Title: PSI 2018/2019 - Condensed Matter - Lecture 3

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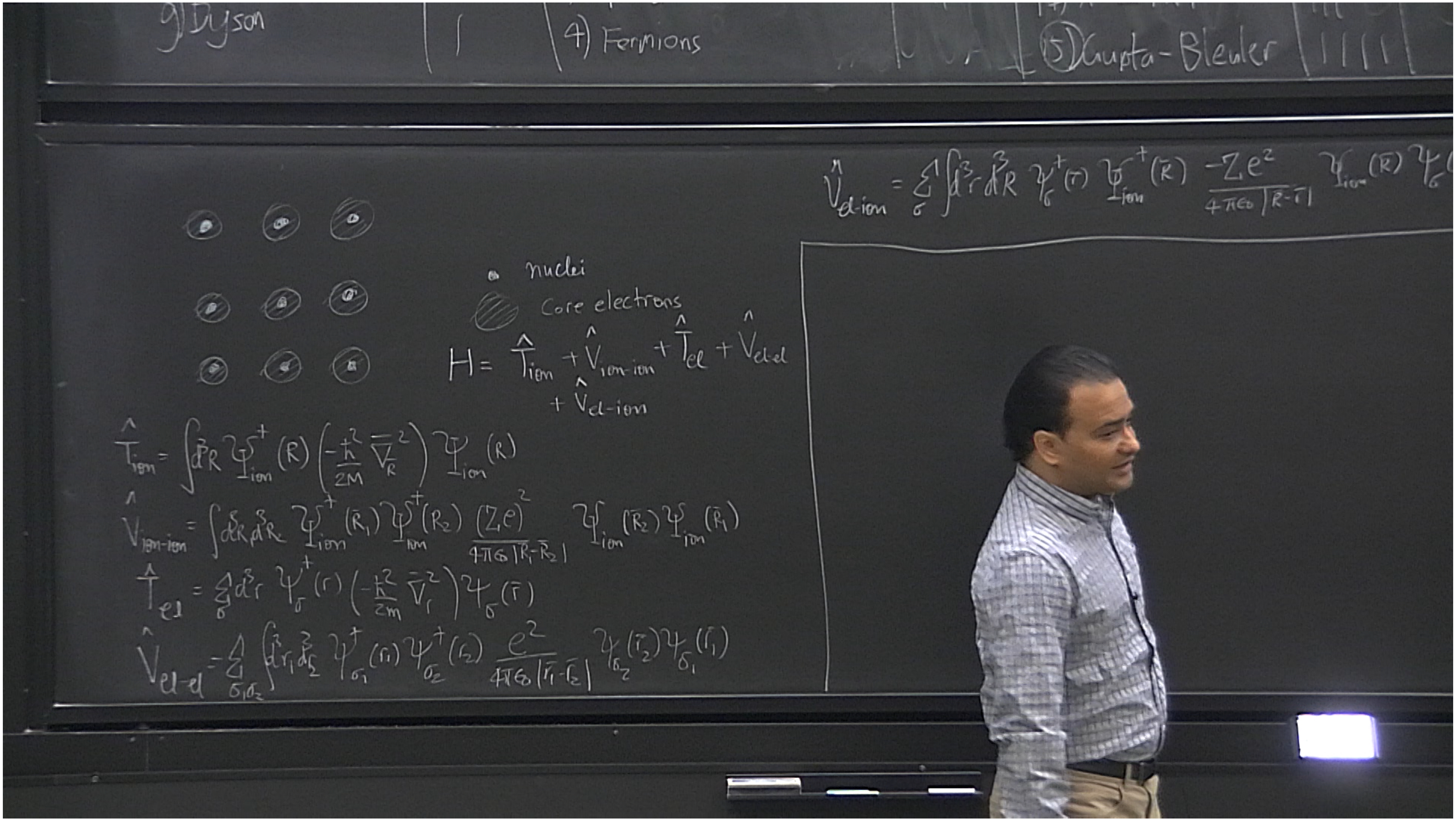
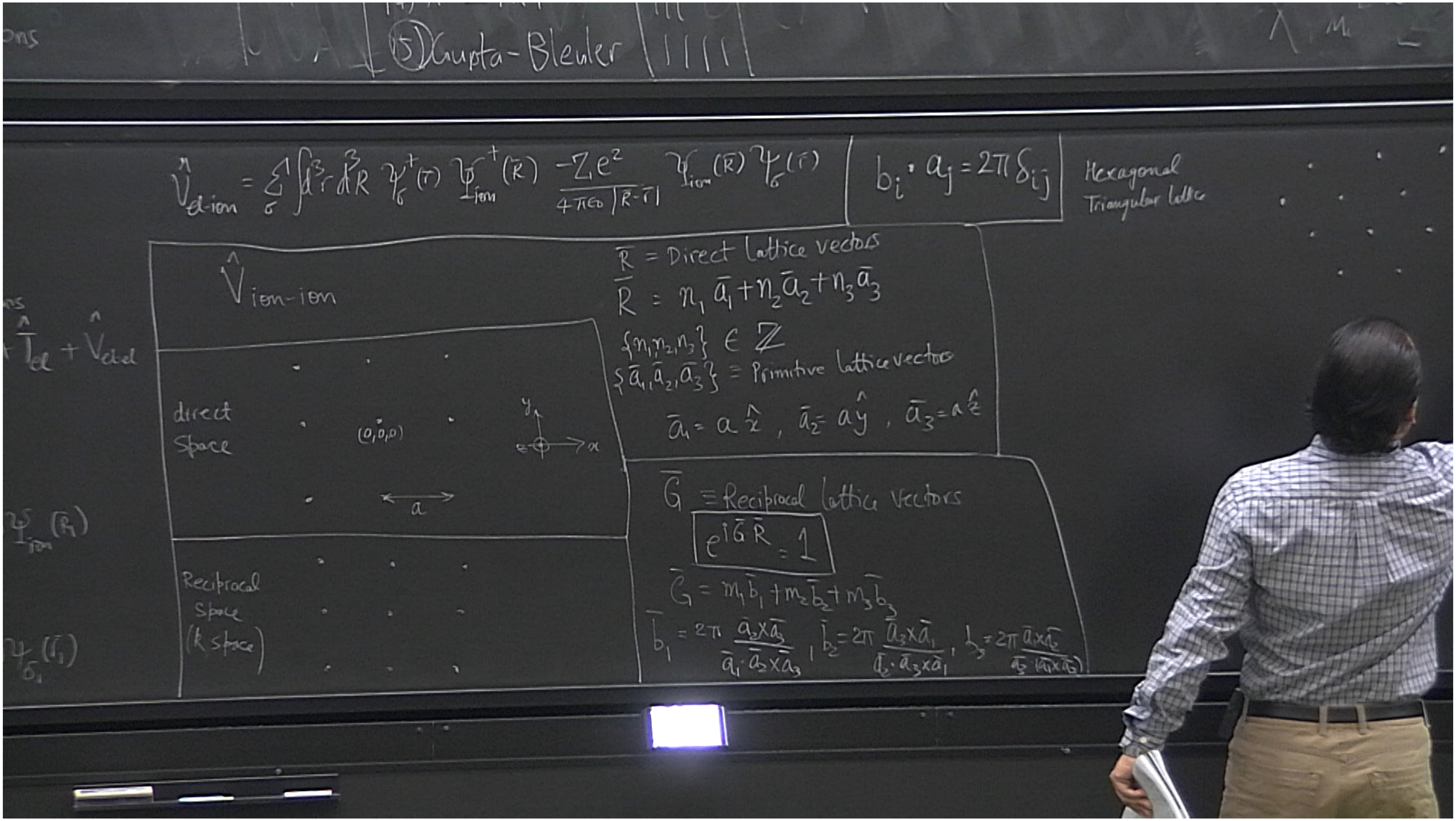
Abstract:


9) Dyson
4) Fermions
15) Gupta-Bleuler
$\hat{V}_{el\text{-}ion} = \sum_\sigma \int d^3r\, d^3R\, \psi^\dagger_\sigma(\bar r)\, \Psi^\dagger_{ion}(\bar R)\, \frac{-Ze^2}{4\pi\epsilon_0 |\bar R - \bar r|}\, \Psi_{ion}(\bar R)\, \psi_\sigma$
nuclei
Core electrons
$H = \hat{T}_{ion} + \hat{V}_{ion\text{-}ion} + \hat{T}_{el} + \hat{V}_{el\text{-}el} + \hat{V}_{el\text{-}ion}$
$\hat{T}_{ion} = \int d^3R\, \Psi^\dagger_{ion}(R) \left(-\frac{\hbar^2}{2M} \bar\nabla^2_R\right) \Psi_{ion}(R)$
$\hat{V}_{ion\text{-}ion} = \int d^3R_1 d^3R_2\, \Psi^\dagger_{ion}(\bar R_1) \Psi^\dagger_{ion}(\bar R_2) \frac{(Z_1 e)^2}{4\pi\epsilon_0 |\bar R_1 - \bar R_2|} \Psi_{ion}(\bar R_2) \Psi_{ion}(\bar R_1)$
$\hat{T}_{el} = \sum_\sigma \int d^3r\, \psi^\dagger_\sigma(\bar r) \left(-\frac{\hbar^2}{2m} \bar\nabla^2_r\right) \psi_\sigma(\bar r)$
$\hat{V}_{el\text{-}el} = \sum_{\sigma_1\sigma_2} \int d^3r_1 d^3r_2\, \psi^\dagger_{\sigma_1}(\bar r_1) \psi^\dagger_{\sigma_2}(\bar r_2) \frac{e^2}{4\pi\epsilon_0 |\bar r_1 - \bar r_2|} \psi_{\sigma_2}(\bar r_2) \psi_{\sigma_1}(\bar r_1)$


(15) Gupta-Bleuler
$\hat{V}_{el\text{-}ion} = \sum_\sigma \int d^3r\, d^3R\, \psi_\sigma^\dagger(\bar r)\, \Psi_{ion}^\dagger(\bar R) \frac{-Z_1 e^2}{4\pi\epsilon_0 |\bar R - \bar r|} \Psi_{ion}(\bar R)\, \psi_\sigma(\bar r)$
$b_i \cdot a_j = 2\pi \delta_{ij}$
Hexagonal
Triangular lattice
$\hat{V}_{ion\text{-}ion}$
$\bar R$ = Direct lattice vectors
$\bar R = n_1 \bar a_1 + n_2 \bar a_2 + n_3 \bar a_3$
$\{n_1, n_2, n_3\} \in \mathbb{Z}$
$\{\bar a_1, \bar a_2, \bar a_3\}$ = Primitive lattice vectors
$\bar a_1 = a\hat x, \quad \bar a_2 = a\hat y, \quad \bar a_3 = a\hat z$
direct Space
(0,0,0)
y
x
a
Reciprocal Space (k space)
$\bar G$ ≡ Reciprocal lattice vectors
$e^{i\bar G \cdot \bar R} = 1$
$\bar G = m_1 \bar b_1 + m_2 \bar b_2 + m_3 \bar b_3$
$\bar b_1 = 2\pi \frac{\bar a_2 \times \bar a_3}{\bar a_1 \cdot \bar a_2 \times \bar a_3}, \quad \bar b_2 = 2\pi \frac{\bar a_3 \times \bar a_1}{\bar a_2 \cdot \bar a_3 \times \bar a_1}, \quad \bar b_3 = 2\pi \frac{\bar a_1 \times \bar a_2}{\bar a_3 \cdot (\bar a_1 \times \bar a_2)}$
$+ \hat T_{el} + \hat V_{el\text{-}el}$

ender

$-\frac{Ze^2}{4\pi\epsilon_0|\bar R-\bar r|}\psi_{ion}(\bar R)\psi_e(\bar r)$

$b_i\cdot a_j = 2\pi\delta_{ij}$

$\bar R$ = Direct lattice vectors

$\bar R = n_1\bar a_1 + n_2\bar a_2 + n_3\bar a_3$

$\{n_1,n_2,n_3\}\in\mathbb{Z}$

$\{\bar a_1,\bar a_2,\bar a_3\}$ = Primitive lattice vectors

$\bar a_1 = a\hat x$, $\bar a_2 = a\hat y$, $\bar a_3 = a\hat z$

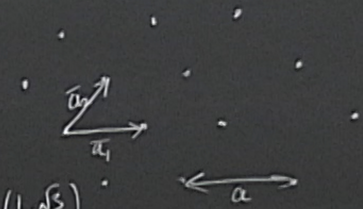
$\bar G$ = Reciprocal lattice vectors

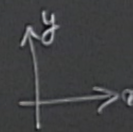
$\boxed{e^{i\bar G\cdot\bar R}=1}$

$\bar G = m_1\bar b_1+m_2\bar b_2+m_3\bar b_3$

$\bar b_1 = 2\pi\frac{\bar a_2\times\bar a_3}{\bar a_1\cdot\bar a_2\times\bar a_3}$, $\bar b_2 = 2\pi\frac{\bar a_3\times\bar a_1}{\bar a_2\cdot\bar a_3\times\bar a_1}$, $\bar b_3=2\pi\frac{\bar a_1\times\bar a_2}{\bar a_3\cdot(\bar a_1\times\bar a_2)}$

Hexagonal
Triangular lattice





$\bar a_1 = a(1,0) = a\hat x$

$\bar a_2 = a(\cos\frac{\pi}{3},\sin\frac{\pi}{3}) = a(\frac12,\frac{\sqrt3}{2})$
$= \frac a2\hat x+\frac{\sqrt3}{2}a\hat y$

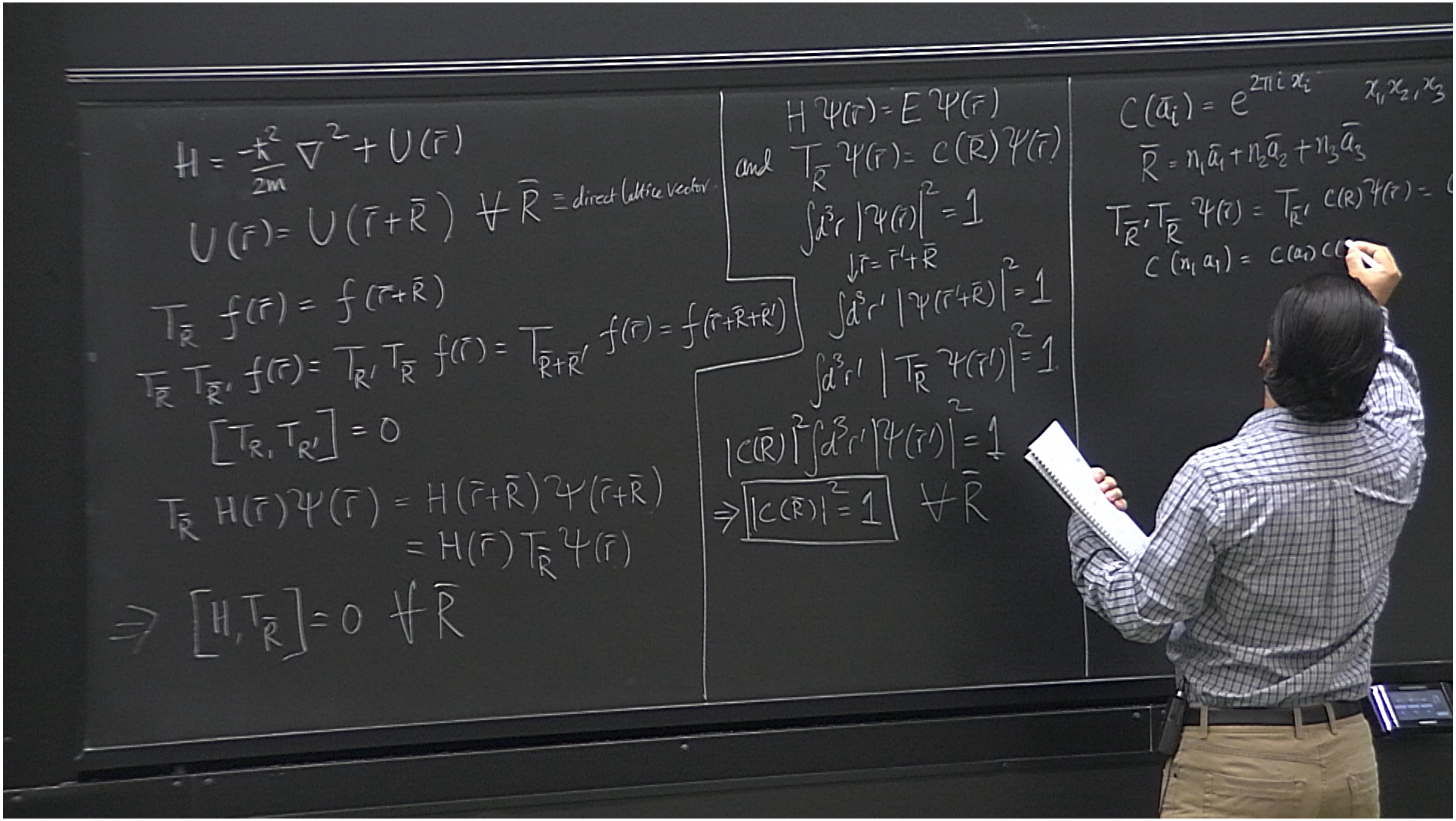
$\bar R = n_1\bar a_1+n_2\bar a_2$

$\bar G = m_1\bar b_1+m_2\bar b_2$

$e^{i\bar G\cdot\bar R}=1 = e^{im_1n_1\bar b_1\cdot\bar a_1}e^{im_1n_2\bar b_1\cdot\bar a_2}e^{im_2n_1\bar b_2\cdot\bar a_1}e^{im_2n_2\bar b_2\cdot\bar a_2}$

$\bar b_2\cdot\bar a_1=0\Rightarrow\bar b_2=\beta\hat y$ use $\bar b_2\cdot\bar a_2=2\pi\Rightarrow\beta\frac{\sqrt3}{2}a=2\pi\Rightarrow\beta=\frac{4\pi}{\sqrt3 a}$

$\bar b_1=\frac{4\pi}{\sqrt3 a}\left(\frac{\sqrt3}{2},-\frac12\right)$


$H = -\frac{\hbar^2}{2m}\nabla^2 + U(\bar{r})$
$U(\bar{r}) = U(\bar{r}+\bar{R}) \;\forall \bar{R}$ ≡ direct lattice vector
$T_{\bar{R}} f(\bar{r}) = f(\bar{r}+\bar{R})$
$T_{\bar{R}} T_{\bar{R}'} f(\bar{r}) = T_{R'} T_{\bar{R}} f(\bar{r}) = T_{\bar{R}+\bar{R}'} f(\bar{r}) = f(\bar{r}+\bar{R}+\bar{R}')$
$[T_R, T_{R'}] = 0$
$T_{\bar{R}} H(\bar{r})\Psi(\bar{r}) = H(\bar{r}+\bar{R})\Psi(\bar{r}+\bar{R}) = H(\bar{r}) T_{\bar{R}} \Psi(\bar{r})$
$\Rightarrow [H, T_{\bar{R}}] = 0 \;\forall \bar{R}$
$H\Psi(\bar{r}) = E\Psi(\bar{r})$
and $T_{\bar{R}}\Psi(\bar{r}) = C(\bar{R})\Psi(\bar{r})$
$\int d^3r\, |\Psi(\bar{r})|^2 = 1$
$\downarrow \bar{r} = \bar{r}' + \bar{R}$
$\int d^3r'\, |\Psi(\bar{r}'+\bar{R})|^2 = 1$
$\int d^3r'\, |T_{\bar{R}}\Psi(\bar{r}')|^2 = 1$
$|C(\bar{R})|^2 \int d^3r'\, |\Psi(\bar{r}')|^2 = 1$
$\Rightarrow \boxed{|C(\bar{R})|^2 = 1} \;\forall \bar{R}$
$C(\bar{a}_i) = e^{2\pi i x_i}$ x_1, x_2, x_3
$\bar{R} = n_1\bar{a}_1 + n_2\bar{a}_2 + n_3\bar{a}_3$
$T_{\bar{R}'} T_{\bar{R}} \Psi(\bar{r}) = T_{\bar{R}'} C(R)\Psi(\bar{r}) =$
$C(n_1 a_1) = C(a_1) C($

$$H\,\Psi(\bar r) = E\,\Psi(\bar r)$$

and $$T_{\bar R}\,\Psi(\bar r) = C(\bar R)\,\Psi(\bar r)$$

$$\int d^3r\, |\Psi(\bar r)|^2 = 1$$

$\bar r = \bar r' + \bar R$

$$\int d^3r'\, |\Psi(\bar r' + \bar R)|^2 = 1$$

$$\int d^3r'\, |T_{\bar R}\,\Psi(\bar r')|^2 = 1$$

$$|C(\bar R)|^2 \int d^3r'\, |\Psi(\bar r')|^2 = 1$$

$$\Rightarrow \boxed{|C(\bar R)|^2 = 1} \quad \forall \bar R$$

$$= f(\bar r + \bar R + \bar R')$$

$$C(\bar a_i) = e^{2\pi i x_i} \qquad x_1, x_2, x_3 \text{ are Real numbers}$$

$$\bar R = n_1 \bar a_1 + n_2 \bar a_2 + n_3 \bar a_3$$

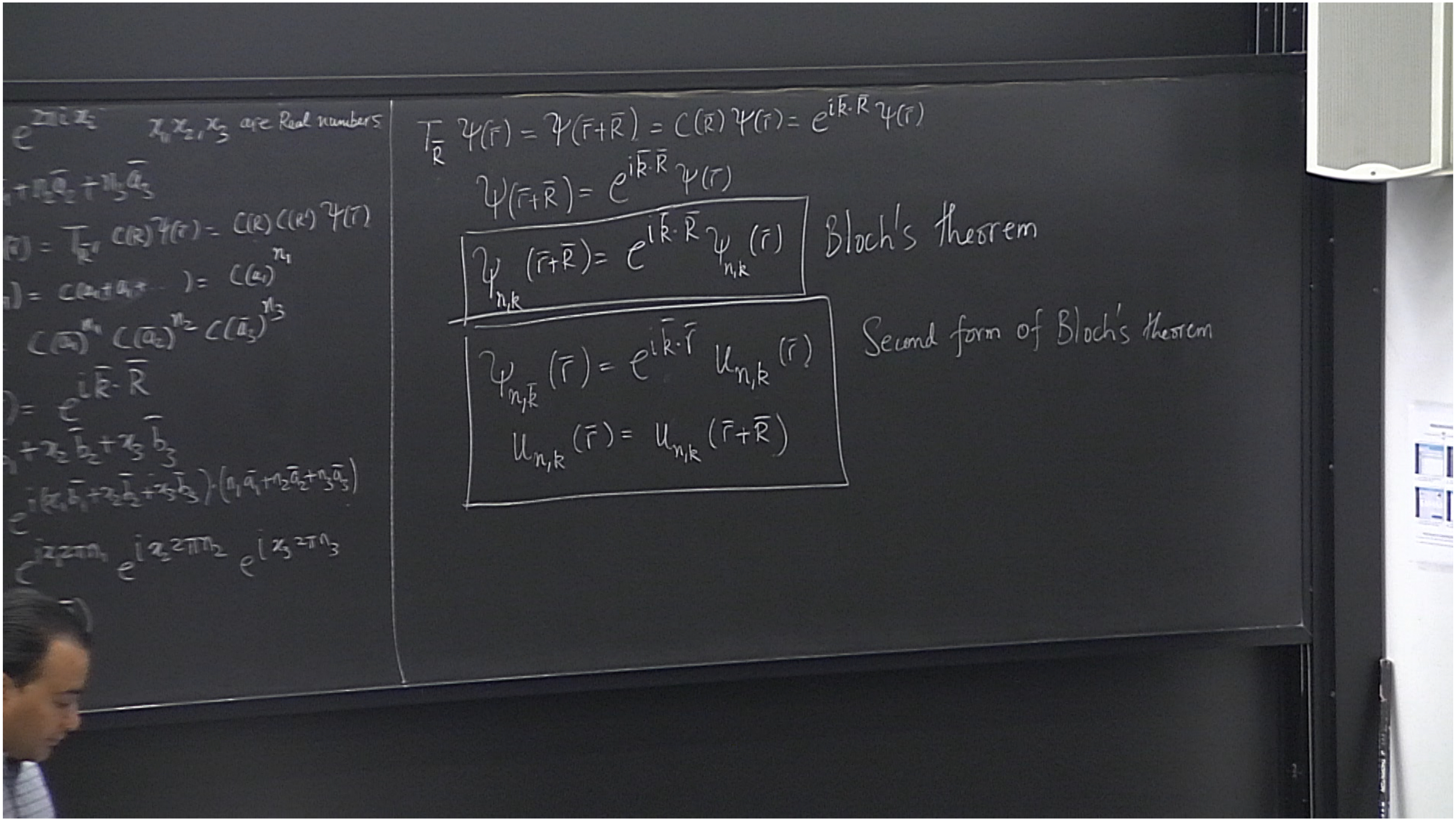
$$T_{\bar R'} T_{\bar R}\,\Psi(\bar r) = T_{\bar R'}\, C(R)\,\Psi(\bar r) = C(R)\,C(R')\,\Psi(\bar r)$$

$$C(n_1 a_1) = C(a_1 + a_1 + \dots) = C(a_1)^{n_1}$$

$$C(\bar R) = C(\bar a_1)^{n_1}\, C(\bar a_2)^{n_2}\, C(\bar a_3)^{n_3}$$

$$C(\bar R) = e^{i \bar k \cdot \bar R}$$

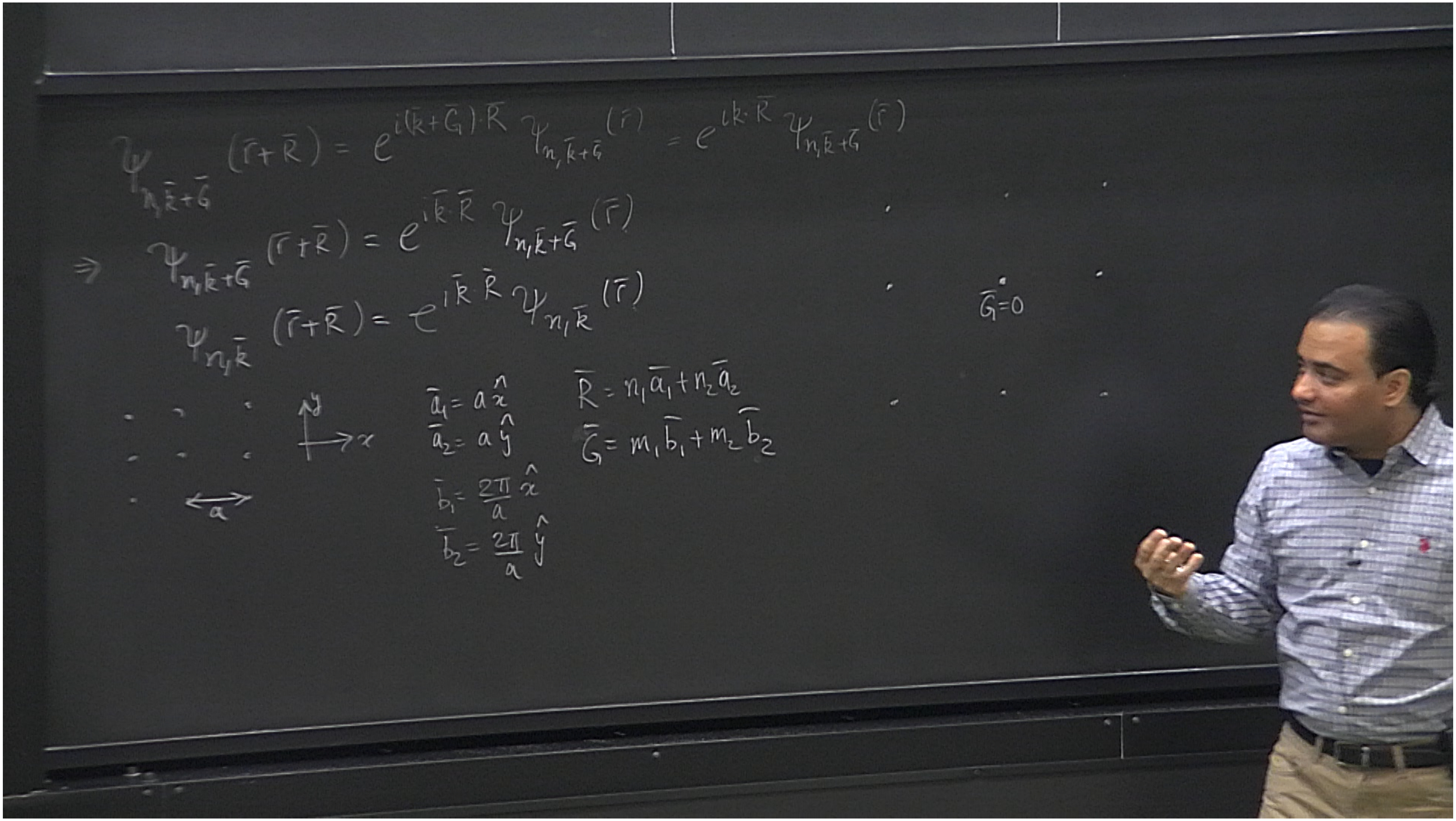
$$\bar k = x_1 \bar b_1 + x_2 \bar b_2 + x_3 \bar b_3$$


x_1, x_2, x_3 are Real numbers
$T_{\bar{R}}\,\psi(\bar{r}) = \psi(\bar{r}+\bar{R}) = C(\bar{R})\,\psi(\bar{r}) = e^{i\bar{k}\cdot\bar{R}}\,\psi(\bar{r})$
$\psi(\bar{r}+\bar{R}) = e^{i\bar{k}\cdot\bar{R}}\,\psi(\bar{r})$
$\psi_{n,k}(\bar{r}+\bar{R}) = e^{i\bar{k}\cdot\bar{R}}\,\psi_{n,k}(\bar{r})$
Bloch's theorem
$\psi_{n,\bar{k}}(\bar{r}) = e^{i\bar{k}\cdot\bar{r}}\,u_{n,k}(\bar{r})$
$u_{n,k}(\bar{r}) = u_{n,k}(\bar{r}+\bar{R})$
Second form of Bloch's theorem

$$\psi_{n,\bar{k}+\bar{G}}(\bar{r}+\bar{R}) = e^{i(\bar{k}+\bar{G})\cdot\bar{R}}\,\psi_{n,\bar{k}+\bar{G}}(\bar{r}) = e^{i\bar{k}\cdot\bar{R}}\,\psi_{n,\bar{k}+\bar{G}}(\bar{r})$$

$$\Rightarrow \psi_{n,\bar{k}+\bar{G}}(\bar{r}+\bar{R}) = e^{i\bar{k}\cdot\bar{R}}\,\psi_{n,\bar{k}+\bar{G}}(\bar{r})$$

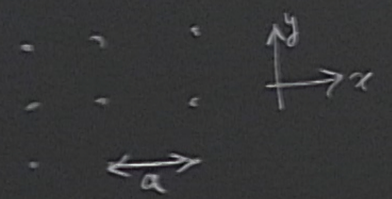
$$\psi_{n,\bar{k}}(\bar{r}+\bar{R}) = e^{i\bar{k}\cdot\bar{R}}\,\psi_{n,\bar{k}}(\bar{r})$$


$\psi_{n,\bar{k}+\bar{G}}(\bar{r}+\bar{R}) = e^{i(\bar{k}+\bar{G})\cdot\bar{R}}\,\psi_{n,\bar{k}+\bar{G}}(\bar{r}) = e^{i\bar{k}\cdot\bar{R}}\,\psi_{n,\bar{k}+\bar{G}}(\bar{r})$
$\Rightarrow \psi_{n,\bar{k}+\bar{G}}(\bar{r}+\bar{R}) = e^{i\bar{k}\cdot\bar{R}}\,\psi_{n,\bar{k}+\bar{G}}(\bar{r})$
$\psi_{n,\bar{k}}(\bar{r}+\bar{R}) = e^{i\bar{k}\cdot\bar{R}}\,\psi_{n,\bar{k}}(\bar{r})$
y
x
a
$\bar{a}_1 = a\hat{x}$
$\bar{a}_2 = a\hat{y}$
$\bar{b}_1 = \frac{2\pi}{a}\hat{x}$
$\bar{b}_2 = \frac{2\pi}{a}\hat{y}$
$\bar{R} = n_1\bar{a}_1 + n_2\bar{a}_2$
$\bar{G} = m_1\bar{b}_1 + m_2\bar{b}_2$
$\bar{G}=0$

$$\psi_{n,\bar k+\bar G}(\bar r+\bar R) = e^{i(\bar k+\bar G)\cdot\bar R}\,\psi_{n,\bar k+\bar G}(\bar r) = e^{i\bar k\cdot\bar R}\,\psi_{n,\bar k+\bar G}(\bar r)$$

$$\Rightarrow\quad \psi_{n,\bar k+\bar G}(\bar r+\bar R) = e^{i\bar k\cdot\bar R}\,\psi_{n,\bar k+\bar G}(\bar r)$$

$$\psi_{n,\bar k}(\bar r+\bar R) = e^{i\bar k\cdot\bar R}\,\psi_{n,\bar k}(\bar r)$$



$\bar a_1 = a\hat x$

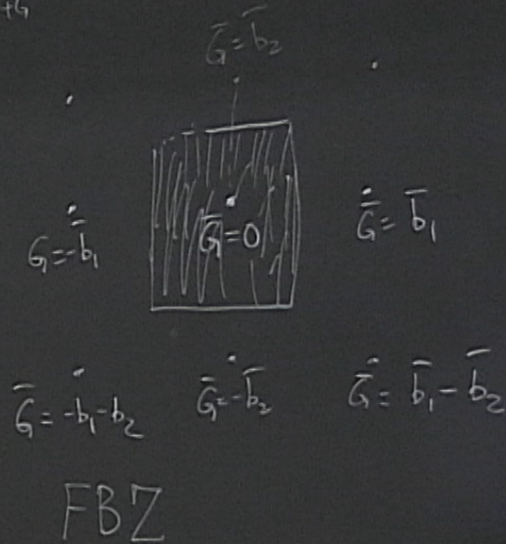
$\bar a_2 = a\hat y$

$\bar b_1 = \frac{2\pi}{a}\hat x$

$\bar b_2 = \frac{2\pi}{a}\hat y$

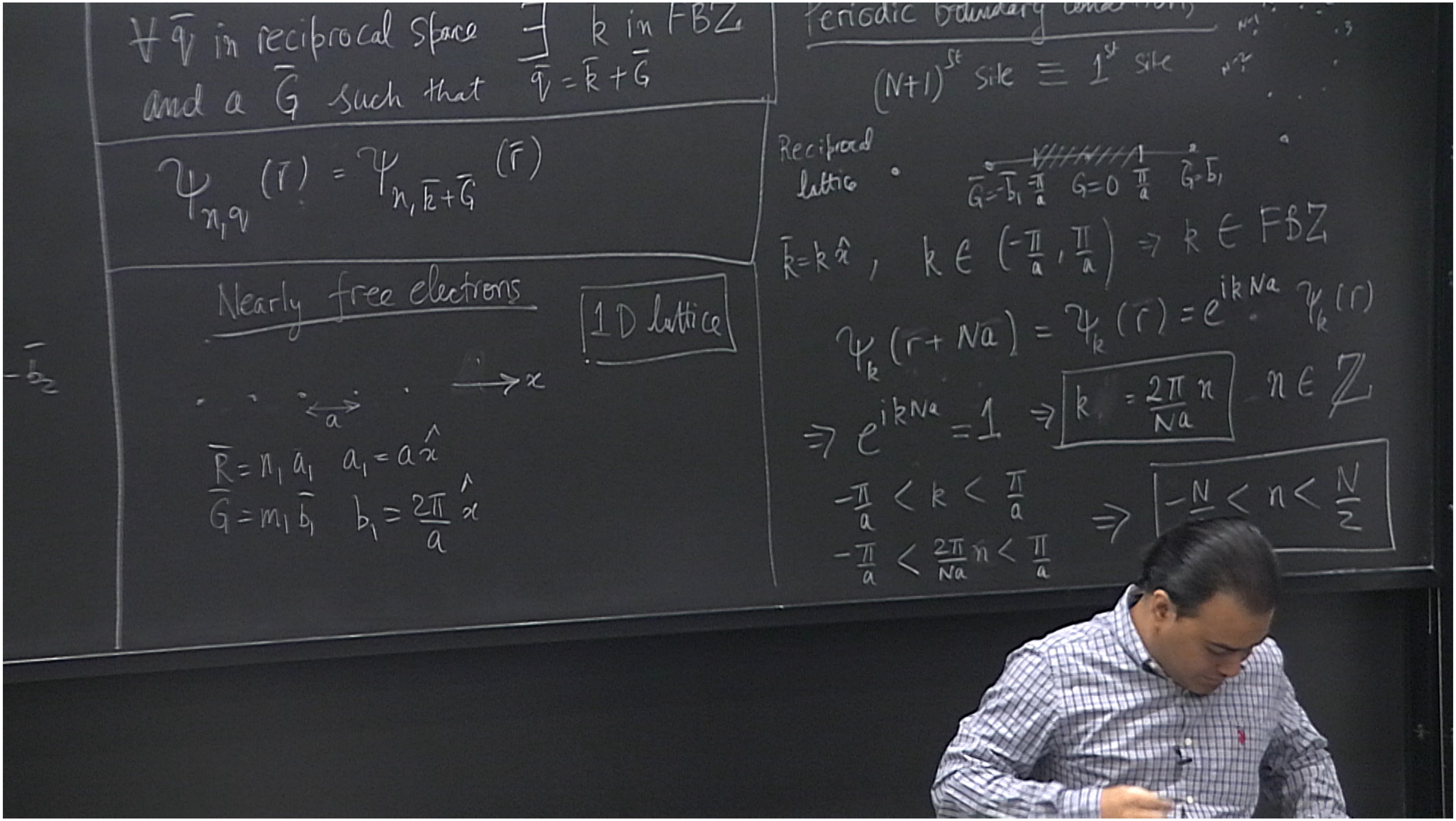
$\bar R = n_1\bar a_1 + n_2\bar a_2$

$\bar G = m_1\bar b_1 + m_2\bar b_2$



$\forall\ \bar q$ in recip

and a $\bar G$


$\forall \bar{q}$ in reciprocal space $\exists$ k in FBZ
and a $\bar{G}$ such that $\bar{q} = \bar{k} + \bar{G}$
$\psi_{n,q}(\bar{r}) = \psi_{n,\bar{k}+\bar{G}}(\bar{r})$
Nearly free electrons
1D lattice
x
a
$\bar{R} = n_1 a_1 \quad a_1 = a\hat{x}$
$\bar{G} = m_1 \bar{b}_1 \quad b_1 = \frac{2\pi}{a}\hat{x}$
Periodic boundary conditions
$(N+1)^{st}$ site $\equiv 1^{st}$ site
Reciprocal lattice
$\bar{G}=-\bar{b}_1 \quad -\frac{\pi}{a} \quad G=0 \quad \frac{\pi}{a} \quad \bar{G}=\bar{b}_1$
$\bar{k} = k\hat{x}, \quad k \in \left(-\frac{\pi}{a}, \frac{\pi}{a}\right) \Rightarrow k \in$ FBZ
$\psi_k(r+Na) = \psi_k(r) = e^{ikNa}\psi_k(r)$
$\Rightarrow e^{ikNa} = 1 \Rightarrow \boxed{k = \frac{2\pi}{Na} n} \quad n \in \mathbb{Z}$
$-\frac{\pi}{a} < k < \frac{\pi}{a}$
$-\frac{\pi}{a} < \frac{2\pi}{Na} n < \frac{\pi}{a}$
$\Rightarrow \boxed{-\frac{N}{2} < n < \frac{N}{2}}$