Title: Explorations in Condensed Matter-7

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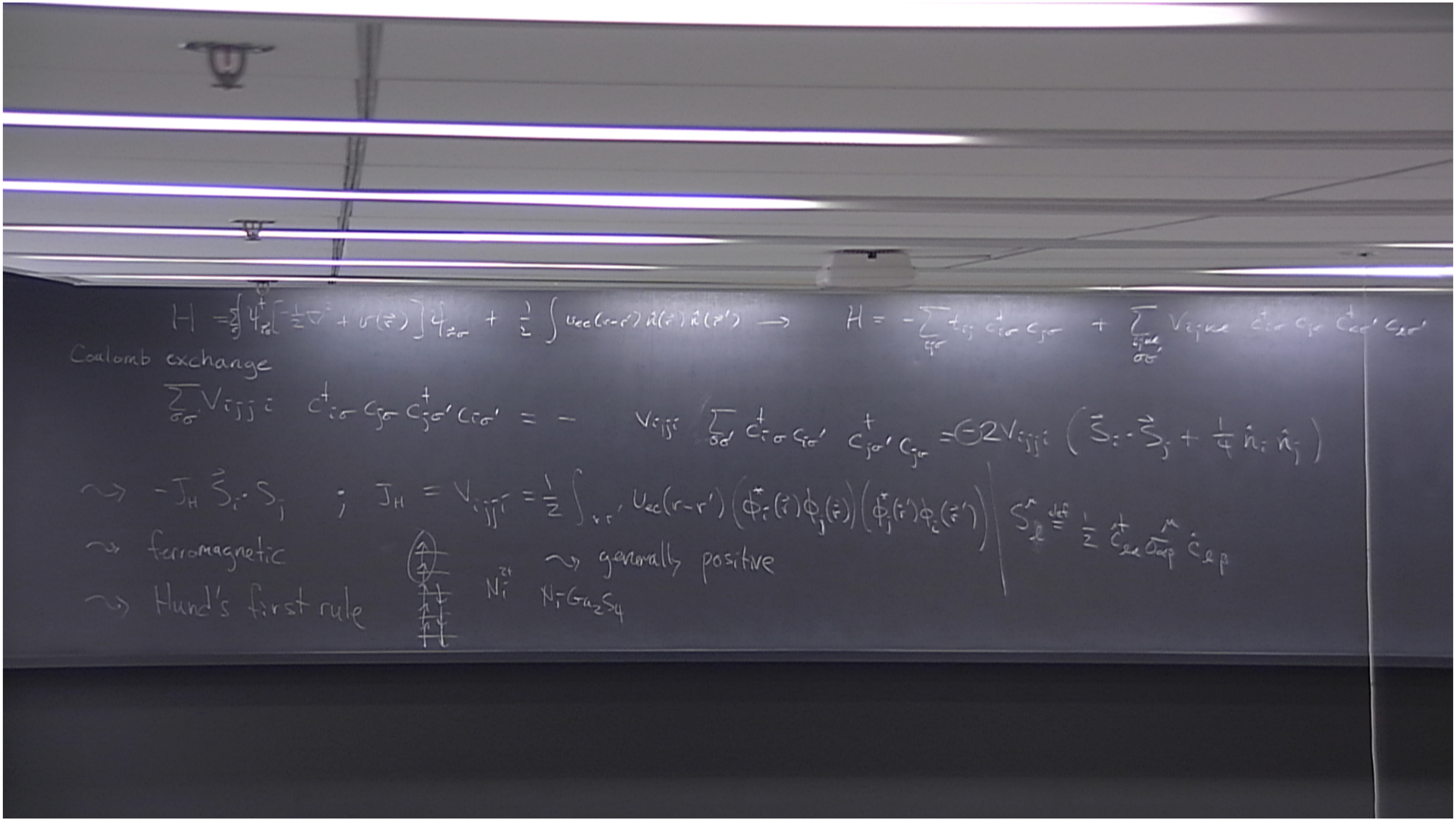
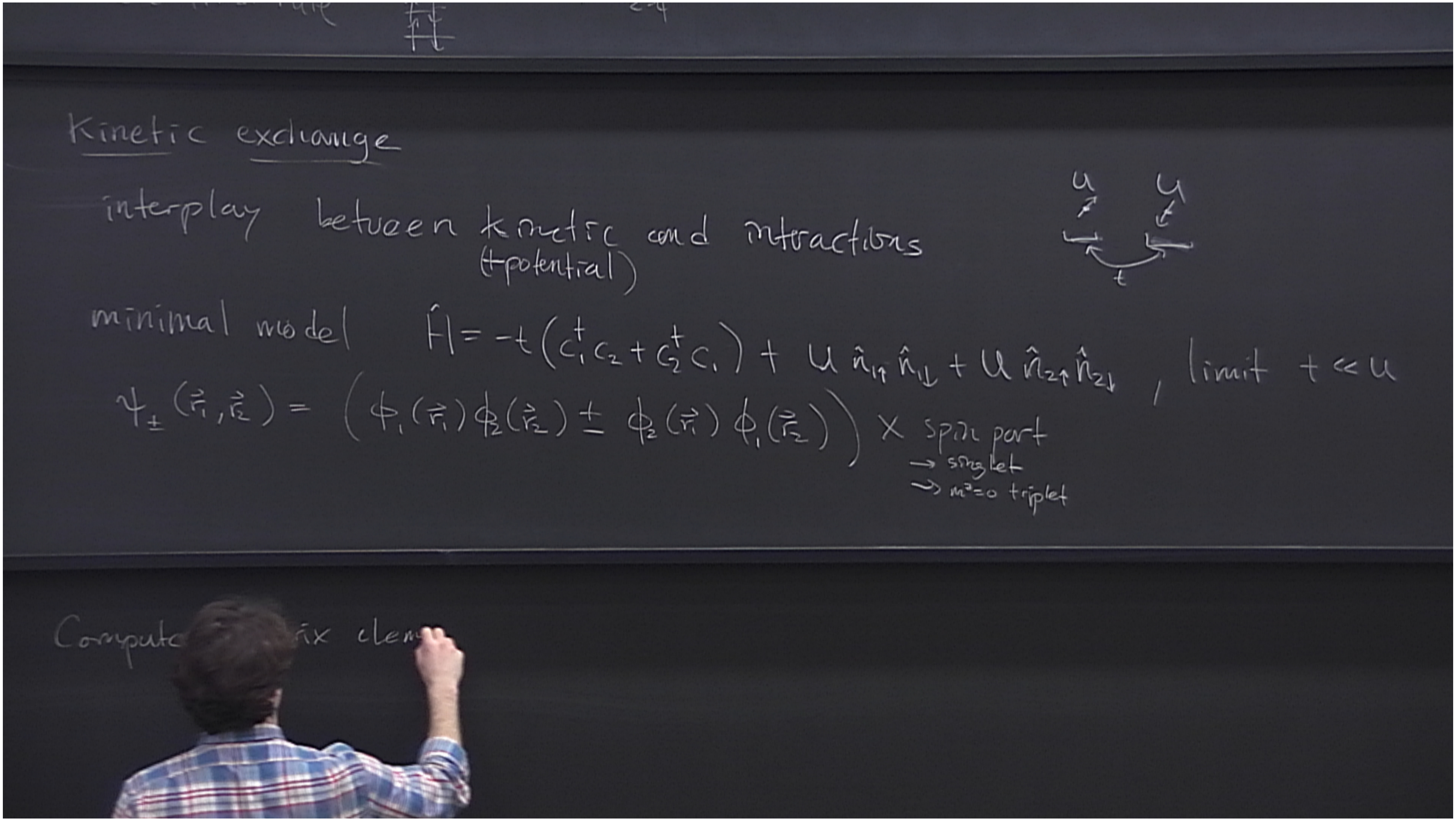
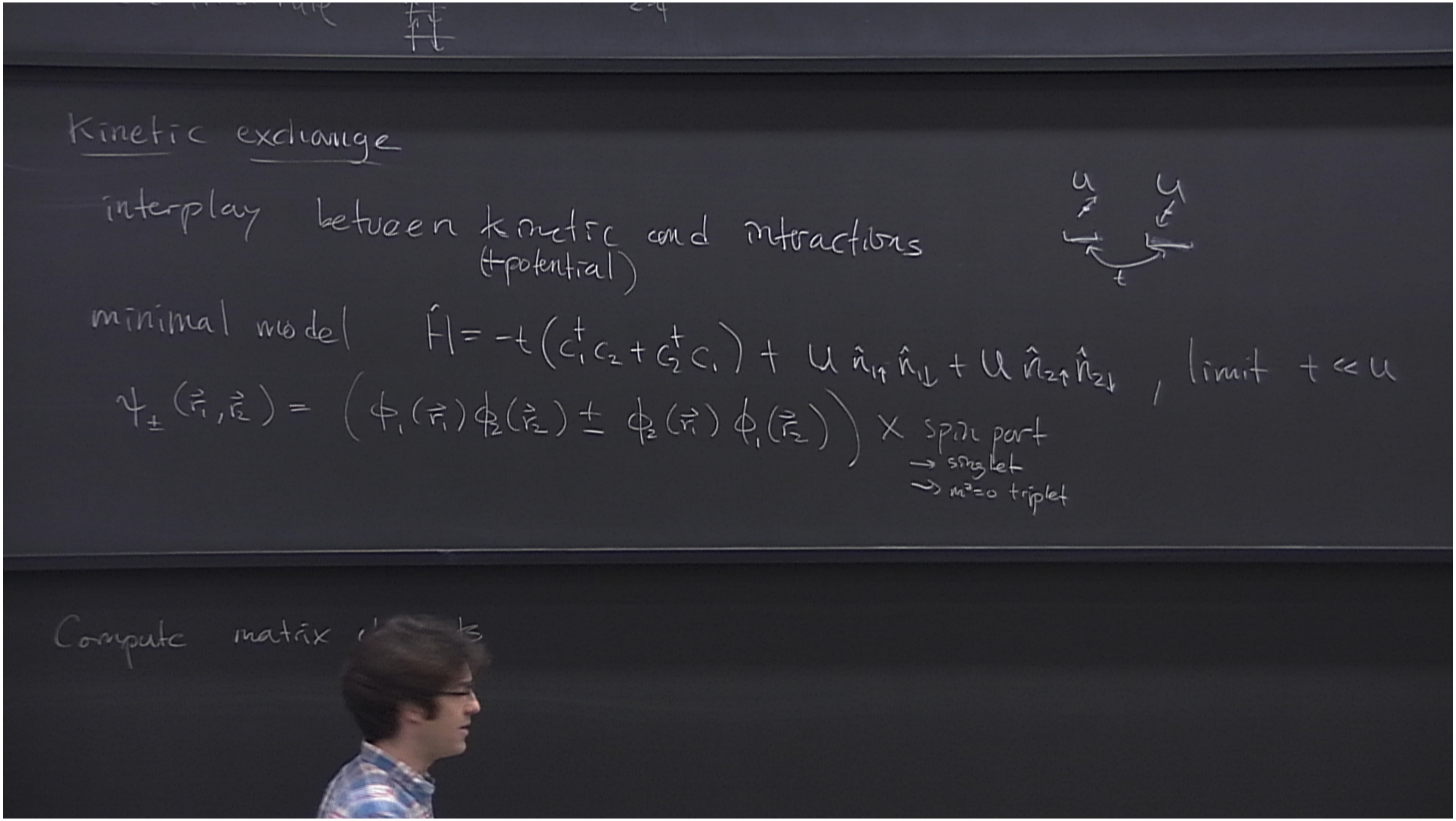
URL: http://pirsa.org/15030042

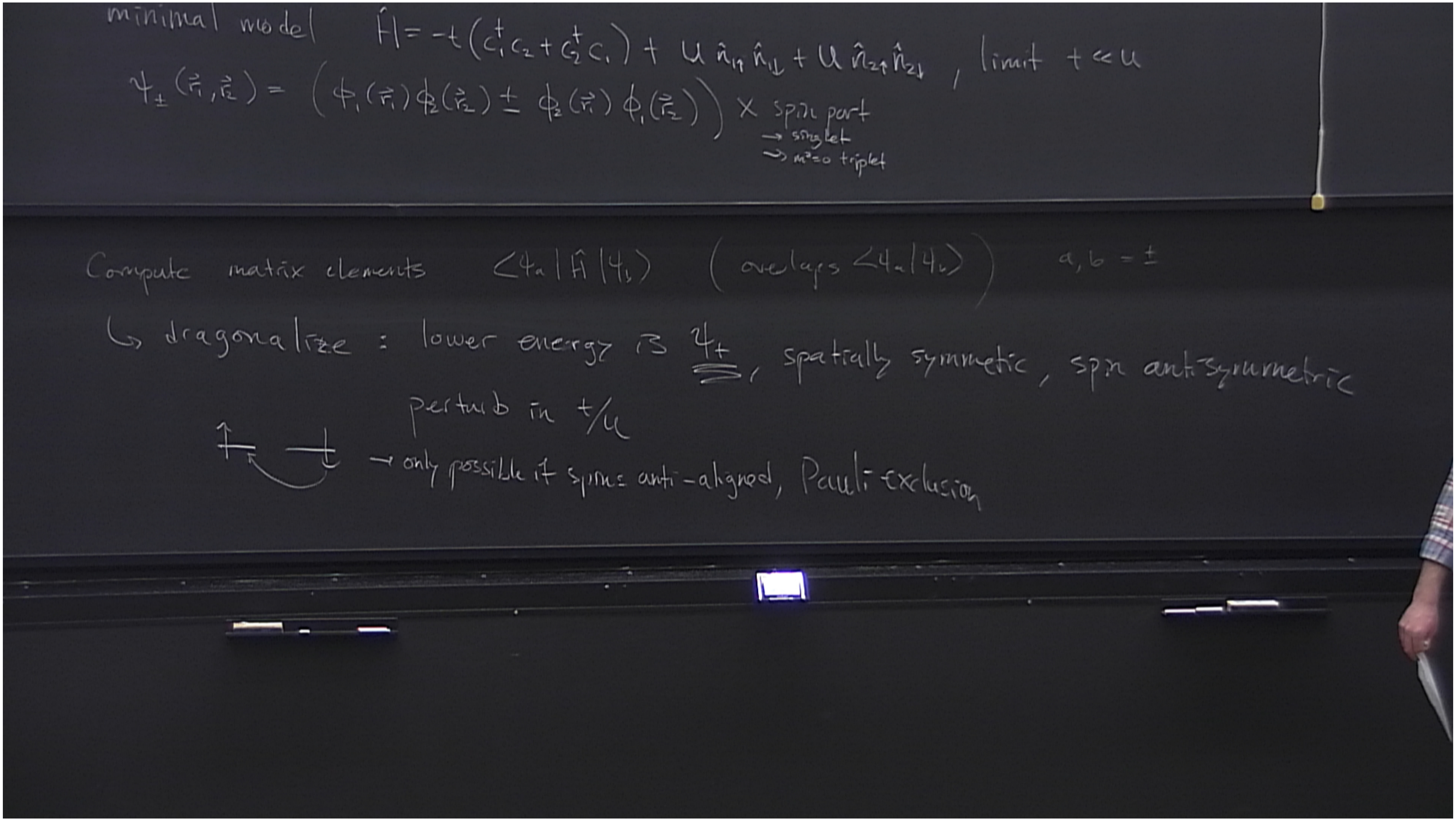
Abstract:

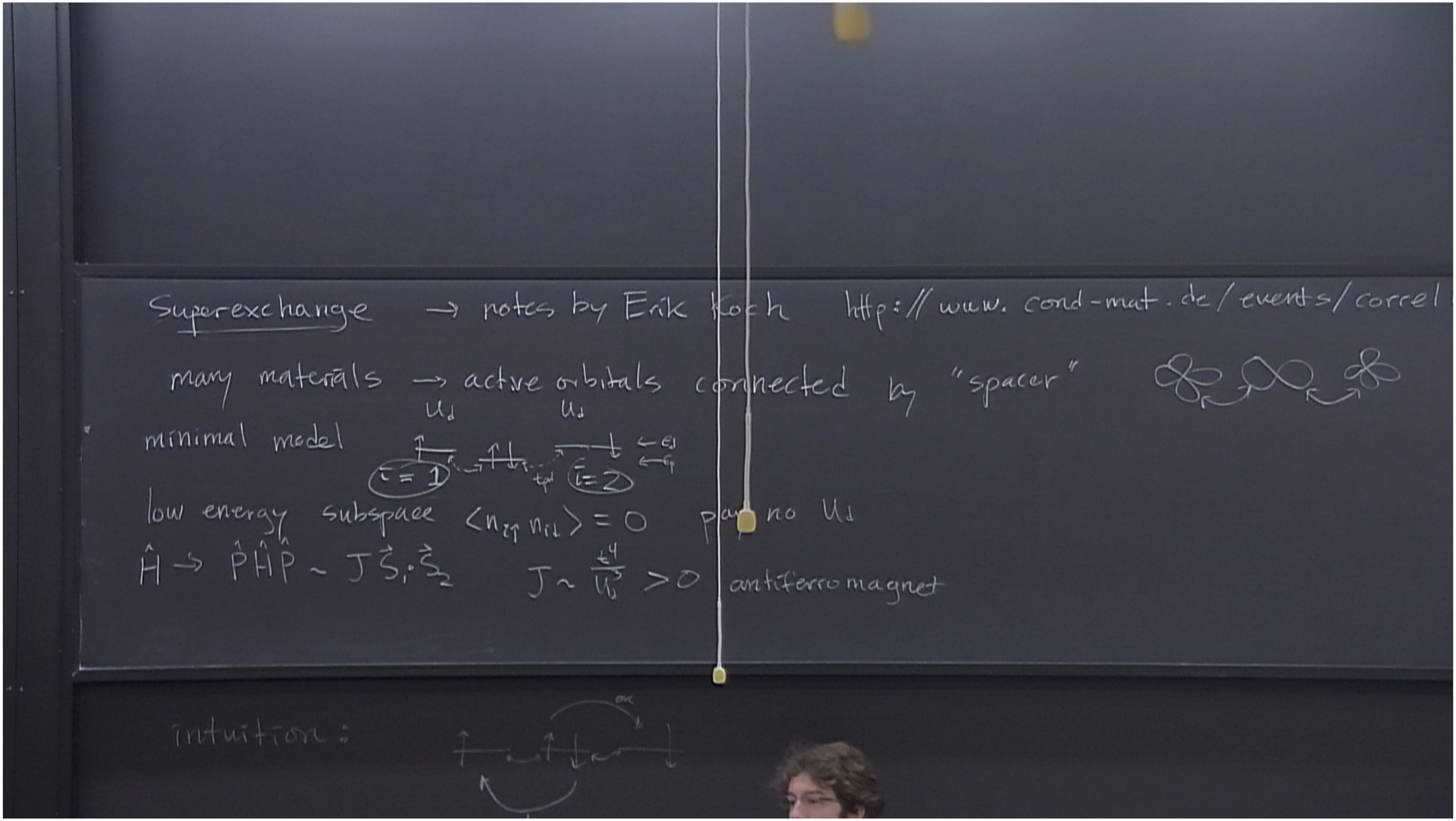


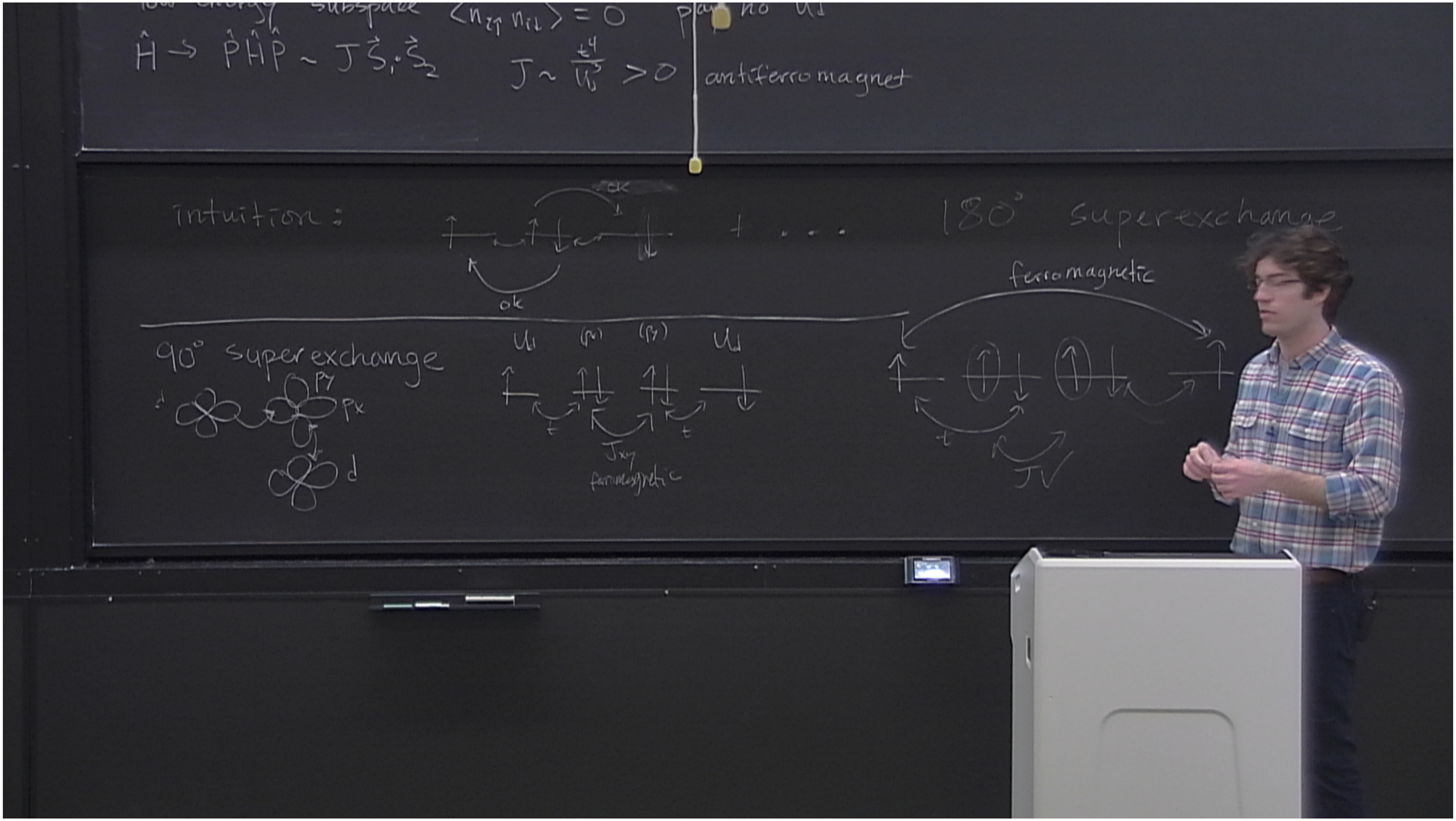
$H = \sum_\sigma \int \psi^\dagger_{r\sigma}[-\frac{1}{2}\nabla^2 + v(\vec r)]\psi_{r\sigma} + \frac{1}{2}\int U_{ee}(r-r')\hat n(\vec r)\hat n(\vec r') \longrightarrow H = -\sum_{ij\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + \sum_{ijkl,\sigma\sigma'} V_{ijkl} c^\dagger_{i\sigma} c_{j\sigma} c^\dagger_{k\sigma'} c_{l\sigma'}$
Coulomb exchange
$\sum_{\sigma\sigma'} V_{ijji} c^\dagger_{i\sigma} c_{j\sigma} c^\dagger_{j\sigma'} c_{i\sigma'} = - V_{ijji}\sum_{\sigma\sigma'} c^\dagger_{i\sigma} c_{i\sigma'} c^\dagger_{j\sigma'} c_{j\sigma} = -2V_{ijji}(\vec S_i\cdot\vec S_j + \frac{1}{4}\hat n_i \hat n_j)$
$\rightsquigarrow -J_H \vec S_i\cdot S_j$; $J_H = V_{ijji} = \frac{1}{2}\int_{rr'} U_{ee}(r-r')(\phi^*_i(\vec r)\phi_j(\vec r))(\phi^*_j(\vec r')\phi_i(\vec r'))$
$S^\mu_\ell \stackrel{def}{=} \frac{1}{2} c^\dagger_{\ell\alpha}\sigma^\mu_{\alpha\beta} c_{\ell\beta}$
⇝ ferromagnetic
⇝ generally positive
⇝ Hund's first rule
Ni^{2+} $NiGa_2S_4$

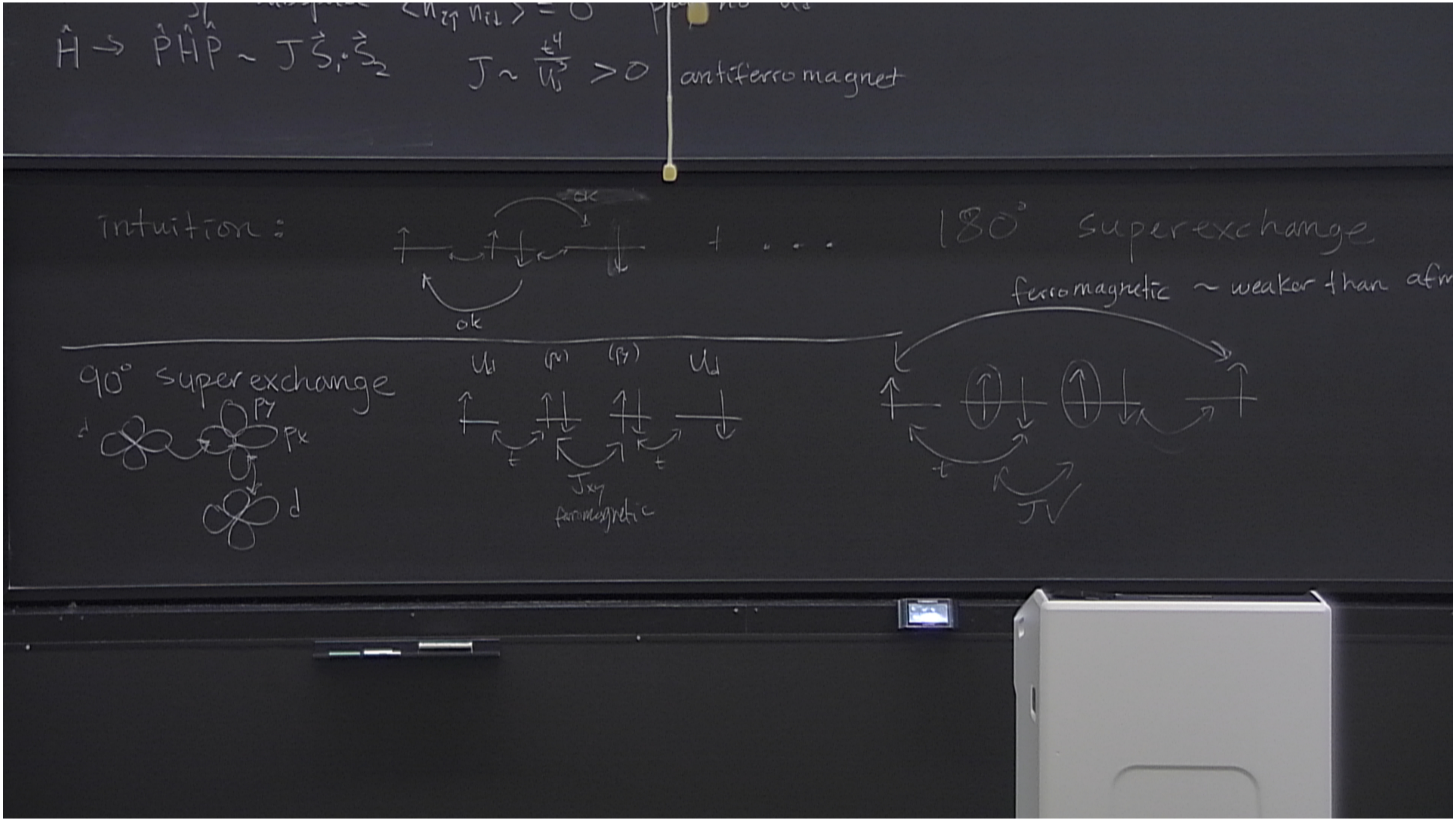

Kinetic exchange
interplay between kinetic (+potential) and interactions
U U
t
minimal model $\hat{H} = -t(c_1^\dagger c_2 + c_2^\dagger c_1) + U \hat{n}_{1\uparrow}\hat{n}_{1\downarrow} + U \hat{n}_{2\uparrow}\hat{n}_{2\downarrow}$, limit $t \ll U$
$\psi_\pm(\vec{r}_1, \vec{r}_2) = \left(\phi_1(\vec{r}_1)\phi_2(\vec{r}_2) \pm \phi_2(\vec{r}_1)\phi_1(\vec{r}_2)\right) \times$ spin part
→ singlet
→ $m^z=0$ triplet
Compute

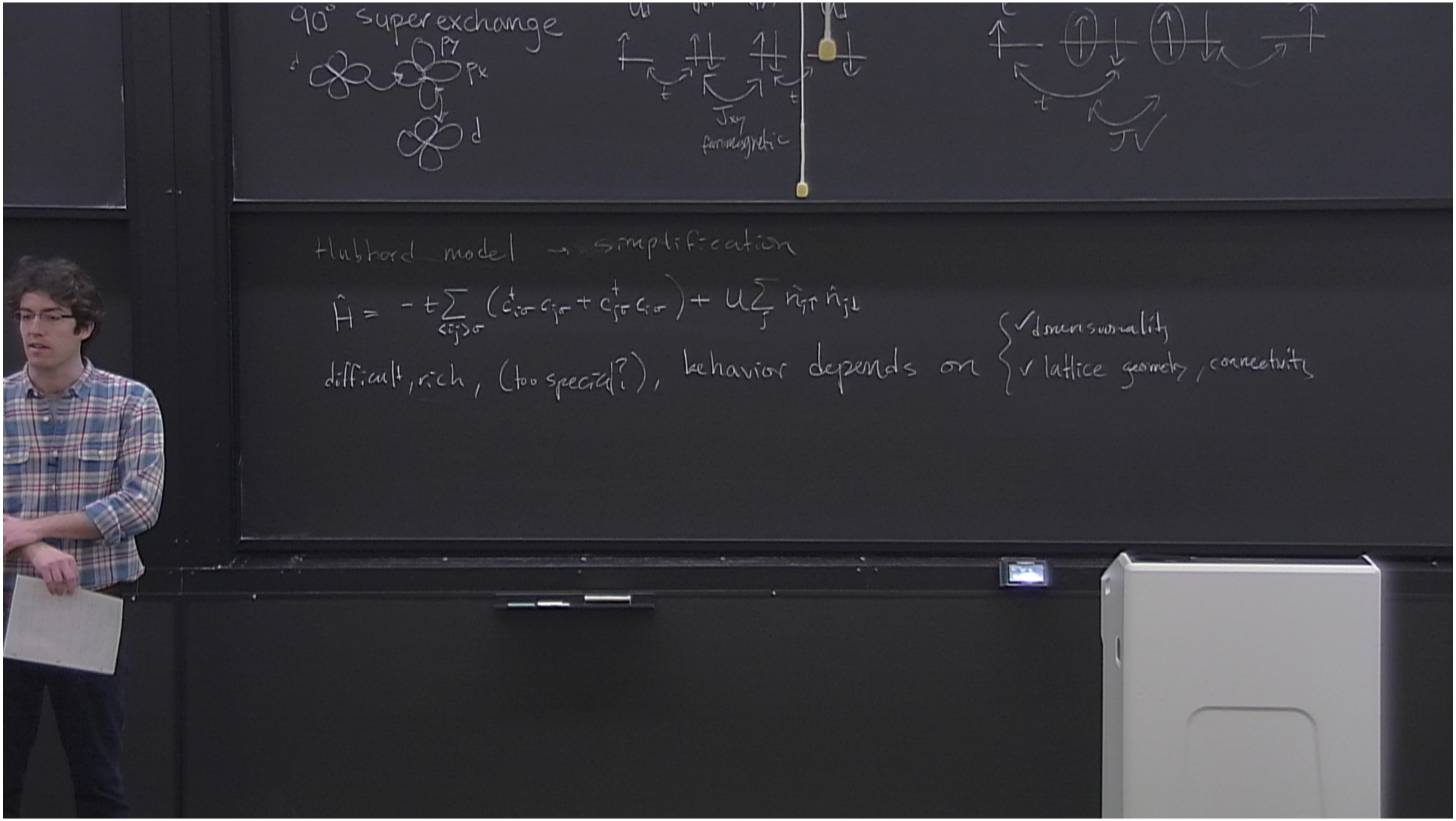

Kinetic exchange
interplay between kinetic and interactions
(+potential)
minimal model $\hat{H} = -t\left(c_1^\dagger c_2 + c_2^\dagger c_1\right) + U\,\hat{n}_{1\uparrow}\hat{n}_{1\downarrow} + U\,\hat{n}_{2\uparrow}\hat{n}_{2\downarrow}$, limit $t \ll U$
$\psi_\pm(\vec{r}_1,\vec{r}_2) = \left(\phi_1(\vec{r}_1)\phi_2(\vec{r}_2) \pm \phi_2(\vec{r}_1)\phi_1(\vec{r}_2)\right) \times$ spin part
→ singlet
→ $m^z=0$ triplet
U
U
t
Compute matrix

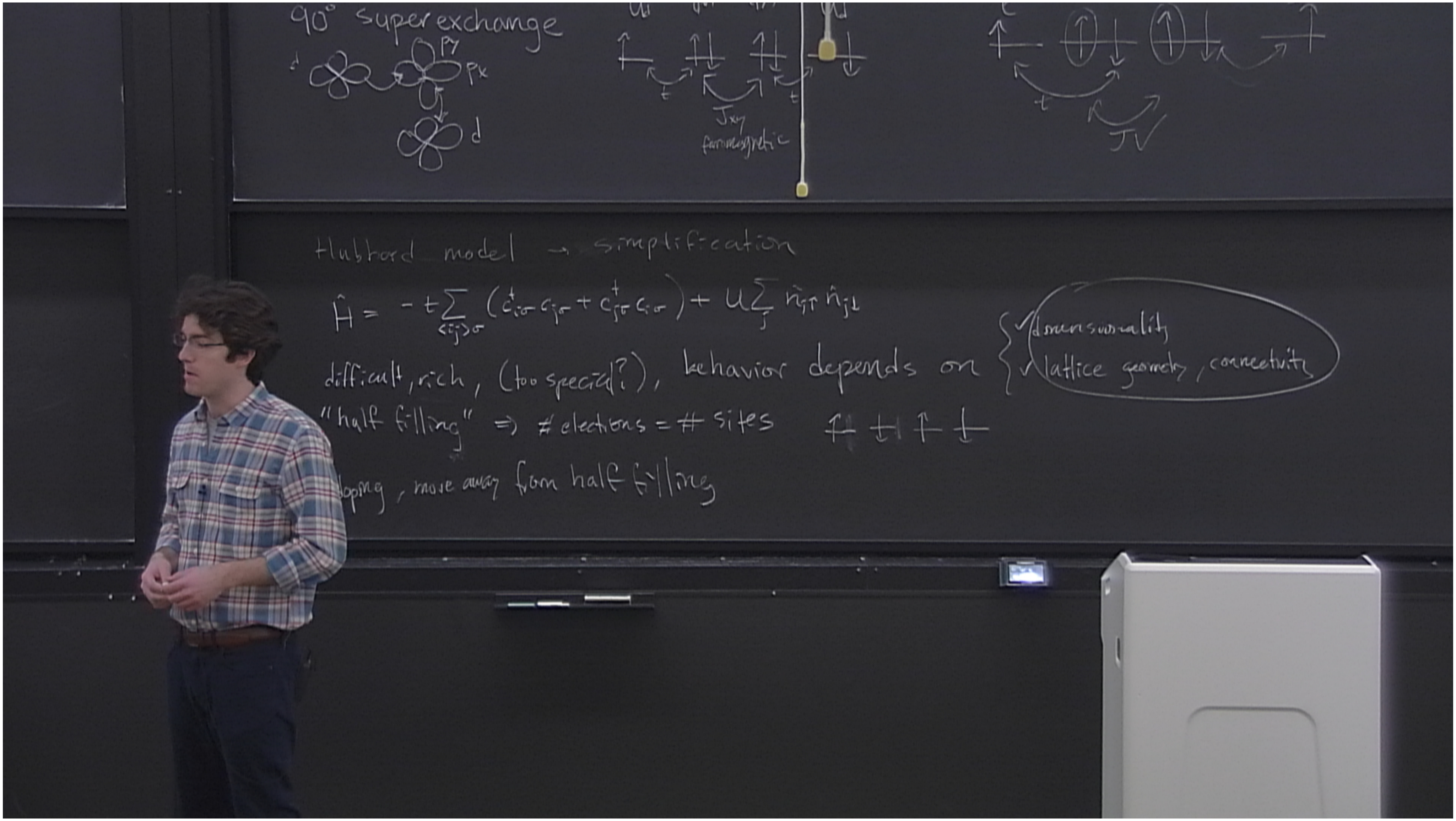

minimal model $\hat{H} = -t(c_1^\dagger c_2 + c_2^\dagger c_1) + U \hat{n}_{1\uparrow}\hat{n}_{1\downarrow} + U \hat{n}_{2\uparrow}\hat{n}_{2\downarrow}$, limit $t \ll U$
$\psi_\pm(\vec{r}_1, \vec{r}_2) = \left(\phi_1(\vec{r}_1)\phi_2(\vec{r}_2) \pm \phi_2(\vec{r}_1)\phi_1(\vec{r}_2)\right) \times$ spin part
→ singlet
→ $m^z=0$ triplet
Compute matrix elements $\langle\psi_a|\hat{H}|\psi_b\rangle$ (overlaps $\langle\psi_a|\psi_b\rangle$) $a,b = \pm$
↳ diagonalize : lower energy is ψ_+, spatially symmetric, spin anti-symmetric
perturb in t/U
→ only possible if spins anti-aligned, Pauli exclusion


Superexchange → notes by Erik Koch http://www.cond-mat.de/events/correl
many materials → active orbitals connected by "spacer"
minimal model
low energy subspace ⟨n_i↑ n_i↓⟩ = 0 ... no U_d
Ĥ → P̂ĤP̂ ~ J S⃗₁·S⃗₂ J ~ t⁴/U_d³ > 0 antiferromagnet
intuition:


antiferromagnet
intuition:
180° superexchange
ferromagnetic
ok
90° superexchange
py
px
d
Jxy
ferromagnetic


antiferromagnet
intuition:
ok
180° superexchange
ferromagnetic ~ weaker than afm
90° superexchange
Jxy
ferromagnetic


90° super exchange
py
px
d
Jxy
ferromagnetic
JV
Hubbard model → simplification
Ĥ = − t Σ_{⟨ij⟩σ} (c†_{iσ} c_{jσ} + c†_{jσ} c_{iσ}) + U Σ_j n̂_{j↑} n̂_{j↓}
difficult, rich, (too special?), behavior depends on
✓ dimensionality
✓ lattice geometry, connectivity


90° super exchange
py
px
d
t
Jxy
ferromagnetic
t
JV
Hubbard model → simplification
$\hat{H} = -t\sum_{\langle ij\rangle\sigma}(c^\dagger_{i\sigma}c_{j\sigma} + c^\dagger_{j\sigma}c_{i\sigma}) + U\sum_j \hat{n}_{j\uparrow}\hat{n}_{j\downarrow}$
difficult, rich, (too special?), behavior depends on
dimensionality
lattice geometry, connectivity
"half filling" ⇒ # electrons = # sites
move away from half filling