

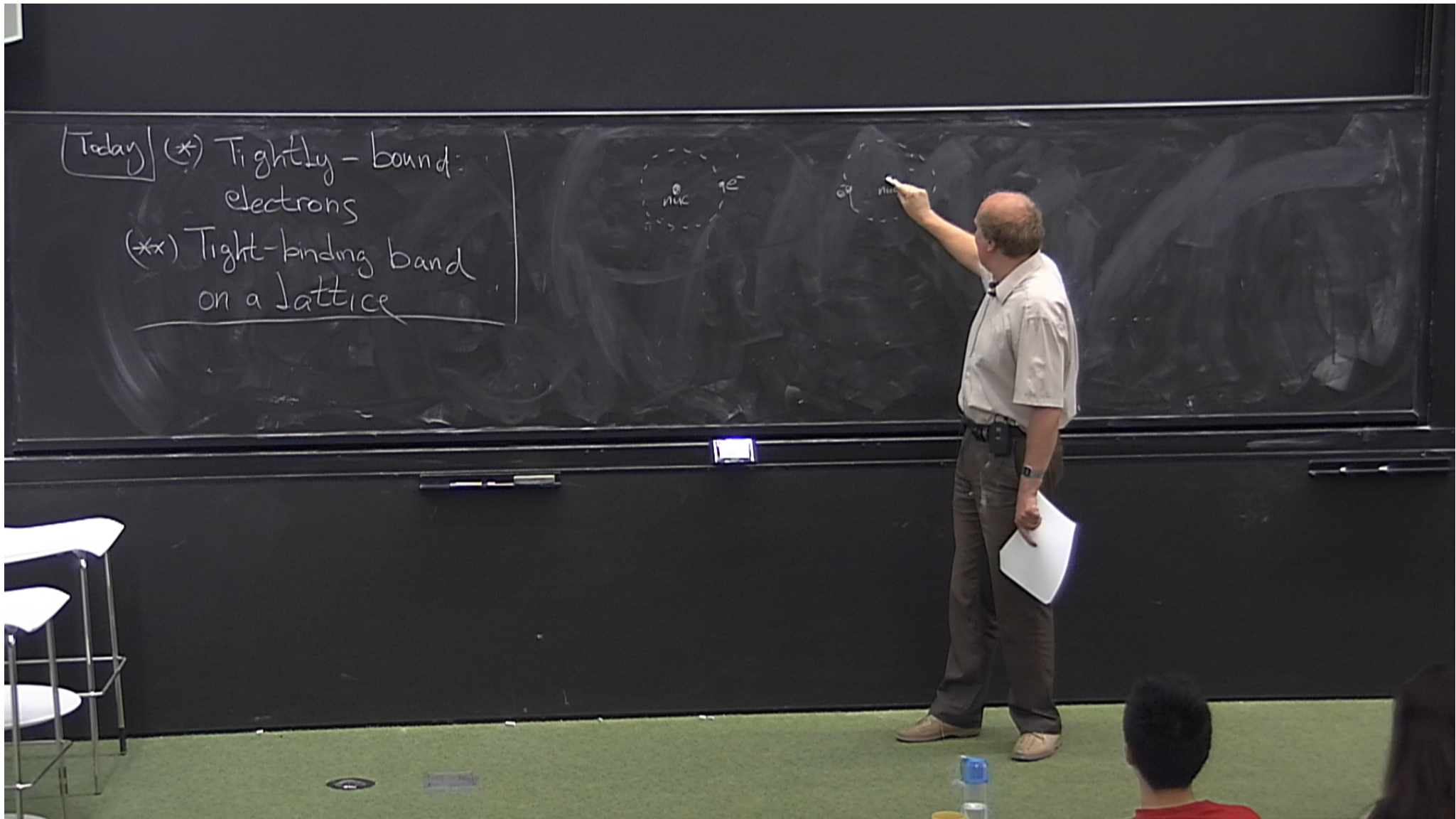
Title: Condensed Matter 101 - Lecture 4

Date: Aug 30, 2012 10:30 AM

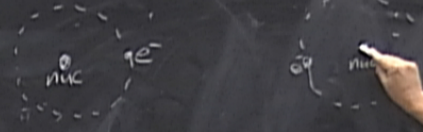
URL: <http://pirsa.org/12080035>

Abstract:

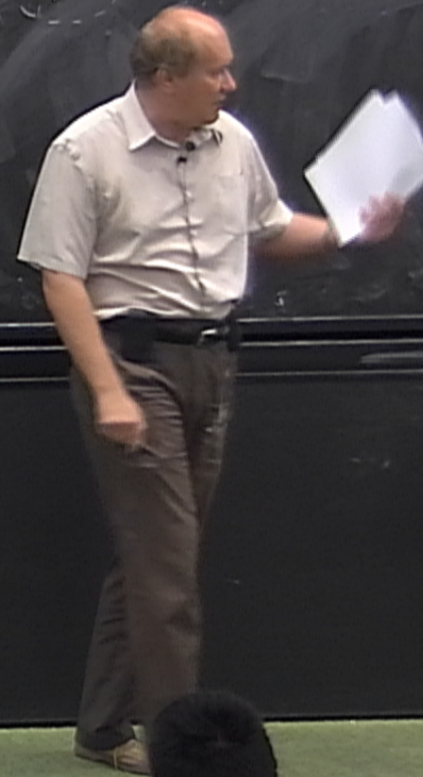
Today (*) Tightly-bound
electrons
(**) Tight-binding band
on a lattice



Today (*) Tightly-bound
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(xx) Tight-binding band
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$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + \sum_n$$

1D system

n labels the sites
 $x = na$

[Today] (*) Tightly-bound electrons

(xx) Tight-binding band on a lattice


$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + \underbrace{\sum_n V(x-na)}_{V(x)} \psi(x) = \epsilon \psi(x)$$

1D system

n labels the sites
 $R-na$

Today (*) Tightly-bound electrons
 (xx) Tight-binding band on a lattice

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + \sum_n V(x-na) \psi(x) = E \psi(x)$$

1D system

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fast $|x| > a$

Today (*) Tightly-bound electrons

(xx) Tight-binding band on a lattice

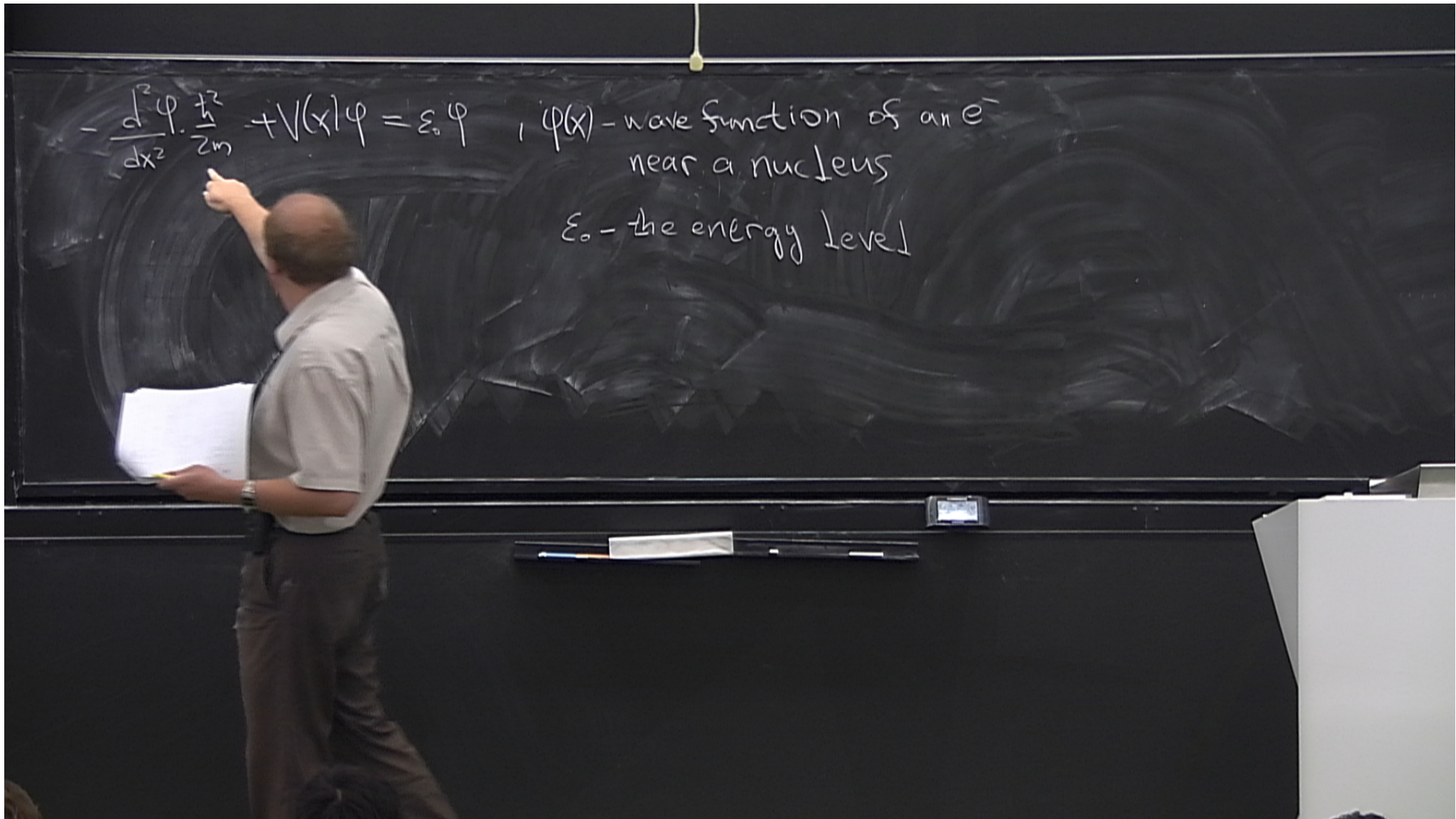

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + \sum_n \underbrace{V(x-na)}_{V(x)} \psi(x) = \epsilon \psi(x)$$

$V(x)$ decays very fast $|x| > a$

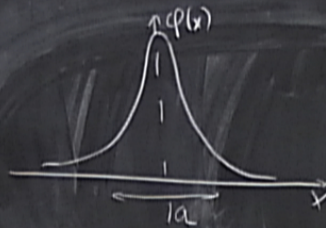
1D system

n labels the sites
 $R-na$





$$-\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} + V(x) \psi = \epsilon_0 \psi, \quad \psi(x) - \text{wave function of an } e^- \text{ near a nucleus}$$



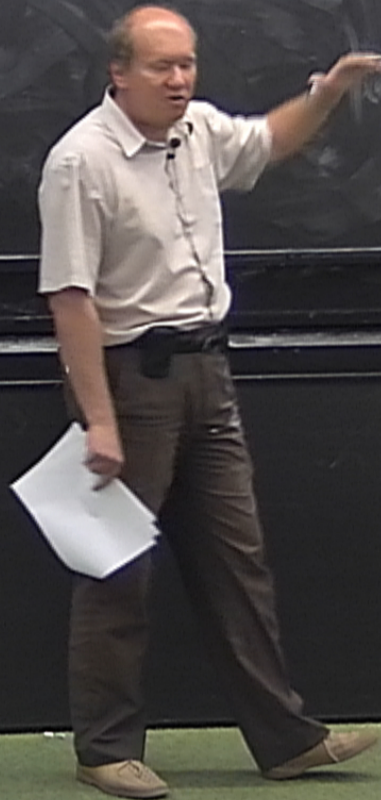
ϵ_0 - the energy level

We need to solve: $-\frac{\hbar^2}{2m} \frac{d^2 \Psi}{dx^2} + \sum_n V(x-na) \Psi(x) = E \Psi(x)$

$\Psi(x)$ are the Bloch's functions, $\Psi_k(x) = e^{ikx} u_k(x)$, $u_k(x) = u_k(x+a)$

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no band index!



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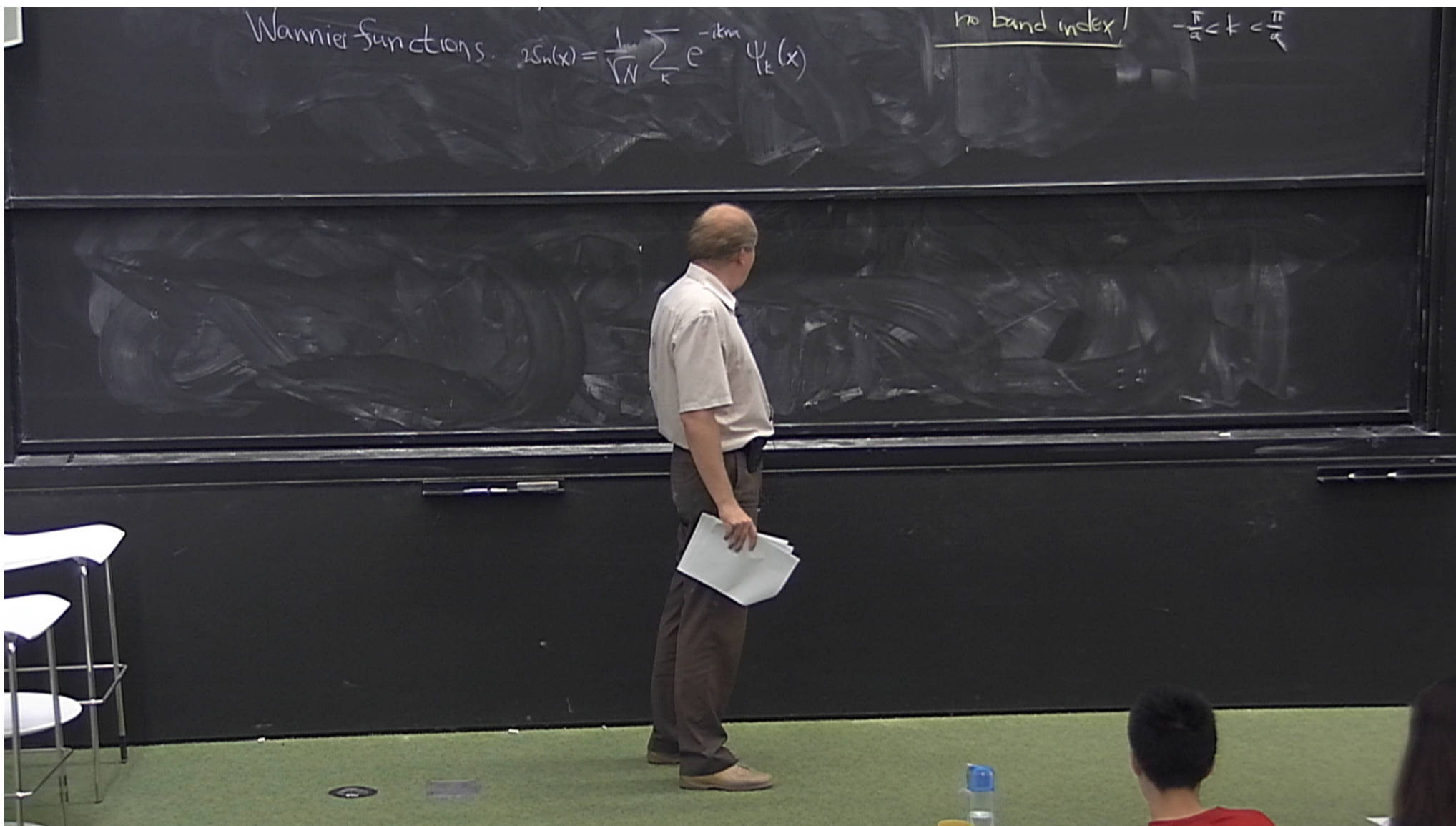
Wannier function

no band index! $-\frac{\pi}{a} < k < \frac{\pi}{a}$

Wannier functions. $\psi_n(x) = \frac{1}{\sqrt{N}} \sum_k e^{-ikn} \psi_k(x)$

no band index!

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Some properties of Wannier functions (1) $\psi_k(x) = \frac{1}{\sqrt{N}}$

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Some properties of Wannier functions

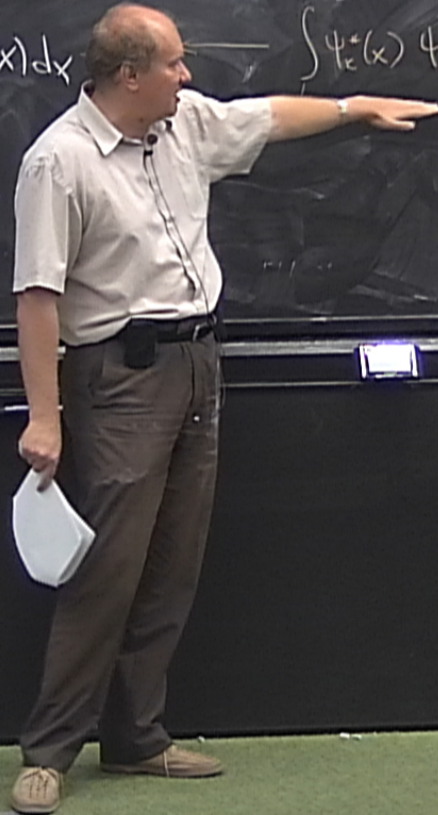
$$(i) \quad \psi_k(x) = \frac{1}{\sqrt{N}} \sum_n e^{ikna} w_n(x) \leftarrow \text{checked using } \sum_n e^{i(k-k')na} = N \delta_{k,k'}$$

$$(ii) \quad \int_L w_n^*(x) w_m(x) dx = \delta_{n,m}$$

Some properties of Wannier functions

(i) $\psi_k(x) = \frac{1}{\sqrt{N}} \sum_n e^{ikna} \psi_n(x) \leftarrow \text{checked using } \sum_n e^{i(k-k')na} = N \delta_{k,k'}$

(ii) $\int_L \psi_n^*(x) \psi_m(x) dx = \delta_{n,m}$ $\int_L \psi_k^*(x) \psi_{k'}(x) dx = \delta_{k,k'}$



$w_n(x)$ is not very close to 0 only near $x=na$ — follows from $w_n(x) = \frac{1}{\sqrt{N}} \sum_F e^{ik(x-na)} u_k(x)$

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We need to solve: $-\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} + \sum_n V(x-na) \psi(x) = \epsilon \psi(x)$

$\psi(x)$ are the Bloch's functions, $\psi_k(x) = e^{ikx} u_k(x)$, $u_k(x) = u_k(x+a)$

Wannier functions: $w_n(x) = \frac{1}{\sqrt{N}} \sum_k e^{-ikna} \psi_k(x)$ no band index! $-\frac{\pi}{a} < k < \frac{\pi}{a}$

Some properties of Wannier functions (i) $\psi_k(x) = \frac{1}{\sqrt{N}} \sum_n e^{ikna} w_n(x)$ ← checked using

(ii) $\int_L w_n^*(x) w_m(x) dx = \delta_{n,m}$ ← $\int_L \psi_k^*(x) \psi_{k'}(x) dx = \delta_{k,k'}$ $\sum_n e^{i(k-k')na} = N \delta_{k,k'}$

iii) $w_n(x)$ is not very close to 0 only near $x=na$ — follows from $w_n(x) = \frac{1}{\sqrt{N}} \sum_F e^{i(x-na)} u_F(x)$

Substitute: $\sum_n \left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x-na) \right) e^{ikna} w_n(x) + \sum_n [U(x$

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$$\sum_n \left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x-na) \right) e^{ikna} \psi_n(x) + \sum_n [U(x) - V(x-na)] e^{ikna} \psi_n(x) = E(k) \sum_n e^{ikna} \psi_n(x)$$

iii) $w_n(x)$ is not very close to 0 only near $x=na$ — follows from $w_n(x) = \frac{1}{\sqrt{N}} \sum_F e^{i(x-na)} u_k(x)$

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formally small $\Rightarrow$ considered
as a perturbation

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$$U(x) - V(x-na) = \sum_m V(x-ma) - V(x-na)$$

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$$\psi_n(x) = \psi_n^{(0)}(x) + \psi_n^{(1)}(x) + \dots$$

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We need to solve: $-\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} + \sum_n V(x-na) \psi(x) = \epsilon \psi(x)$

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$$\sum_n \left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x-na) - \epsilon \right) \psi_n^{(1)}(x) e^{ikna} = \underbrace{(\epsilon(k) - \epsilon_0)}_{\epsilon^{(1)}(k)} \sum_n e^{ikna} \psi(x-na) - \sum_n h_n(x) e^{ikna} \psi(x-na)$$

(iii) $\psi_n(x)$ is not very close to 0 only near $x=na$ ← follows from $\psi_n(x) = \frac{1}{\sqrt{N}} \sum_k e^{ik(x-na)} u_k(x)$

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Multiply by $\psi^*(x)$ and integrate $\int dx$

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Multiply by $\psi^*(x)$ and integrate $\int dx$

$$\text{LHS of } (x) = \int dx \psi^*(x) \sum_n \left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \right)$$

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$$\begin{aligned} \text{LHS of } (x) &= \int dx \psi^*(x) \sum_n \left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x-na) - \epsilon_0 \right) w_n^{(1)}(x) e^{ikna} dx = \\ &= \int dx w_n^{(1)*}(x) \sum_n \left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} - \epsilon_0 + V(x-na) \right) \psi^*(x) e^{ikna} dx \end{aligned}$$

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$$(x) \sum_n \left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x-na) - \epsilon_0 \right) w_n^{(1)}(x) e^{ikna} = \underbrace{(\epsilon(k) - \epsilon_0)}_{\epsilon^{(1)}(k)} \sum_n e^{ikna} \psi(x-na) - \sum_n h_n(x) e^{ikna} \psi(x-na)$$

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$$\begin{aligned} \text{LHS of (x)} &= \int dx \psi^*(x) \sum_n \left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x-na) - \epsilon_0 \right) w_n^{(1)}(x) e^{ikna} dx = \\ &= \int dx \sum_n w_n^{(1)*}(x) \left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} - \epsilon_0 + V(x-na) \right) \psi(x) e^{ikna} dx = \int dx \sum_n w_n^{(1)*}(x) [V(x-na) - V(x)] \psi(x) e^{ikna} \end{aligned}$$

We need to solve: $-\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} + \sum_n V(x-na) \psi(x) = \epsilon \psi(x)$

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$$(x) \sum_n \left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x-na) - \epsilon_0 \right) w_n^{(1)}(x) e^{ikna} = \underbrace{(\epsilon(k) - \epsilon_0)}_{\epsilon^{(1)}(k)} \sum_n e^{ikna} \psi(x-na) - \sum_n h_n(x) e^{ikna} \psi(x-na)$$

Multiply by $\psi^*(x)$ and integrate $\int dx$

$$\begin{aligned} \text{LHS of } (x) &= \int dx \psi^*(x) \sum_n \left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x-na) - \epsilon_0 \right) w_n^{(1)}(x) e^{ikna} dx = \\ &= \int dx \sum_n w_n^{(1)}(x) \left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} - \epsilon_0 + V(x-na) \right) \psi^*(x) e^{ikna} dx = \int dx \sum_n \underbrace{w_n^{(1)}(x)}_{\neq 0 \text{ around } na} [V(x-na) - V(x)] \psi^*(x) e^{ikna} \end{aligned}$$

We need to solve: $-\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} + \sum_n V(x-na) \psi(x) = \epsilon \psi(x)$

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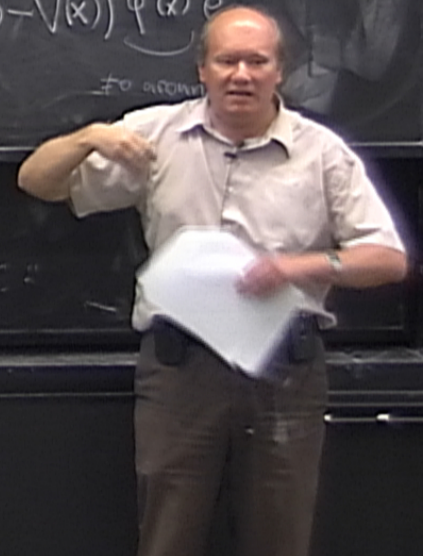
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higher order of smallness $\Downarrow \approx 0$
 $\neq 0$ around na

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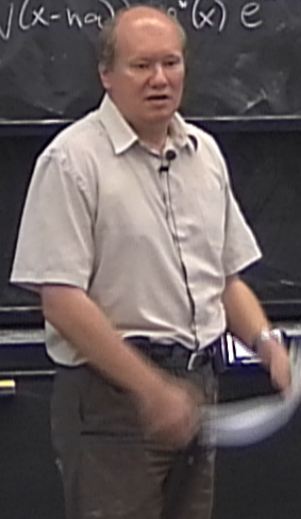
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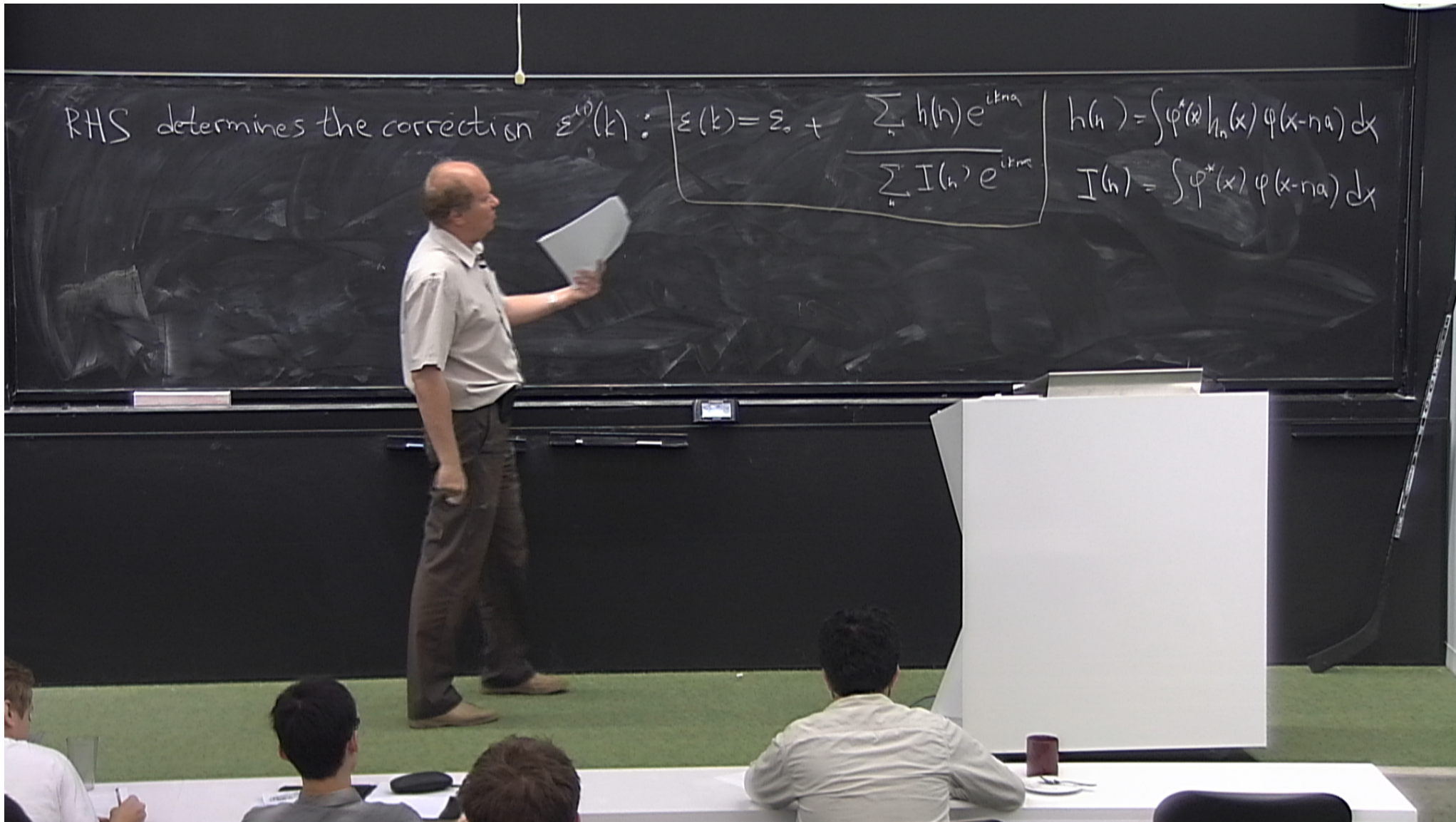
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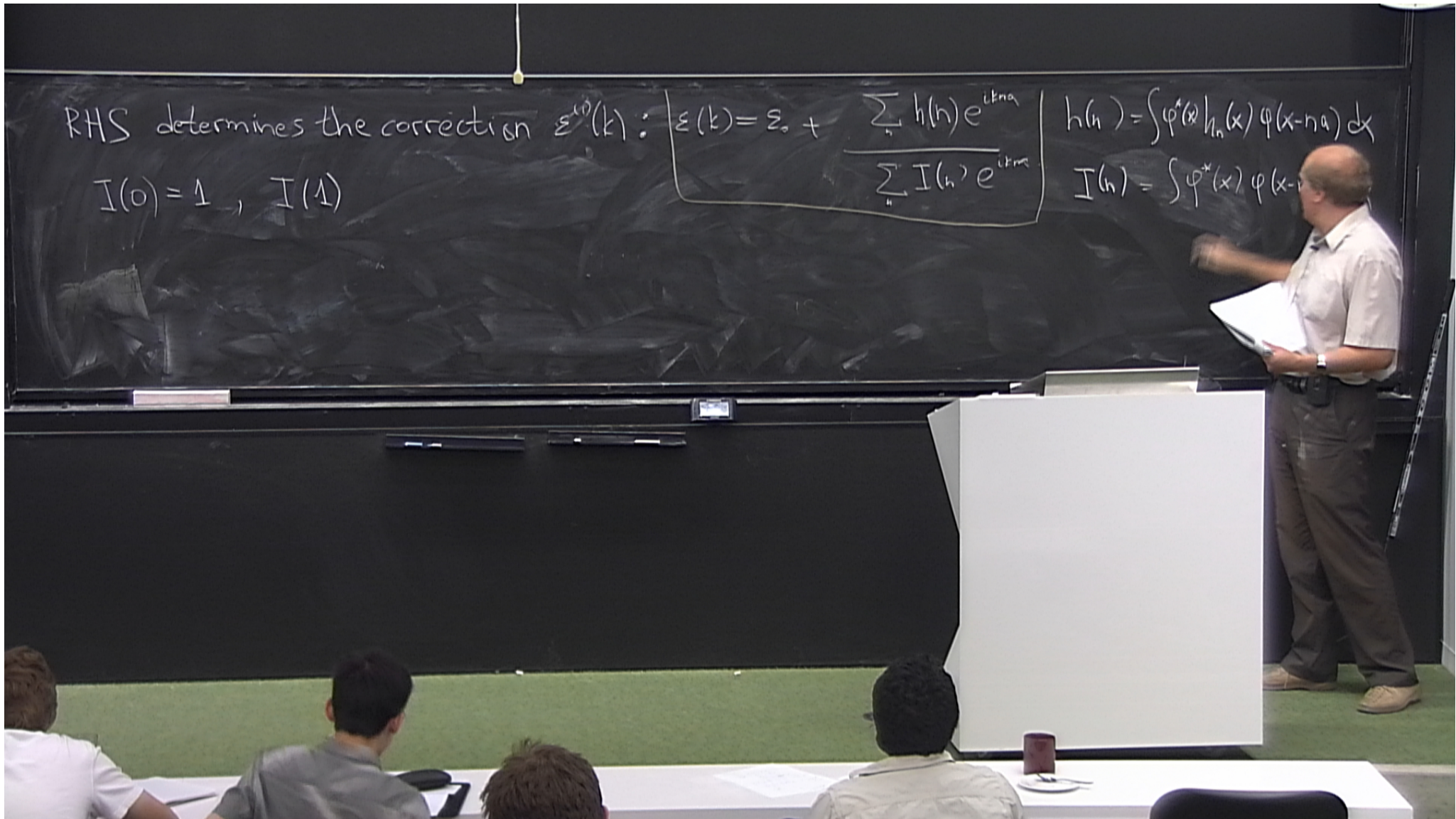


RHS determines the correction $\varepsilon^{(1)}(k)$: $\varepsilon(k) = \varepsilon_0 + \frac{\sum_n h(n) e^{ikna}}{\sum_n I(n) e^{ikna}} \quad \left| \quad h(n) = \int \varphi^*(x) h_n(x) \right.$



RHS determines the correction $\varepsilon^{(1)}(k)$:

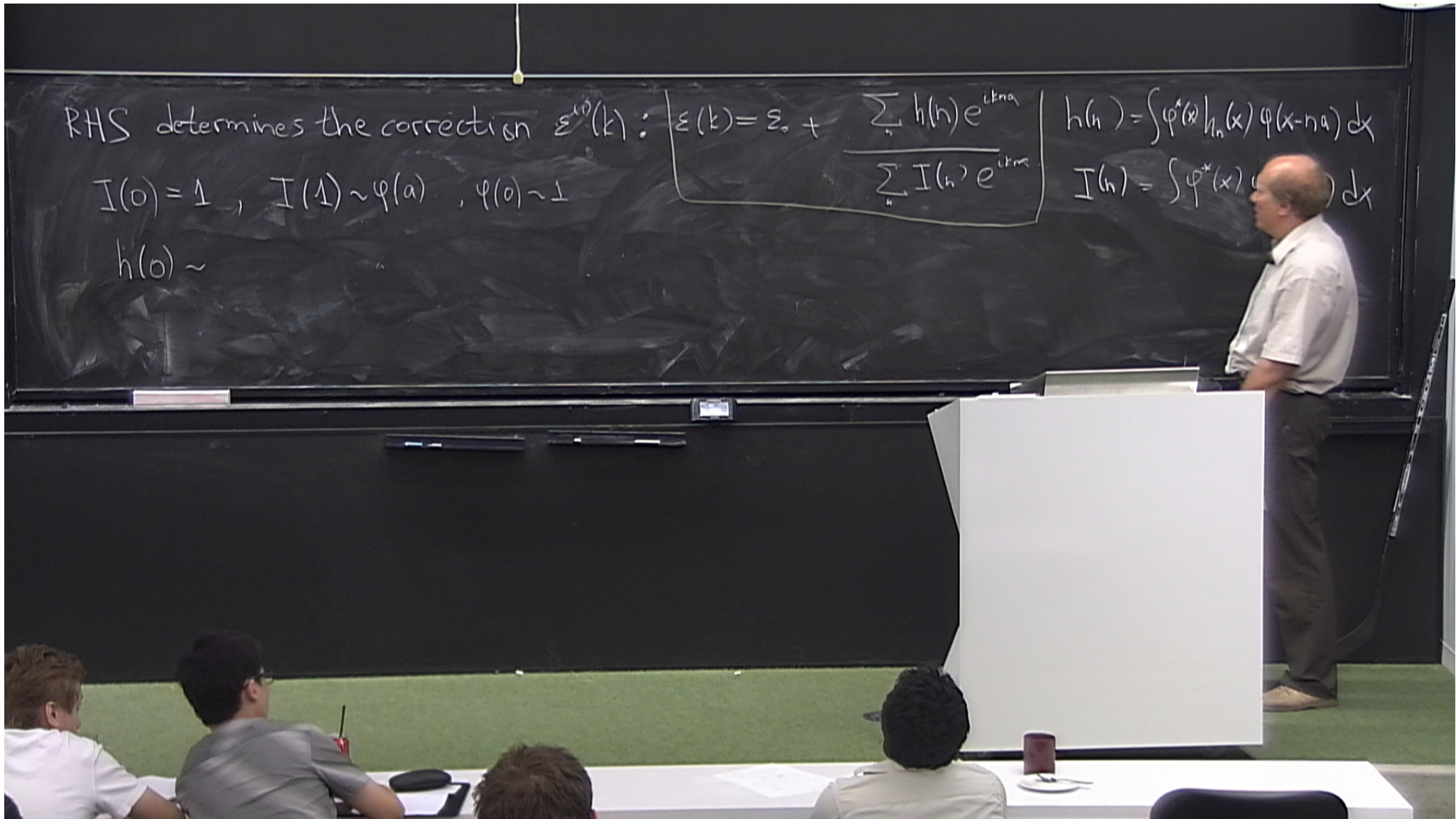
$$\varepsilon(k) = \varepsilon_0 + \frac{\sum_n h(n) e^{ikna}}{\sum_n I(n) e^{ikna}} \quad \left| \begin{array}{l} h(n) = \int \varphi^*(x) h_n(x) \varphi(x-na) dx \\ I(n) = \int \varphi^*(x) \varphi(x-na) dx \end{array} \right.$$



RHS determines the correction $\epsilon^{(1)}(k)$:
 $I(0) = 1, I(1)$

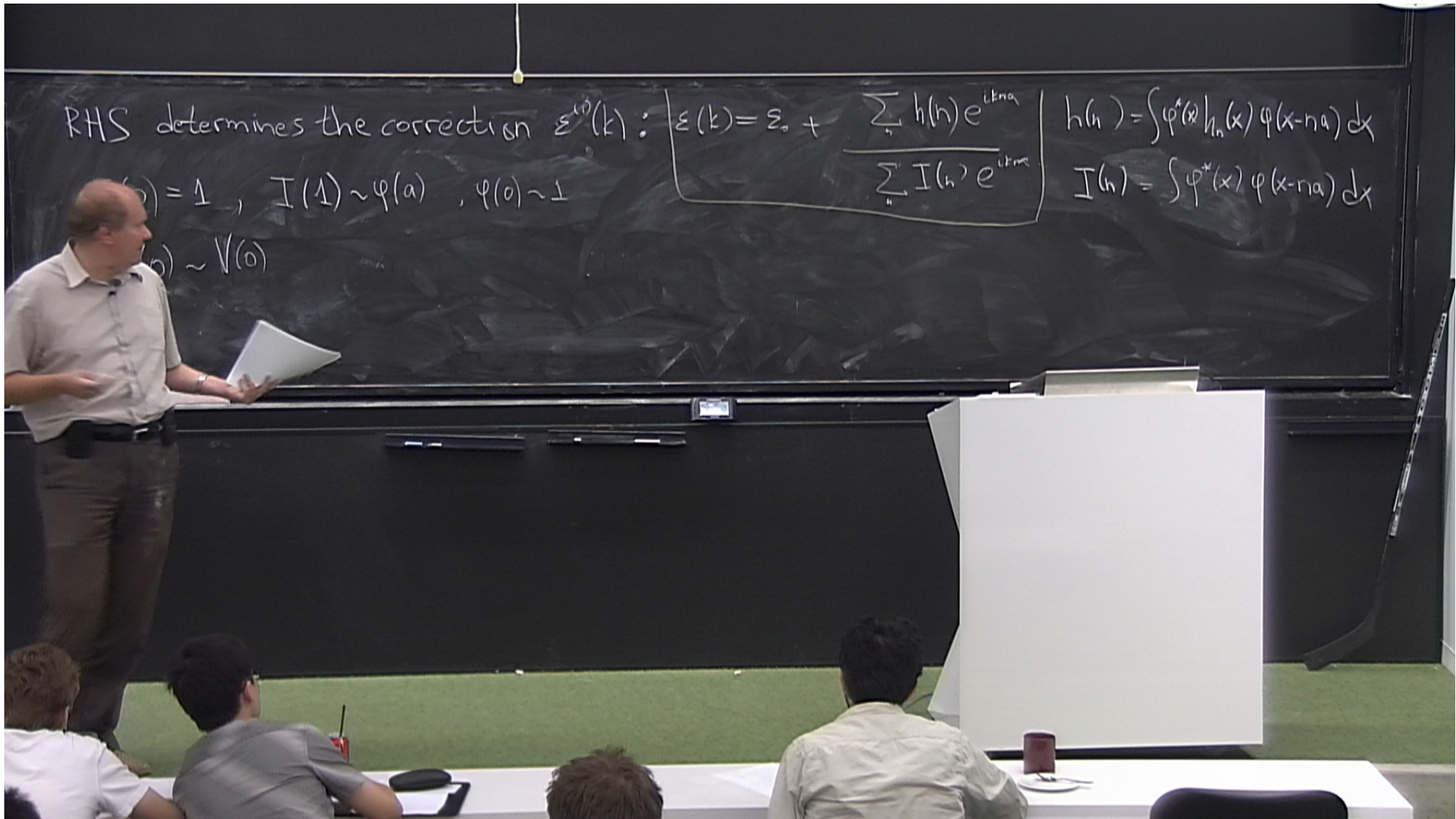
$$\epsilon(k) = \epsilon_0 + \frac{\sum_n h(n) e^{ikna}}{\sum_n I(n) e^{ikm}}$$

$$h(n) = \int \varphi^*(x) h_n(x) \varphi(x-na) dx$$
$$I(n) = \int \varphi^*(x) \varphi(x-na) dx$$



RHS determines the correction $\epsilon^{(1)}(k)$:
 $I(0) = 1$, $I(1) \sim \varphi(a)$, $\varphi(0) \sim 1$
 $h(0) \sim$

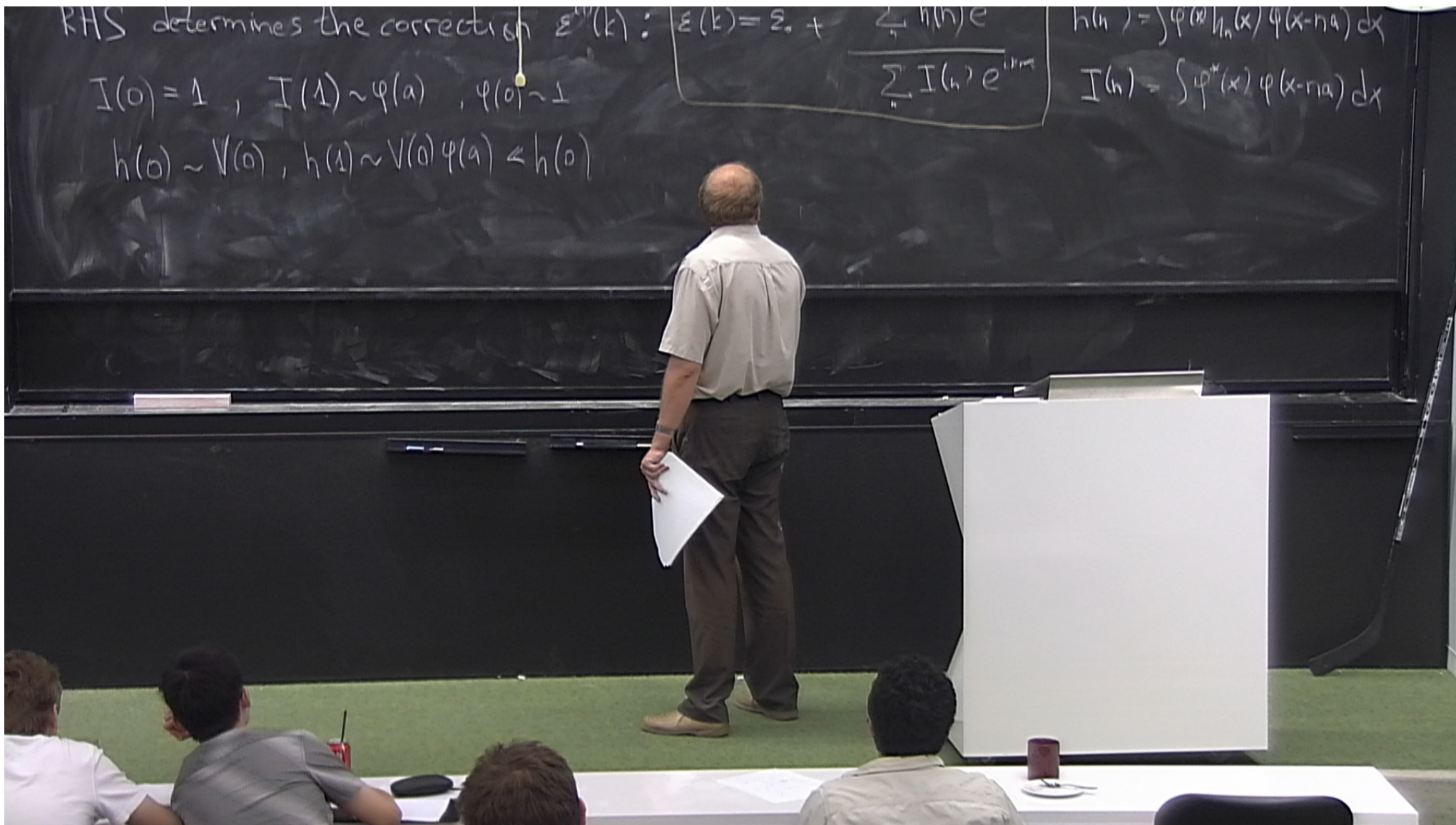
$$\epsilon(k) = \epsilon_0 + \frac{\sum_n h(n) e^{ikna}}{\sum_n I(n) e^{ikna}} \quad \left| \begin{array}{l} h(n) = \int \varphi^*(x) h_n(x) \varphi(x-na) dx \\ I(n) = \int \varphi^*(x) \varphi(x-na) dx \end{array} \right.$$

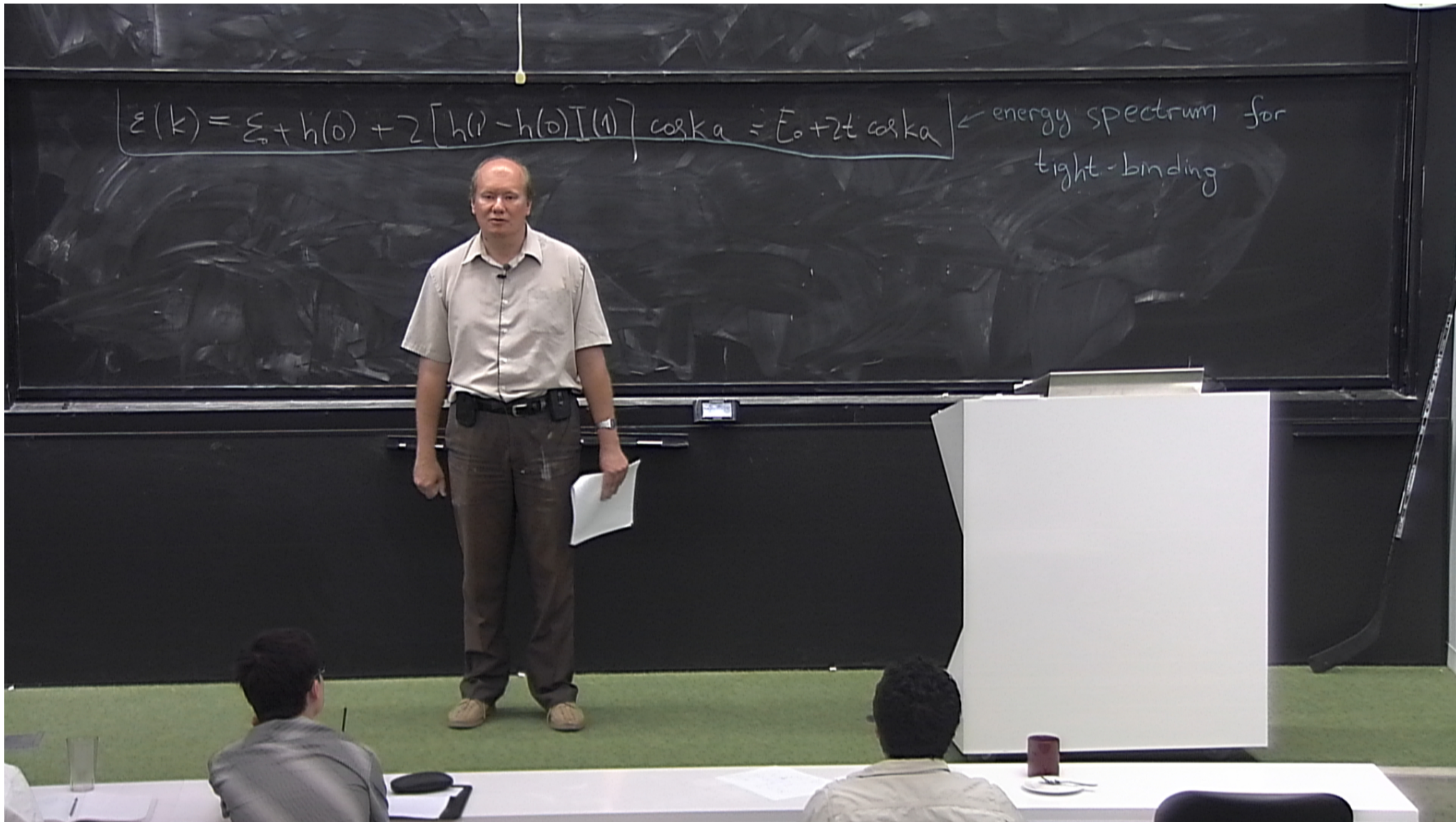


RHS determines the correction $\epsilon^{(1)}(k)$:

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$\psi(0) = 1$, $I(1) \sim \varphi(a)$, $\varphi(0) \sim 1$
 $\psi(0) \sim V(0)$





We need to solve: $-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + \sum_n V(x-na) \psi(x) = \epsilon \psi(x)$

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Wannier functions: $\phi_n(x) = \frac{1}{\sqrt{N}} \sum_k e^{-ikna} \psi_k(x)$

no band index! $-\frac{\pi}{a} < k < \frac{\pi}{a}$

$$H = \sum_{n\sigma} E_0 c_{n\sigma}^\dagger c_{n\sigma} + t \sum_{\langle n, n' \rangle} (c_{n\sigma}^\dagger c_{n'\sigma} + c_{n'\sigma}^\dagger c_{n\sigma})$$

$$c_{n\sigma}^\dagger = \frac{1}{\sqrt{N}} \sum_k c_{k\sigma}^\dagger e^{-ikna}$$

$$c_{n\sigma} = \frac{1}{\sqrt{N}} \sum_k c_{k\sigma} e^{ikna}$$

$$\frac{0}{a} \rightarrow \frac{0}{a} \quad R=na$$

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$$\vec{R} = na$$

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$$H = \sum_{n\sigma} E_0 c_{n\sigma}^\dagger c_{n\sigma} + t \sum_{\sigma} (c_{n\sigma} c_{n+1,\sigma}^\dagger + c_{n+1,\sigma}^\dagger c_{n\sigma})$$

$$c_{n\sigma}^\dagger = \frac{1}{\sqrt{N}} \sum_k c_{k\sigma}^\dagger e^{-ikna}$$

$$c_{n\sigma} = \frac{1}{\sqrt{N}} \sum_k c_{k\sigma} e^{ikna}$$

$$H = \sum_k c_{k\sigma}^\dagger c_{k\sigma} \epsilon(k) \quad R=na$$

$$\epsilon(k) = E_0 + 2t \cos ka$$