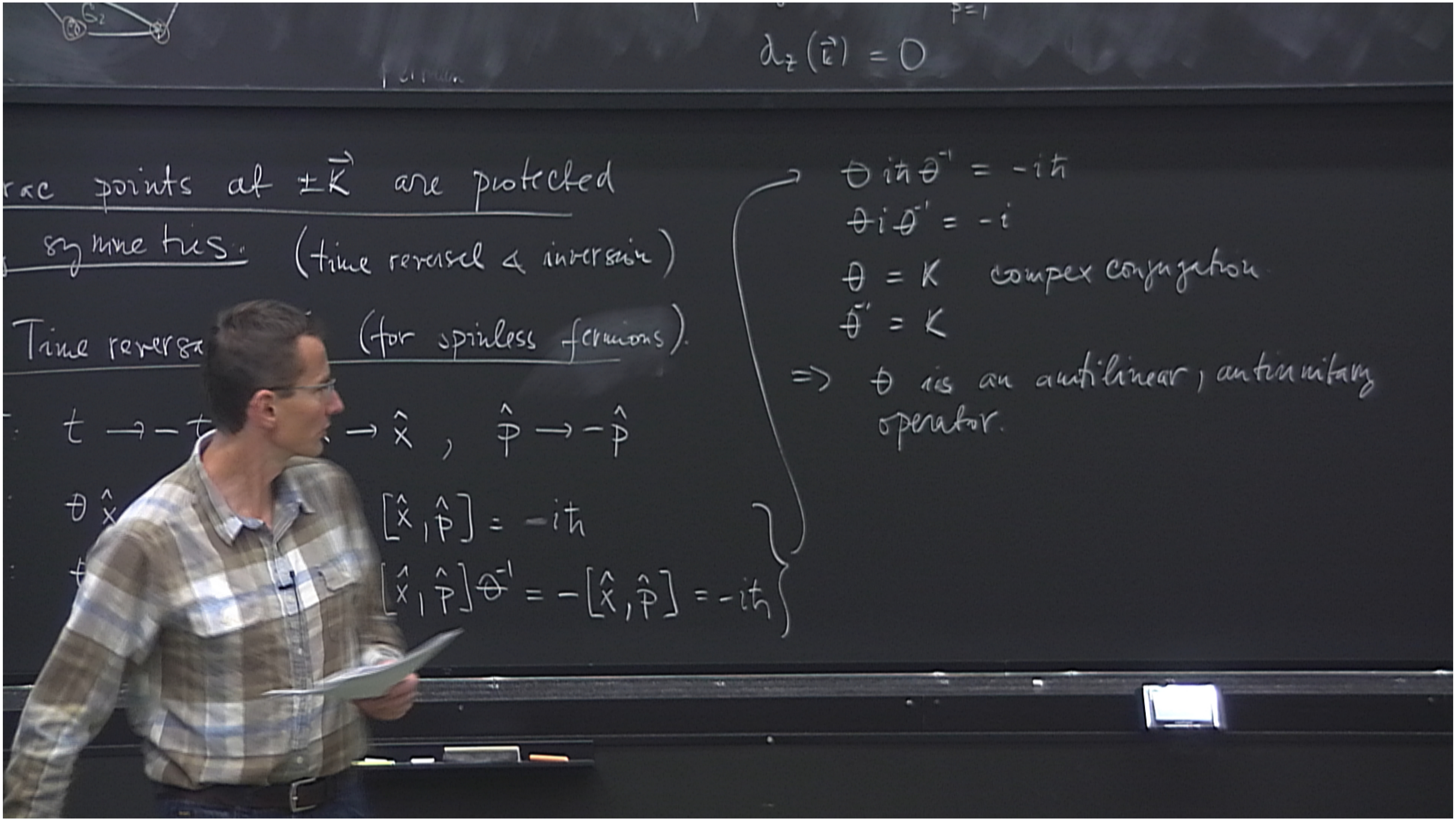
$\Theta\, i\hbar\, \Theta^{-1} = -i\hbar$
$\Theta\, i\, \Theta^{-1} = -i$
$\Theta = K$ compex conjugation
$\Theta^{-1} = K$
$\Theta[\hat{x}, \hat{p}]\Theta^{-1} = -[\hat{x}, \hat{p}] = -i\hbar$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points at $\pm\vec{K}$ are protected
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Time revers (for spinless fermions)
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$[\hat{x}, \hat{p}] = -i\hbar$
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$\theta i\hbar\theta^{-1} = -i\hbar$
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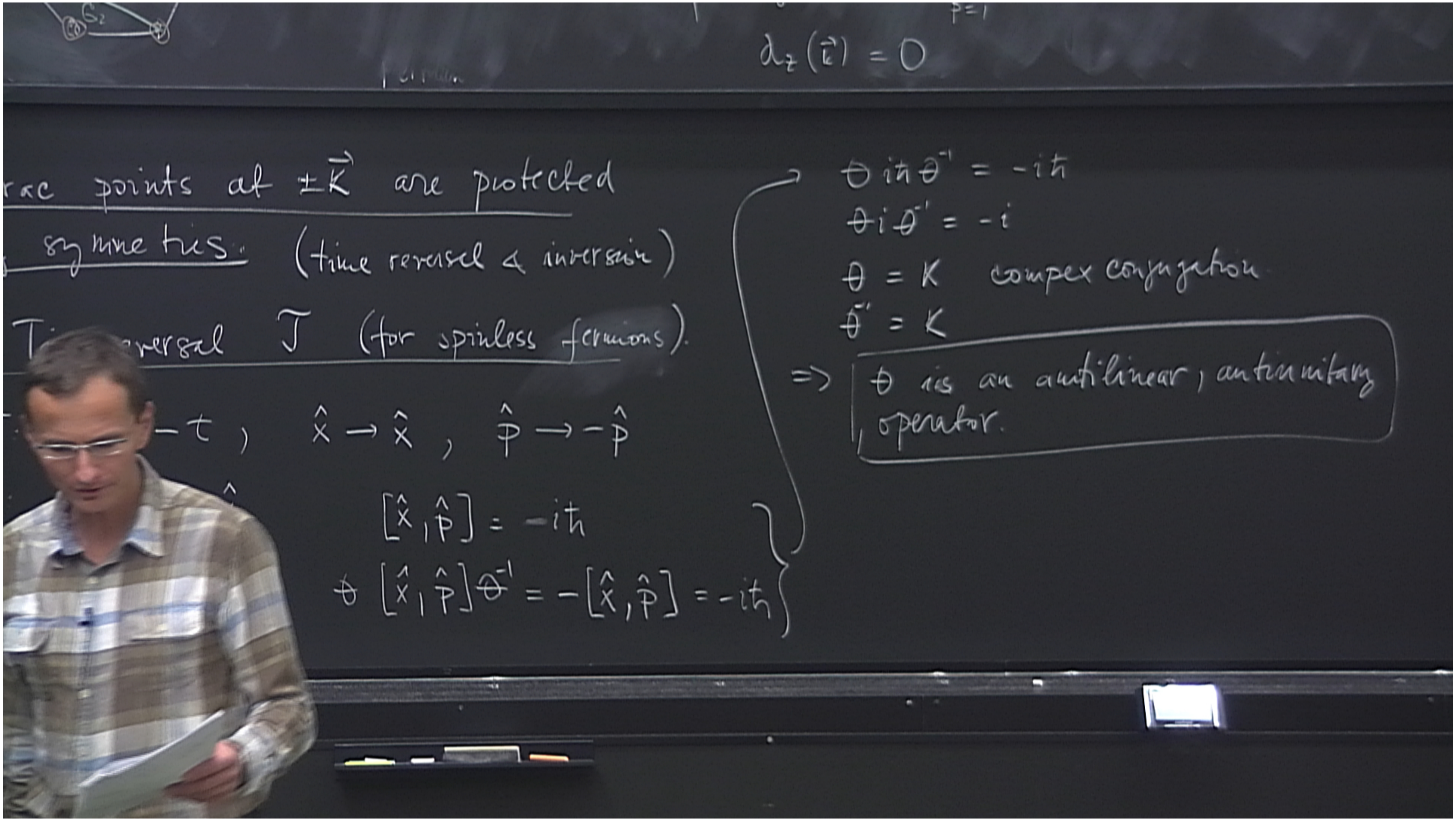
$\theta = K$ compex conjugation
$\theta^{-1} = K$
$\Rightarrow$ θ is an antilinear, antiunitary operator.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...rac points at $\pm\vec{K}$ are protected
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- Time reversal in crystals

$$H = \sum_{k} c^{+}_{\alpha k} \, \mathcal{H}^{\alpha\beta}(\vec{k}) \, c_{\beta k}$$

...opagation

...inear, antiunitary

• Time reversal in crystals

$$H = \sum_{k} c^{+}_{\alpha k} \mathcal{H}^{\alpha\beta}(\vec{k})\, c_{\beta k}$$ Bloch Hamiltonian

$$\Theta c_i \Theta^{-1} = c_i$$

...opagation

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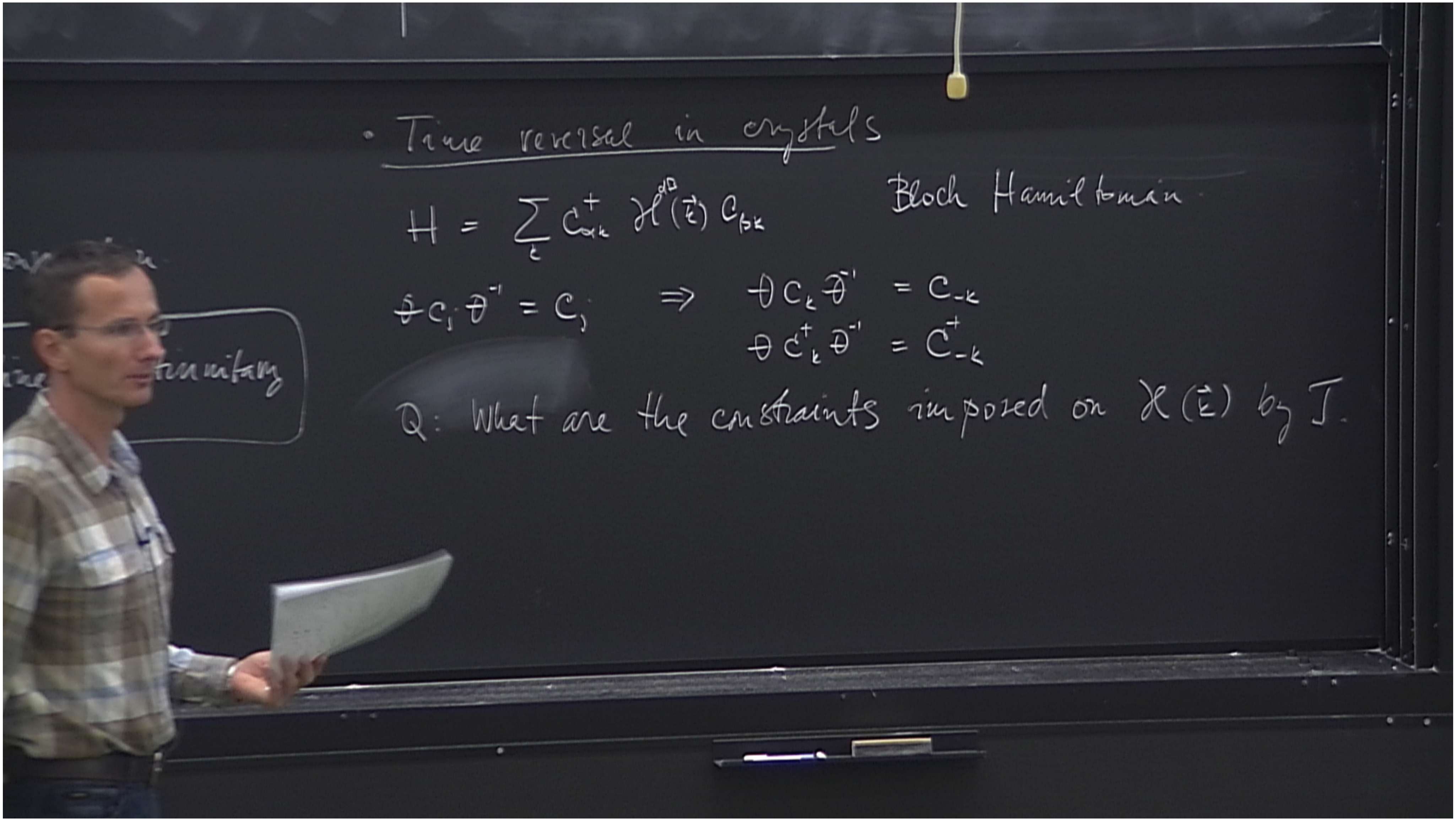
...agation

$\boxed{\text{...inear, antiunitary}}$


• Time reversal in crystals
$H = \sum_k c^+_{\alpha k} \mathcal{H}^{\alpha\beta}(\vec{k}) c_{\beta k}$
Bloch Hamiltonian
$\Theta c_i \Theta^{-1} = c_i \Rightarrow \Theta c_k \Theta^{-1} = c_{-k}$
$\Theta c^+_k \Theta^{-1} = c^+_{-k}$
Q: What are the constraints imposed on $\mathcal{H}(\vec{k})$ by T.

...agation

...inear, antiunitary

• Time reversal in crystals

$$H = \sum_k c^\dagger_{\alpha k} \mathcal{H}^{\alpha\beta}(\vec{k})\, c_{\beta k}$$ Bloch Hamiltonian

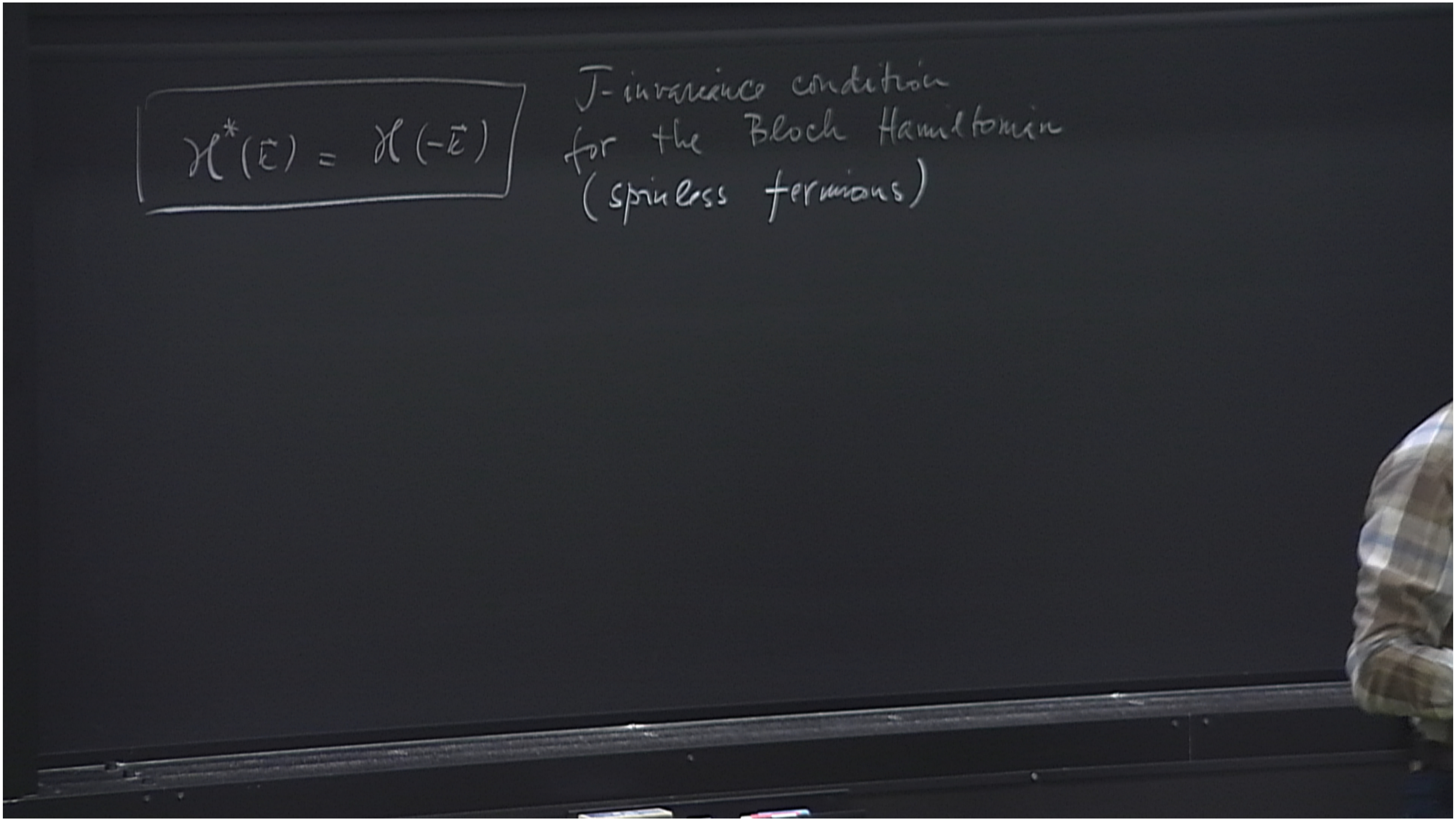
$$\Theta c_i \Theta^{-1} = c_i \quad \Rightarrow \quad \Theta c_k \Theta^{-1} = c_{-k}$$

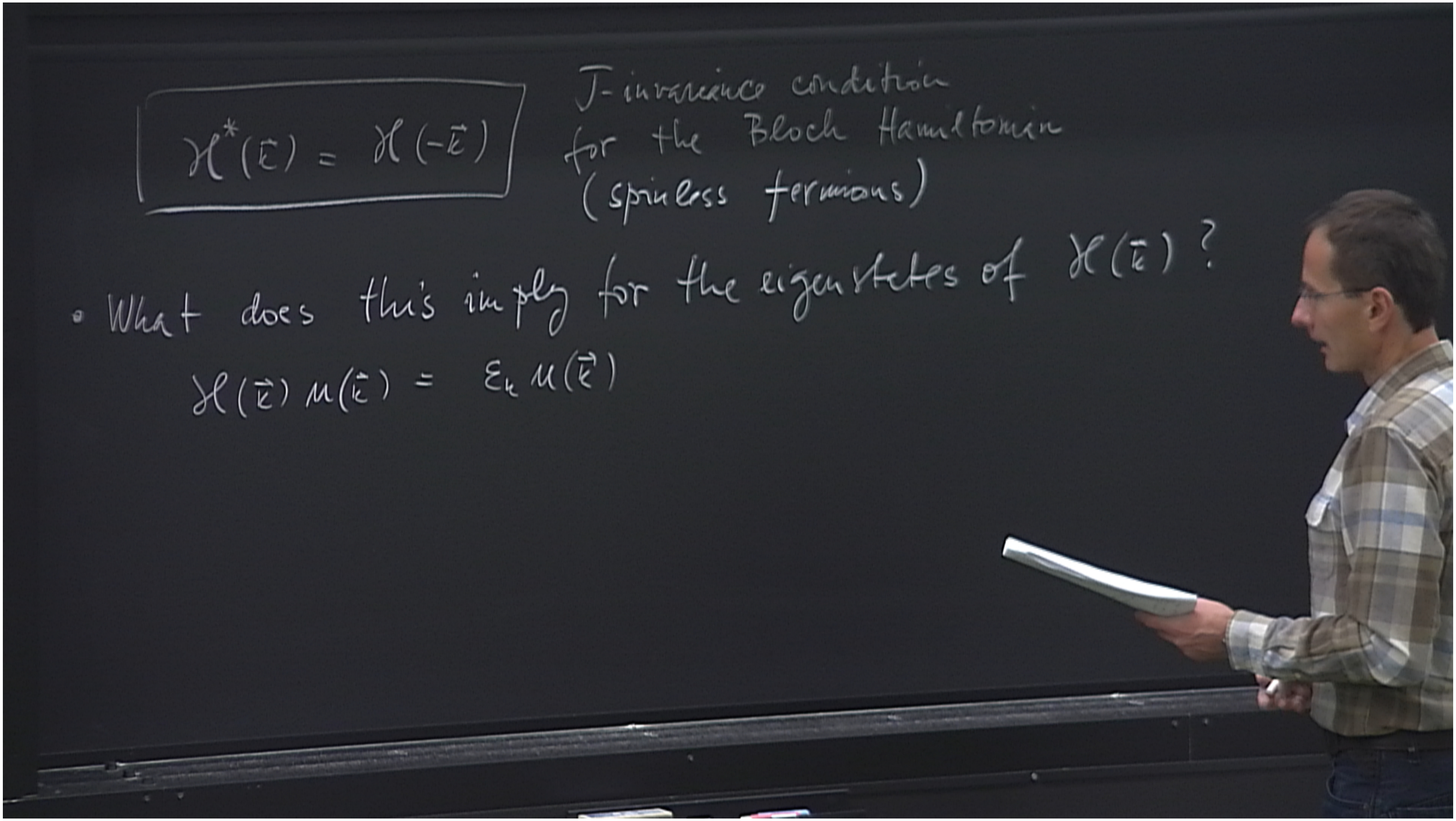
$$\Theta c^\dagger_k \Theta^{-1} = c^\dagger_{-k}$$

Q: What are the constraints imposed on $\mathcal{H}(\vec{k})$ by T.

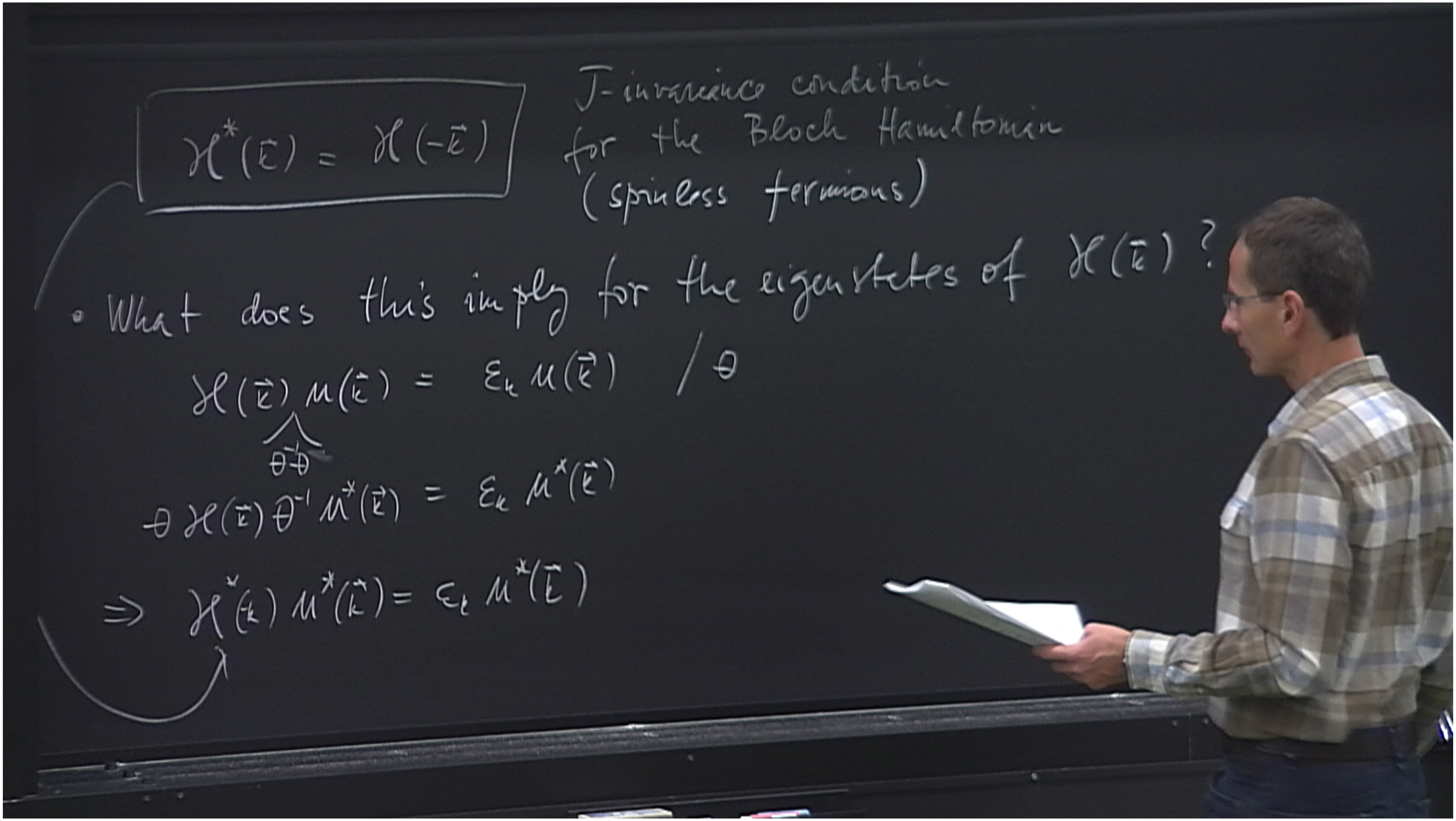
$$\Theta H \Theta^{-1} = H$$

$$\Rightarrow \sum_k c^\dagger_{-k}\, \Theta \mathcal{H}(\vec{k}) \Theta^{-1} c_{-k} = \sum_k c^\dagger_k\, \mathcal{H}(\vec{k})\, c_k$$


$\boxed{\mathcal{H}^*(\vec{k}) = \mathcal{H}(-\vec{k})}$
T-invariance condition
for the Bloch Hamiltonian
(spinless fermions)



$\boxed{\mathcal{H}^*(\vec{k}) = \mathcal{H}(-\vec{k})}$
T-invariance condition
for the Bloch Hamiltonian
(spinless fermions)
• What does this imply for the eigenstates of $\mathcal{H}(\vec{k})$?
$\mathcal{H}(\vec{k})\, u(\vec{k}) = \varepsilon_k\, u(\vec{k})$


$\boxed{\mathcal{H}^*(\vec{k}) = \mathcal{H}(-\vec{k})}$
T-invariance condition for the Bloch Hamiltonian (spinless fermions)
• What does this imply for the eigenstates of $\mathcal{H}(\vec{k})$?
$\mathcal{H}(\vec{k})\, u(\vec{k}) = \varepsilon_k\, u(\vec{k}) \quad / \Theta$
$\Theta^{-1}\Theta$
$\Theta\, \mathcal{H}(\vec{k})\, \Theta^{-1}\, u^*(\vec{k}) = \varepsilon_k\, u^*(\vec{k})$
$\Rightarrow \mathcal{H}^*(\vec{k})\, u^*(\vec{k}) = \varepsilon_k\, u^*(\vec{k})$

$$\boxed{\mathcal{H}^*(\vec{k}) = \mathcal{H}(-\vec{k})}$$

T-invariance condition for the Bloch Hamiltonian (spinless fermions)

- What does this imply for the eigenstates of $\mathcal{H}(\vec{k})$?

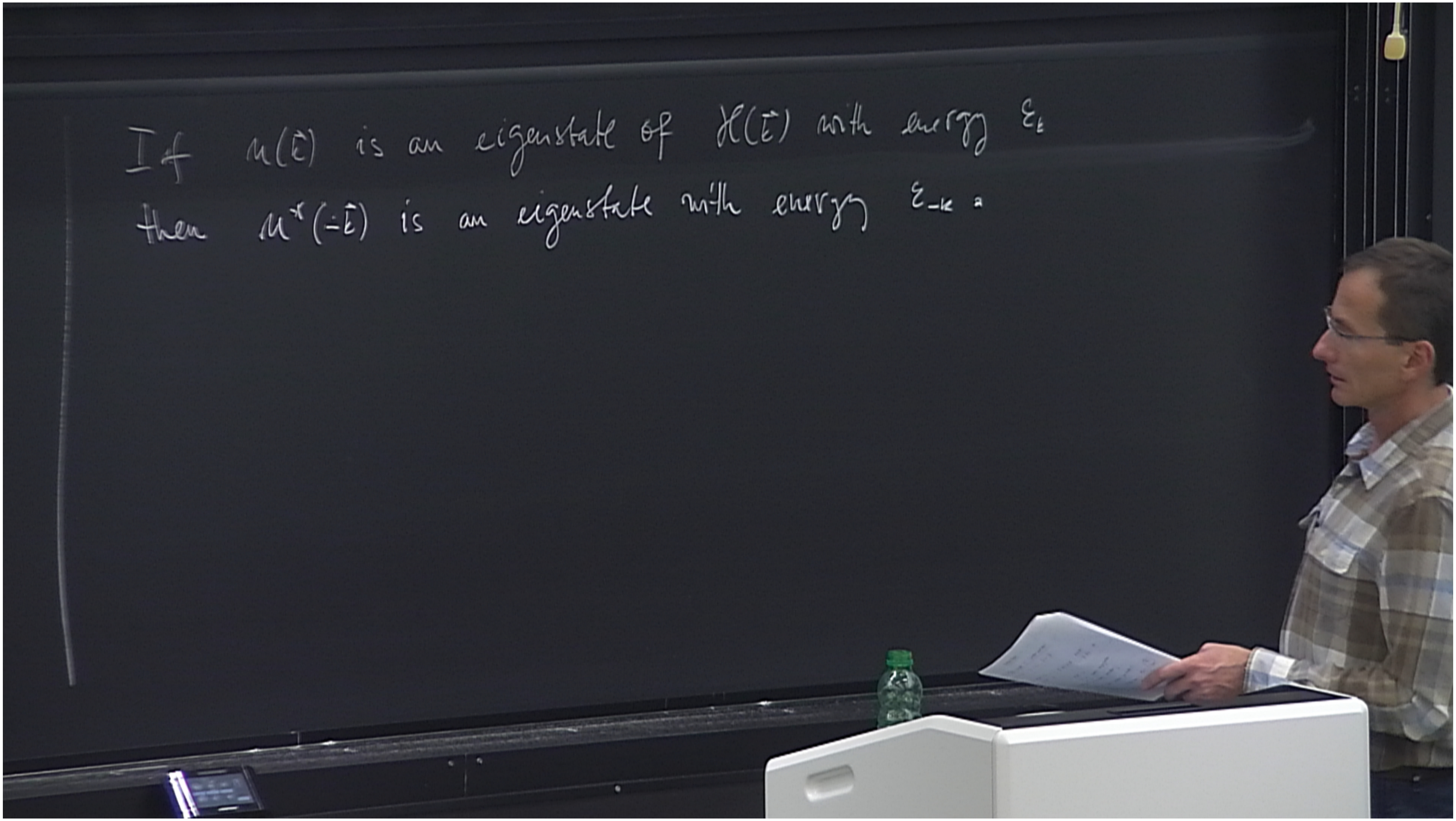
$$\mathcal{H}(\vec{k})\, u(\vec{k}) = \varepsilon_k\, u(\vec{k}) \quad / \Theta$$

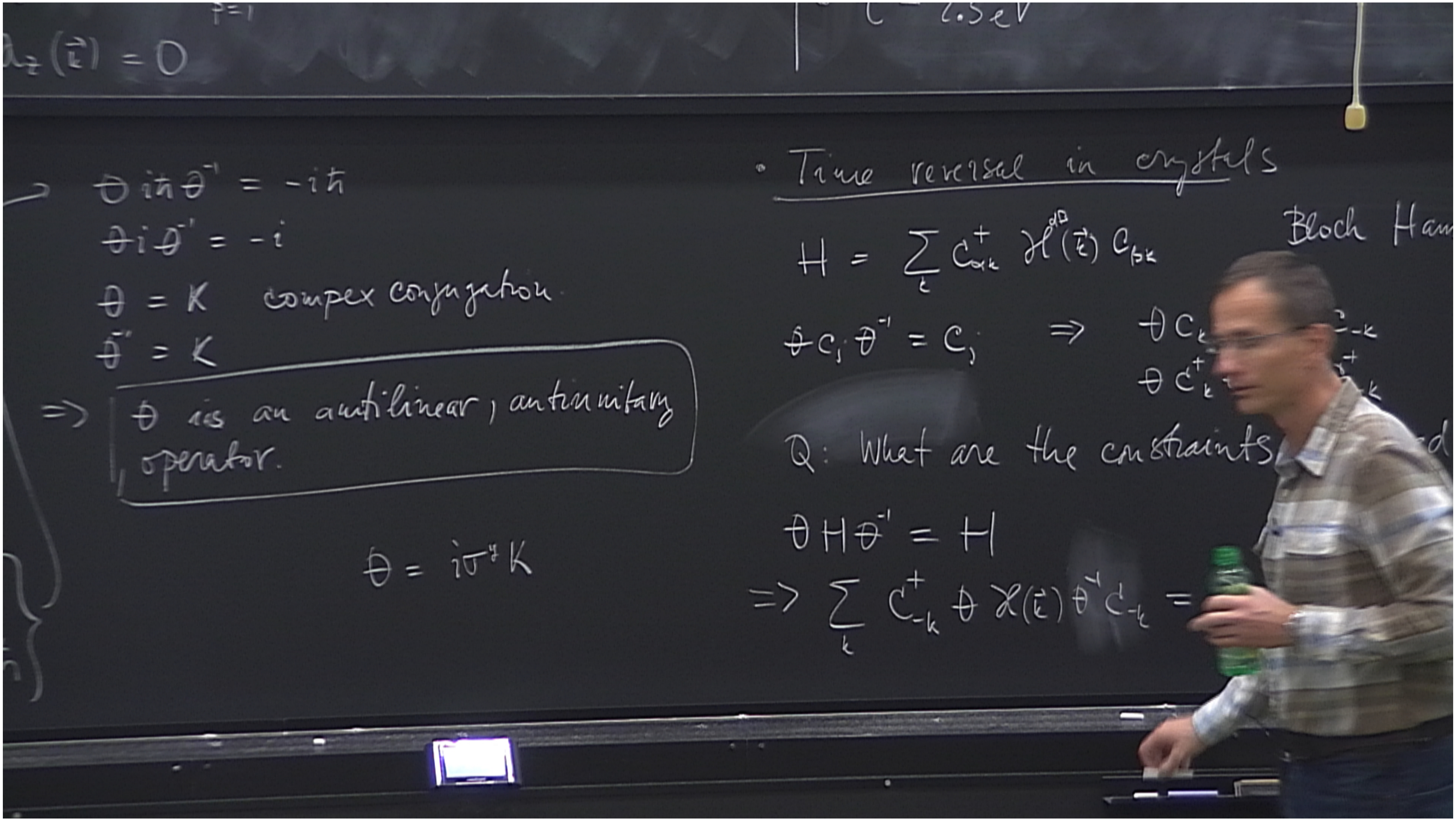
$$\Theta^{-1}\Theta$$

$$\Theta\, \mathcal{H}(\vec{k})\, \Theta^{-1}\, u^*(\vec{k}) = \varepsilon_k\, u^*(\vec{k})$$

$$\Rightarrow \mathcal{H}^*(k)\, u^*(\vec{k}) = \varepsilon_k\, u^*(\vec{k})$$

$$\Rightarrow \boxed{\mathcal{H}(k)\, u^*(-\vec{k}) = \varepsilon_{-k}\, u^*(-\vec{k})}$$


If $u(\vec{k})$ is an eigenstate of $\mathcal{H}(\vec{k})$ with energy ε_k
then $u^*(-\vec{k})$ is an eigenstate with energy ε_{-k} .



$\theta i\hbar \theta^{-1} = -i\hbar$
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$\theta = i\sigma^y K$
• Time reversal in crystals
Bloch Ham
$H = \sum_k C^+_{\alpha k} \mathcal{H}^{\alpha\beta}(\vec{k}) C_{\beta k}$
$\theta c_j \theta^{-1} = c_j$ $\Rightarrow$
Q: What are the constraints
$\theta H \theta^{-1} = H$
$\Rightarrow \sum_k C^+_{-k} \theta \mathcal{H}(\vec{k}) \theta^{-1} C_{-k} =$