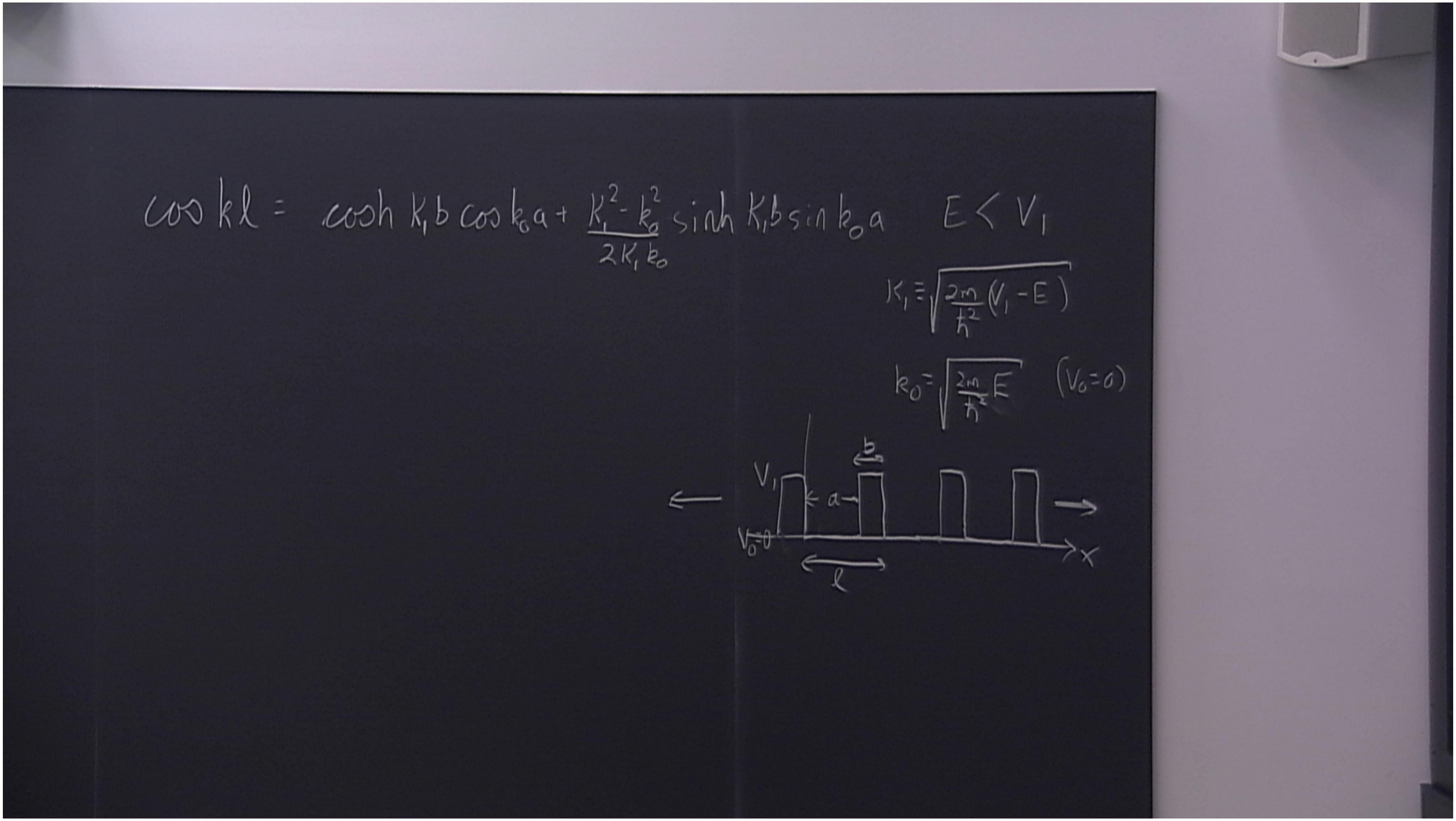
Title: PSI 2016/2017 Condensed Matter - Lecture 4

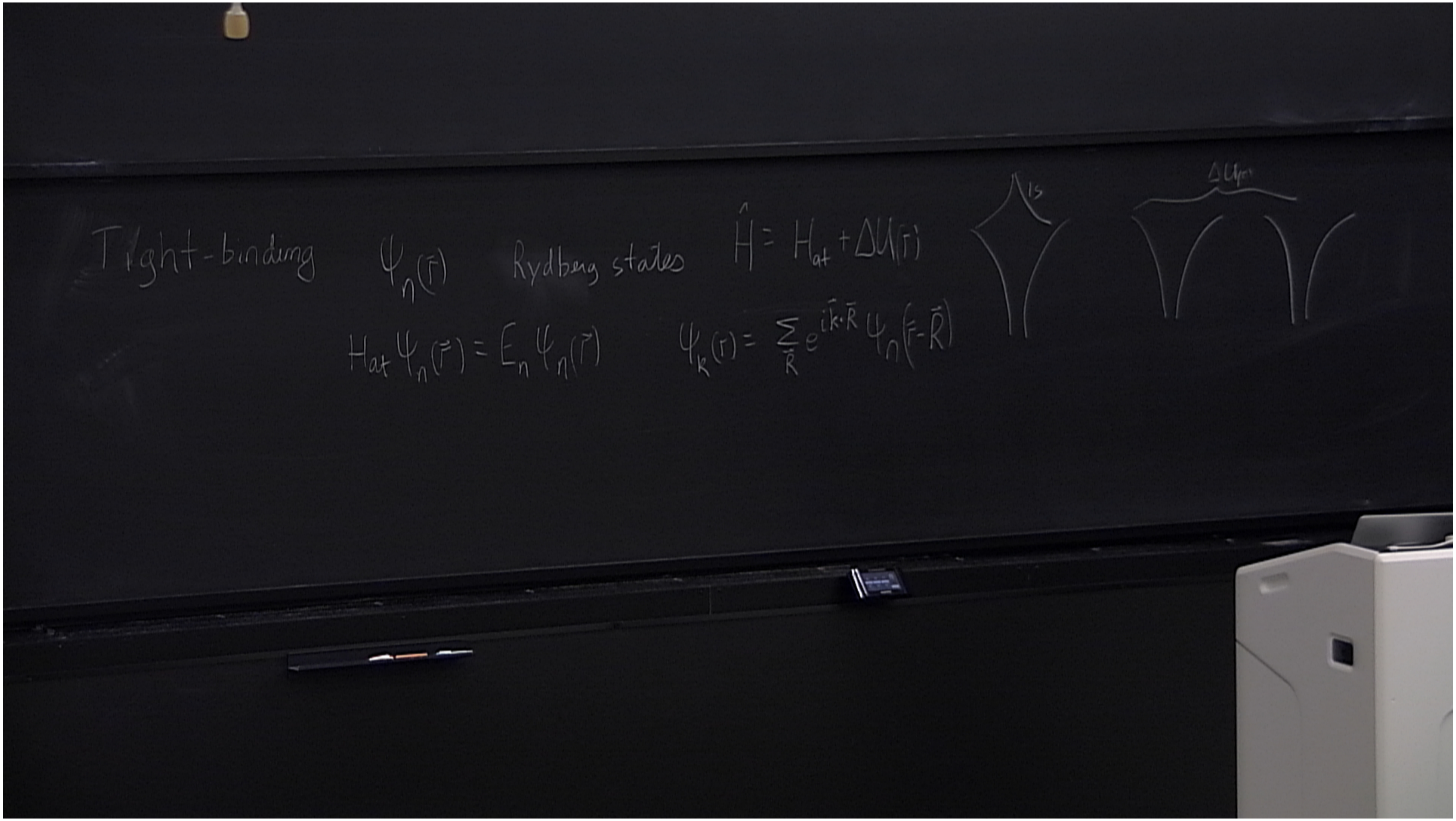
Date: Nov 10, 2016 10:45 AM

URL: http://pirsa.org/16110055

Abstract:


Rydberg states


$\cos kl = \cosh K_1 b \cos k_0 a + \frac{K_1^2 - k_0^2}{2K_1 k_0} \sinh K_1 b \sin k_0 a$
$E < V_1$
$K_1 \equiv \sqrt{\frac{2m}{\hbar^2}(V_1 - E)}$
$k_0 = \sqrt{\frac{2m}{\hbar^2} E}$
$(V_0 = 0)$
V_1
a
b
$V_0 = 0$
l
x


Tight-binding
$\psi_n(\vec{r})$
Rydberg states
$\hat{H} = H_{at} + \Delta U(\vec{r})$
1s
$\Delta U(\vec{r})$
$H_{at}\psi_n(\vec{r}) = E_n \psi_n(\vec{r})$
$\psi_k(\vec{r}) = \sum_{\vec{R}} e^{i\vec{k}\cdot\vec{R}} \psi_n(\vec{r}-\vec{R})$

Other extreme: tight-binding

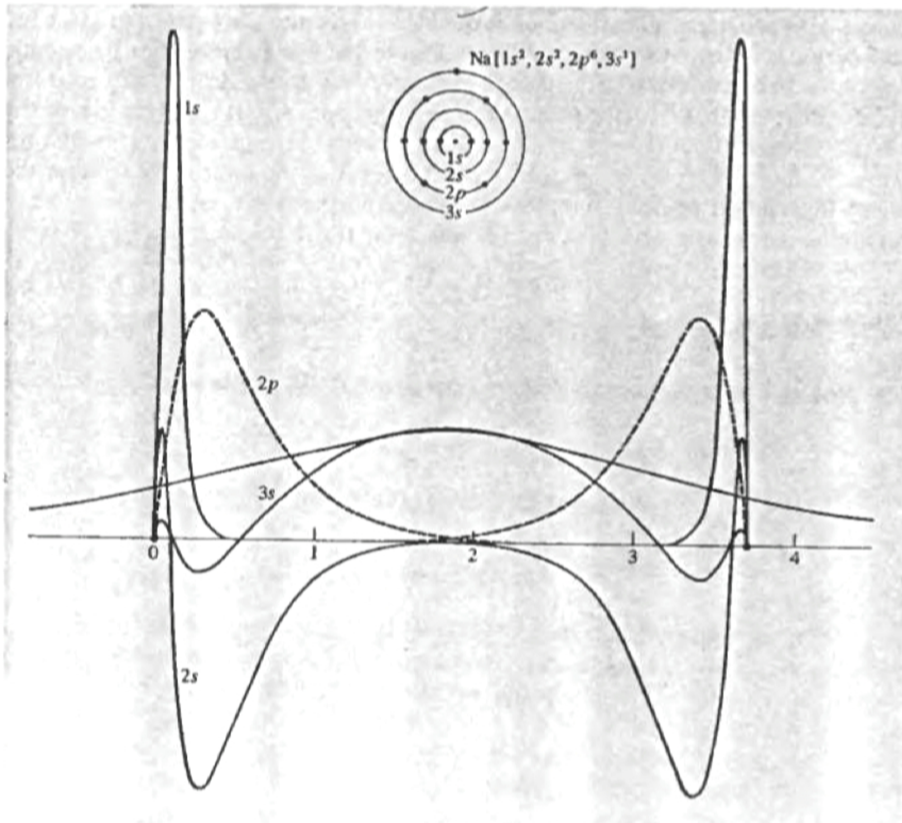


Figure 10.1

Calculated electron wave functions for the levels of atomic sodium, plotted about two nuclei separated by the nearest-neighbor distance in metallic sodium, 3.7 Å. The solid curves are $r\psi(r)$ for the 1*s*, 2*s*, and 3*s* levels. The dashed curve is *r* times the radial wave function for the 2*p* levels. Note how the 3*s* curves overlap extensively, the 2*s* and 2*p* curves overlap only a little, and the 1*s* curves have essentially no overlap. The curves are taken from calculations by D. R. Hartree and W. Hartree, *Proc. Roy. Soc.* **A193**, 299 (1948). The scale on the *r*-axis is in angstroms.

Fig. 10.1 from Ashcroft and Mermin

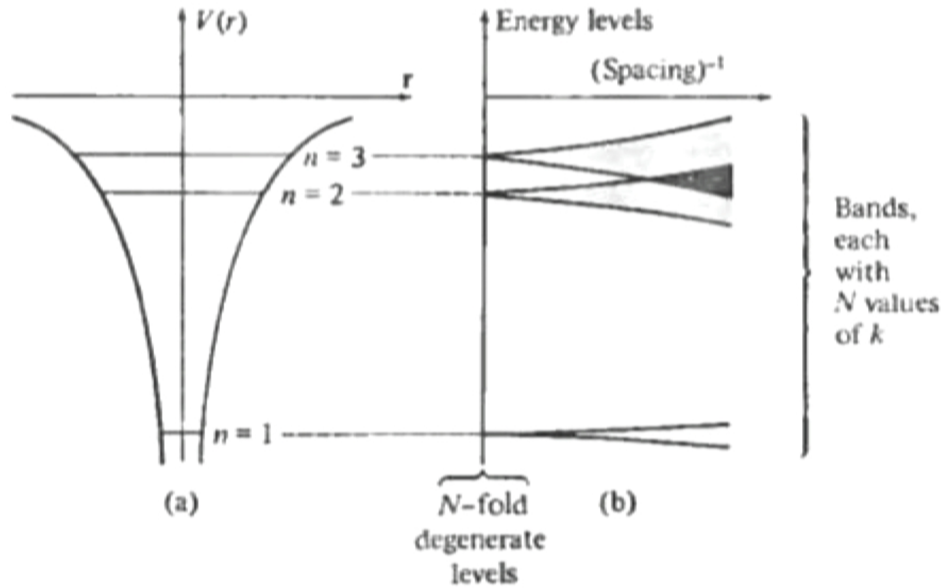


Figure 10.4

(a) Schematic representation of nondegenerate electronic levels in an atomic potential. (b) The energy levels for N such atoms in a periodic array, plotted as a function of mean inverse interatomic spacing. When the atoms are far apart (small overlap integrals) the levels are nearly degenerate, but when the atoms are closer together (larger overlap integrals), the levels broaden into bands.

Fig. 10.4 from Ashcroft and Mermin

NRC Research Press

ARTICLE

The importance of basis states: an example using the hydrogen basis

Lindsay Forestell and Frank Marsiglio

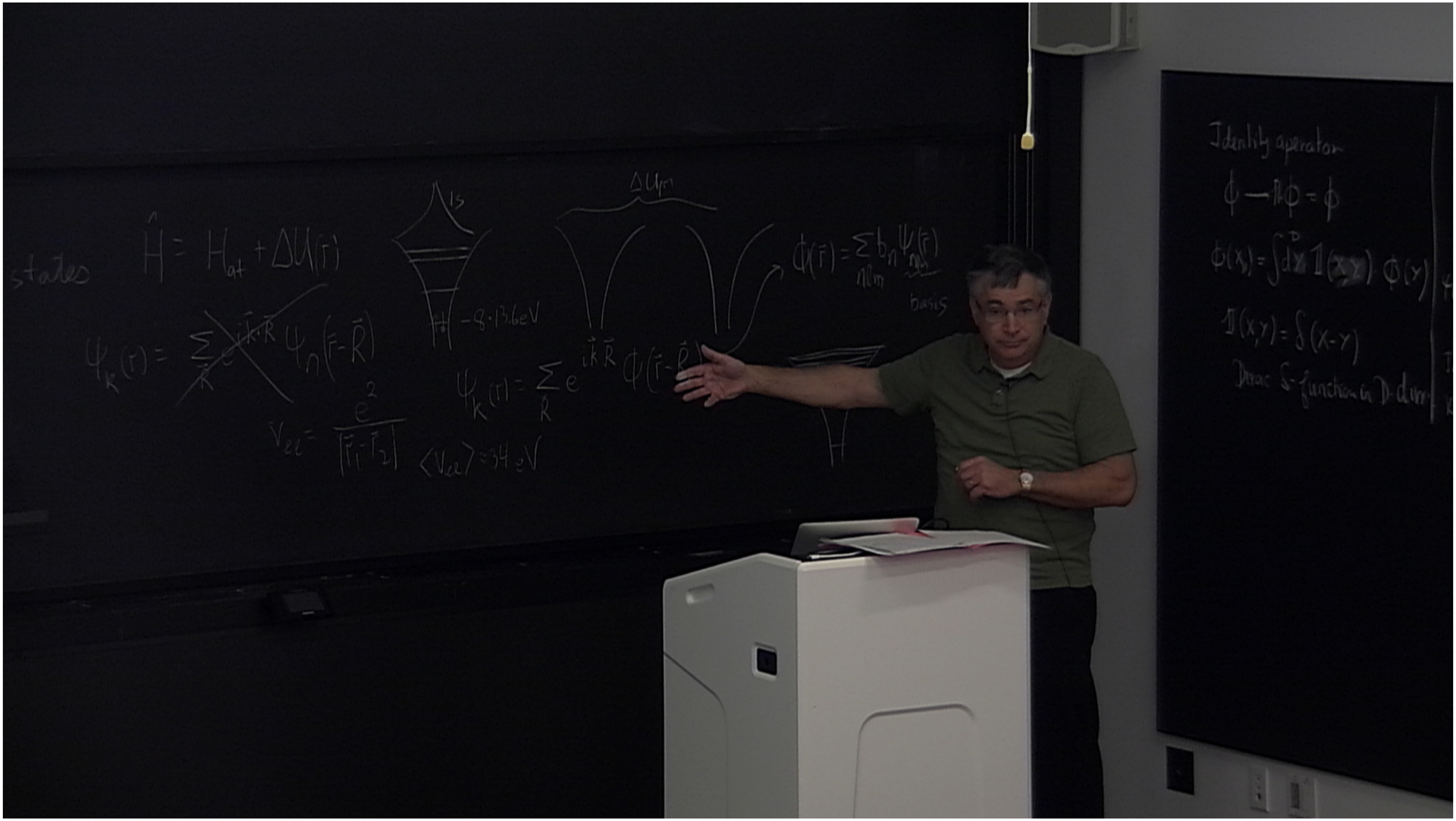
Can. J. Phys. 93: 1009–1014 (2015) dx.doi.org/10.1139/cjp-2014-0726

IOP PUBLISHING EUROPEAN JOURNAL OF PHYSICS

Eur. J. Phys. 34 (2013) 111–128 doi:10.1088/0143-0807/34/1/111

The spectral decomposition of the helium atom two-electron configuration in terms of hydrogenic orbitals

Joel Hutchinson[1], Marc Baker[1] and Frank Marsiglio[1,2,3]


states
Ĥ = H_at + ΔU(r)
Ψ_k(r) = Σ_R e^{ik·R} Ψ_n(r - R)
-8·13.6eV
ΔU(r)
Ψ_k(r) = Σ_R e^{ik·R} φ(r - R)
φ(r) = Σ_{nlm} b_n Ψ_nlm(r)
basis
V_ee = e^2 / |r_1 - r_2|
⟨V_ee⟩ = 34 eV
Identity operator
φ → 1φ = φ
φ(x) = ∫ d^D y 1(x,y) · φ(y)
1(x,y) = δ(x-y)
Dirac δ-function in D-dim

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The spectral decomposition of the helium atom two-electron configuration in terms of hydrogenic orbitals

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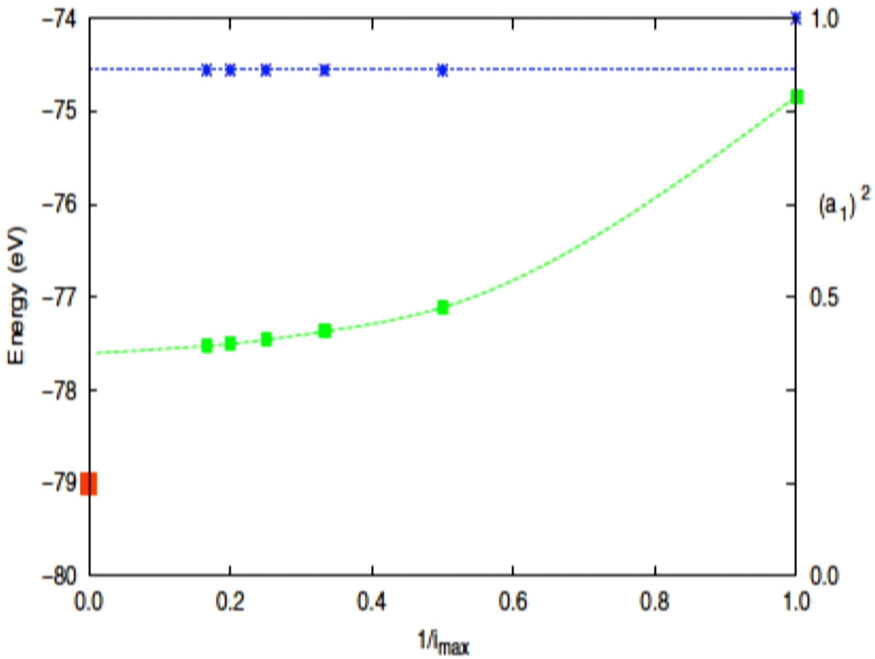
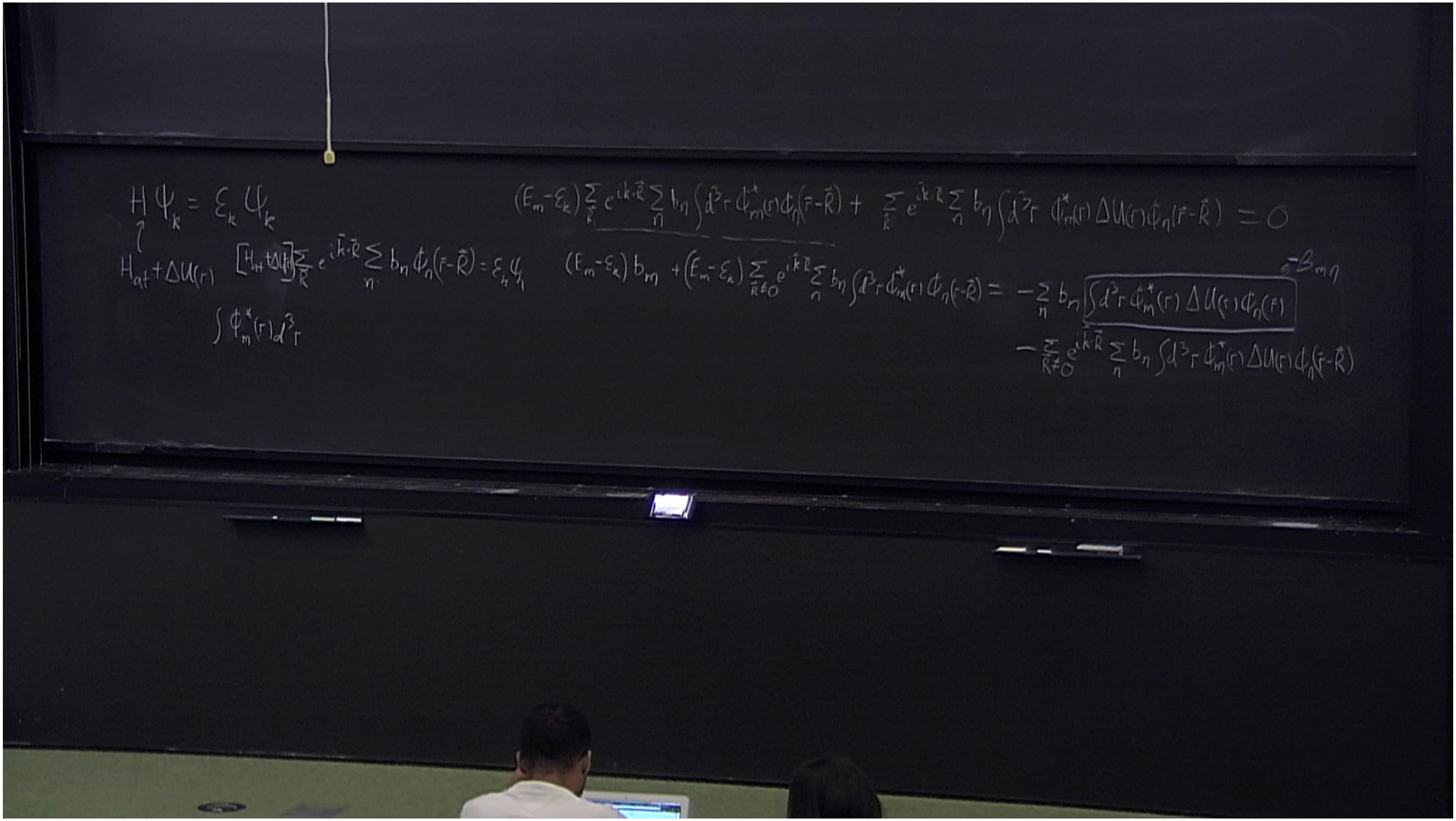




$H\psi_k = \varepsilon_k \psi_k$
$H_{at} + \Delta U(r)$
$[H_{at} + \Delta U(r)] \sum_{\vec{R}} e^{i\vec{k}\cdot\vec{R}} \sum_n b_n \phi_n(\vec{r}-\vec{R}) = \varepsilon_k \psi_k$
$\int \phi_m^*(r) d^3r$
$(E_m - \varepsilon_k) \sum_{\vec{R}} e^{ik\cdot\vec{R}} \sum_n b_n \int d^3r\, \phi_m^*(r)\phi_n(\vec{r}-\vec{R}) + \sum_{\vec{R}} e^{ik\cdot R} \sum_n b_n \int d^3r\, \phi_m^*(r)\Delta U(r)\phi_n(\vec{r}-\vec{R}) = 0$
$(E_m - \varepsilon_k) b_m + (E_m - \varepsilon_k) \sum_{\vec{R}\neq 0} e^{i\vec{k}\vec{R}} \sum_n b_n \int d^3r\, \phi_m^*(r)\phi_n(\vec{r}-\vec{R}) = -\sum_n b_n \int d^3r\, \phi_m^*(r)\Delta U(r)\phi_n(\vec{r})$
$= -\beta_{mn}$
$-\sum_{\vec{R}\neq 0} e^{i\vec{k}\vec{R}} \sum_n b_n \int d^3r\, \phi_m^*(r)\Delta U(r)\phi_n(\vec{r}-\vec{R})$

$$(E_m - \mathcal{E}_k)\sum_{\vec R}$$

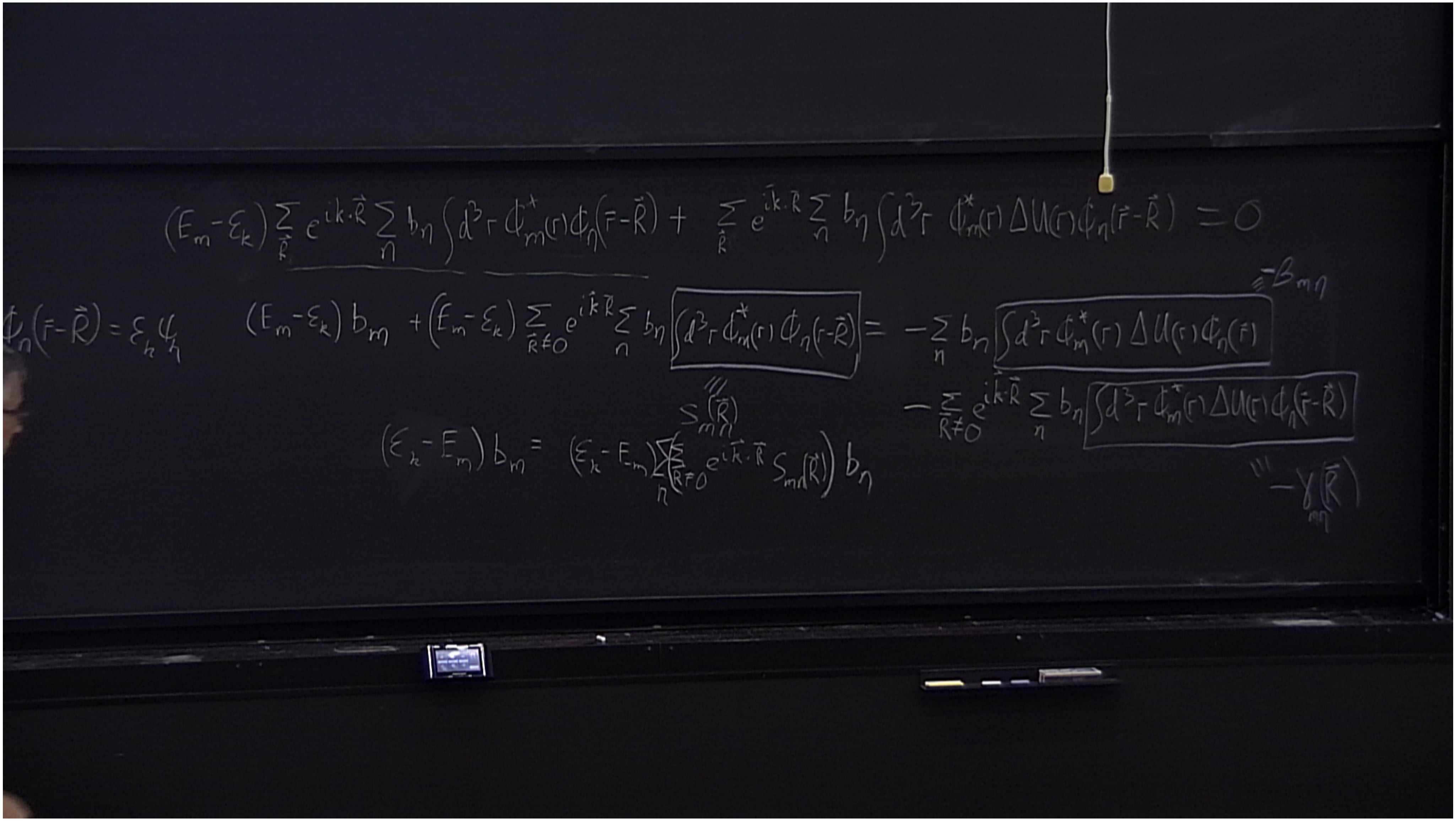
$$H\psi_k = \mathcal{E}_k \psi_k$$

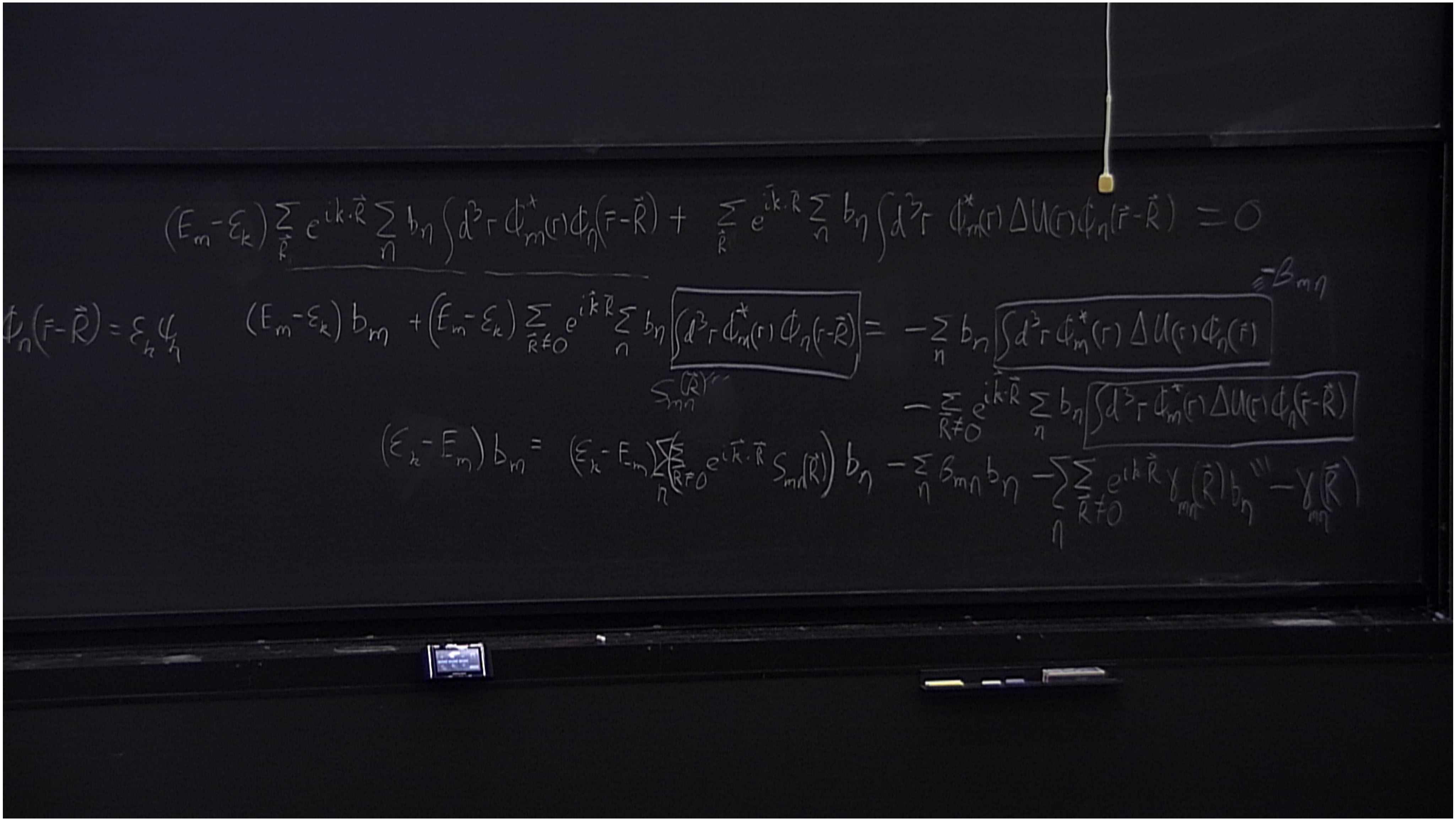
$$H_{at} + \Delta U(r)$$

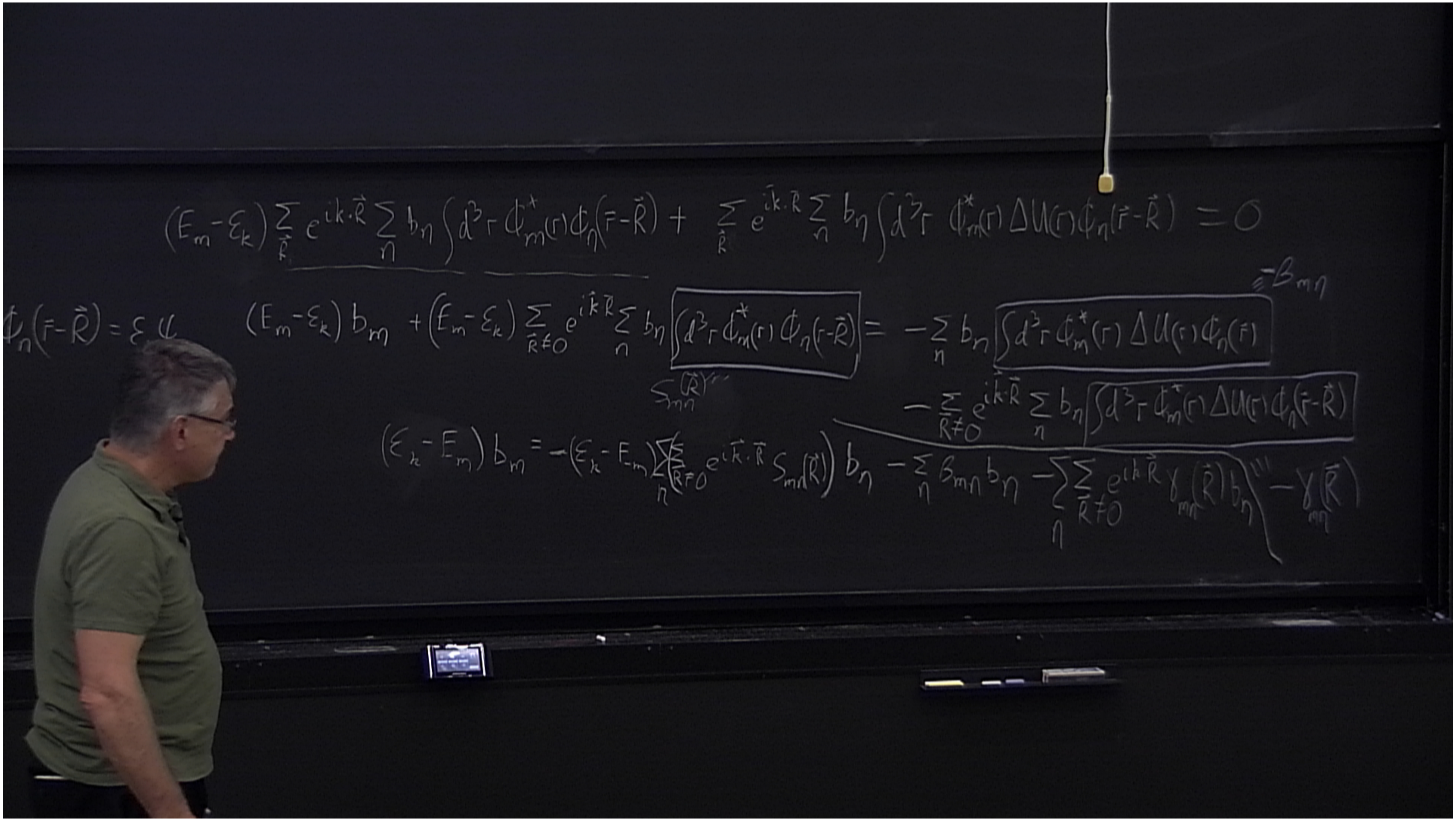
$$\left[H_{at} + \Delta U(r)\right] \sum_{\vec R} e^{i\vec k\cdot\vec R} \sum_{n} b_n \phi_n(\vec r - \vec R) = \mathcal{E}_k \psi_k$$

$$(E_m$$

$$\int \phi_m^*(\vec r)\, d^3 r$$


$(E_m-\varepsilon_k)\sum_{\vec R} e^{i\vec k\cdot\vec R}\sum_n b_n\int d^3r\,\phi_m^*(r)\phi_n(\vec r-\vec R) + \sum_{\vec R} e^{i\vec k\cdot\vec R}\sum_n b_n\int d^3r\,\phi_m^*(r)\Delta U(r)\phi_n(\vec r-\vec R) = 0$
$\phi_n(\vec r-\vec R)=\varepsilon_n\phi_n$
$(E_m-\varepsilon_k)b_m + (E_m-\varepsilon_k)\sum_{\vec R\neq 0} e^{i\vec k\cdot\vec R}\sum_n b_n\int d^3r\,\phi_m^*(r)\phi_n(\vec r-\vec R) = -\sum_n b_n\int d^3r\,\phi_m^*(r)\Delta U(r)\phi_n(r)$
$-\sum_{\vec R\neq 0} e^{i\vec k\cdot\vec R}\sum_n b_n\int d^3r\,\phi_m^*(r)\Delta U(r)\phi_n(\vec r-\vec R)$
$\equiv S_{mn}(\vec R)$
$\equiv -\beta_{mn}$
$\equiv -\gamma_{mn}(\vec R)$
$(\varepsilon_k-E_m)b_m = (\varepsilon_k-E_m)\sum_n\left(\sum_{\vec R\neq 0} e^{i\vec k\cdot\vec R}S_{mn}(\vec R)\right)b_n$


$(E_m-\varepsilon_k)\sum_{\vec R} e^{i\vec k\cdot\vec R}\sum_n b_n\int d^3r\,\phi_m^*(r)\phi_n(\vec r-\vec R) + \sum_{\vec R} e^{i\vec k\cdot\vec R}\sum_n b_n\int d^3r\,\phi_m^*(r)\Delta U(r)\phi_n(\vec r-\vec R) = 0$
$\phi_n(\vec r-\vec R) = \varepsilon_k\psi_k$
$\equiv -\beta_{mn}$
$(E_m-\varepsilon_k)b_m + (E_m-\varepsilon_k)\sum_{\vec R\neq 0} e^{i\vec k\cdot\vec R}\sum_n b_n\int d^3r\,\phi_m^*(r)\phi_n(\vec r-\vec R) = -\sum_n b_n\int d^3r\,\phi_m^*(r)\Delta U(r)\phi_n(r)$
$S_{mn}(\vec R)$
$-\sum_{\vec R\neq 0} e^{i\vec k\cdot\vec R}\sum_n b_n\int d^3r\,\phi_m^*(r)\Delta U(r)\phi_n(\vec r-\vec R)$
$(\varepsilon_k-E_m)b_m = (\varepsilon_k-E_m)\sum_n\Big(\sum_{\vec R\neq 0} e^{i\vec k\cdot\vec R}S_{mn}(\vec R)\Big)b_n - \sum_n\beta_{mn}b_n - \sum_n\sum_{\vec R\neq 0} e^{i\vec k\cdot\vec R}\gamma_{mn}(\vec R)b_n$
$-\gamma_{mn}(\vec R)$


(E_m - ε_k) Σ_R e^{ik·R} Σ_n b_n ∫d³r φ*_m(r) φ_n(r - R) + Σ_R e^{ik·R} Σ_n b_n ∫d³r φ*_m(r) ΔU(r) φ_n(r - R) = 0
φ_n(r - R) = ε φ
(E_m - ε_k) b_m + (E_m - ε_k) Σ_{R≠0} e^{ik·R} Σ_n b_n ∫d³r φ*_m(r) φ_n(r - R) = - Σ_n b_n ∫d³r φ*_m(r) ΔU(r) φ_n(r)
≡ -β_mn
S_mn(R)
- Σ_{R≠0} e^{ik·R} Σ_n b_n ∫d³r φ*_m(r) ΔU(r) φ_n(r - R)
(ε_k - E_m) b_m = -(ε_k - E_m) (Σ_n Σ_{R≠0} e^{ik·R} S_mn(R)) b_n - Σ_n β_mn b_n - Σ_n Σ_{R≠0} e^{ik·R} γ_mn(R) b_n
- γ_mn(R)

$$H\psi_k = \mathcal{E}_k \psi_k$$

$$H_{at} + \Delta U(r)$$

$$[H_{at} + \Delta U(r)] \sum_{\vec R} e^{i\vec k\cdot\vec R} \sum_n b_n \phi_n(\vec r - \vec R) = \mathcal{E}_k \psi_k$$

$$\int \phi_m^*(r)\, d^3r$$

$$(E_m - \mathcal{E}_k)\, b_m + (E_m - \mathcal{E}_k) \sum_{\vec R\neq 0} e^{i\vec k\cdot\vec R} \sum_n b_n \int d^3r\, \phi_m^*(r)\phi_n(\vec r - \vec R) = -\sum_n b_n \int d^3r\, \phi_m^*(r)\, \Delta U(r)\, \phi_n(r) - \sum_{\vec R\neq 0} e^{i\vec k\cdot\vec R} \sum_n b_n \int d^3r\, \phi_m^*(r)\, \Delta U(r)\, \phi_n(\vec r - \vec R)$$

$S_{mn}(\vec R)$, $-\beta_{mn}$

$$(\mathcal{E}_k - E_m)\, b_m = -(\mathcal{E}_k - E_m) \sum_n \sum_{\vec R\neq 0} e^{i\vec k\cdot\vec R} S_{mn}(\vec R)\, b_n - \sum_n \beta_{mn} b_n - \sum_n \sum_{\vec R\neq 0} e^{i\vec k\cdot\vec R} \gamma_{mn}(\vec R)\, b_n$$

$-\gamma_{mn}(\vec R)$

$$\psi_{100}(\vec r) = \frac{1}{\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2} e^{-Zr/a_0}$$

just consider the 1s states

$m = 1s$

but also in $\sum_n$, consider only 1s

$$S(\vec R) = \int d^3r\, \psi_{100}^*(\vec r)\, \psi_{100}(\vec r - \vec R)$$

$$(\mathcal{E}_k - E_{1s})\, b_{1s} = -(\mathcal{E}_k - E_{1s}) \sum_{\vec R\neq 0} S(\vec R)\, e^{i\vec k\cdot\vec R}\, b_{1s} - \beta\, b_{1s} - \sum_{\vec R\neq 0} e^{i\vec k\cdot\vec R}\, \gamma(\vec R)\, b_{1s}$$

$$\mathcal{E}_k = E_{1s} - \frac{\beta + \sum_{\vec R\neq 0} e^{i\vec k\cdot\vec R}\, \gamma(\vec R)}{1 + \sum_{\vec R\neq 0} S(\vec R)\, e^{i\vec k\cdot\vec R}}$$

$H_{at} + \Delta U(r)$ $\quad [H_{at} + \Delta U(r)] \sum_{\vec{R}} e^{i\vec{k}\cdot\vec{R}} \sum_n b_n \phi_n(\vec{r}-\vec{R}) = \varepsilon_k \psi_k$

$\int \phi_m^*(r) d^3r$

$(E_m - \varepsilon_k) b_m + (E_m - \varepsilon_k) \sum_{\vec{R}\neq 0} e^{i\vec{k}\cdot\vec{R}} \sum_n b_n \int d^3r\, \phi_m^*(r) \phi_n(\vec{r}-\vec{R}) = -\sum_n b_n \int d^3r\, \phi_m^*(r) \Delta U(r) \phi_n \ldots$

$S_{mn}(\vec{R})$

$- \sum_{\vec{R}\neq 0} e^{i\vec{k}\cdot\vec{R}} \sum_n b_n \int d^3r\, \phi_m^*(r) \Delta \ldots$

$(\varepsilon_k - E_m) b_m = -(\varepsilon_k - E_m) \sum_n \left(\sum_{\vec{R}\neq 0} e^{i\vec{k}\cdot\vec{R}} S_{mn}(\vec{R}) \right) b_n - \sum_n \beta_{mn} b_n - \sum_n \sum_{\vec{R}\neq 0} e^{i\vec{k}\cdot\vec{R}} \gamma_{mn}(\vec{R}) \ldots$

$\psi_{100}(\vec{r}) = \frac{1}{\sqrt{\pi}} \left(\frac{Z}{a_0}\right)^{3/2} e^{-Zr/a_0}$ | just consider the 1s states $m = 1s$

but also in $\sum_n$, consider only 1s

$S(\vec{R}) = \int d^3r\, \psi_{100}^*(\vec{r}) \psi_{100}(\vec{r}-\vec{R})$

$Z = 11$

$R = 3.7\,\text{Å}$

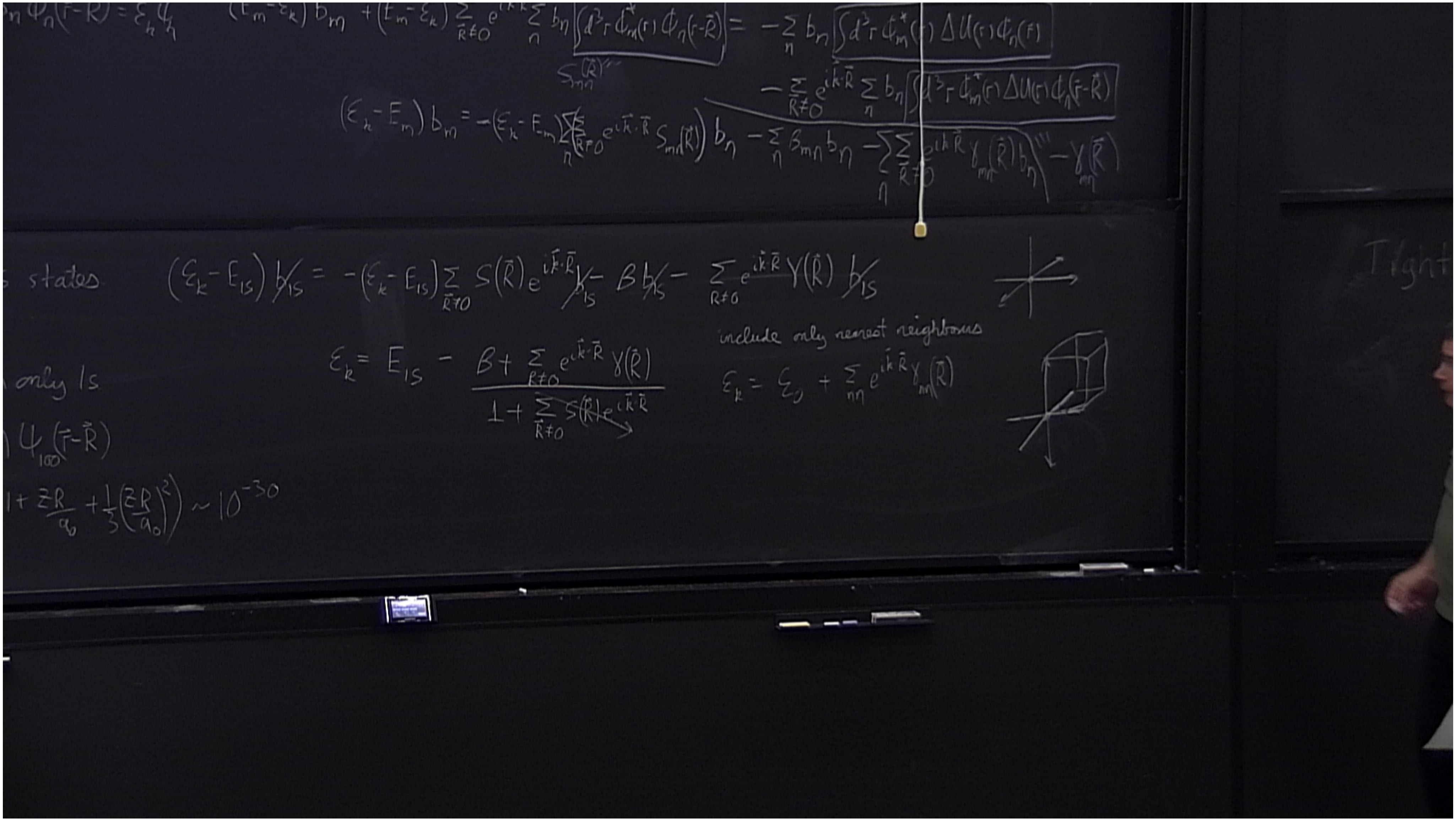
$a_0 = 0.529\,\text{Å}$

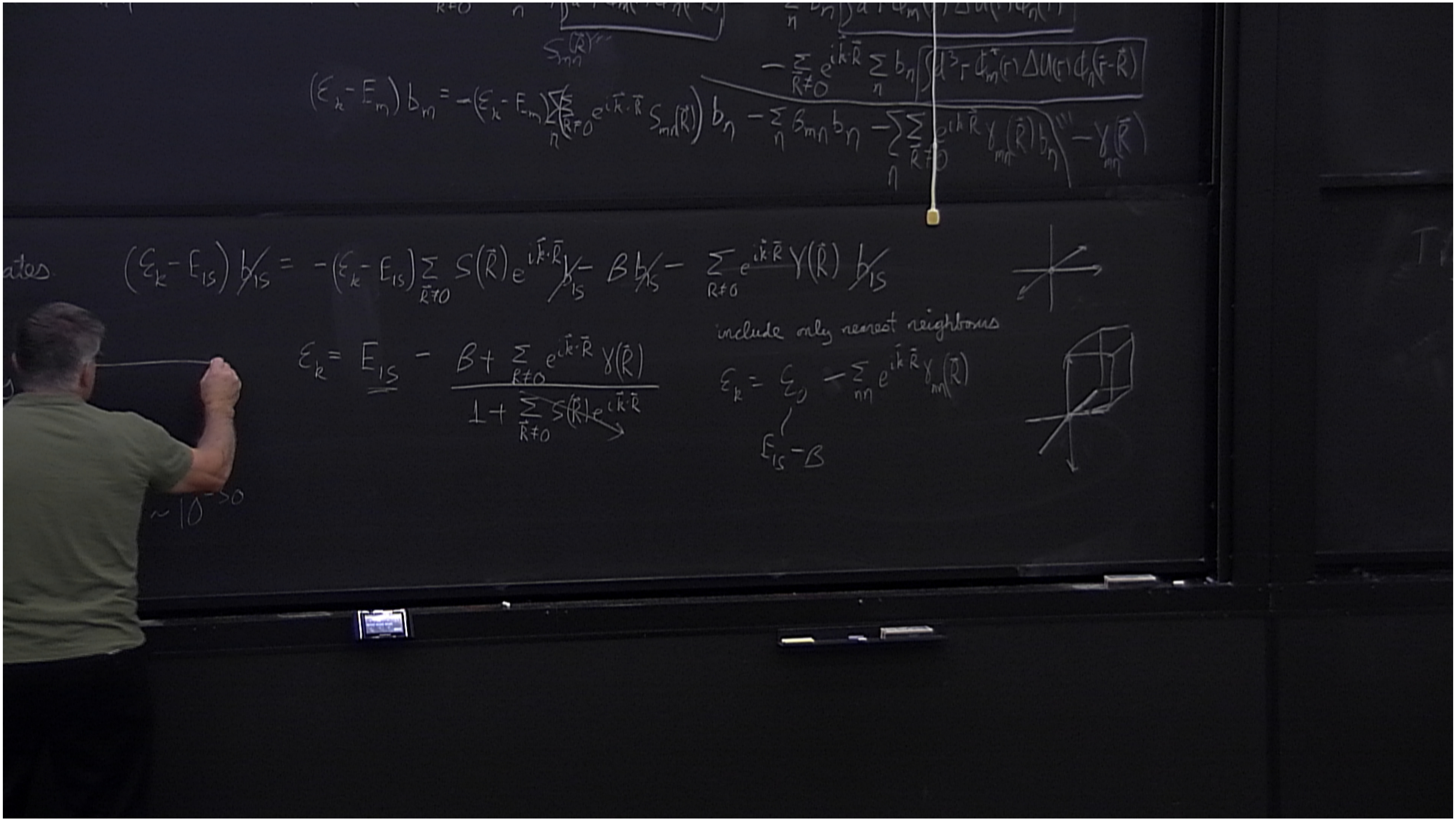
$S(R_{nn}) = e^{-ZR/a_0} \left(1 + \frac{ZR}{a_0} + \frac{1}{3}\left(\frac{ZR}{a_0}\right)^2 \right) \sim 10^{-30}$

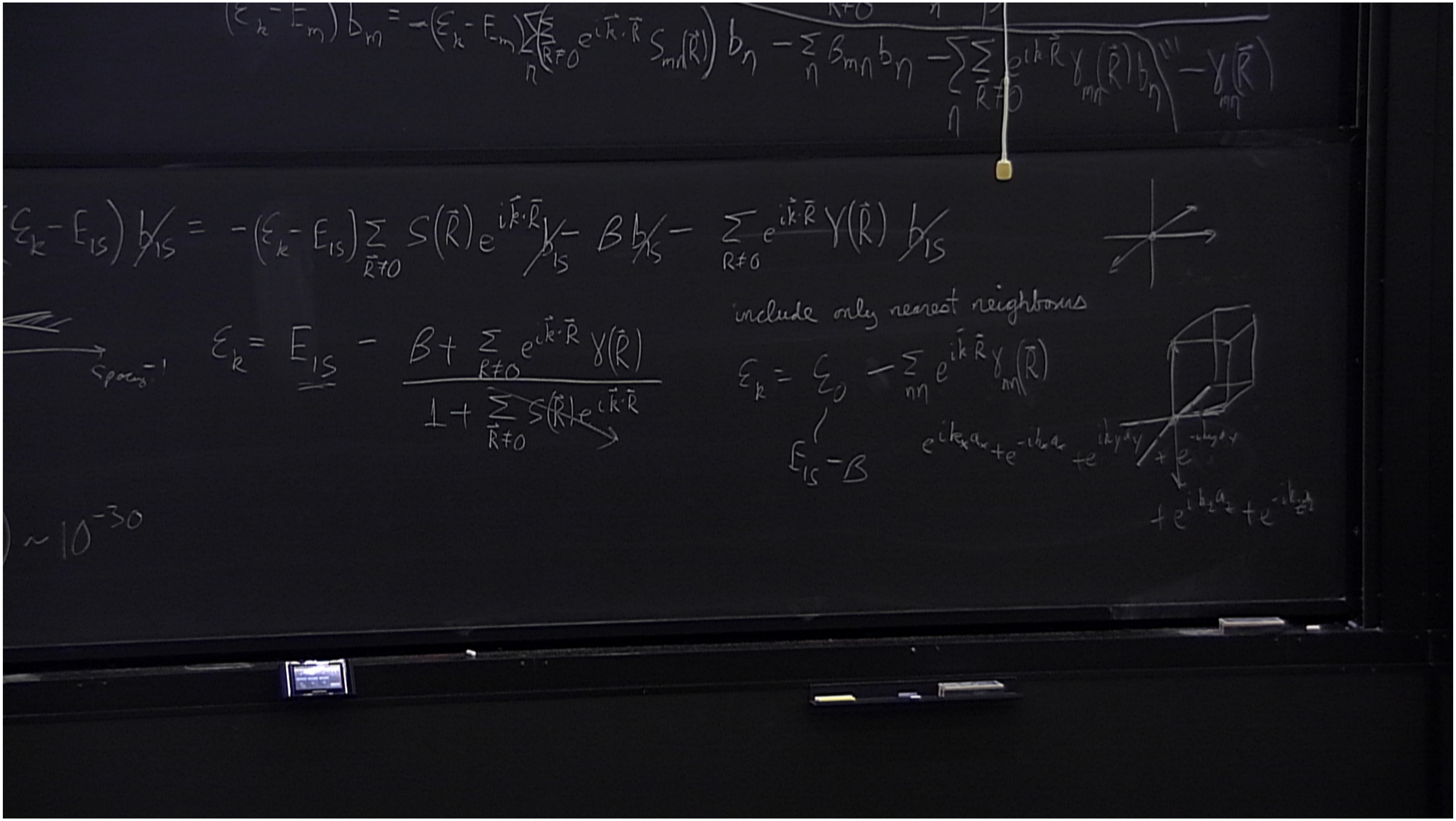
$(\varepsilon_k - E_{1s}) b_{1s} = -(\varepsilon_k - E_{1s}) \sum_{\vec{R}\neq 0} S(\vec{R}) e^{i\vec{k}\cdot\vec{R}} b_{1s} - \beta b_{1s} - \sum_{R\neq 0} e^{i\vec{k}\cdot\vec{R}} \gamma(\vec{R})\, b_{1s}$

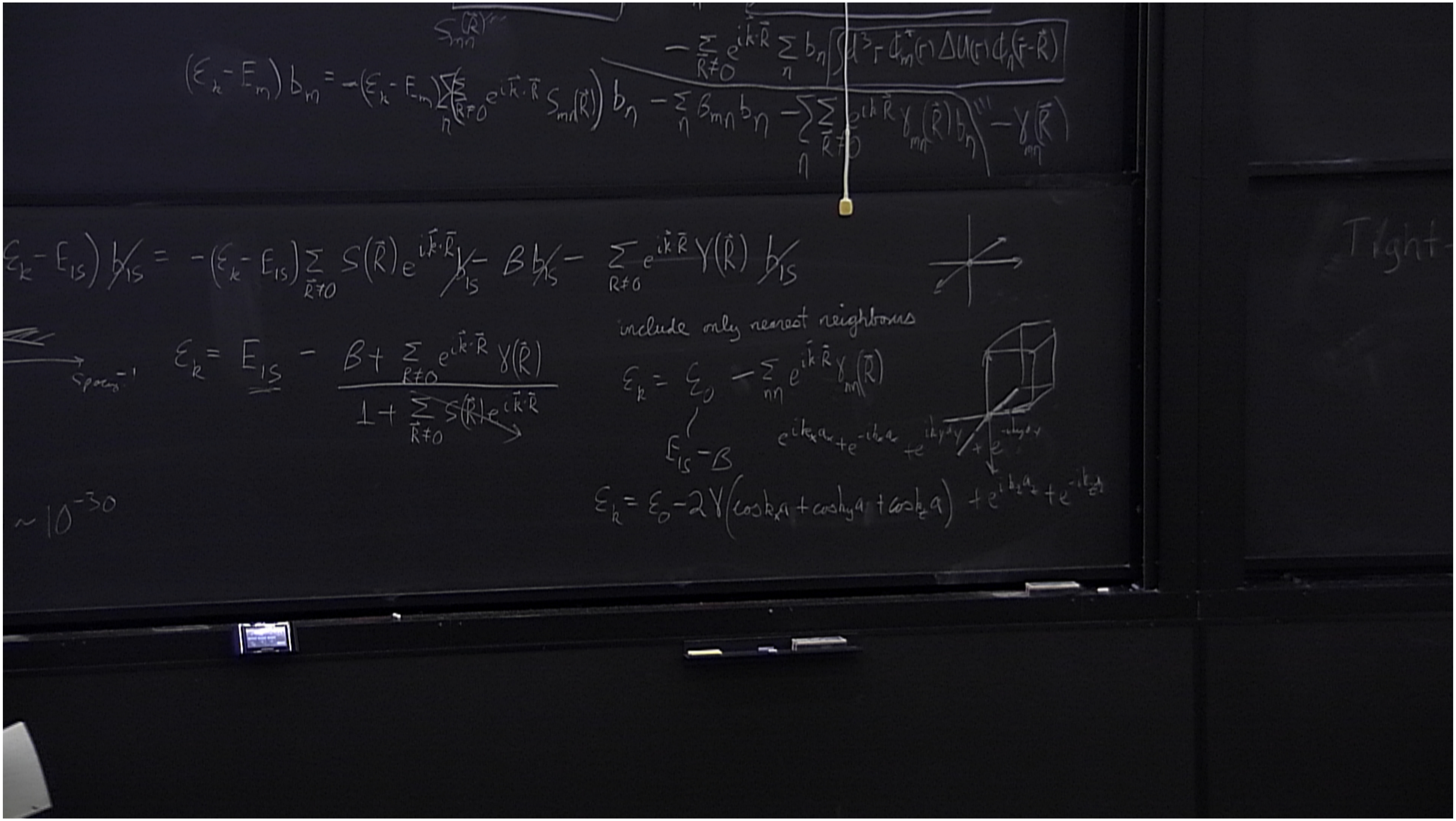
include only nearest neighbours

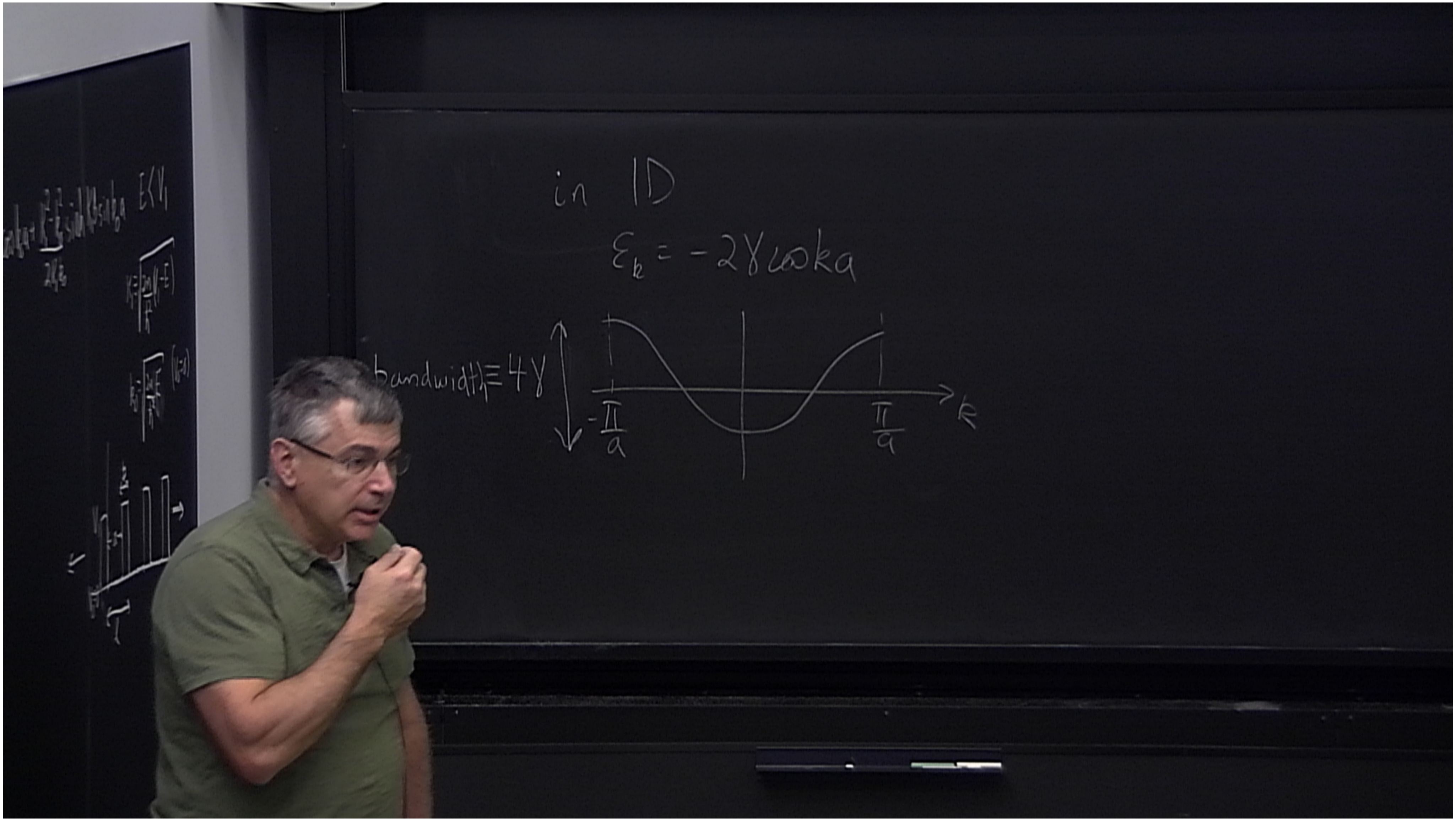
$$\varepsilon_k = E_{1s} - \frac{\beta + \sum_{\vec{R}\neq 0} e^{i\vec{k}\cdot\vec{R}} \gamma(\vec{R})}{1 + \sum_{\vec{R}\neq 0} S(\vec{R}) e^{i\vec{k}\cdot\vec{R}}}$$

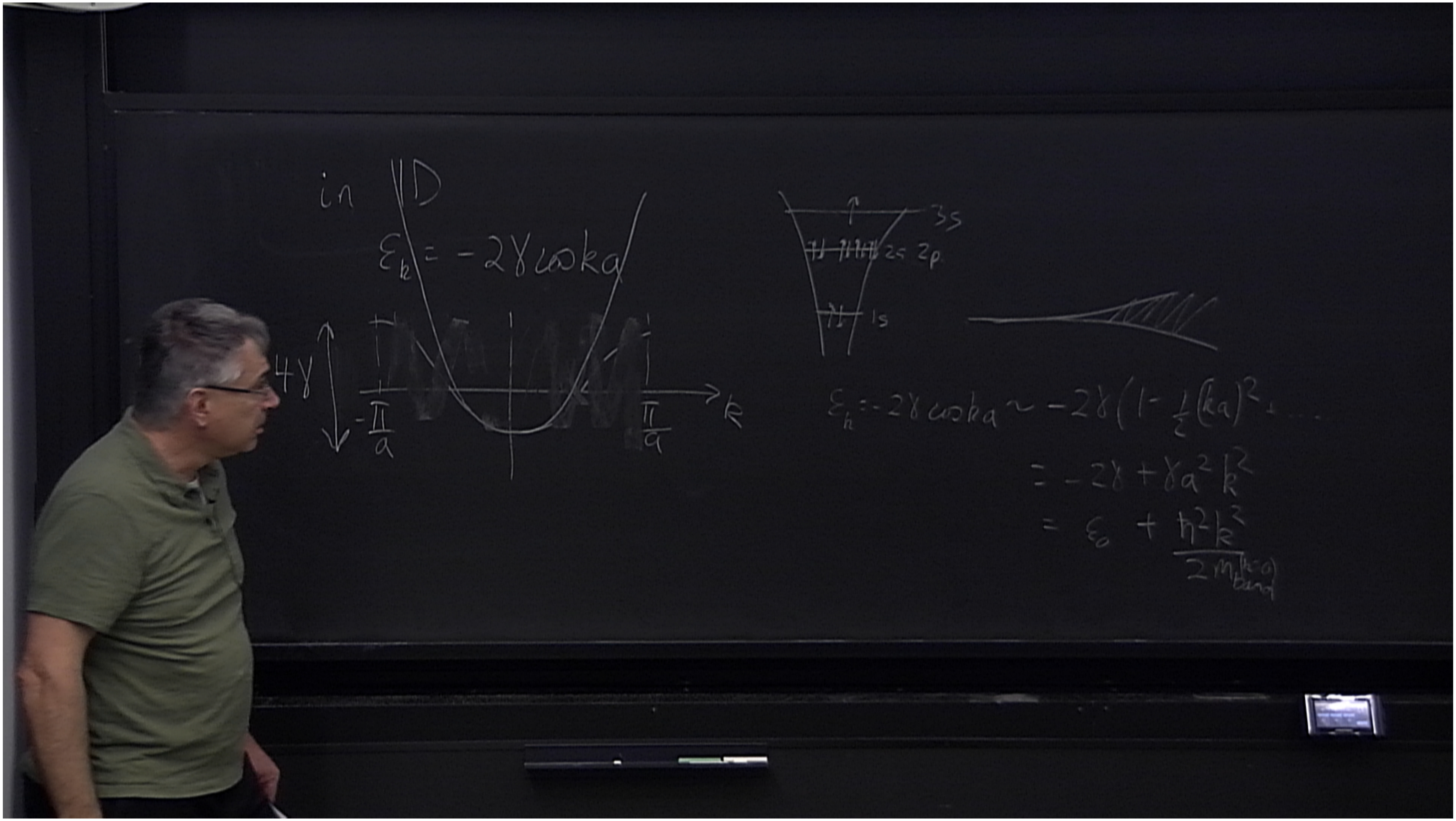

states
$(\varepsilon_k - E_{1s}) b_{1s} = -(\varepsilon_k - E_{1s}) \sum_{\vec{R}\neq 0} S(\vec{R}) e^{i\vec{k}\cdot\vec{R}} b_{1s} - \beta b_{1s} - \sum_{R\neq 0} e^{i\vec{k}\cdot\vec{R}} \gamma(\vec{R}) b_{1s}$
$\varepsilon_k = E_{1s} - \frac{\beta + \sum_{\vec{R}\neq 0} e^{i\vec{k}\cdot\vec{R}} \gamma(\vec{R})}{1 + \sum_{\vec{R}\neq 0} S(\vec{R}) e^{i\vec{k}\cdot\vec{R}}}$
include only nearest neighbours
$\varepsilon_k = \varepsilon_0 + \sum_{nn} e^{i\vec{k}\cdot\vec{R}} \gamma_{nn}(\vec{R})$
only 1s
$\sim 10^{-30}$

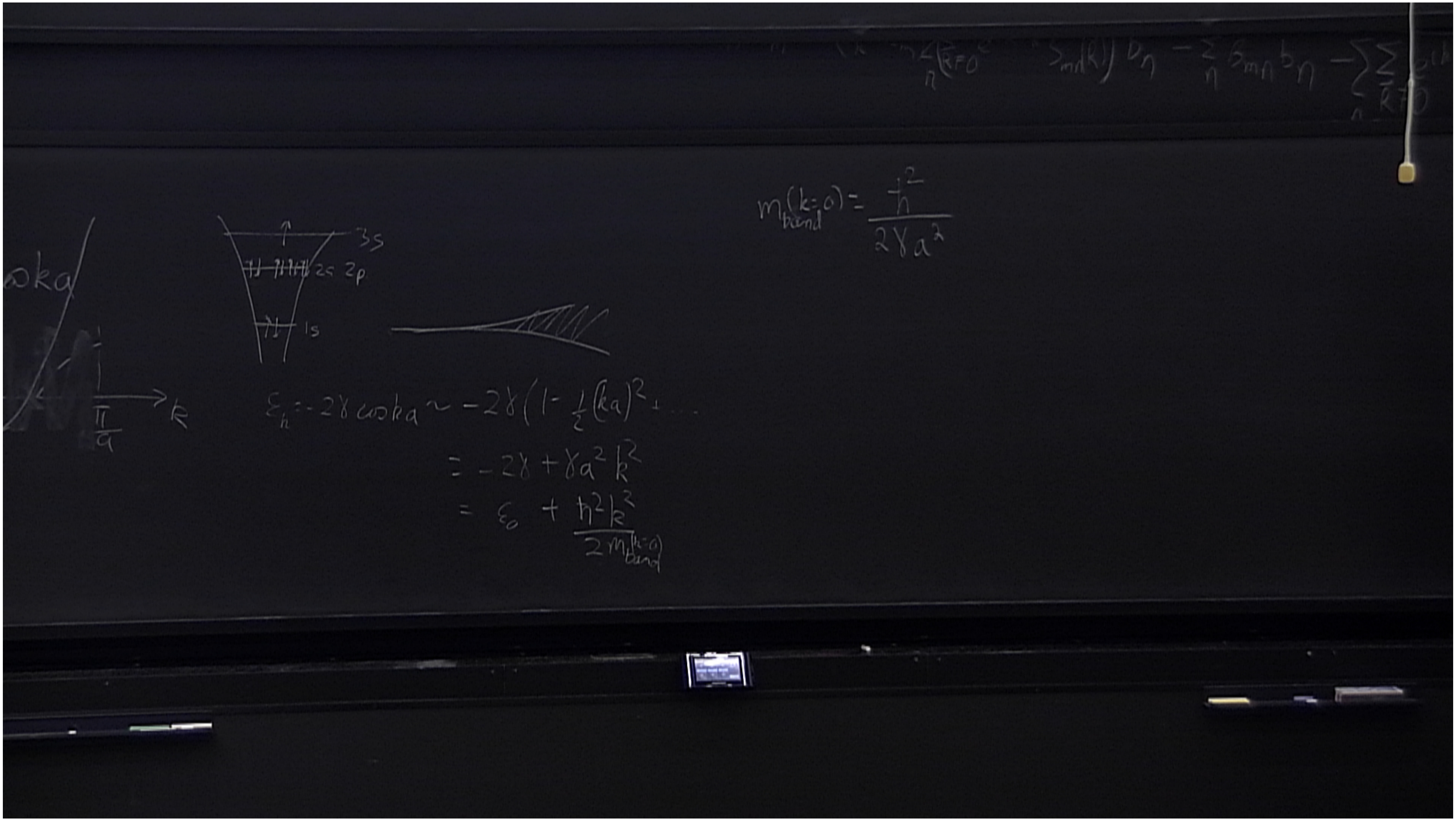

include only nearest neighbors

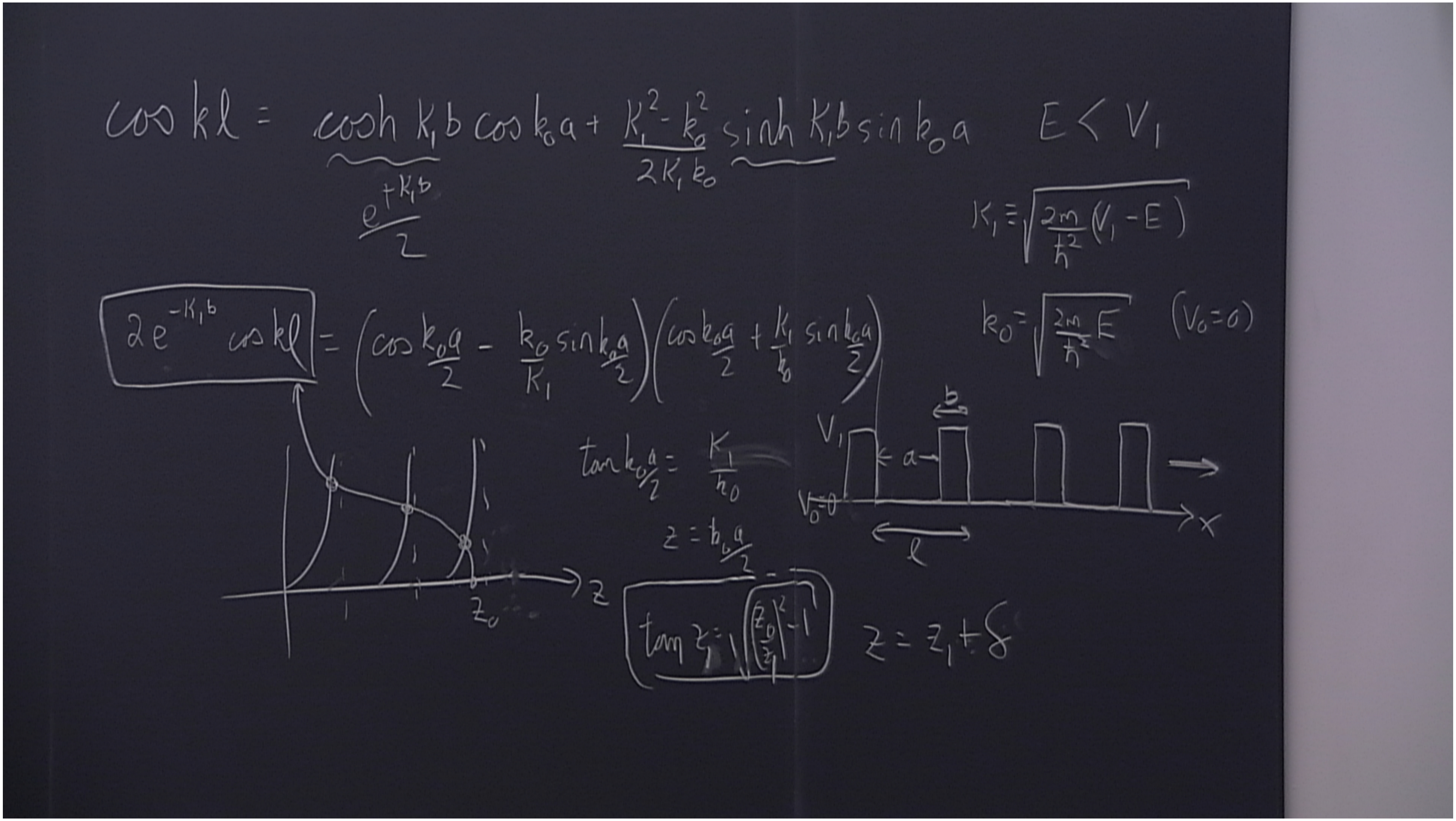

include only nearest neighbours
~10^-30


include only nearest neighbors
Tight-
~10^-30

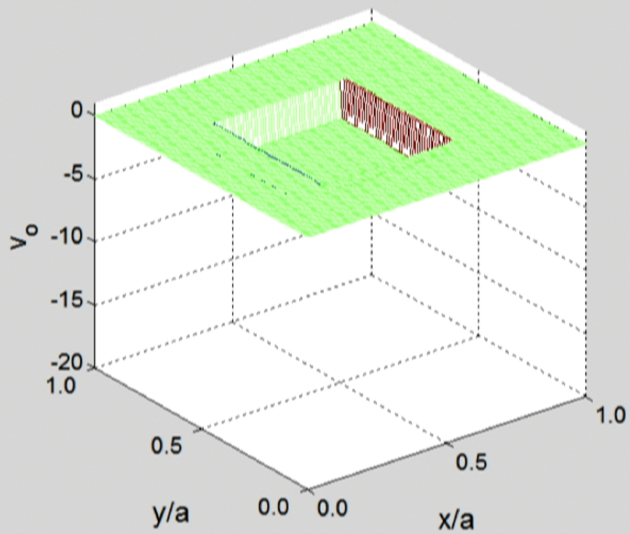

in 1D
$\varepsilon_k = -2\gamma \cos ka$
bandwidth ≡ 4γ
$-\frac{\pi}{a}$
$\frac{\pi}{a}$
k

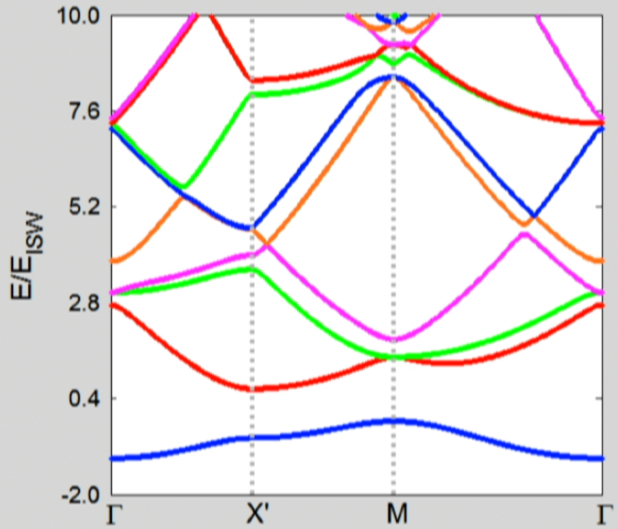

in 1D
ε_k = -2γ cos ka
4γ
-π/a
π/a
k
3s
2s 2p
1s
ε_k = -2γ cos ka ~ -2γ(1 - ½(ka)² + ...
= -2γ + γa²k²
= ε_0 + ħ²k²/2m_band

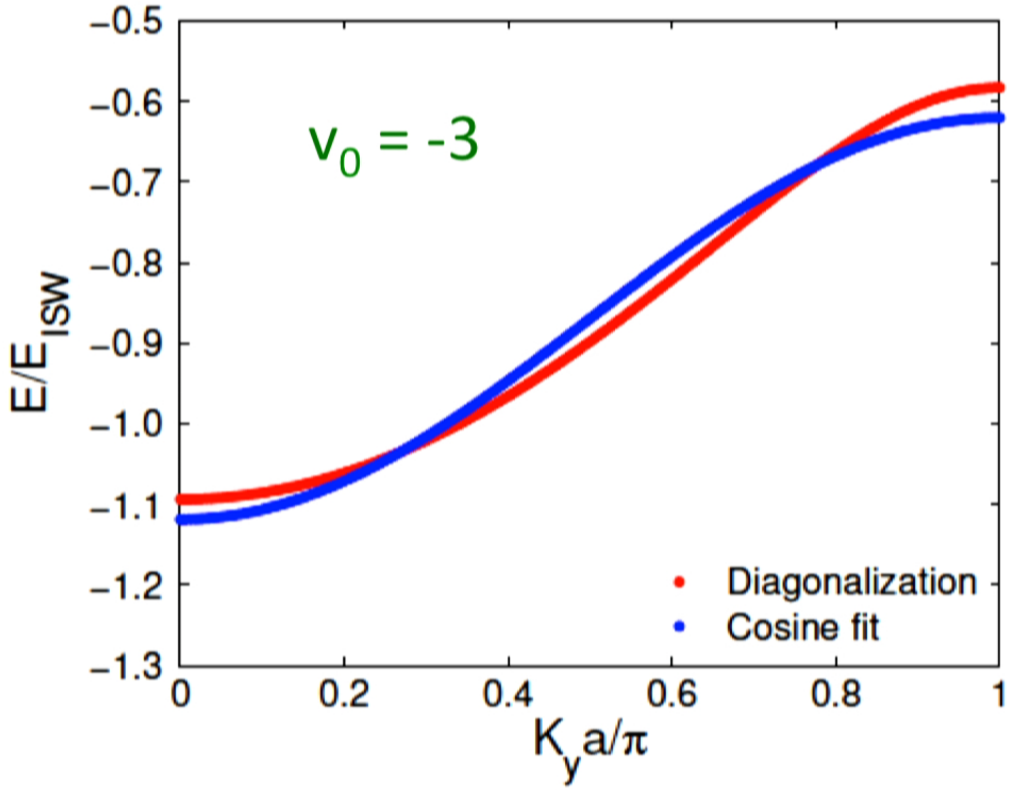

3s
2s 2p
1s
m_band(k=0) = ħ²/2γa²
ε_k = -2γ cos ka ≈ -2γ(1 - ½(ka)² + ...)
= -2γ + γa²k²
= ε_0 + ħ²k²/2m_band(k=0)


cos kl = cosh K1b cos k0a + (K1^2 - k0^2)/(2K1k0) sinh K1b sin k0a
E < V1
e^{+K1b}/2
K1 ≡ √(2m/ħ^2 (V1 - E))
k0 = √(2m/ħ^2 E)
(V0 = 0)
2e^{-K1b} cos kl = (cos k0a/2 - k0/K1 sin k0a/2)(cos k0a/2 + K1/k0 sin k0a/2)
tan k0a/2 = K1/k0
z = k0a/2
tan z = √((z0/z)^2 - 1)
z = z1 + δ
z0
z
V1
V0=0
a
b
l
x

Tight-binding

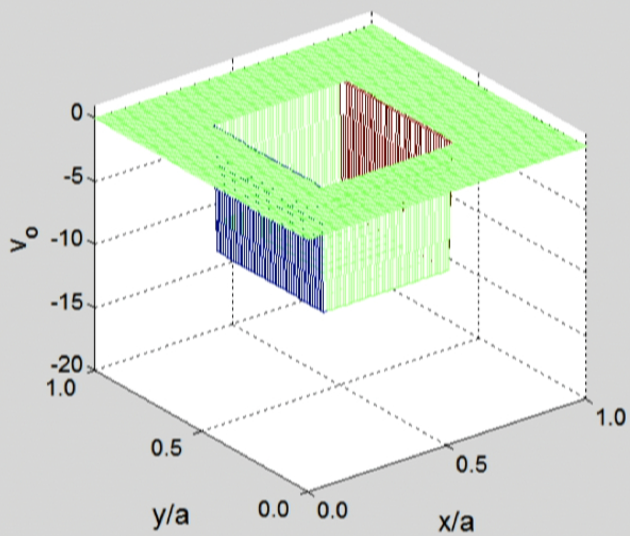


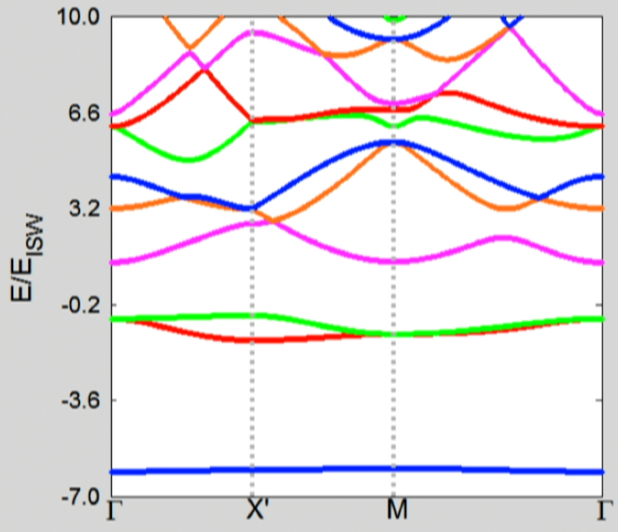




(b) $v_0 = -3, R^2 = 0.9854$

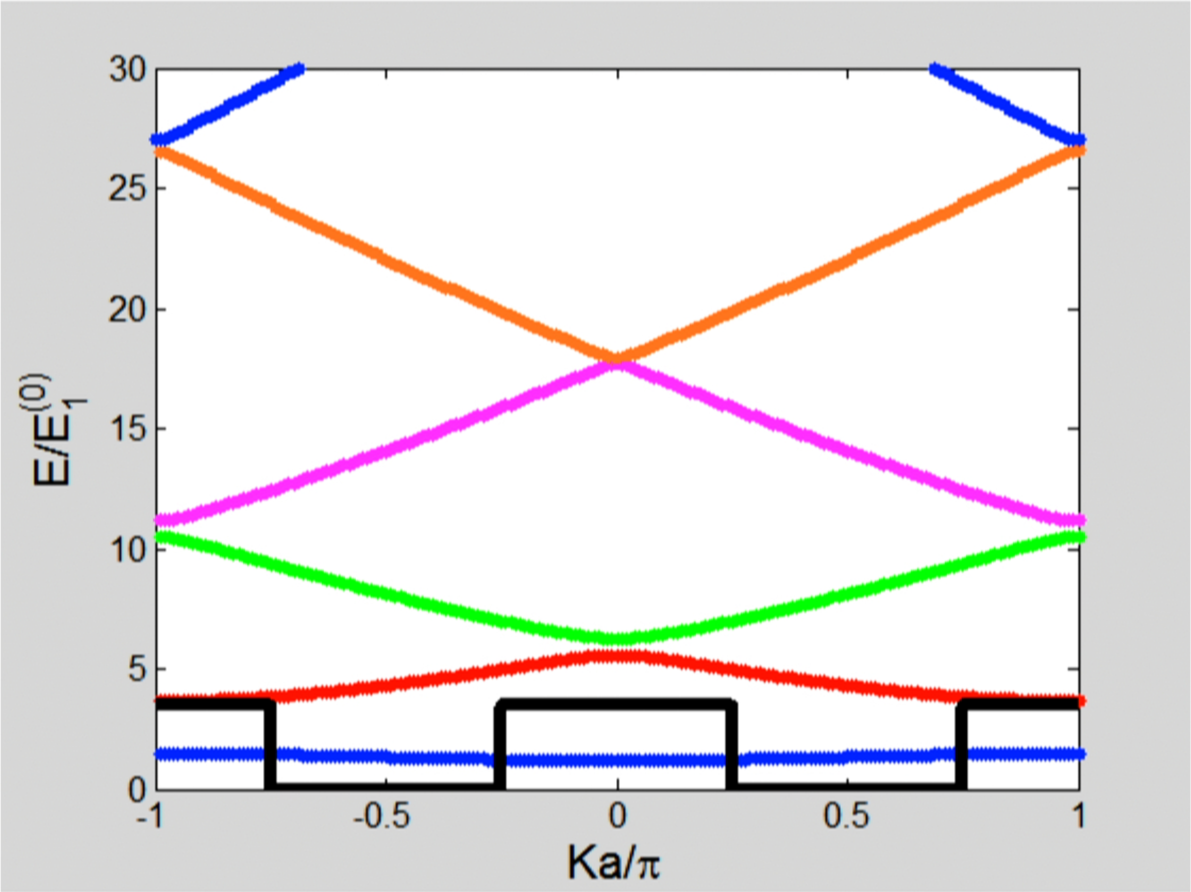
Tight-binding





Stick to 1D

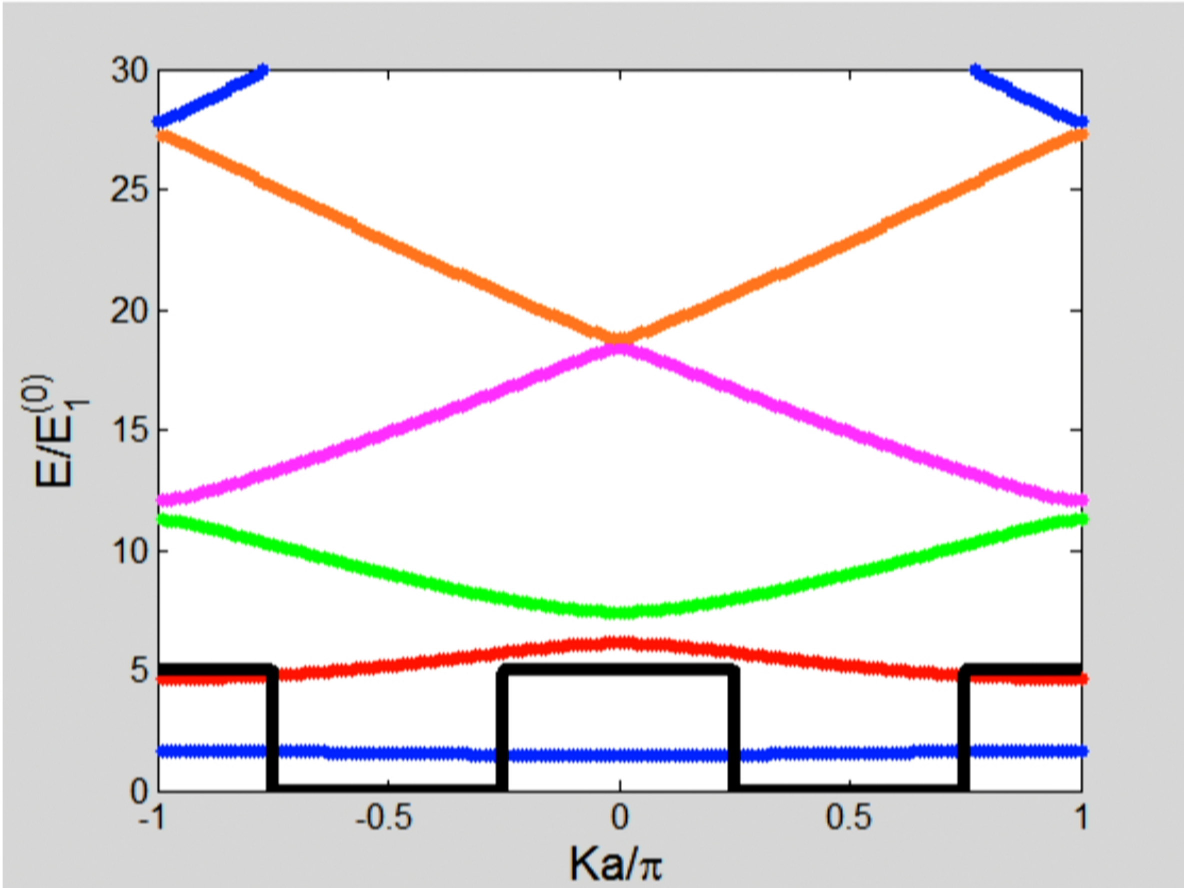
Change the barrier height



Pavelich MSc Thesis

Stick to 1D

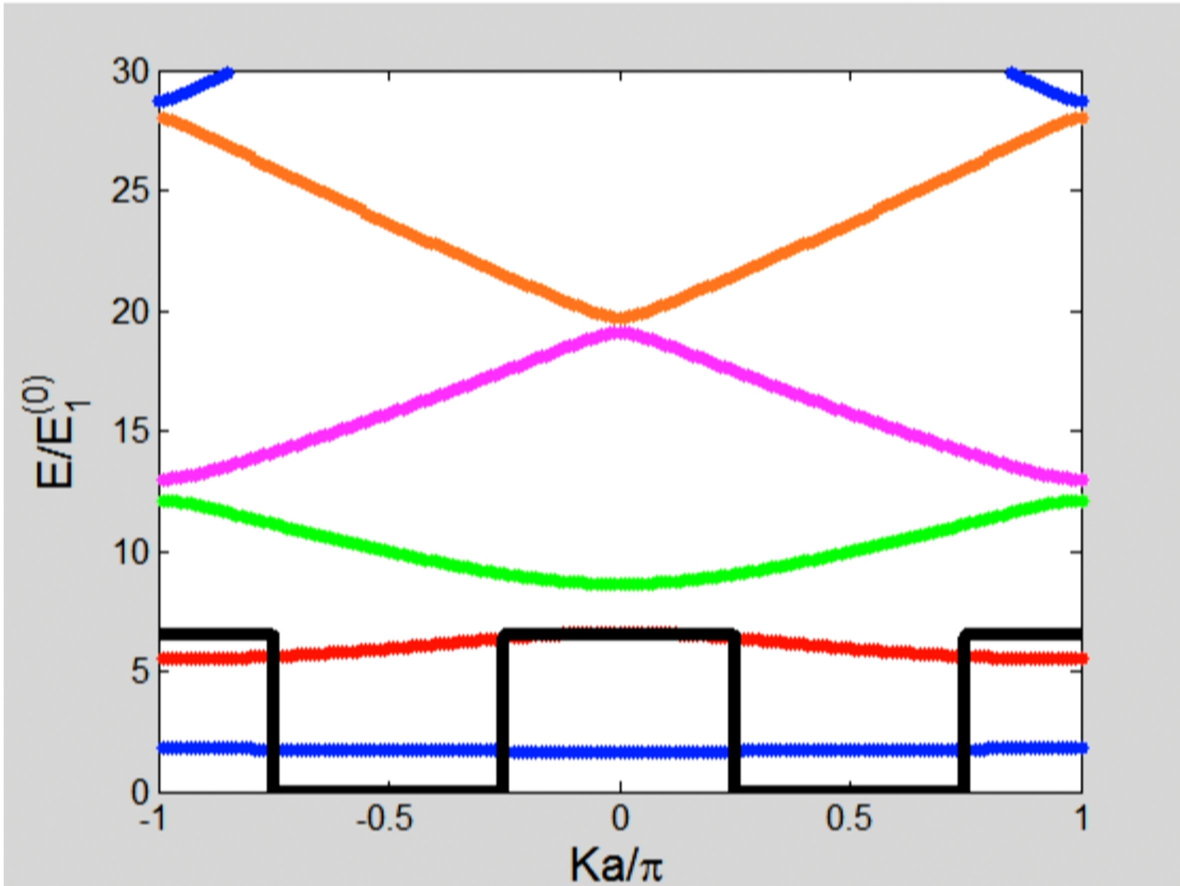
Change the barrier height



Pavelich MSc Thesis

Stick to 1D

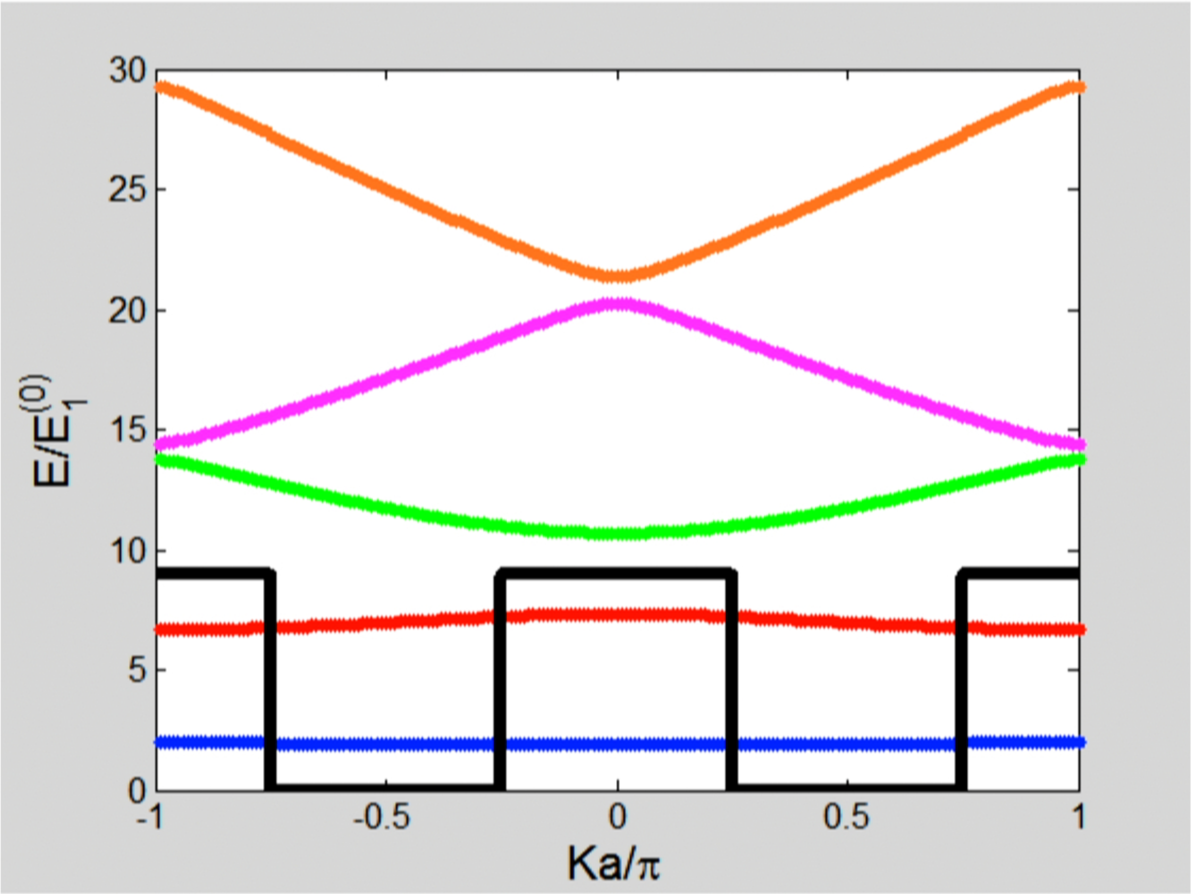
Change the barrier height



Pavelich MSc Thesis

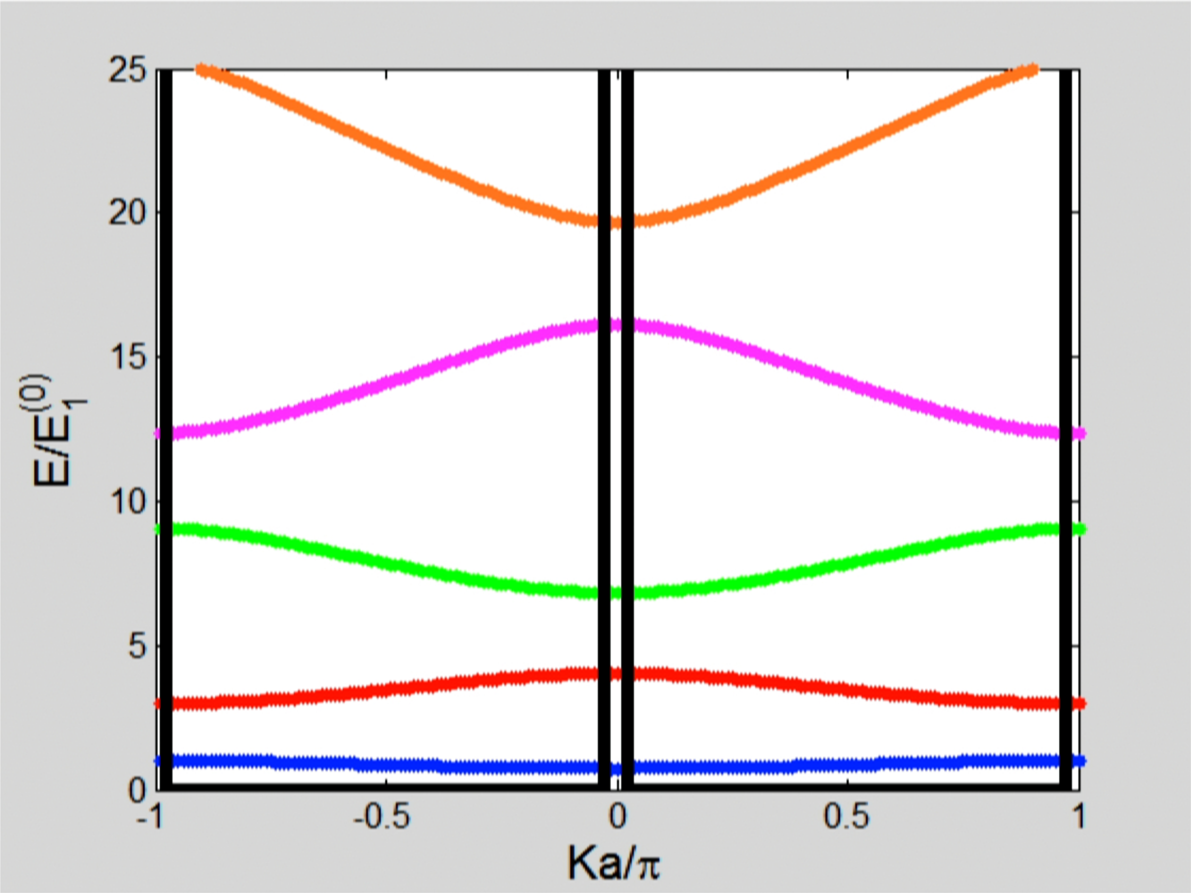
Stick to 1D

Change the barrier height



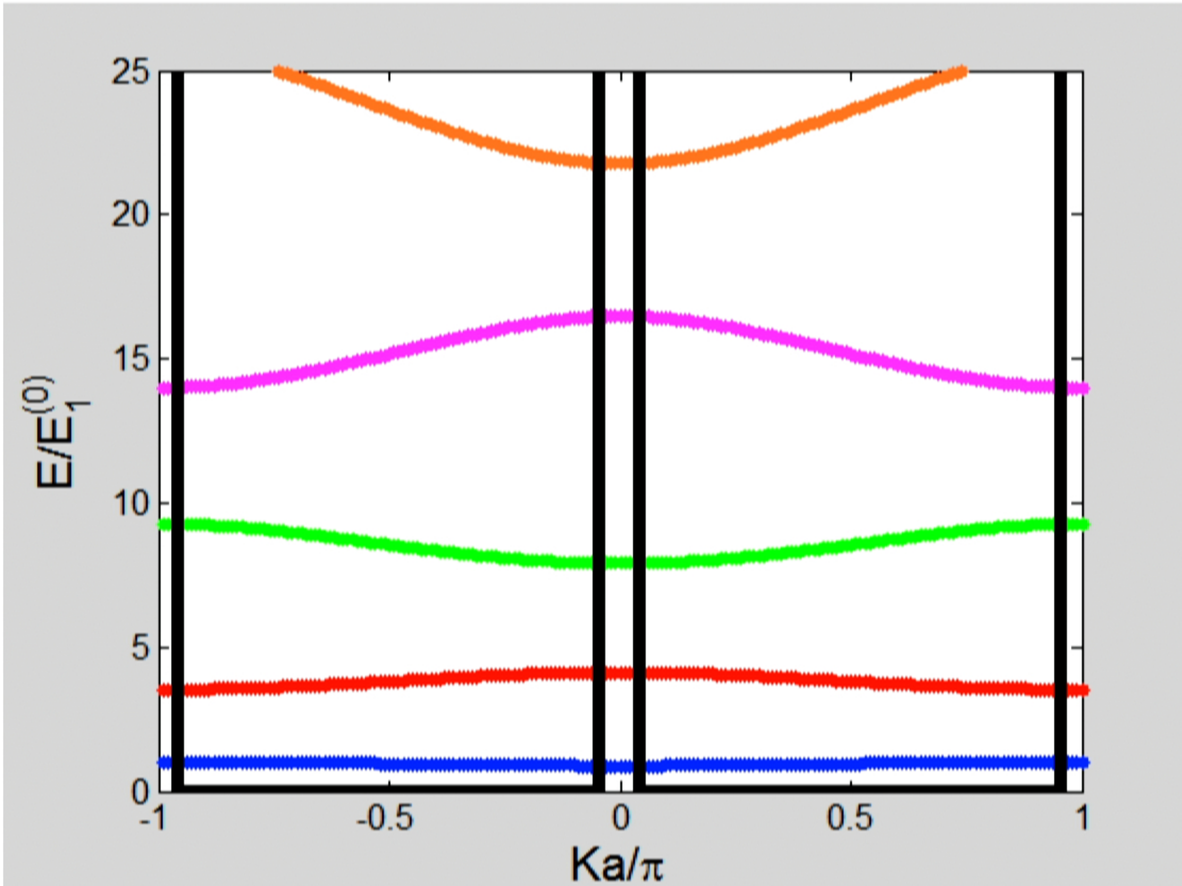
Pavelich MSc Thesis

Stick to 1D Change the barrier width



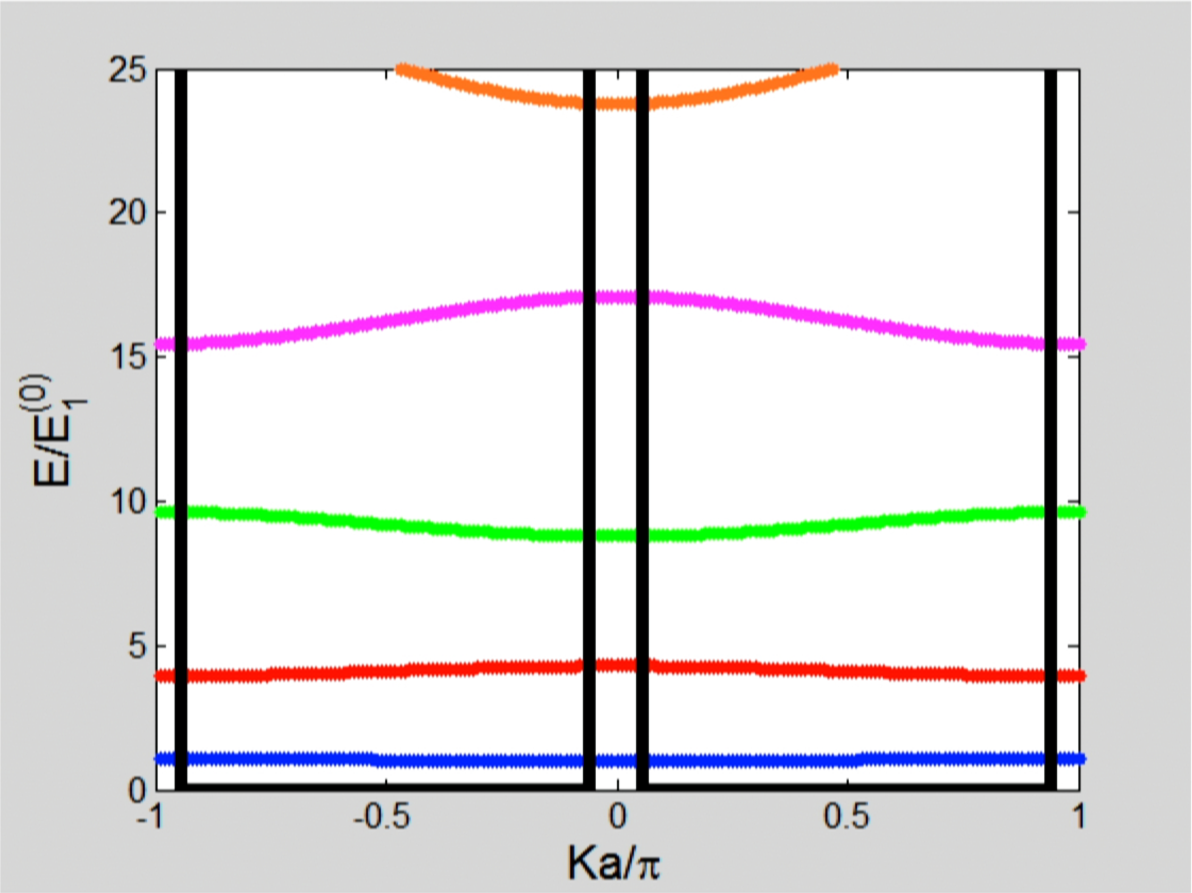
$V_0 = 40\ E_1^{(0)}$

Stick to 1D Change the barrier width



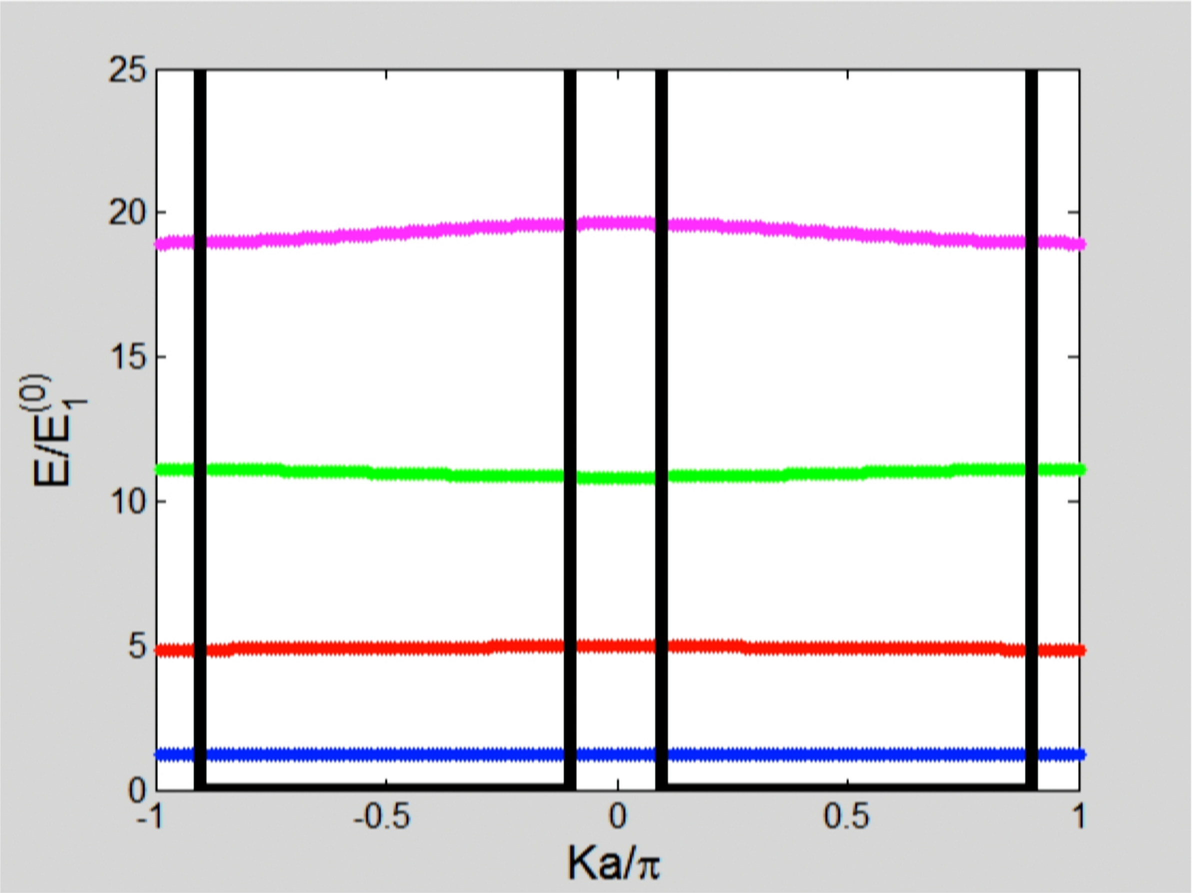
$V_0 = 40\ E_1^{(0)}$

Stick to 1D Change the barrier width



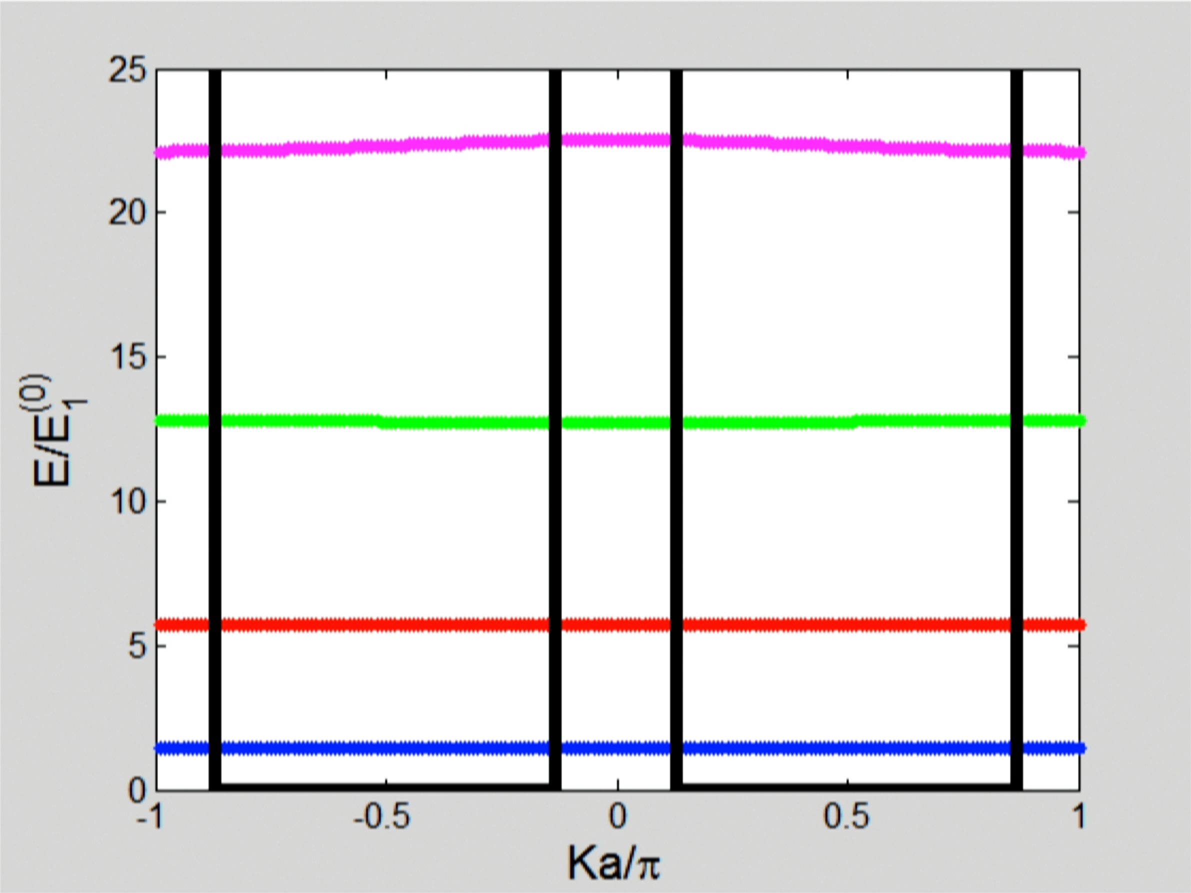
$V_0 = 40\ E_1^{(0)}$

Stick to 1D Change the barrier width



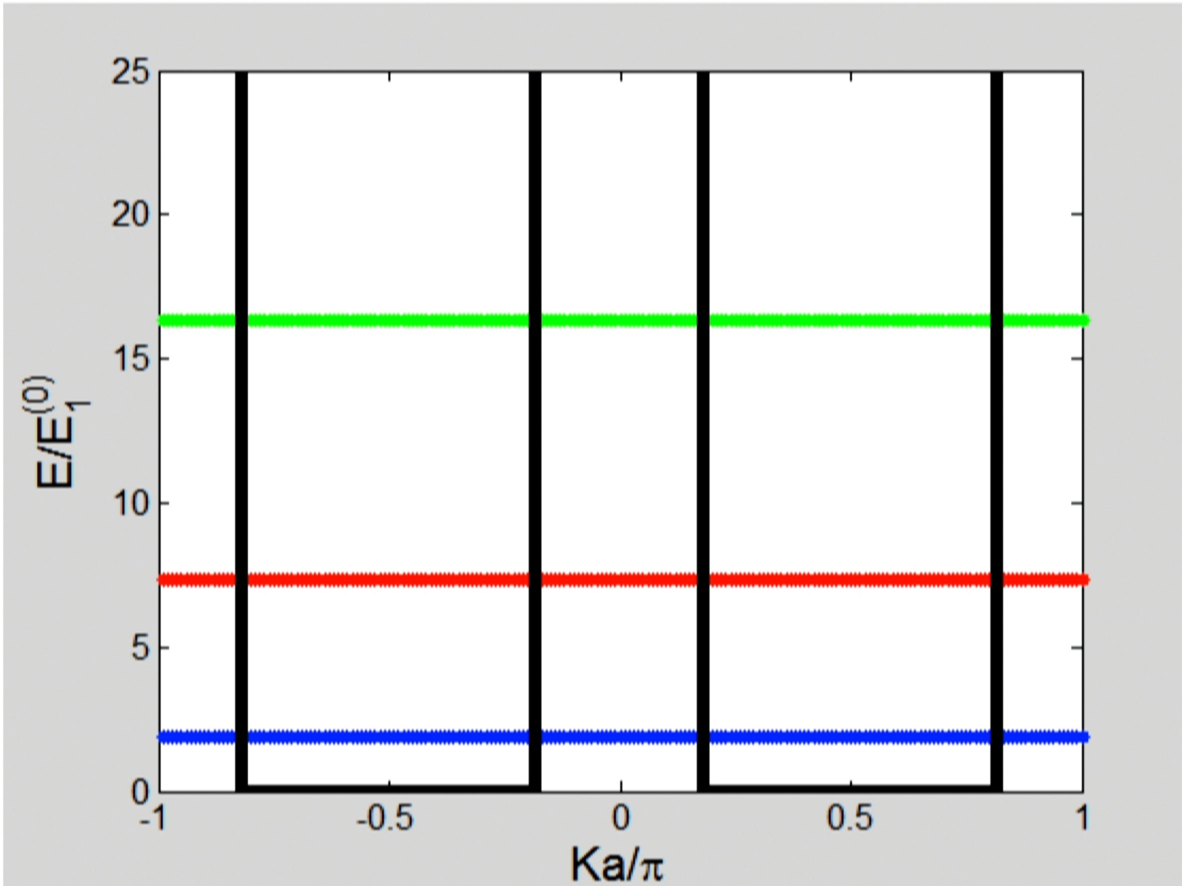
$V_0 = 40\ E_1^{(0)}$

Stick to 1D Change the barrier width



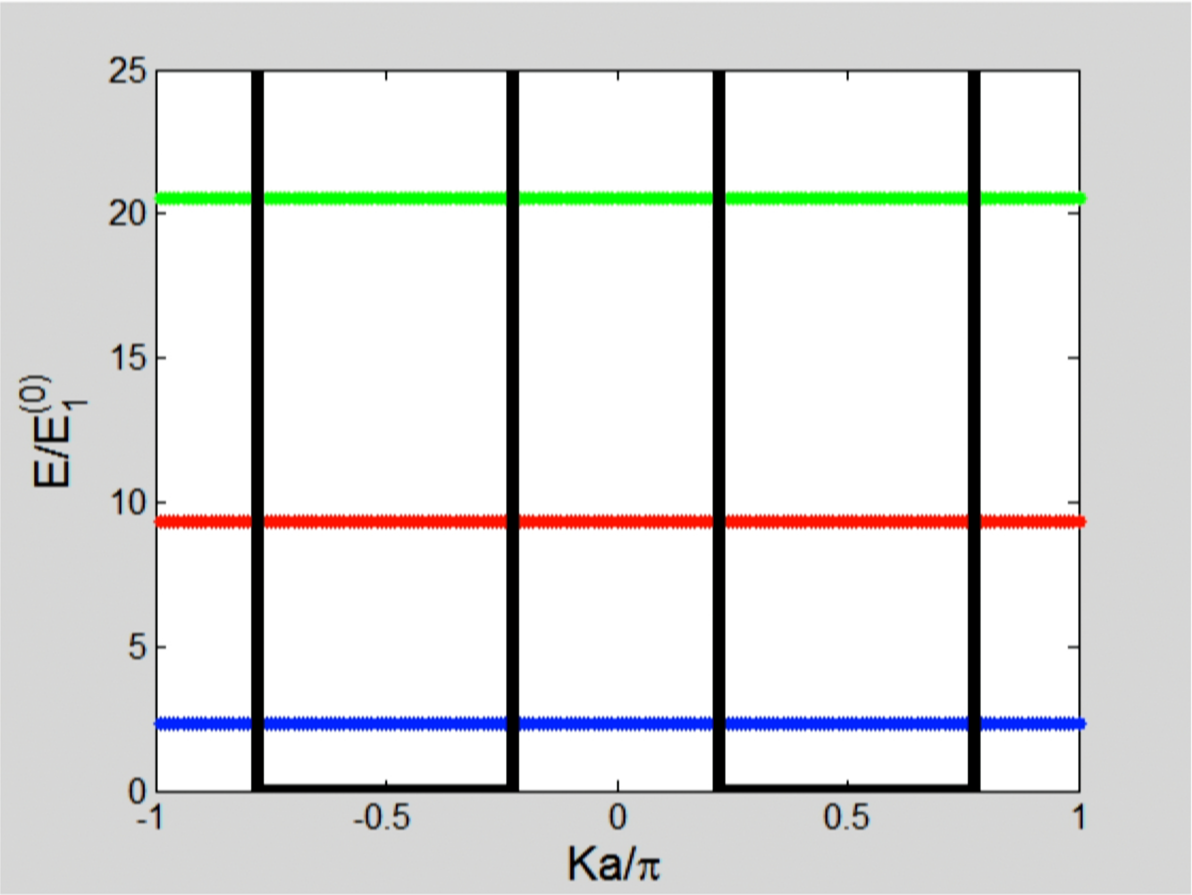
$V_0 = 40\ E_1^{(0)}$

Stick to 1D Change the barrier width



$V_0 = 40\ E_1^{(0)}$

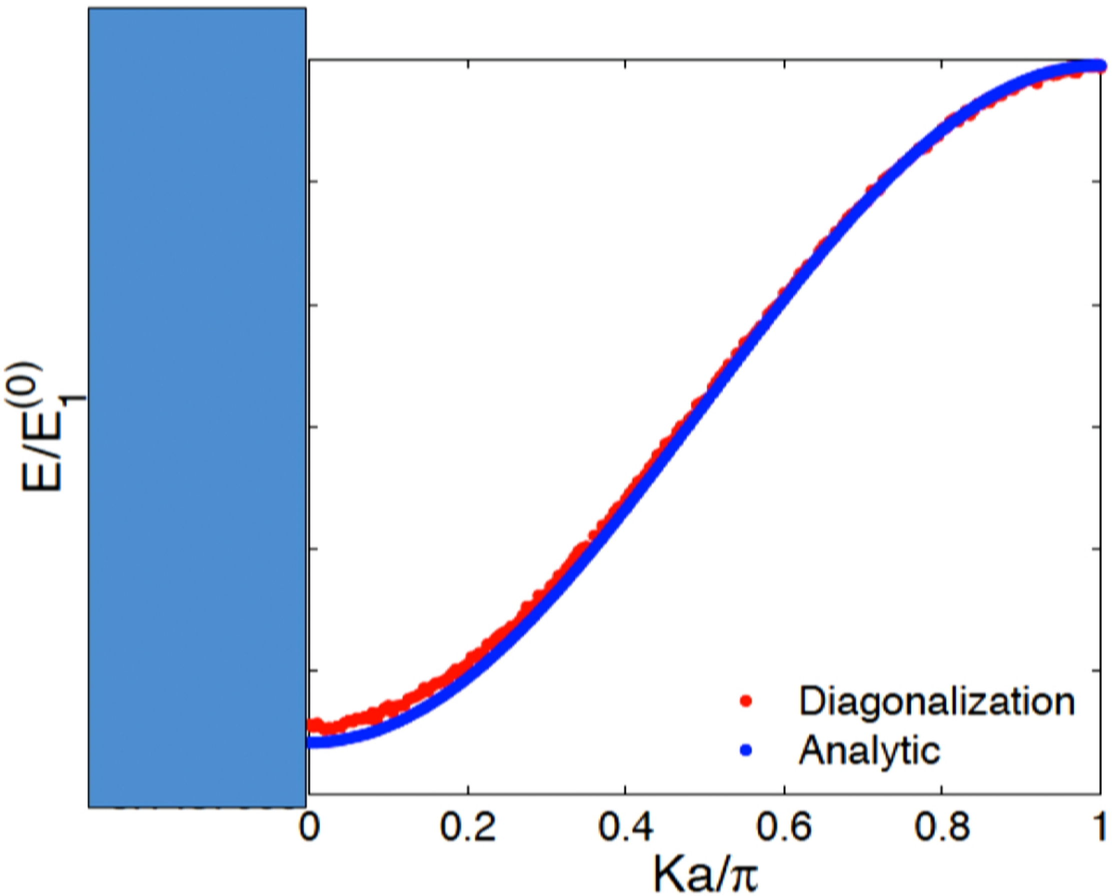
Stick to 1D Change the barrier width



$V_0 = 40\ E_1^{(0)}$

1D

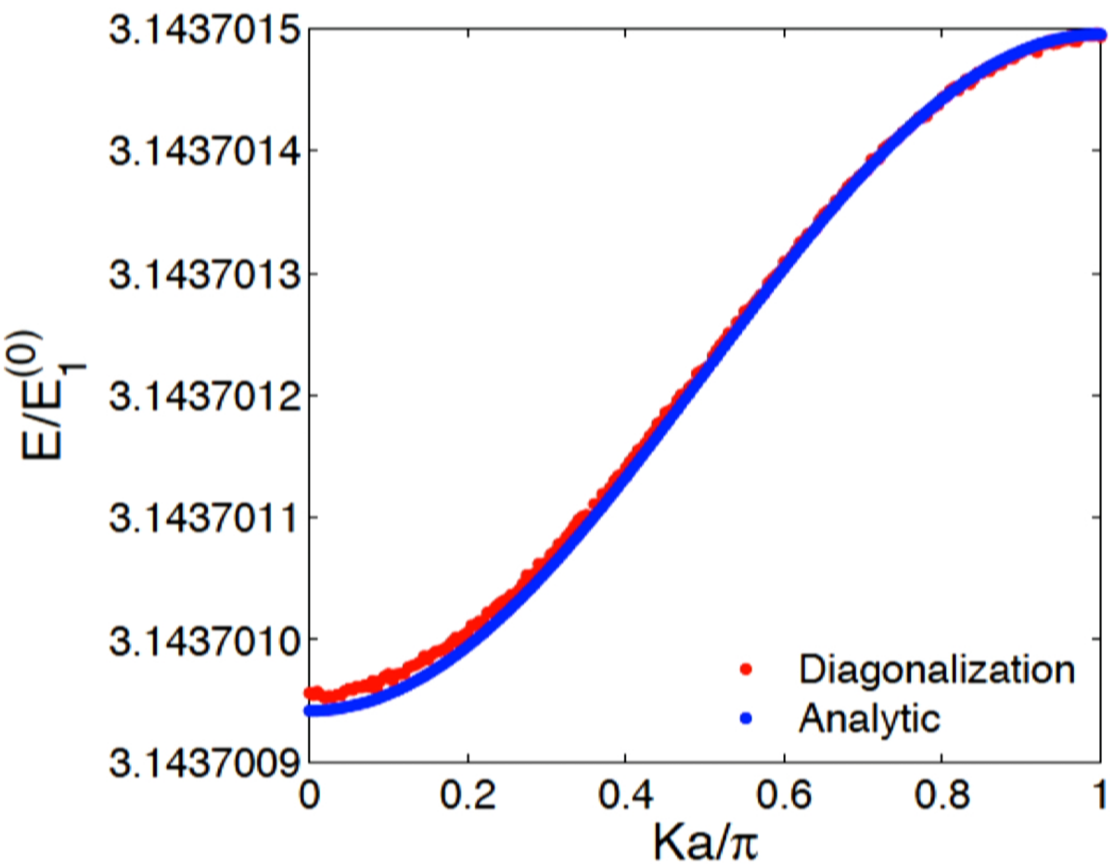
Pavelich thesis (unpublished)



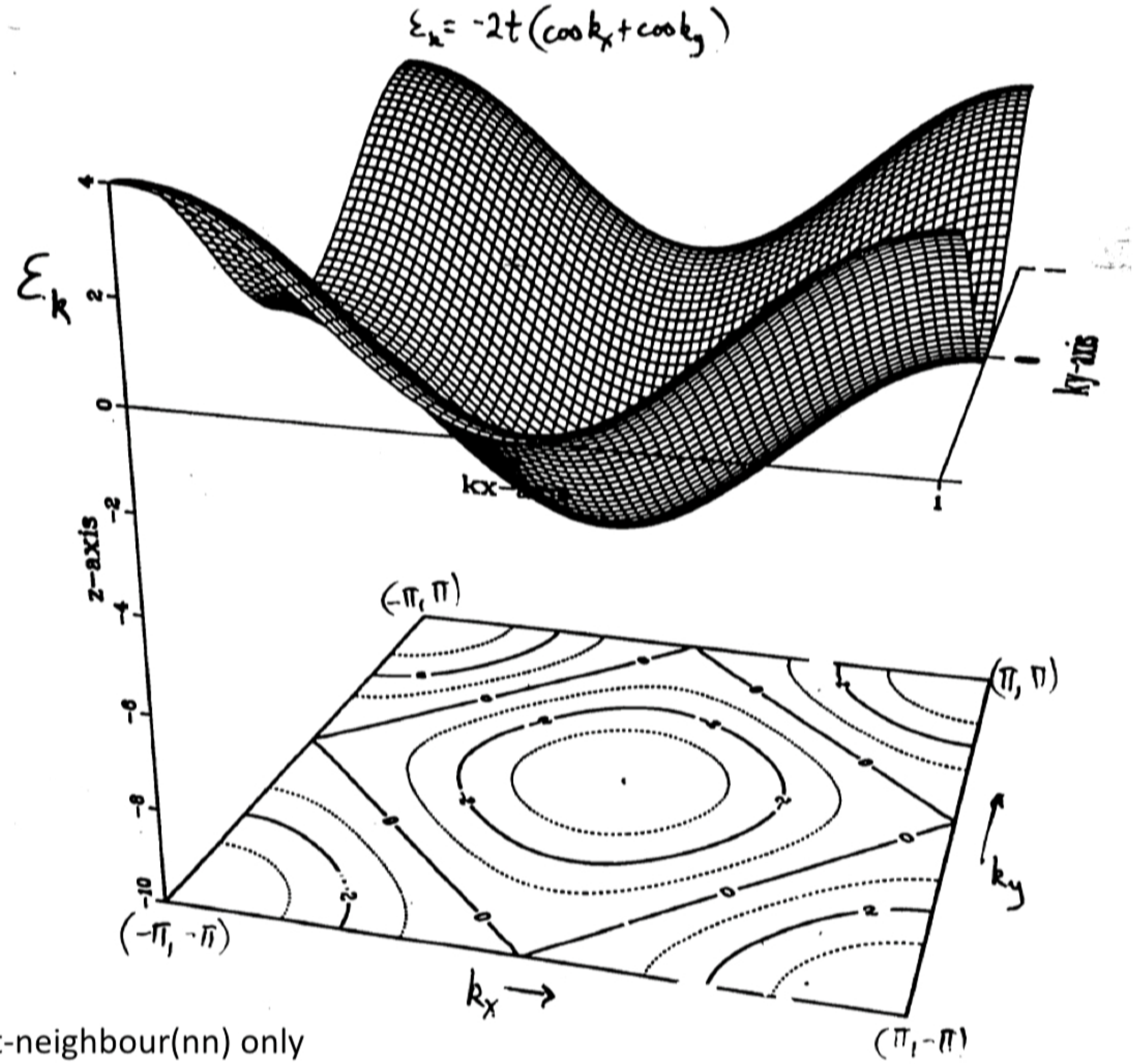
(f) $v_0 = 100,\ \alpha = 0.887$

1D

Pavelich thesis (unpublished)



(f) $v_0 = 100,\ \alpha = 0.887$

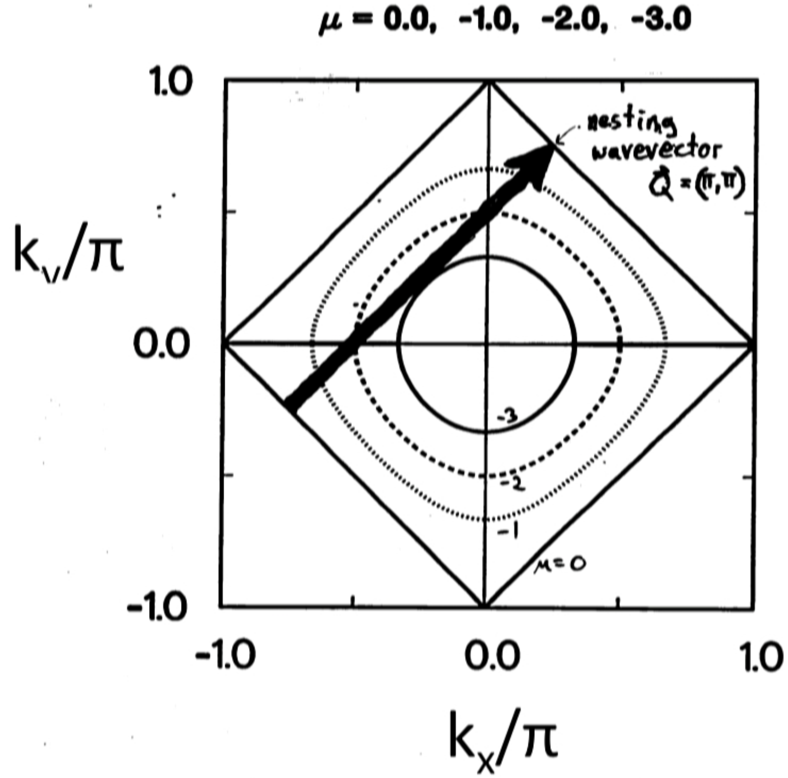


2D nearest-neighbour(nn) only

$t \equiv 1$

Nesting

ONE wavevector maps a large piece of the Fermi surface onto another large piece of the Fermi surface.



- actually not good for superconductivity
- good for charge density wave (CDW) or spin density wave (SDW)

$$g(E) = \int_{-\infty}^{+\infty} \left(\frac{dk}{2\pi}\right)^D \delta(E - E_k)$$

$$E_k = E_g + \frac{\hbar^2 k^2}{2m^*}$$

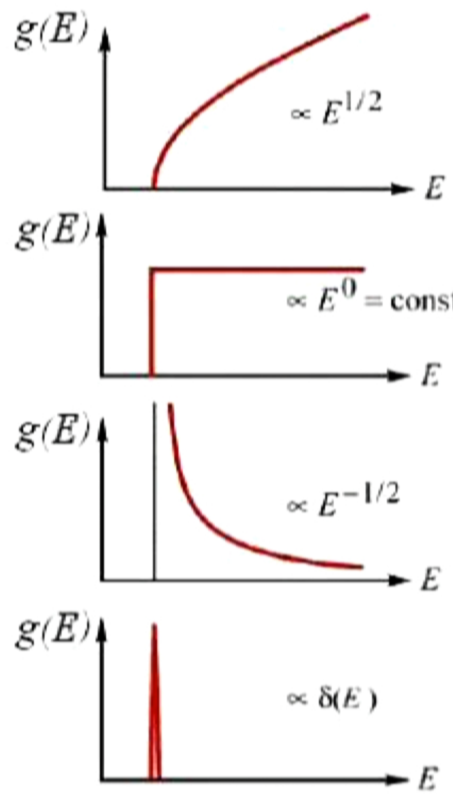
$$g(E) = \int_{-\infty}^{+\infty} \left(\frac{dk}{2\pi}\right)^{D} \delta(E - E_k)$$

3-D (bulk) $g(E) = \frac{1}{2\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{\frac{3}{2}}\sqrt{E_g - E}$

2-D (slab) $g(E) = \frac{m^*}{\pi\hbar^2}\sigma(E_g - E)$

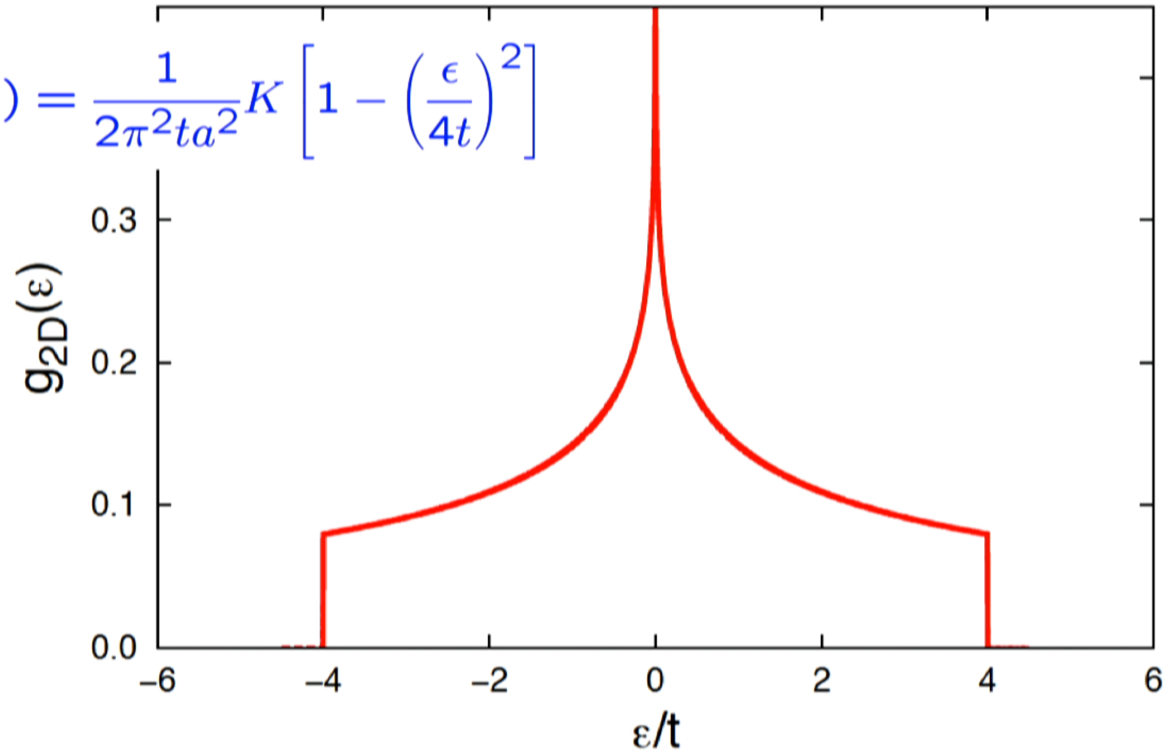
1-D (wire) $g(E) = \frac{m^*}{\pi\hbar}\sqrt{\frac{m^*}{2(E_g - E)}}$

0-D (dot) $g(E) = 2\delta(E_g - E)$



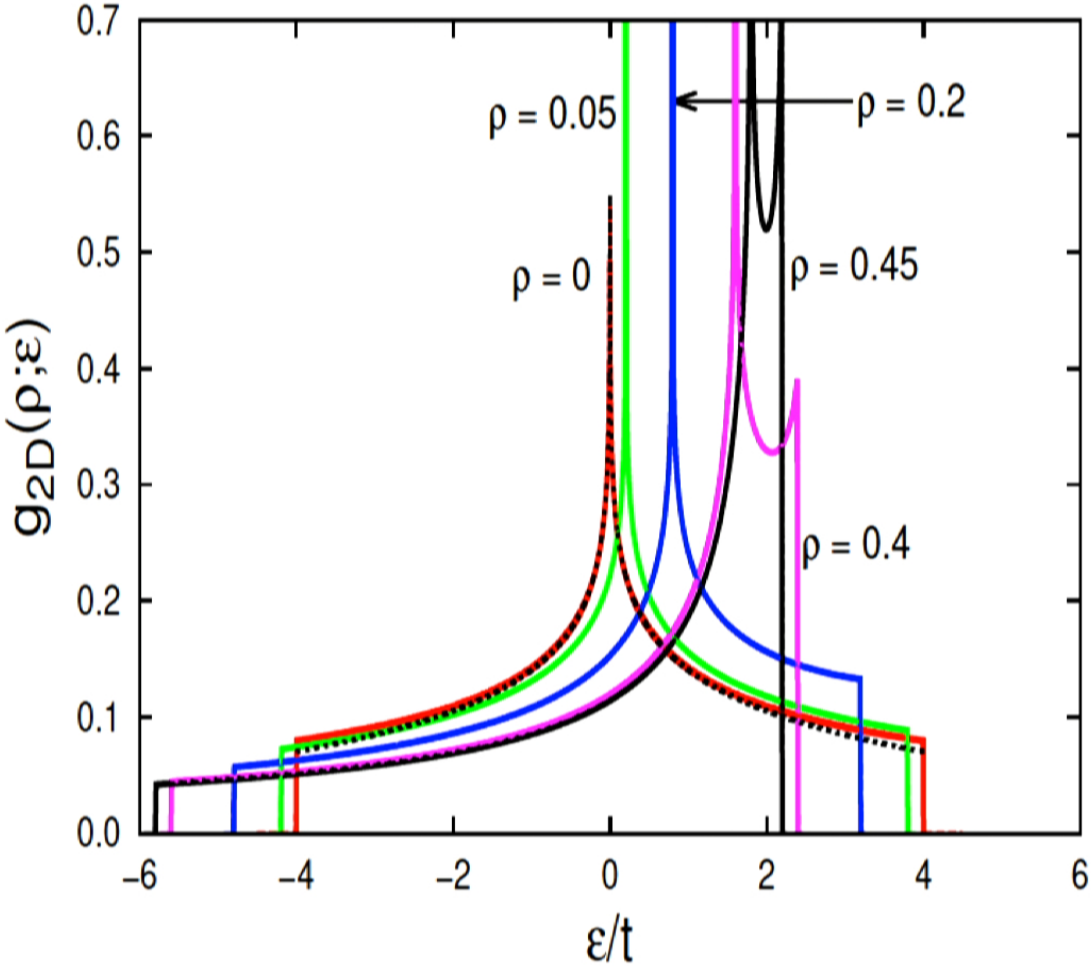
2D Density of States, with NN hopping ($t_2 = 0$)

$$g_{2D}(\epsilon) = \frac{1}{2\pi^2 t a^2} K\left[1 - \left(\frac{\epsilon}{4t}\right)^2\right]$$



2D Density of States, with , NNN hopping t_2 $\rho \equiv t_2/t$

$$\epsilon_k = -2t\,[\cos(k_x a) + \cos(k_y a)] - 4t_2 \cos(k_x a)\cos(k_y a)$$



Three Dimensions (NN)

$$\epsilon_k = -2t_s\left[\cos(k_x a) + \cos(k_y a) + \cos(k_z a)\right] \quad [\mathrm{sc}]$$

SC

$$\epsilon_k = -8t_b\left[\cos(\frac{k_x a}{2})\cos(\frac{k_y a}{2})\cos(\frac{k_z a}{2})\right] \quad [\mathrm{bcc}]$$

BCC

$$\epsilon_k = -4t_f\left[\cos(\frac{k_x a}{2})\cos(\frac{k_y a}{2}) + \cos(\frac{k_x a}{2})\cos(\frac{k_z a}{2}) + \cos(\frac{k_y a}{2})\cos(\frac{k_z a}{2})\right]$$

FCC

Three Dimensions

$$\epsilon_k = -2t_s\left[\cos(k_x a) + \cos(k_y a) + \cos(k_z a)\right]$$
$$-4t_{s2}\Big[\cos(k_x a)\cos(k_y a) + \cos(k_x a)\cos(k_z a) + \cos(k_y a)\cos(k_z a)\Big] \quad \text{[sc NNN]} \qquad \text{(A4)}$$

SC

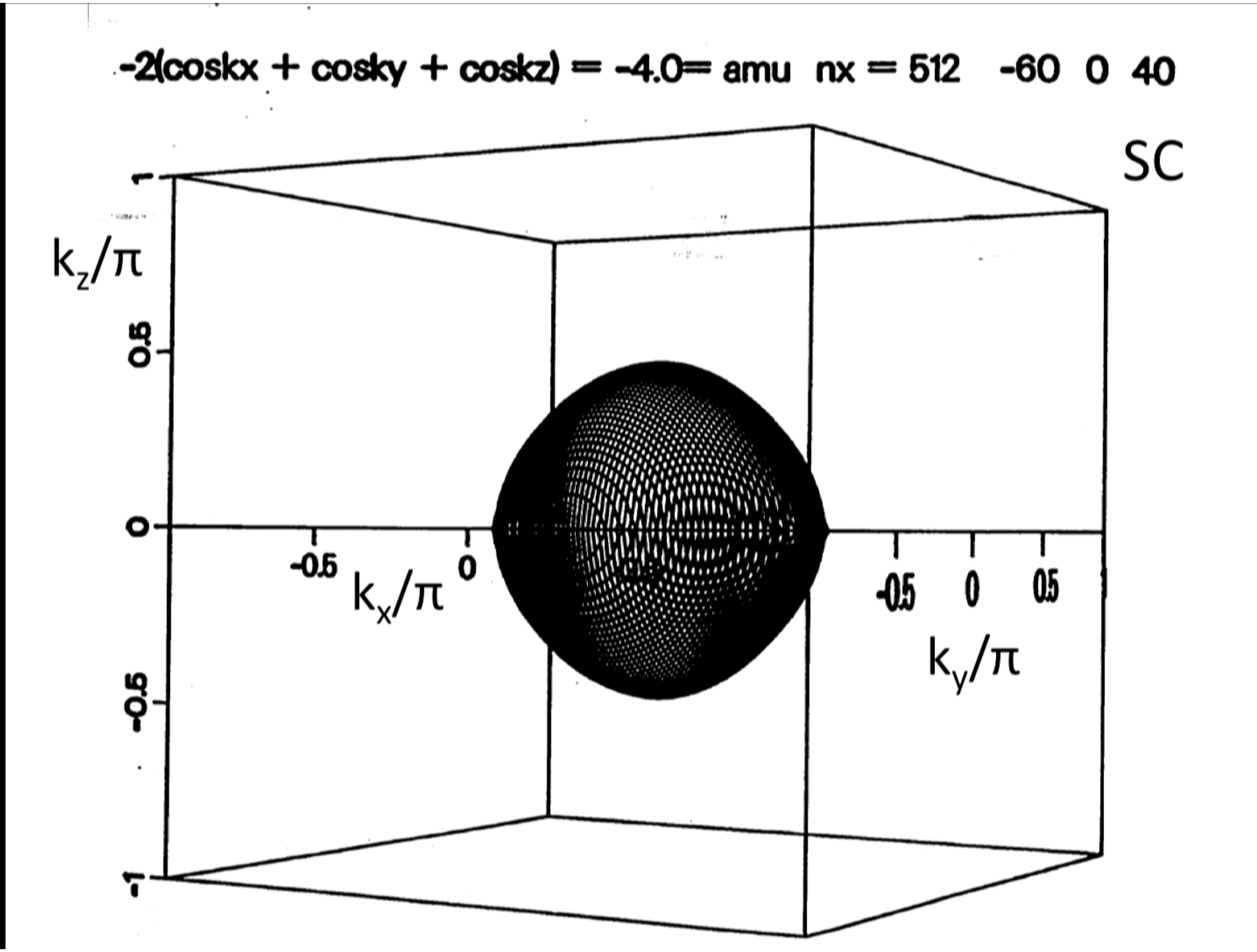
$$\epsilon_k = -8t_b\left[\cos(\frac{k_x a}{2})\cos(\frac{k_y a}{2})\cos(\frac{k_z a}{2})\right] \quad \text{[bcc NNN]}$$
$$-2t_{b2}\left[\cos(k_x a) + \cos(k_y a) + \cos(k_z a)\right] \qquad \text{(A5)}$$

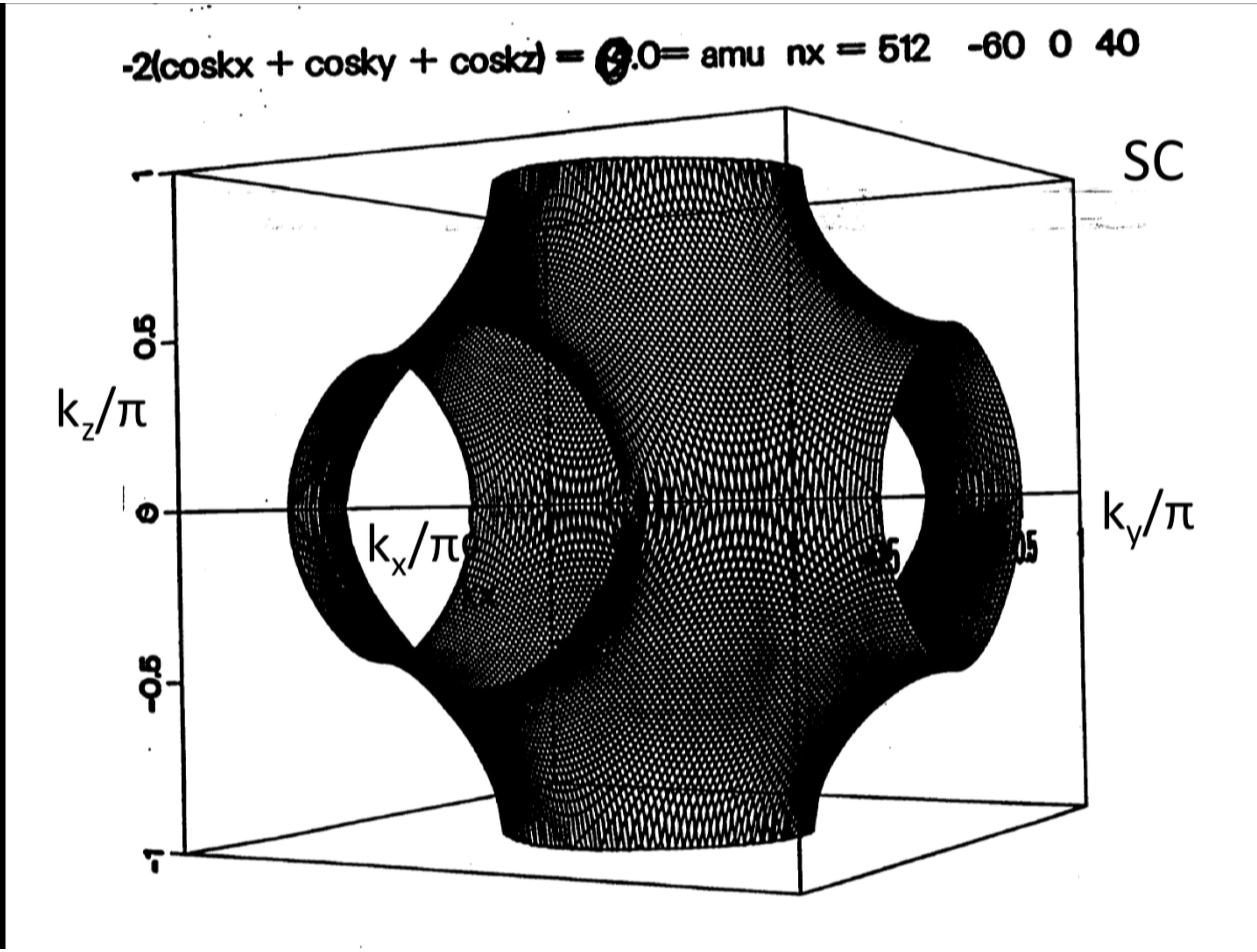
BCC

$$\epsilon_k = -4t_f\Big[\cos(\frac{k_x a}{2})\cos(\frac{k_y a}{2}) + \cos(\frac{k_x a}{2})\cos(\frac{k_z a}{2}) + \cos(\frac{k_y a}{2})\cos(\frac{k_z a}{2})\Big] \quad \text{[fcc NNN]}$$
$$-2t_{f2}\left[\cos(k_x a) + \cos(k_y a) + \cos(k_z a)\right]. \qquad \text{(A6)}$$

FCC

Dispersions?


-2(coskx + cosky + coskz) = -4.0= amu nx = 512 -60 0 40
SC
k_z/π
1
0.5
0
-0.5
-1
-0.5
0
k_x/π
-0.5
0
0.5
k_y/π


-2(coskx + cosky + coskz) =
.0= amu nx = 512 -60 0 40
SC
1
0.5
k_z/π
0
-0.5
-1
k_x/π
k_y/π

What do the densities of states look like?

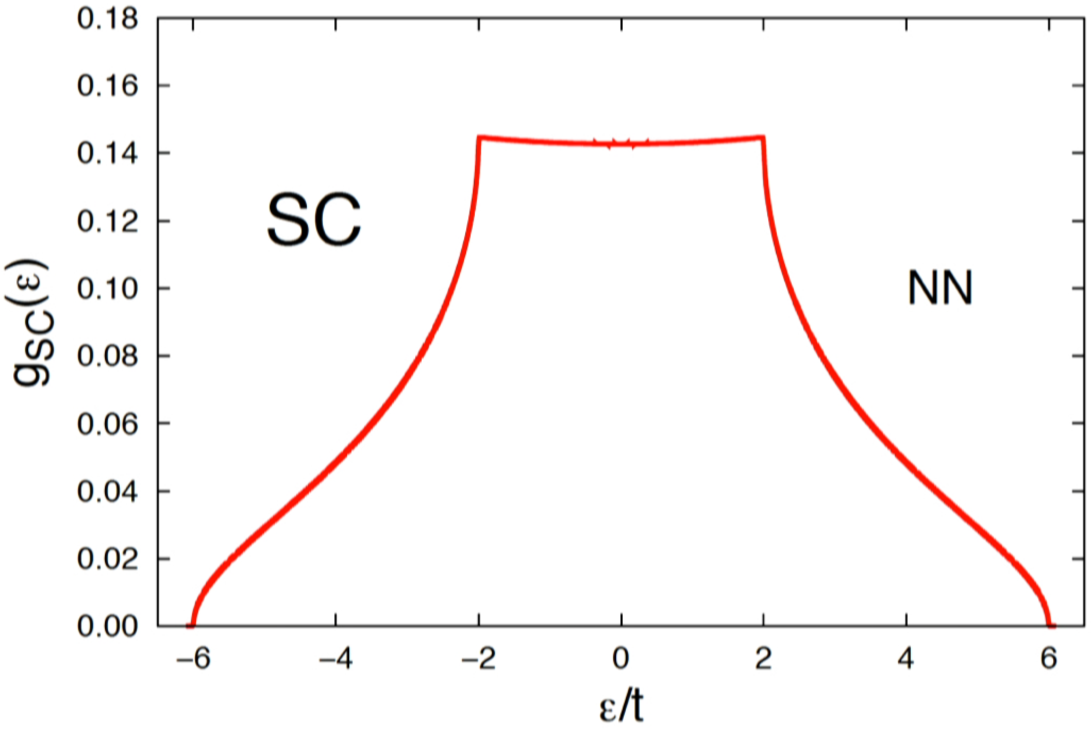
J. Phys. Chem. Solids Pergamon Press 1969. Vol. 30, pp. 609–626. Printed in Great Britain.

THE DENSITY OF STATES OF SOME SIMPLE EXCITATIONS IN SOLIDS

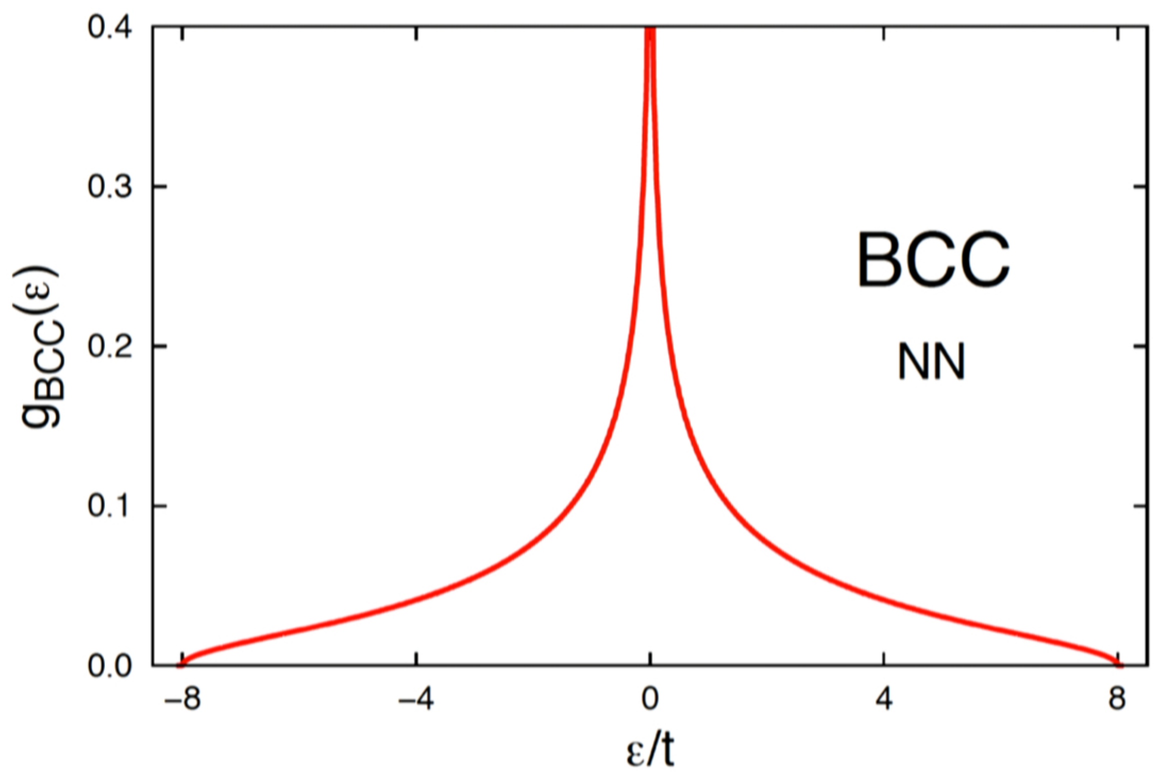
RAINER J. JELITTO
Institut für Theoretische Physik der Universität Kiel, Germany

(*Received* 4 *March* 1966)

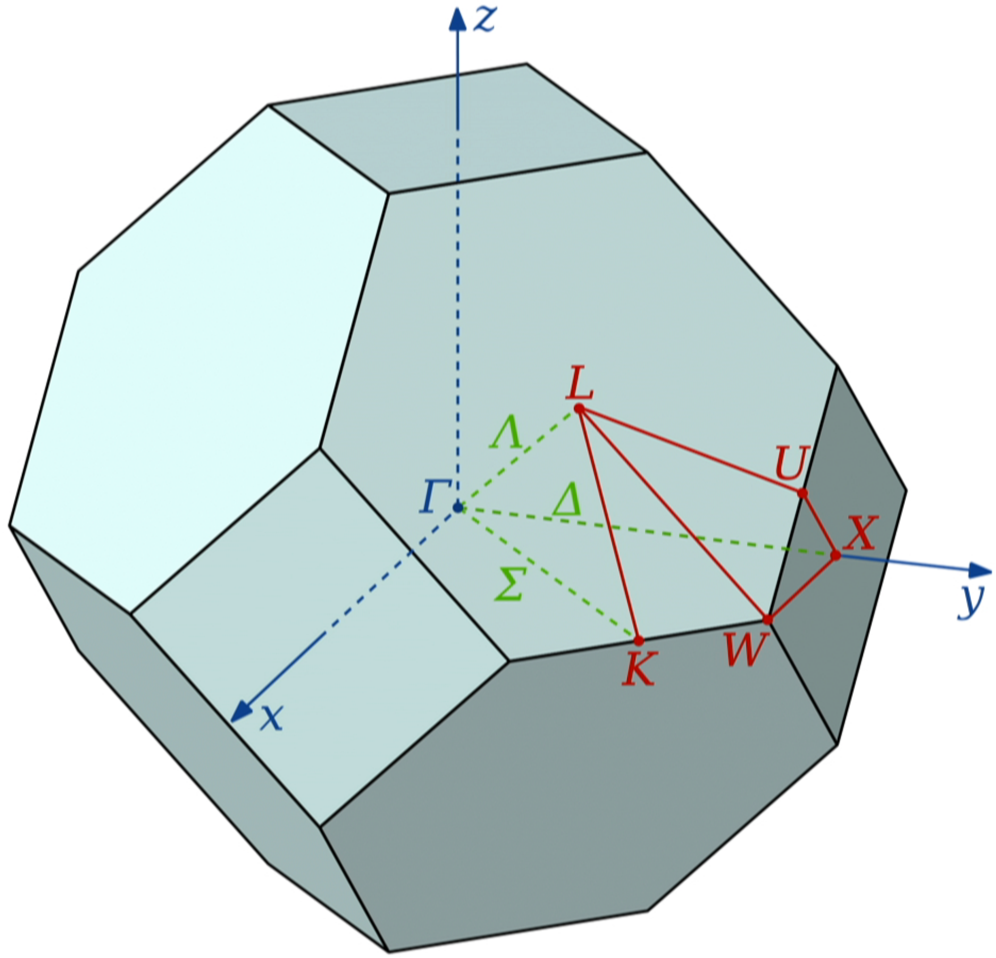
The nearest-neighbour (NN) cases:



The nearest-neighbour (NN) cases:



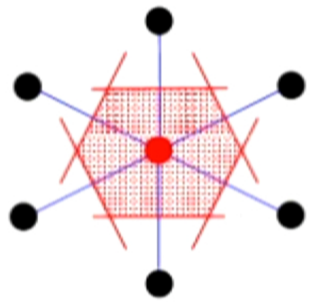
First Brillouin Zone for FCC



FIRST BRILLOUIN ZONES

The Wigner-Seitz cell of the reciprocal lattice is called the first Brillouin zone (FBZ).

Wigner-Seitz cell: primitive cell with lattice point at its center

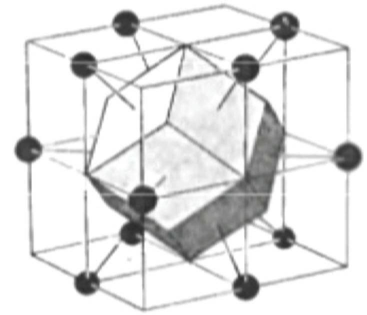


enclosed region is W-S cell for 2D hexagonal lattice

d.l. FCC
r.l. BCC
1st Brillouin zone:

truncated octahedron

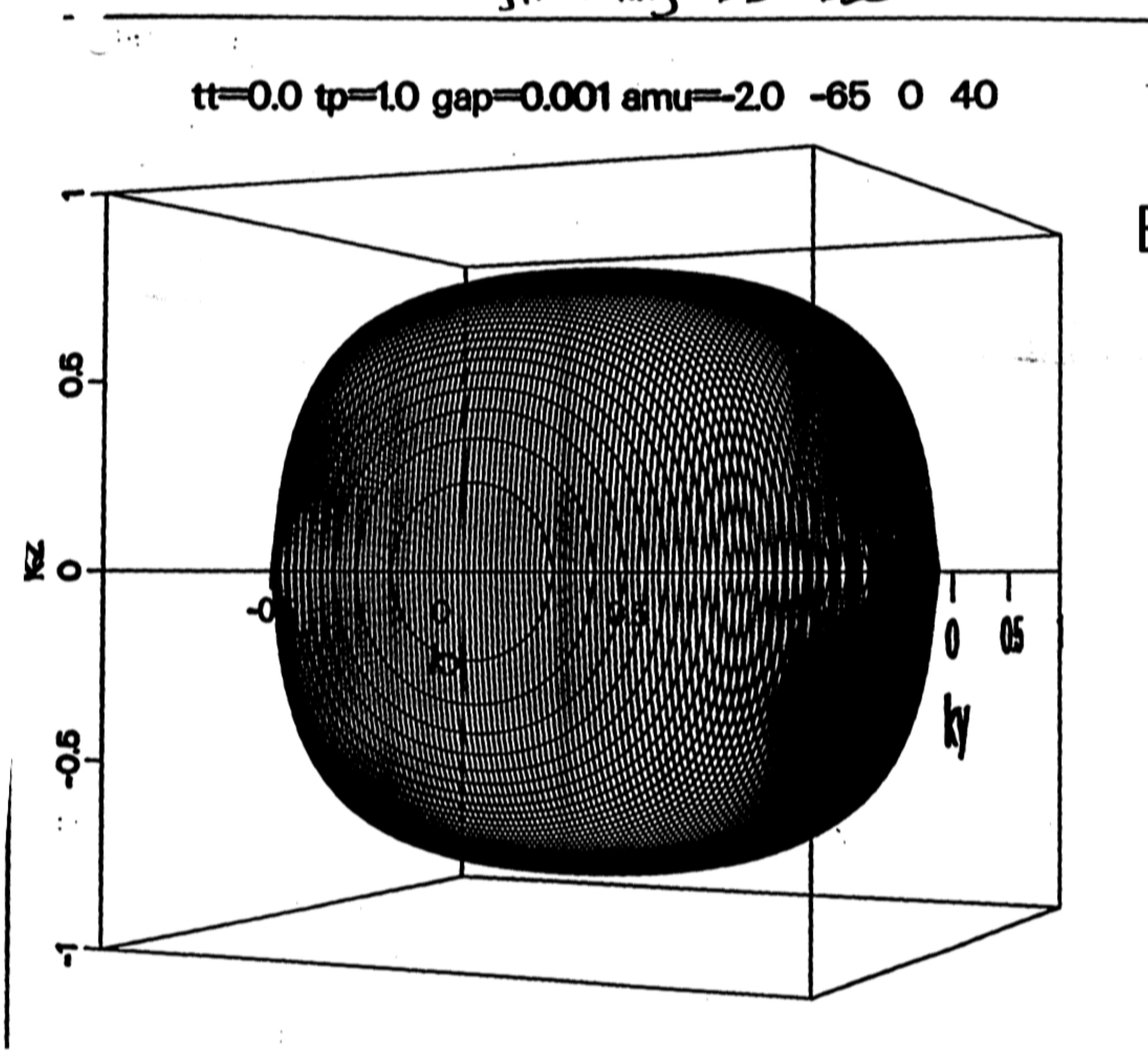
d.l. BCC
r.l. FCC
1st Brillouin zone:



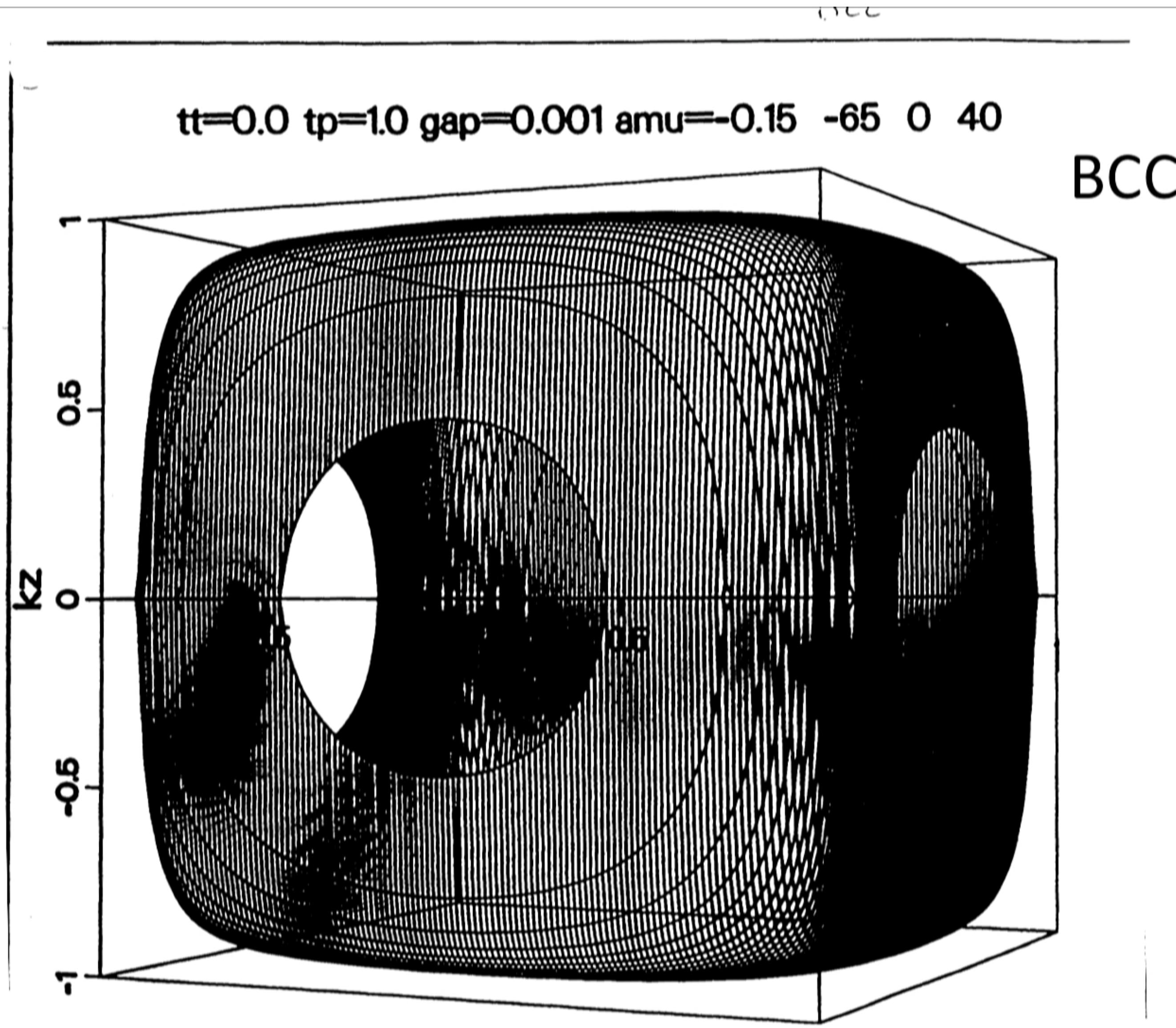
rhombic dodecahedron

268

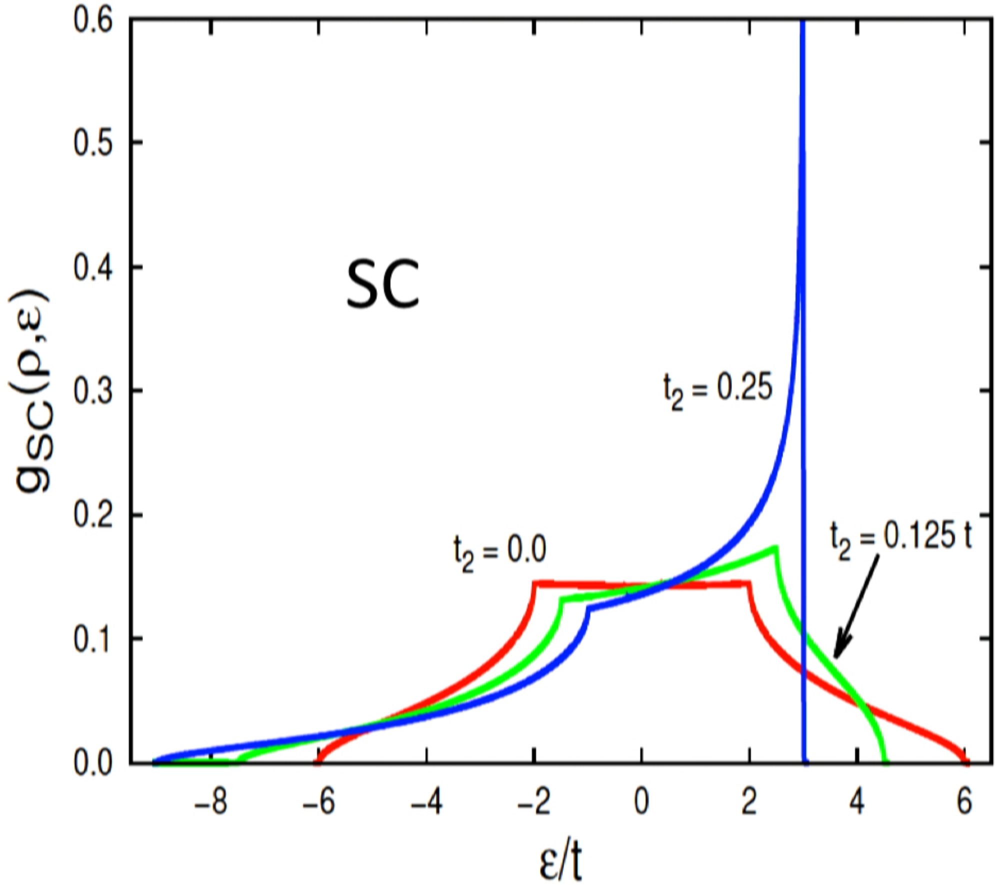
Tight-binding 3D BCC



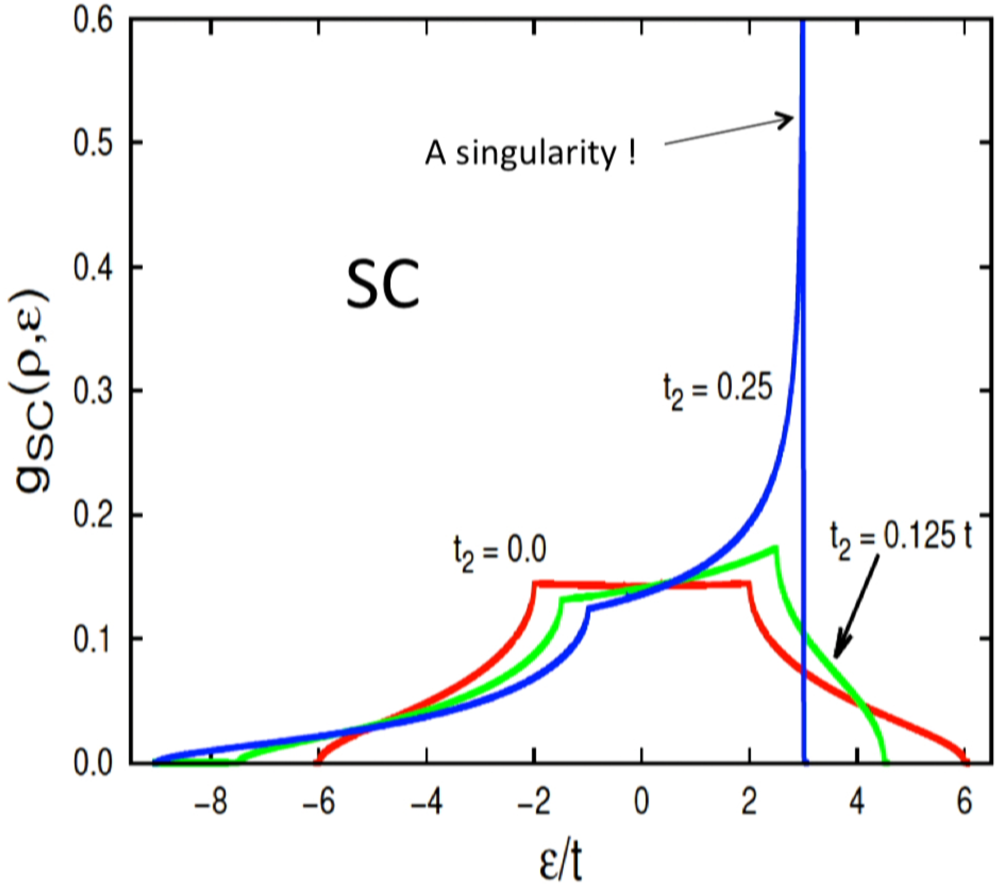
BCC


tt=0.0 tp=1.0 gap=0.001 amu=-0.15 -65 0 40
BCC
kz
1
0.5
0
-0.5
-1

What does next-nearest neighbour (NNN) hopping do to the densities of states?



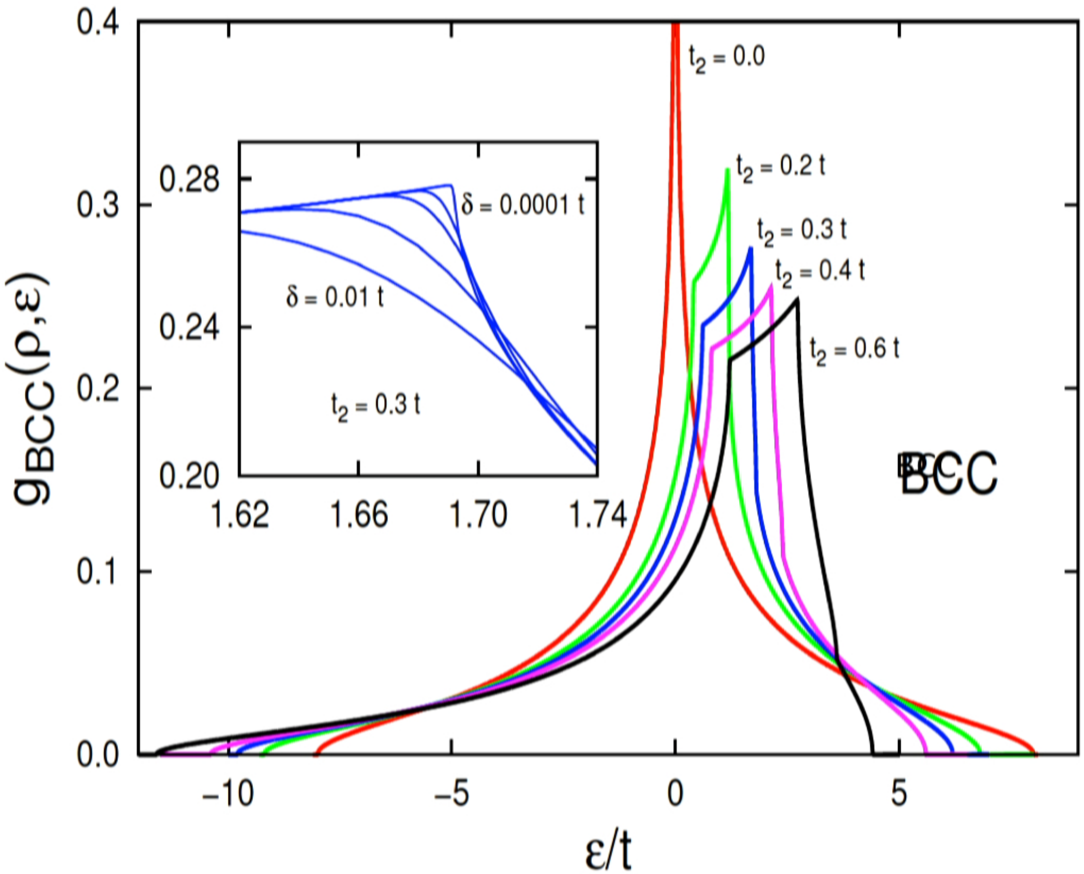
What does next-nearest neighbour (NNN) hopping do to the densities of states?



What does next-nearest neighbour (NNN) hopping do to the densities of states?

BCC

What does next-nearest neighbour (NNN) hopping do to the densities of states?



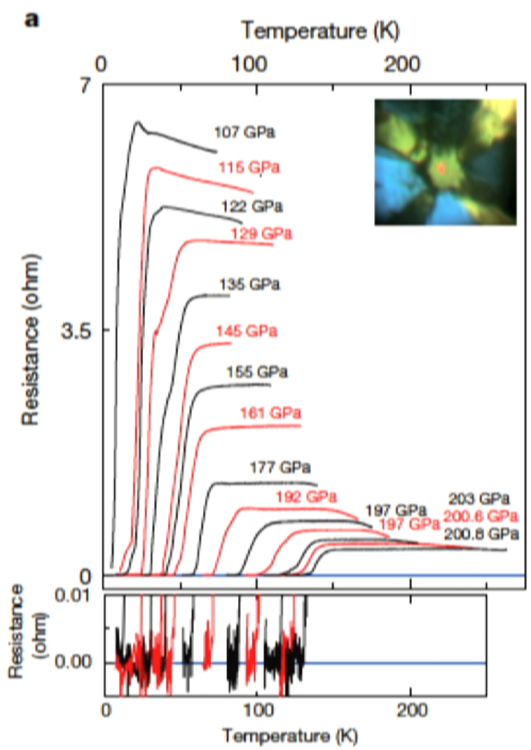
What does next-nearest neighbour (NNN) hopping do to the densities of states?

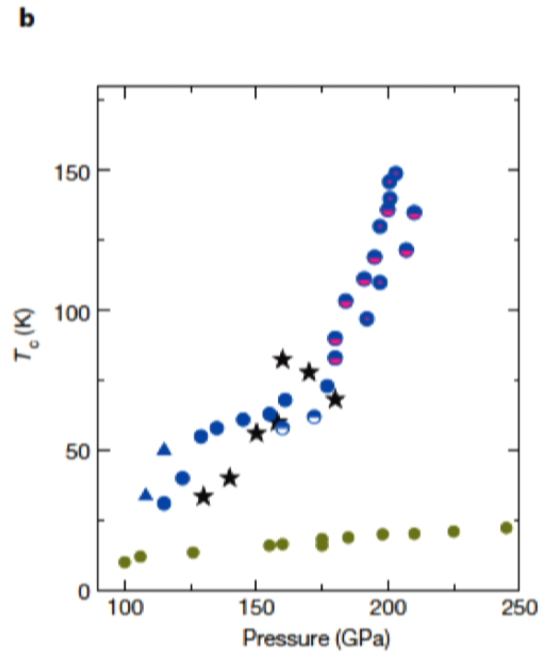
FCC

doi:10.1038/nature14964

Conventional superconductivity at 203 kelvin at high pressures in the sulfur hydride system

A. P. Drozdov[1]*, M. I. Eremets[1]*, I. A. Troyan[1], V. Ksenofontov[2] & S. I. Shylin[2]

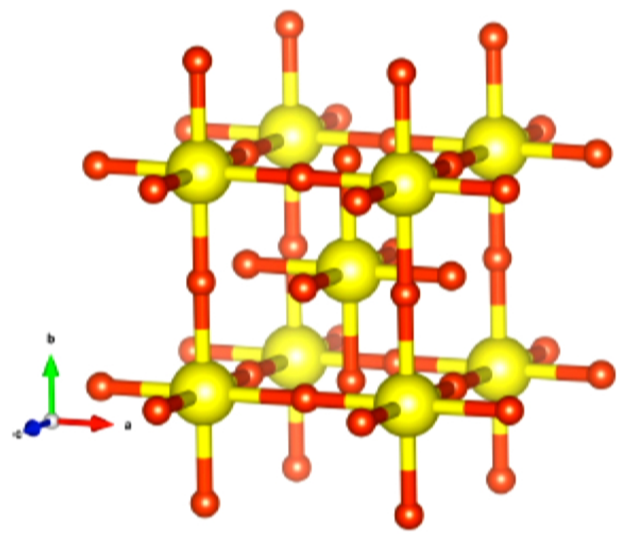




PHYSICAL REVIEW B **93**, 104526 (2016)

Van Hove singularities and spectral smearing in high-temperature superconducting H_3S

Yundi Quan and Warren E. Pickett*
Department of Physics, University of California Davis, Davis, California 95616, USA
(Received 3 September 2015; published 25 March 2016)



A. Importance of sulfur

FIG. 1. Crystal structure of $Im\bar{3}m$ H_3S. Nearest neighbor S-H bonds are shown. At this nearest neighbor level, the structure consists of two interleaved ReO_3 sublattices, displaced relative to one another by the body-centering vector $(1,1,1)a/2$.

See also Sano et al. Phys.Rev. B93, 094525-1-16 (2016)

PHYSICAL REVIEW B **93**, 104526 (2016)

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singularities at energies $\epsilon_{lo} < \epsilon_{hi}$

$$N(E) = \begin{cases} a_1\sqrt{|b_1 - \epsilon|} + c_1\epsilon + d_1 & \epsilon < \epsilon_{lo} \\ a_2\epsilon + b_2 & \\ a_3\sqrt{|\epsilon + b_3|} + c_3\epsilon + d_3 & \end{cases}$$

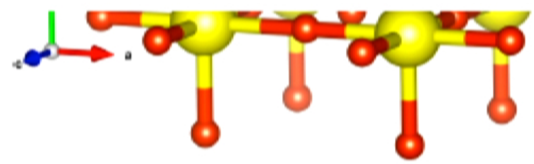

FIG. 1. Crystal structure of $Im\bar{3}m$ H_3S. Nearest bonds are shown. At this nearest neighbor level, the str of two interleaved ReO_3 sublattices, displaced relative by the body-centering vector $(1,1,1)a/2$.

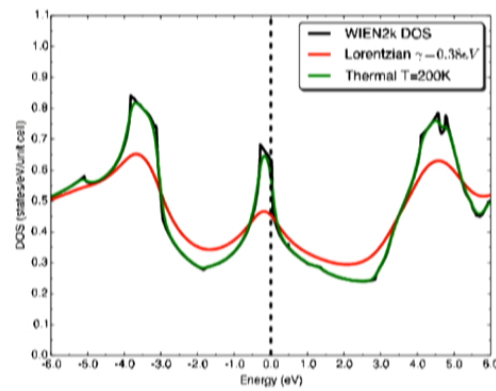

FIG. 8. H_3S density of states without broadening (black line, Wien2k DOS), with thermal broadening at 200 K (green line, which is hard to distinguish from the unbroadened one), and the virtual phonon broadened effective DOS $N(E)$ using a Lorentzian halfwidth of 0.38 eV (red line). Note the large drop in the value at the Fermi energy (dashed vertical line).

See also Sano et al. Phys.Rev. B93, 094525-1-16 (2016)