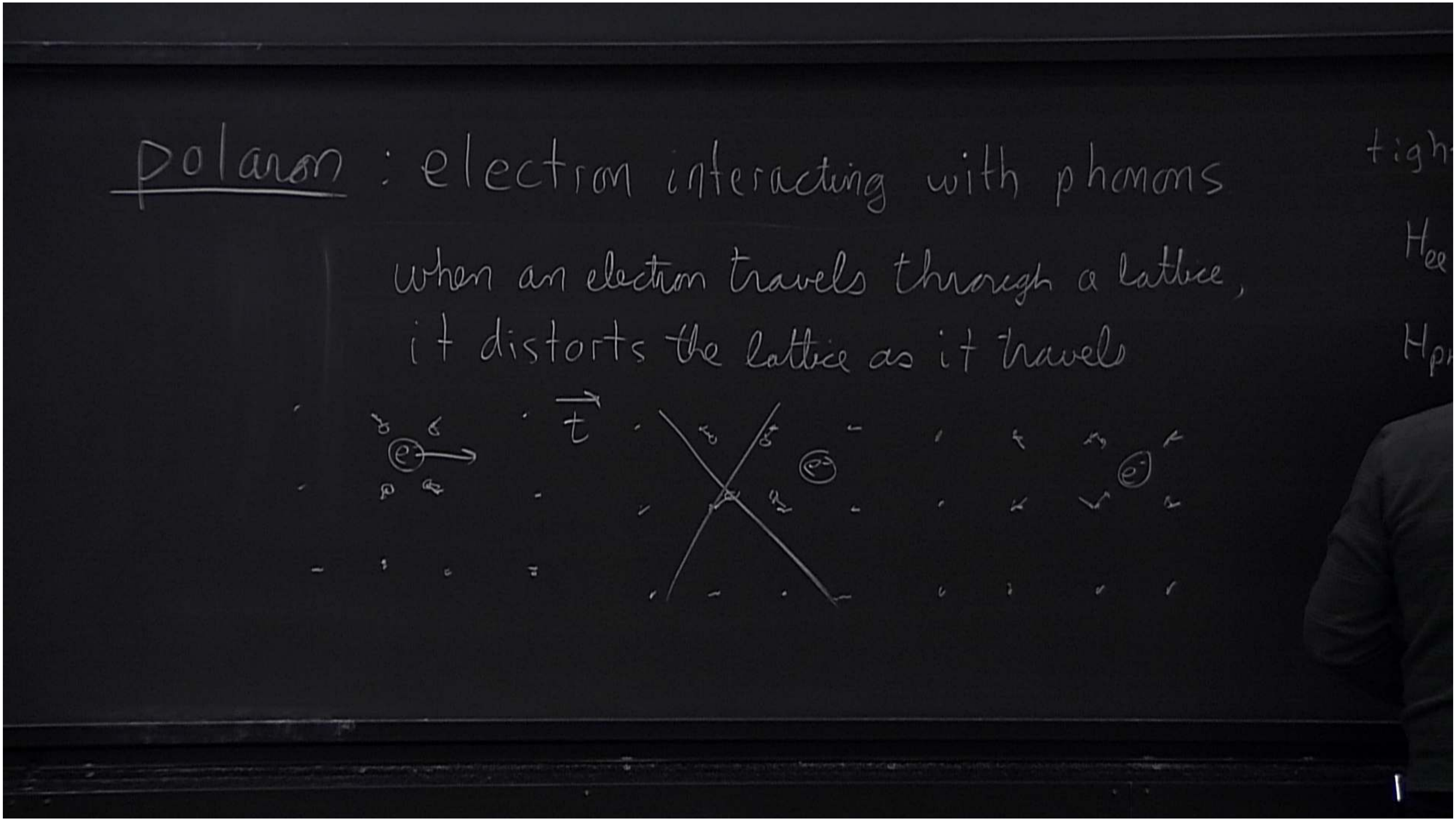
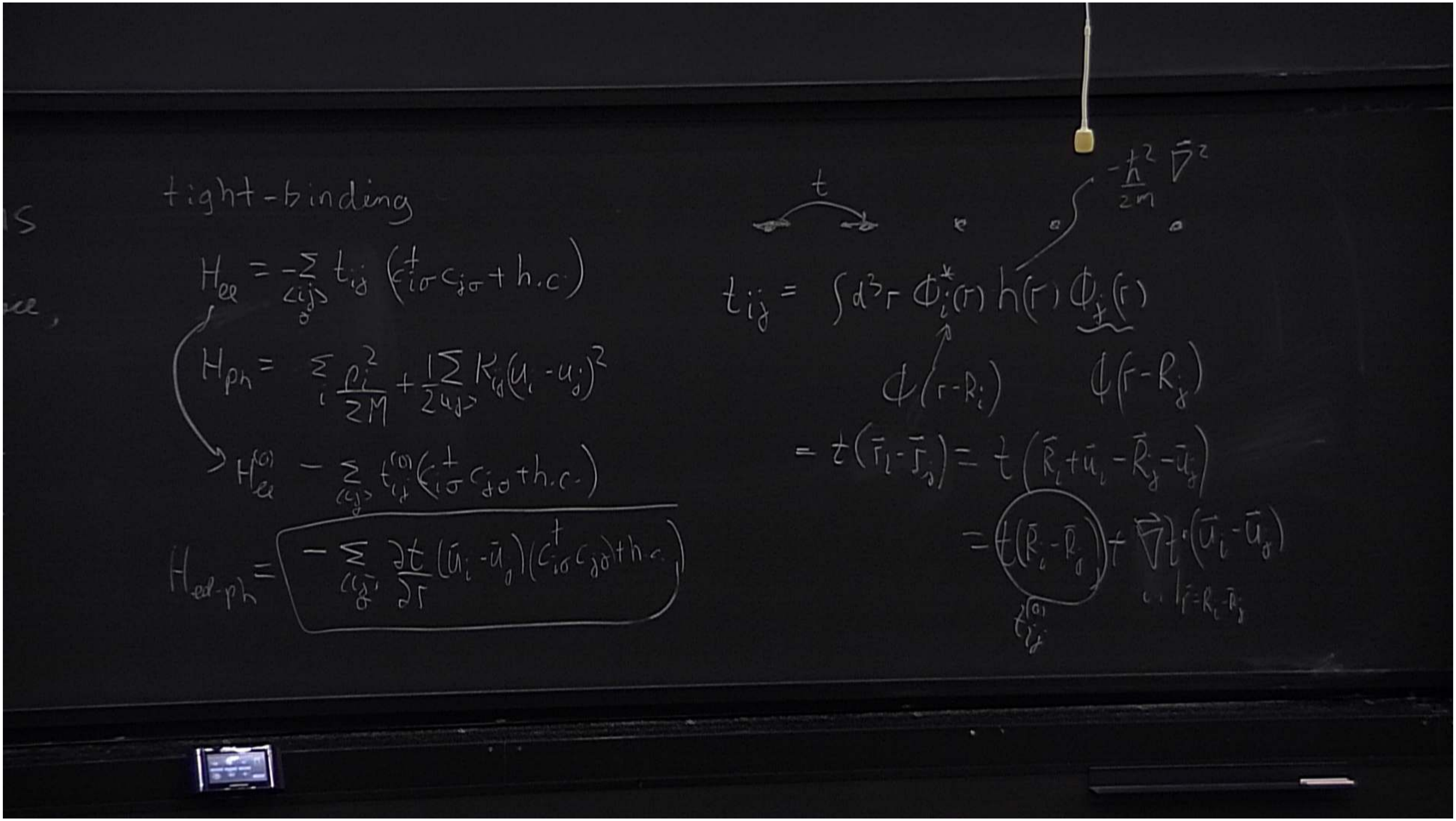
Title: PSI 2016/2017 Condensed Matter - Lecture 8

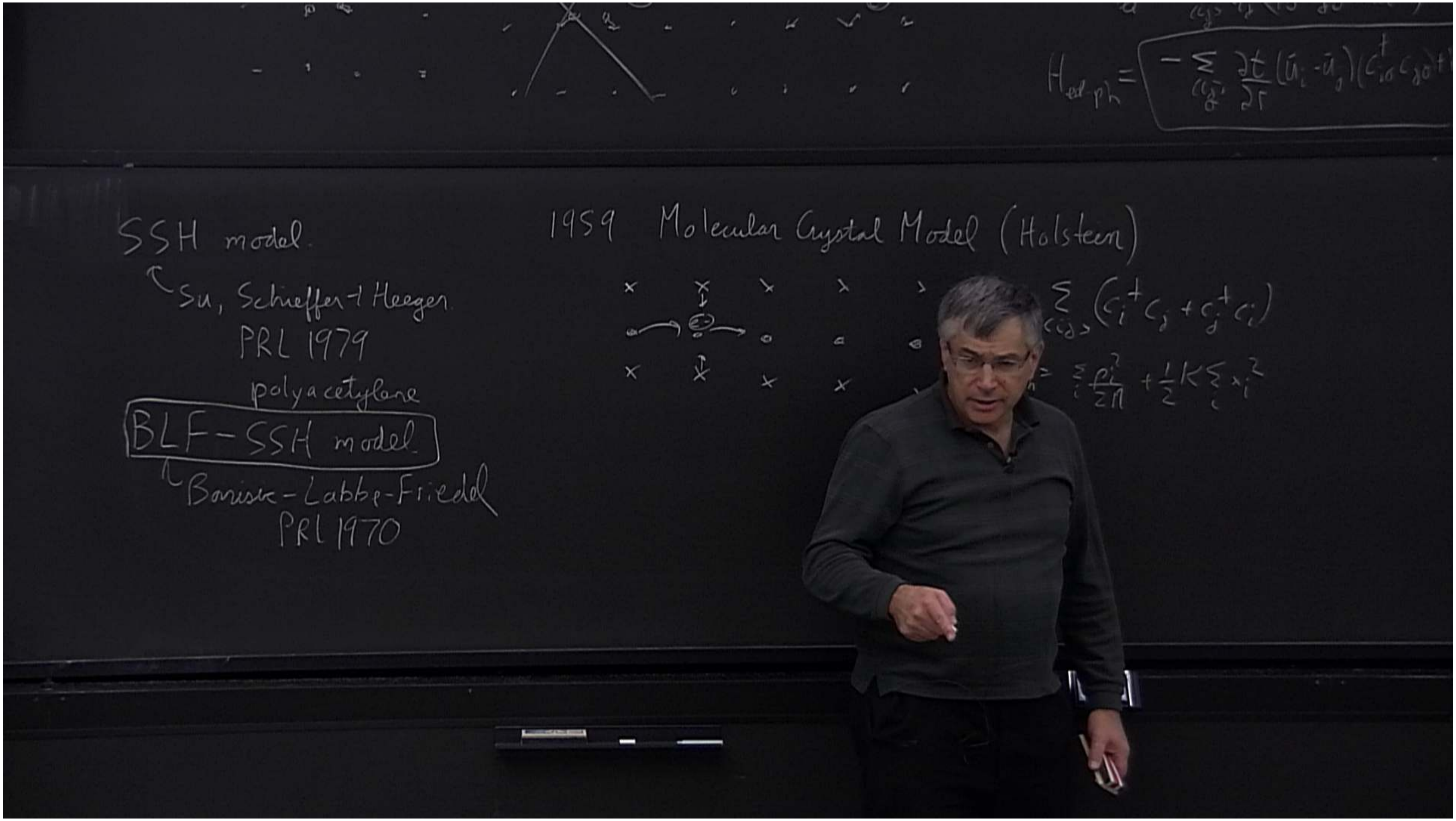
Date: Nov 16, 2016 10:45 AM

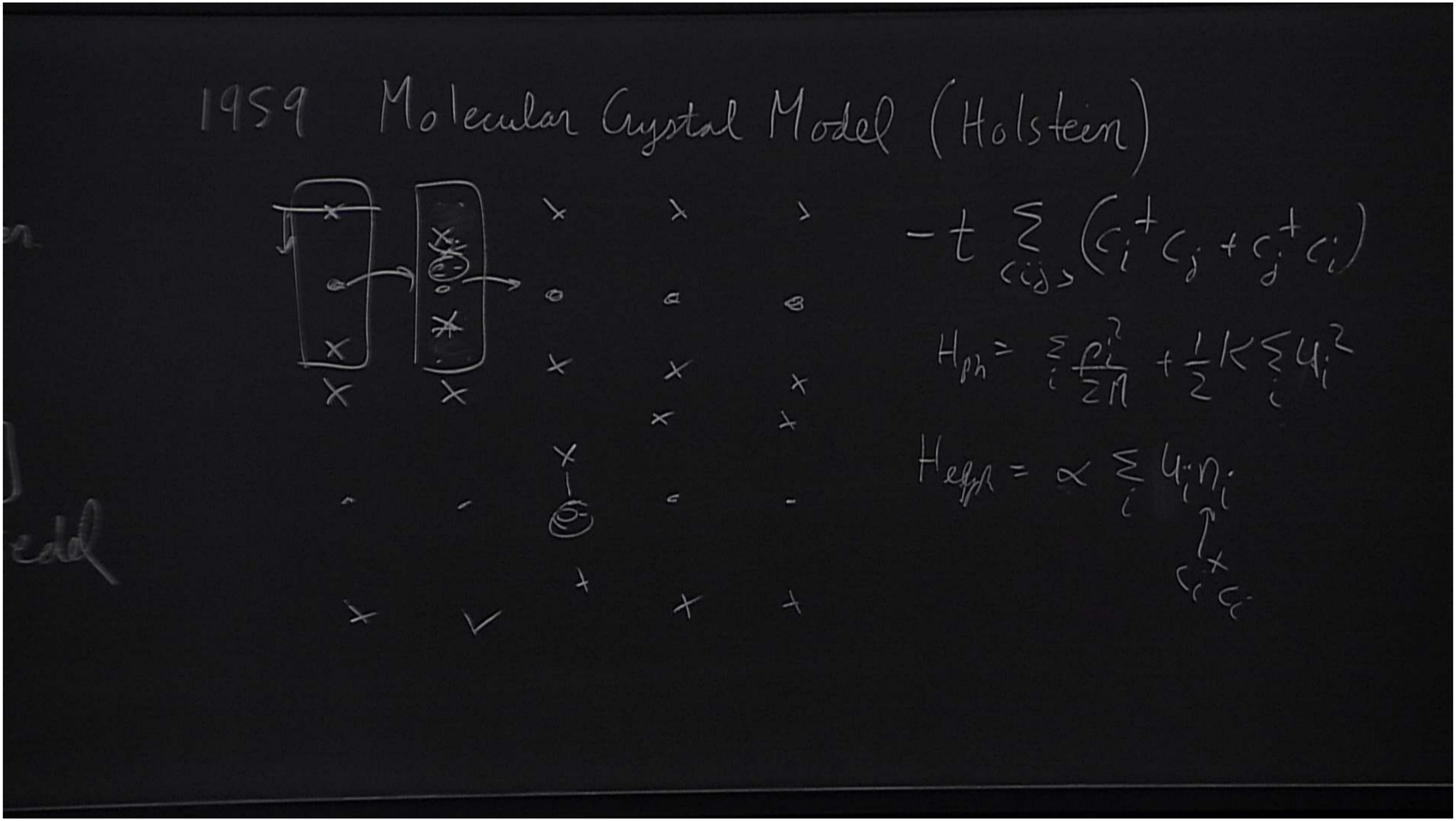
URL: http://pirsa.org/16110059

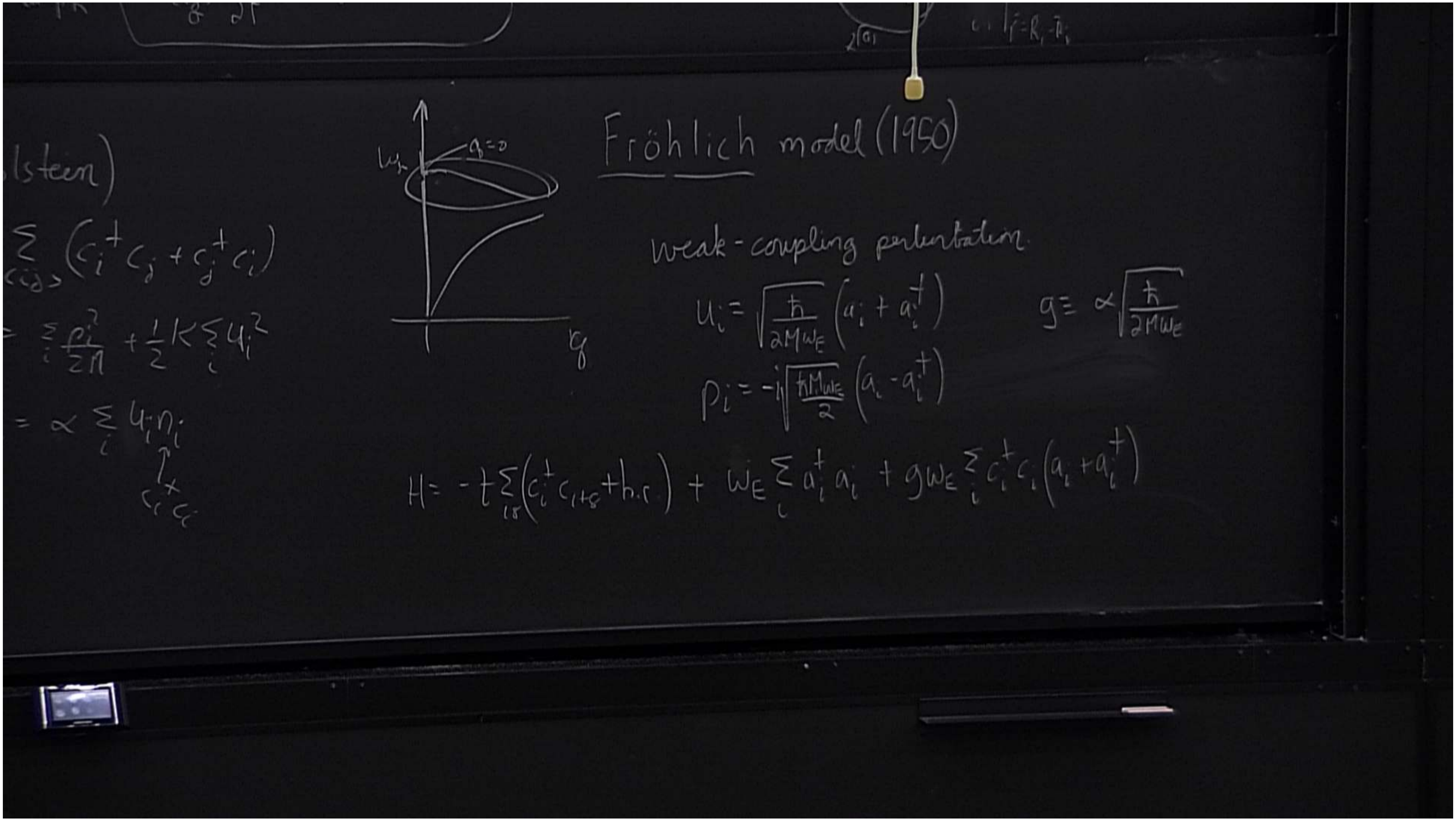
Abstract:

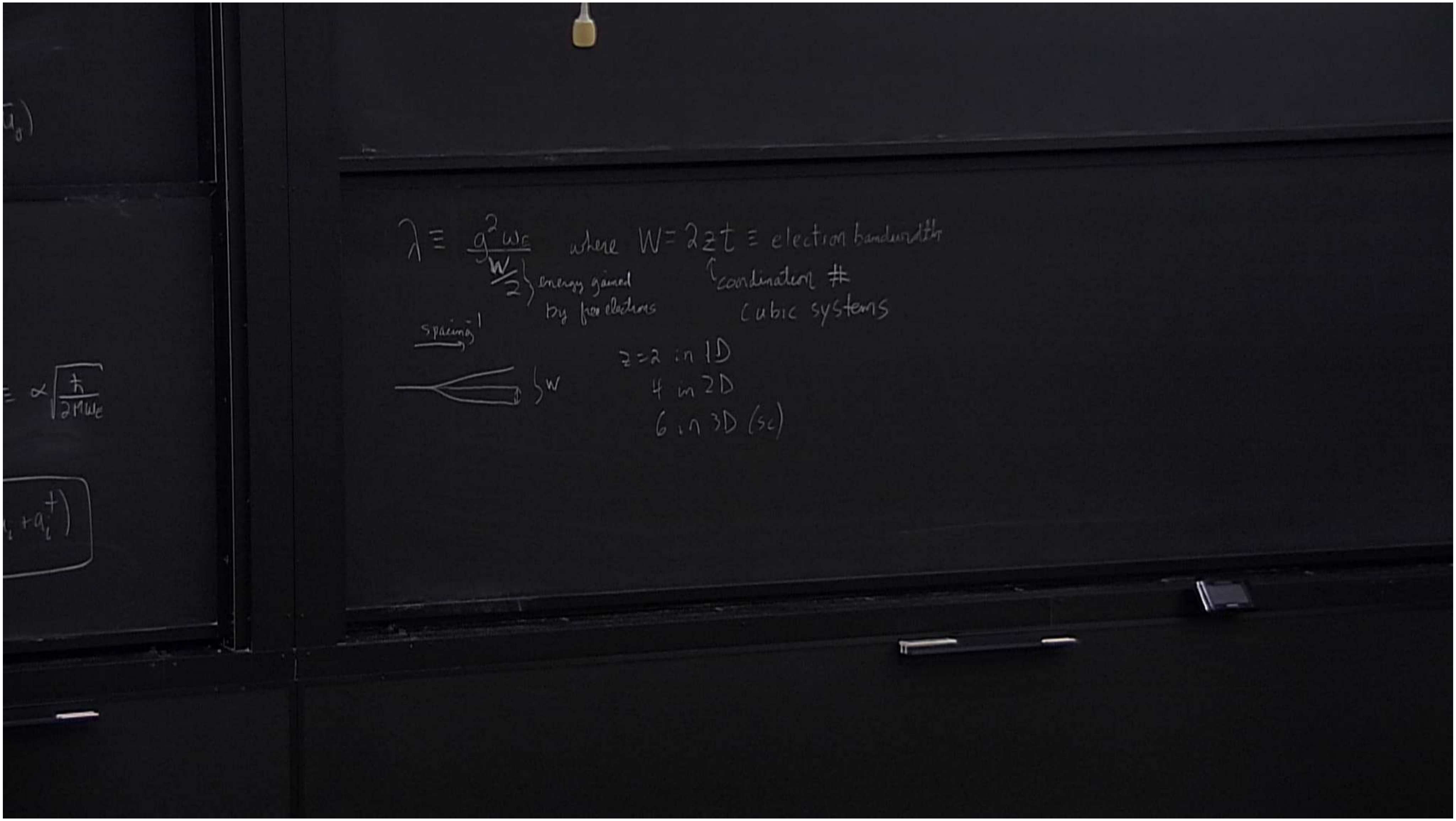

polaron : electron interacting with phonons
when an electron travels through a lattice,
it distorts the lattice as it travels
t
e
H_{ee}

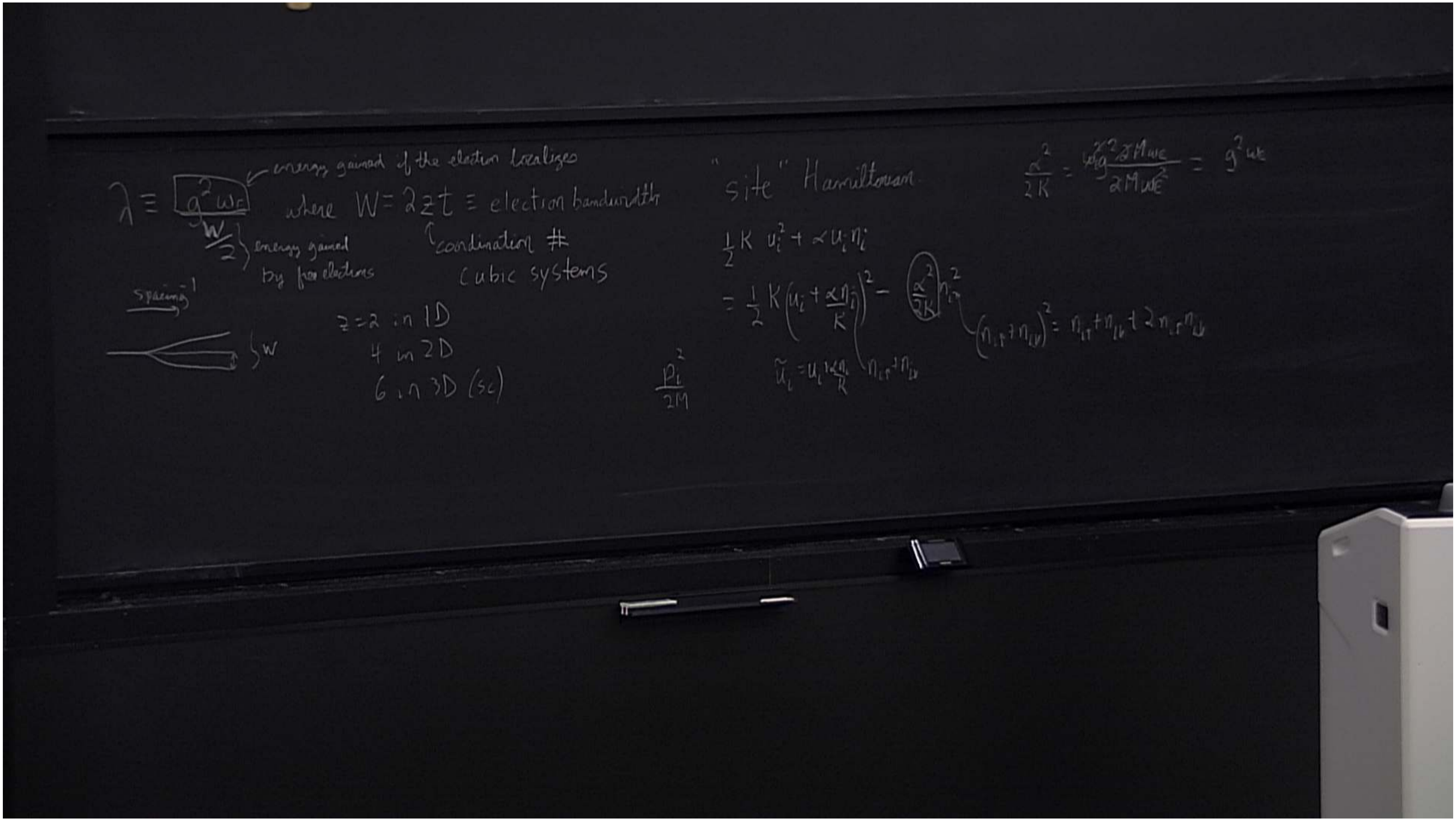

tight-binding
$H_{ee} = -\sum_{\langle ij \rangle, \sigma} t_{ij} (c^\dagger_{i\sigma} c_{j\sigma} + h.c.)$
$H_{ph} = \sum_i \frac{p_i^2}{2M} + \frac{1}{2} \sum_{\langle ij \rangle} K_{ij} (u_i - u_j)^2$
$H^{(0)}_{ee} - \sum_{\langle ij \rangle} t^{(0)}_{ij} (c^\dagger_{i\sigma} c_{j\sigma} + h.c.)$
$H_{el-ph} = -\sum_{\langle ij \rangle, \sigma} \frac{\partial t}{\partial r} (\bar{u}_i - \bar{u}_j)(c^\dagger_{i\sigma} c_{j\sigma}) + h.c.$
t
$-\frac{\hbar^2}{2m} \vec{\nabla}^2$
$t_{ij} = \int d^3r \, \Phi^*_i(r) \, h(r) \, \Phi_j(r)$
$\Phi(r - R_i)$
$\Phi(r - R_j)$
$= t(\bar{r}_i - \bar{r}_j) = t(\bar{R}_i + \bar{u}_i - \bar{R}_j - \bar{u}_j)$
$= t(\bar{R}_i - \bar{R}_j) + \vec{\nabla} t \cdot (\bar{u}_i - \bar{u}_j)$
$t^{(0)}_{ij}$
$|_{r = R_i - R_j}$


SSH model
Su, Schrieffer + Heeger
PRL 1979
polyacetylene
BLF-SSH model
Barisic-Labbe-Friedel
PRL 1970
1959 Molecular Crystal Model (Holstein)


1959 Molecular Crystal Model (Holstein)
$-t \sum_{\langle ij \rangle} (c_i^\dagger c_j + c_j^\dagger c_i)$
$H_{ph} = \sum_i \frac{p_i^2}{2M} + \frac{1}{2} K \sum_i u_i^2$
$H_{e\text{-}ph} = \alpha \sum_i u_i n_i$
$c_i^\dagger c_i$


Fröhlich model (1950)
weak-coupling perturbation
u_i = √(ħ/2Mω_E) (a_i + a_i†)
p_i = −i √(ħMω_E/2) (a_i − a_i†)
g ≡ α √(ħ/2Mω_E)
H = −t Σ_iδ (c_i† c_i+δ + h.c.) + ω_E Σ_i a_i† a_i + gω_E Σ_i c_i† c_i (a_i + a_i†)
lsteen)
= α Σ_i u_i n_i


λ ≡ g²ω_E / (W/2)
energy gained by free electrons
where W = 2zt ≡ electron bandwidth
coordination #
cubic systems
spacing⁻¹
W
z = 2 in 1D
4 in 2D
6 in 3D (sc)


energy gained if the electron localizes
λ ≡ g² ω_E / (W/2)
where W = 2zt ≡ electron bandwidth
coordination #
energy gained by free electrons
cubic systems
spacing⁻¹
W
z = 2 in 1D
4 in 2D
6 in 3D (sc)
"site" Hamiltonian
½ K u_i² + α u_i n_i
= ½ K (u_i + α n_i / K)² − (α²/2K) n_i²
(n_i↑ + n_i↓)² = n_i↑ + n_i↓ + 2 n_i↑ n_i↓
n_i↑ + n_i↓
ũ_i = u_i + α n_i / K
p_i² / 2M
α² / 2K = g² ω_E

$$H = \underbrace{\sum_k \epsilon_k c_k^\dagger c_k + \omega_E \sum_q a_q^\dagger a_q}_{\hat{H}_0} + \underbrace{\frac{g\omega_E}{\sqrt{N}} \sum_{kq} c_{k+q}^\dagger c_k \left(a_q + a_{-q}^\dagger\right)}_{H_{pert.}}$$

2nd order

$$\Delta E_p^{(2)} = \sum_n \frac{\left|\langle n\, H_{pert} | \phi_p^{(0)} \rangle\right|^2}{E_p^{(0)} - E_n} \qquad \left(\sum_n \to \sum_{k',q'}\right)$$

$$|\phi_p^{(0)}\rangle = c_p^\dagger |0\rangle \otimes |0\rangle$$

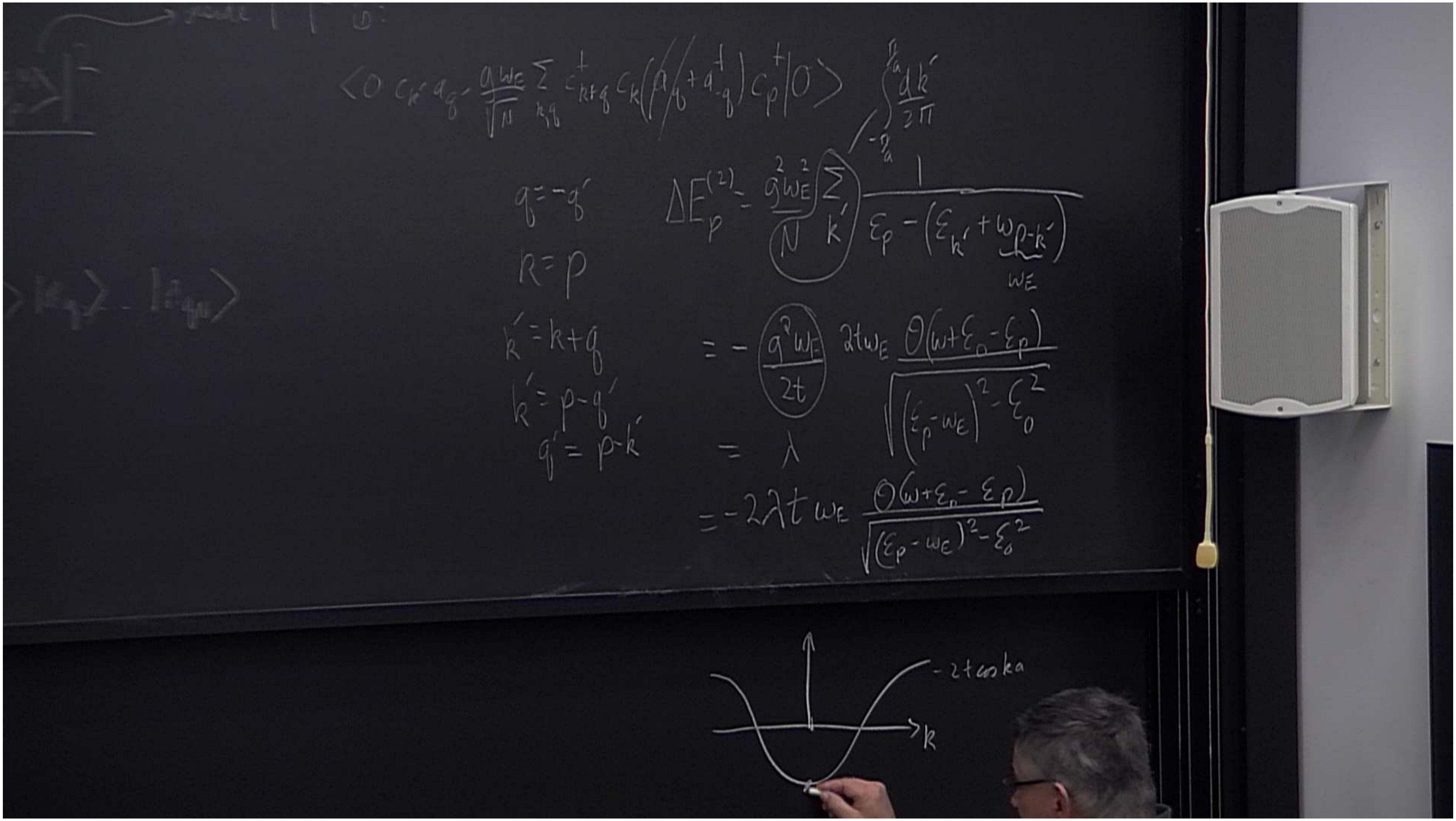
$$\Delta E^{(1)} = 0 = \langle \phi_p^{(0)}\, H_{pert}\, \phi_p^{(0)} \rangle$$

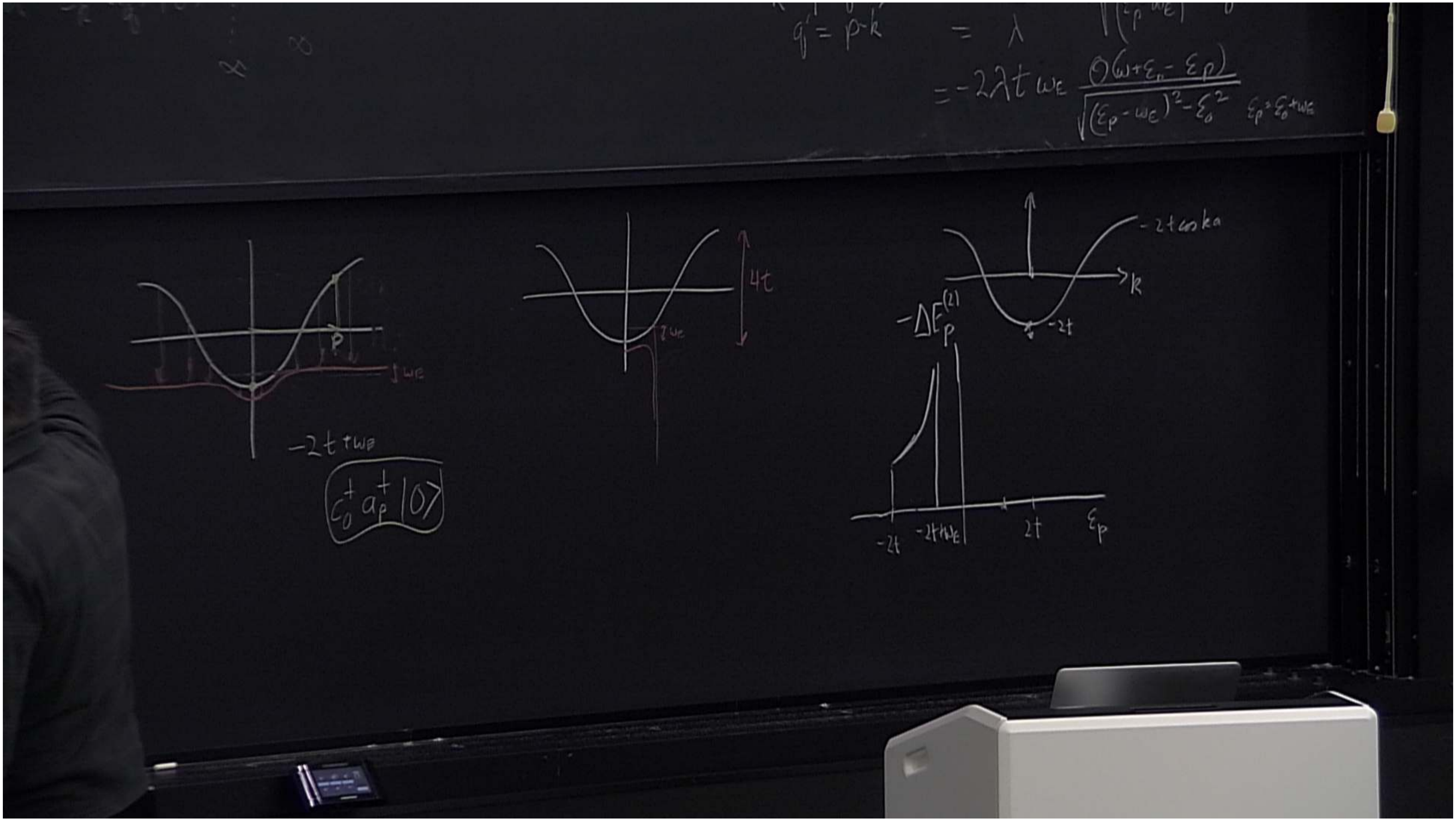
$n \equiv$ excited states

$$c_{k'}^\dagger |0\rangle \otimes |n_{q_1}\rangle |n_{q_2}\rangle |n_{q_3}\rangle \ldots |n_{q_N}\rangle$$

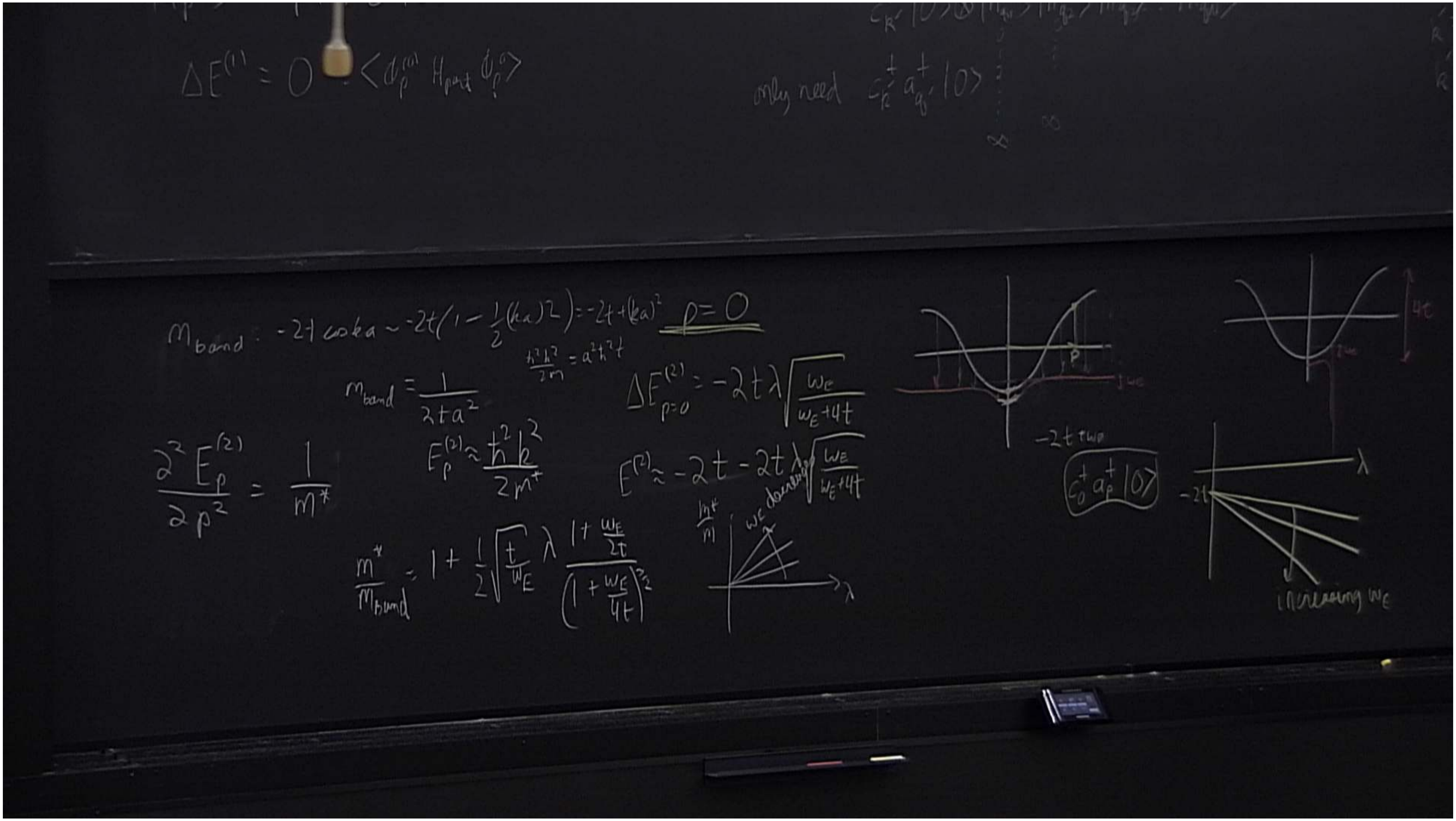
($n_{q_i} = 0, \ldots, \infty$)

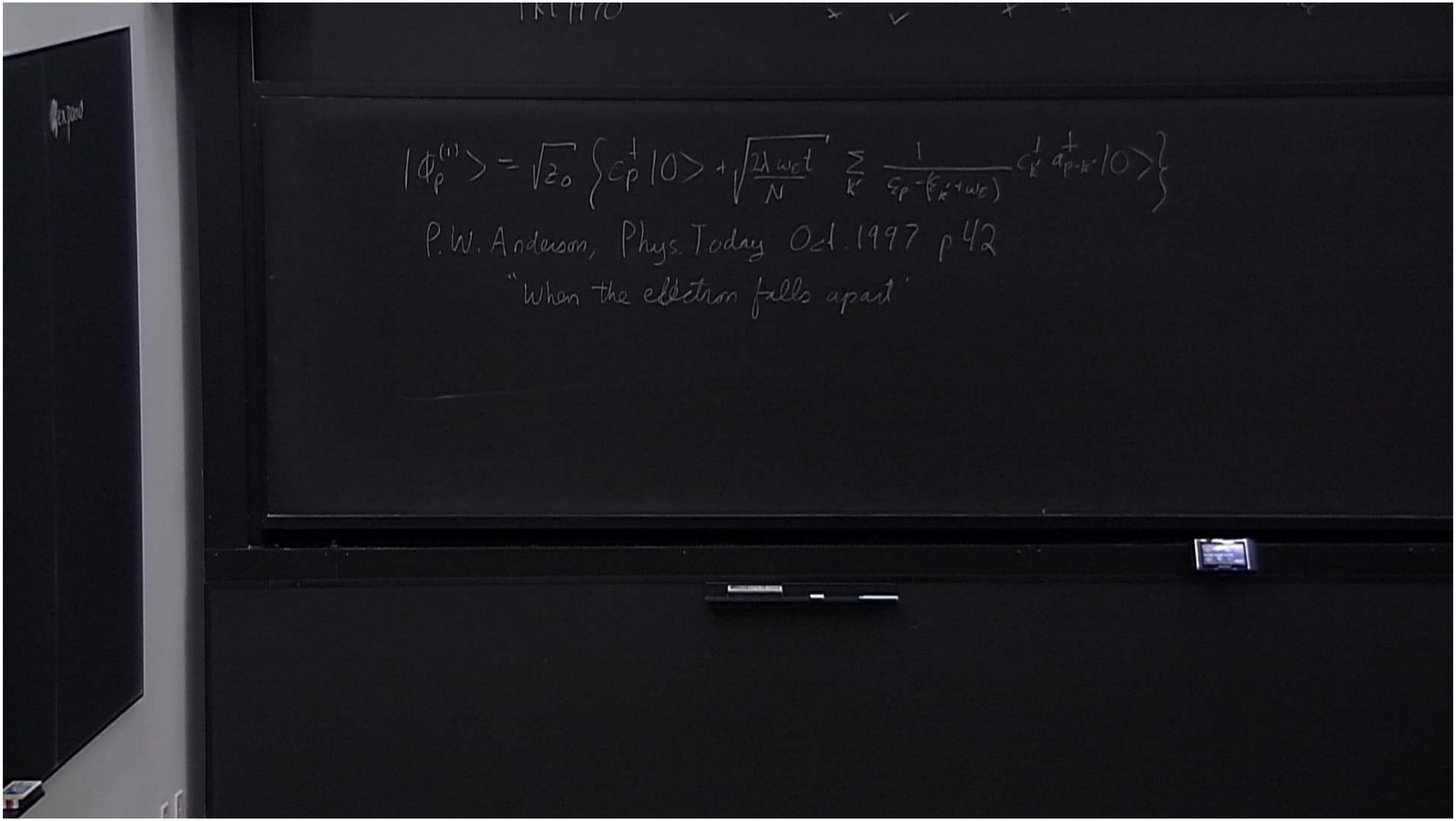
only need $c_{k'}^\dagger a_{q'}^\dagger |0\rangle$


⟨0 c_k' a_q' - g w_E/√N Σ_{k,q} c†_{k+q} c_k (a_q + a†_{-q}) c†_p |0⟩
∫_{-π/a}^{π/a} dk'/2π
q = -q'
k = p
k' = k+q
k' = p-q'
q' = p-k'
ΔE_p^{(2)} = g² w_E² / N Σ_{k'} 1 / (ε_p - (ε_{k'} + ω_{p-k'}))
w_E
= -(g² w_E / 2t) 2t w_E θ(ω+ε_0-ε_p) / √((ε_p-w_E)² - ε_0²)
= λ
= -2λt w_E θ(ω+ε_0-ε_p) / √((ε_p-w_E)² - ε_0²)
-2t cos ka
k

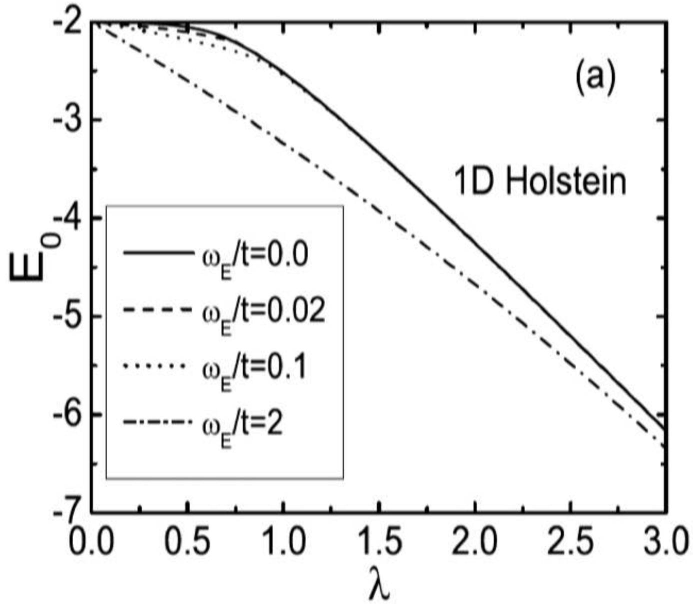


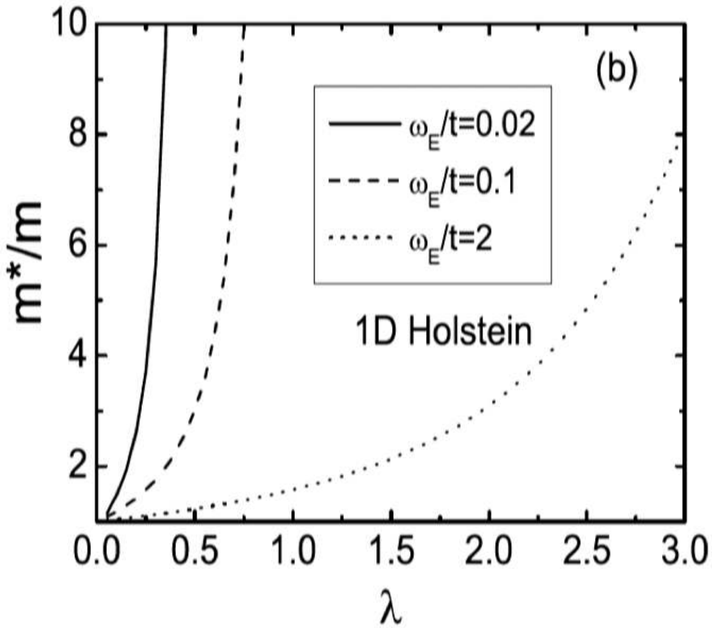
q' = p-k
4t
-2t cos ka
k
-2t
P
-2t +wE
2t
ε_p


ΔE^(1) = 0 = <φ_p^(0) H_pert φ_p^(0)>
only need c_k'^† a_q'^† |0>
m_band : -2t cos ka ~ -2t(1 - 1/2 (ka)^2) = -2t + t(ka)^2
p = 0
ħ^2k^2/2m = a^2k^2t
m_band = 1/(2ta^2)
ΔE^(2)_(p=0) = -2tλ √(w_E/(w_E+4t))
∂^2 E_p^(2) / ∂p^2 = 1/m*
E_p^(2) ≈ ħ^2k^2/2m*
E^(2) ≈ -2t - 2tλ √(w_E/(w_E+4t))
m*/m_band ≈ 1 + 1/2 √(t/w_E) λ (1 + w_E/2t)/(1 + w_E/4t)^(3/2)
m*/m
w_E decreasing
λ
4t
-2t + w_E
c_0^† a_p^† |0>
-2t
λ
increasing w_E


$|\Phi_p^{(1)}\rangle = \sqrt{z_0}\left\{c_p^\dagger|0\rangle + \sqrt{\frac{2\lambda\omega_c t}{N}}\sum_{k'}\frac{1}{\varepsilon_p-(\varepsilon_{k'}+\omega_c)}c_{k'}^\dagger a_{p-k'}^\dagger|0\rangle\right\}$
P.W. Anderson, Phys. Today Oct. 1997 p 42
"When the electron falls apart"

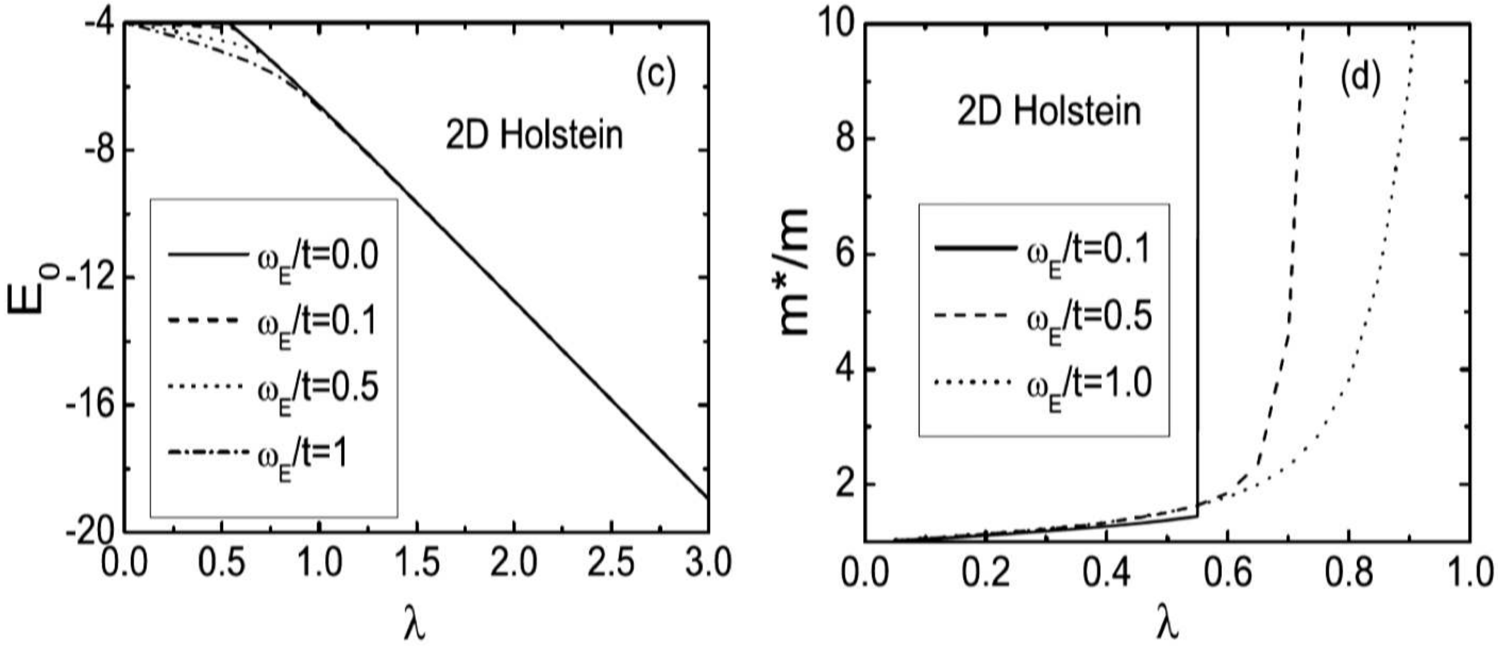
Polarons: 1D





J Supercond Nov Magn (2012) 25:1313–1317
DOI 10.1007/s10948-012-1601-6

Polarons: 2D



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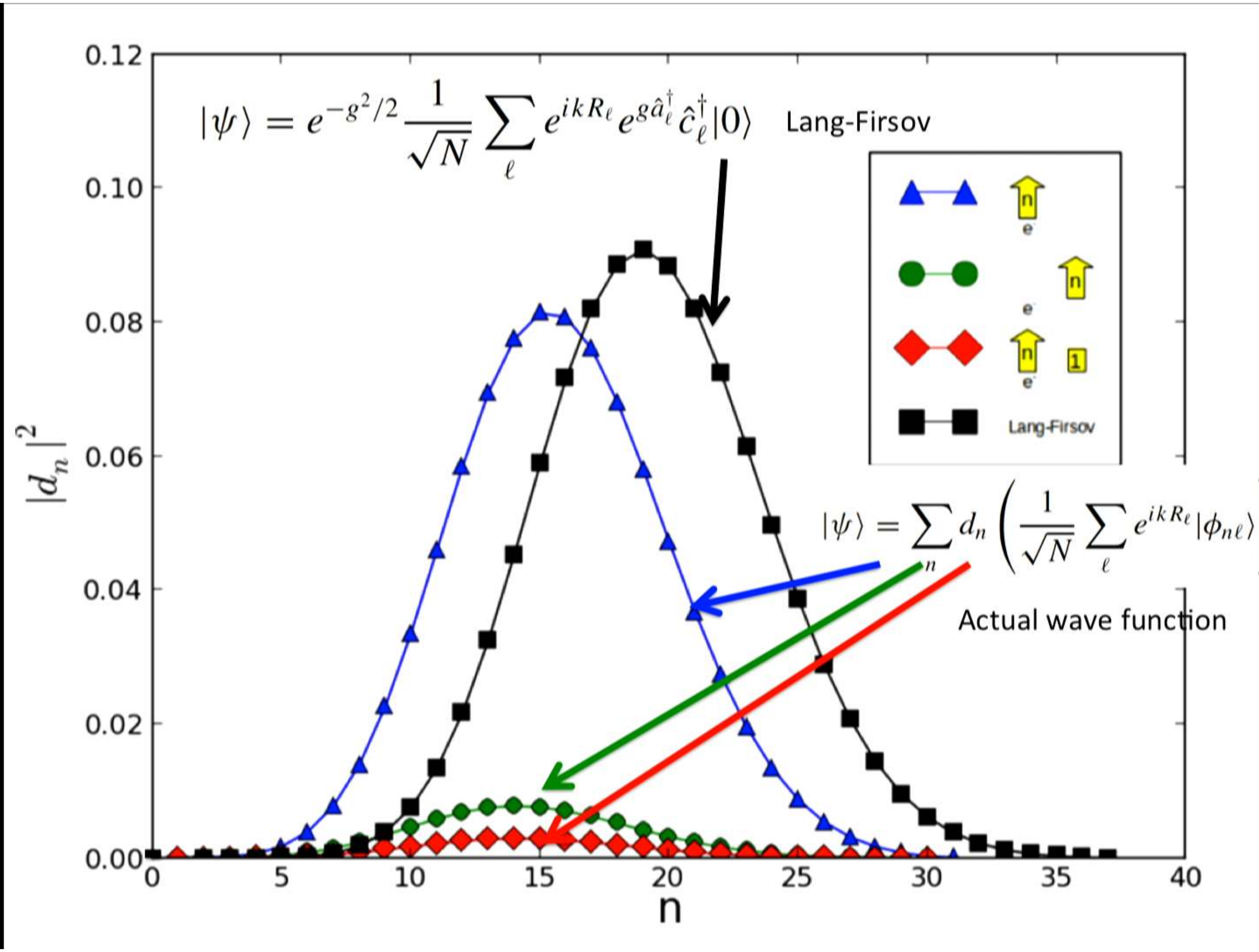
$|\psi\rangle = e^{-g^2/2}\frac{1}{\sqrt{N}}\sum_\ell e^{ikR_\ell}e^{g\hat{a}_\ell^\dagger}\hat{c}_\ell^\dagger|0\rangle$
Lang-Firsov
Lang-Firsov
$|\psi\rangle = \sum_n d_n \left(\frac{1}{\sqrt{N}}\sum_\ell e^{ikR_\ell}|\phi_{n\ell}\rangle\right)$
Actual wave function
$|d_n|^2$
n