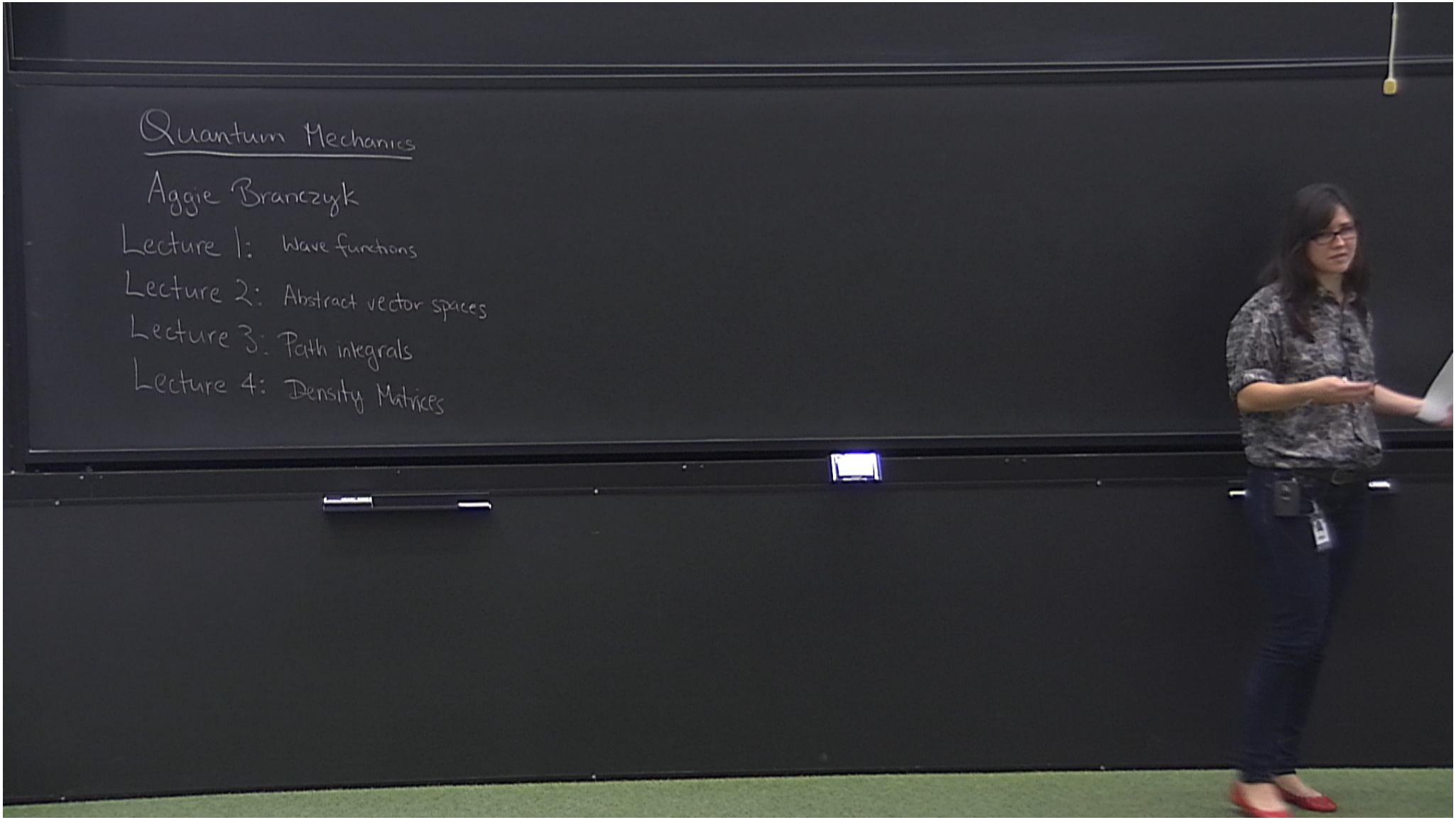
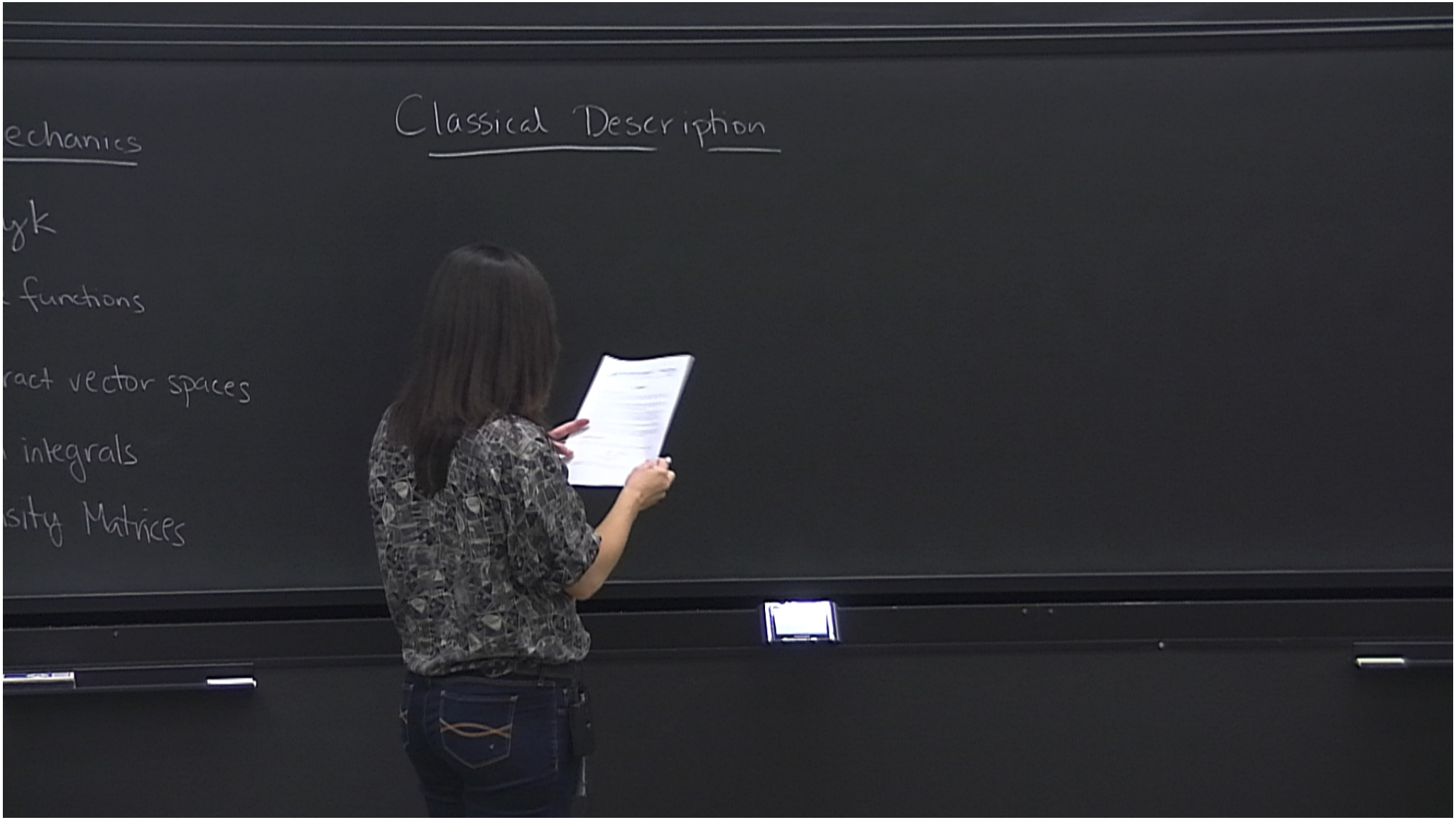
Title: Quantum Mechanics

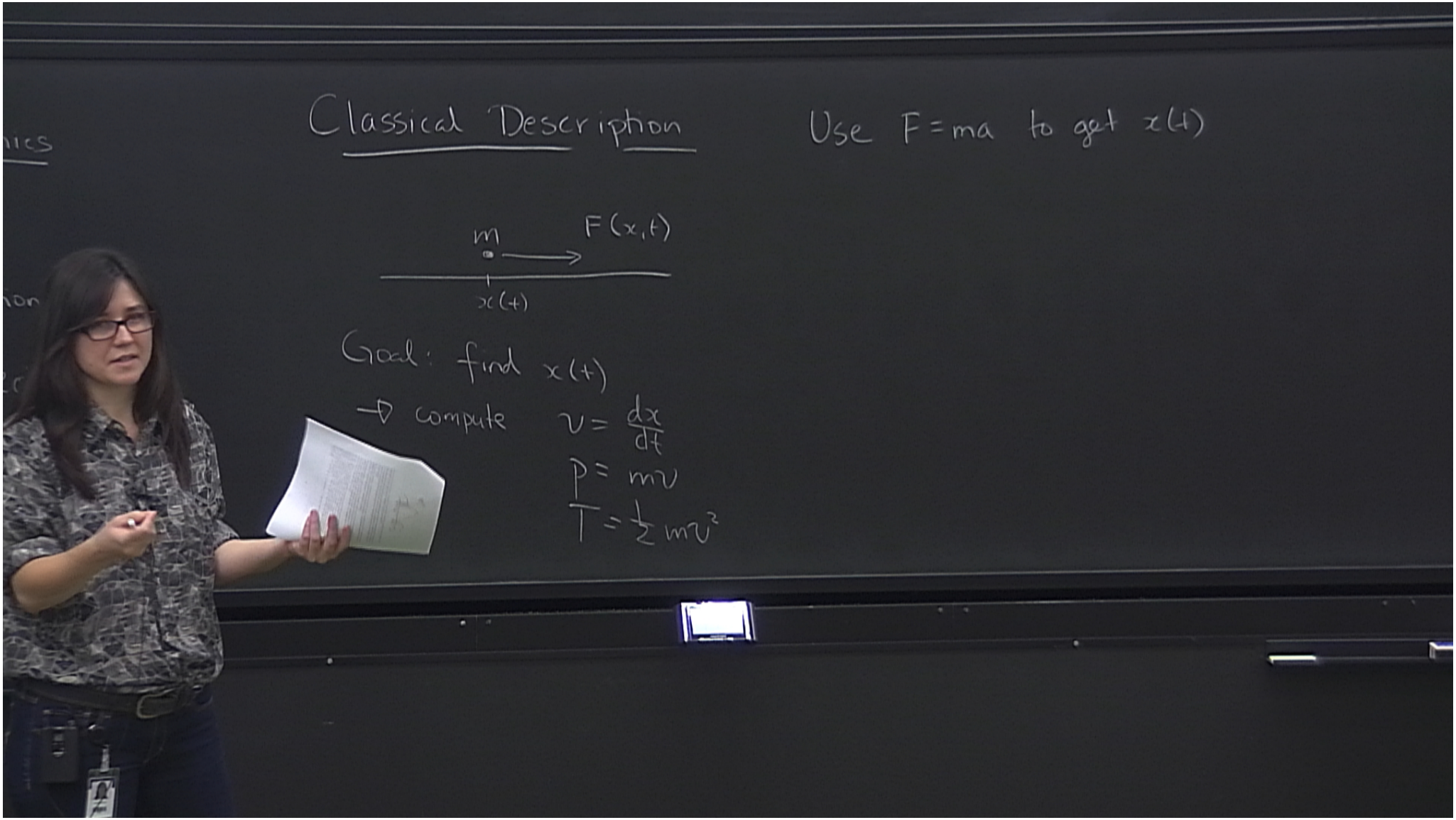
Date: Aug 11, 2015 10:30 AM

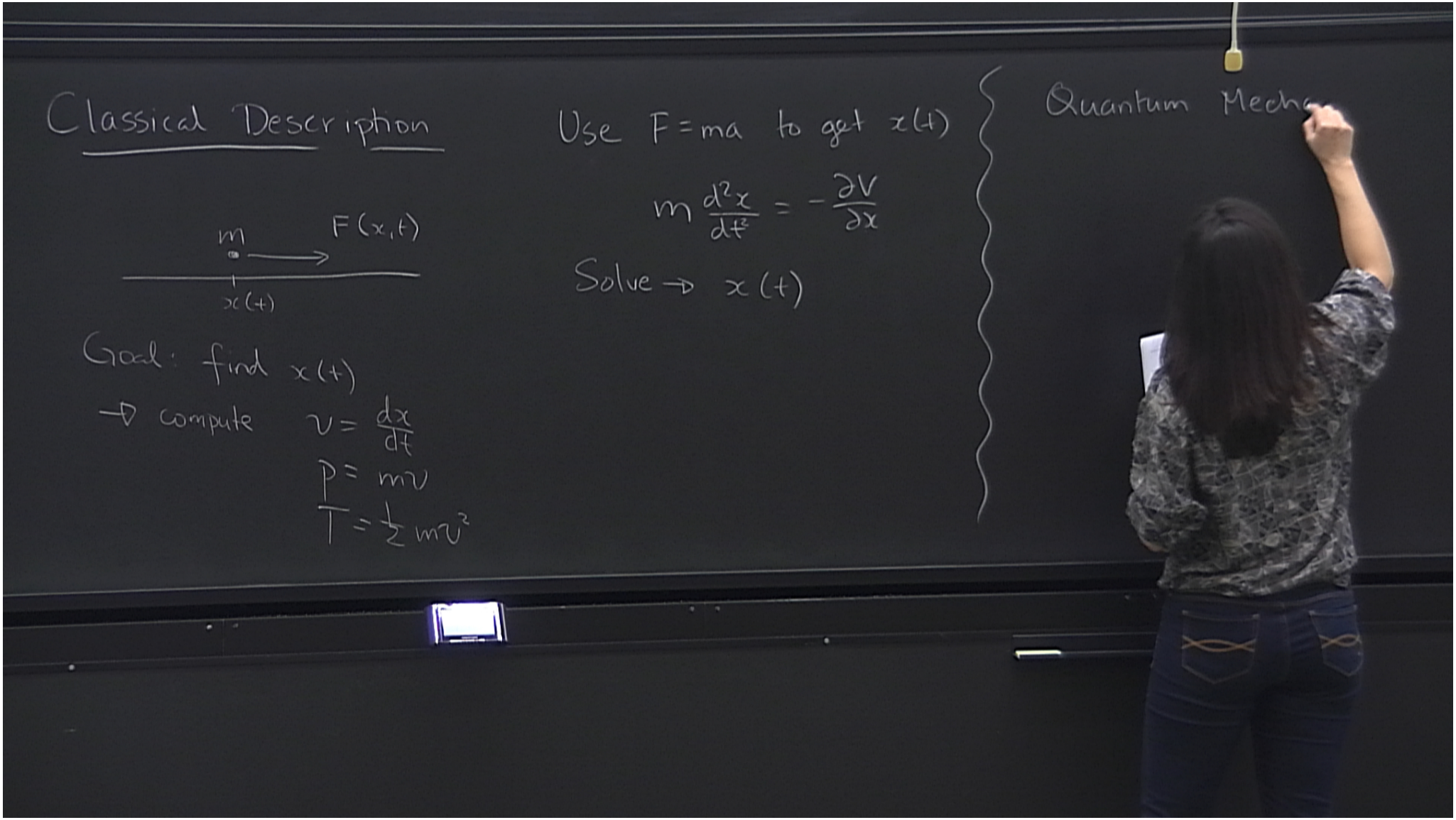
URL: http://pirsa.org/15080092

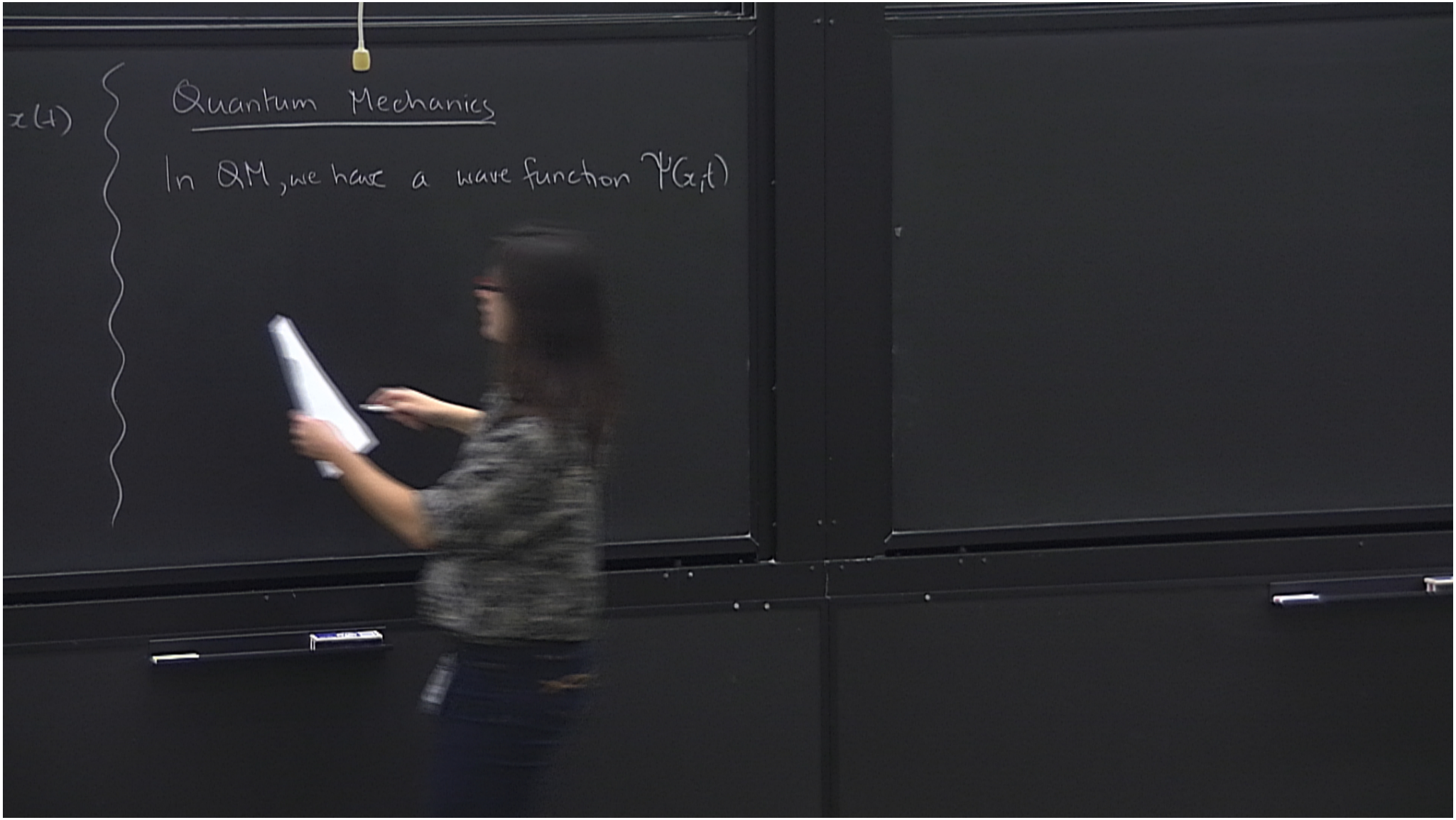
Abstract:


Quantum Mechanics
Aggie Branczyk
Lecture 1: Wave functions
Lecture 2: Abstract vector spaces
Lecture 3: Path integrals
Lecture 4: Density Matrices


Classical Description
echanics
yk
functions
ract vector spaces
integrals
sity Matrices


Classical Description
Use F = ma to get x(t)
m
F(x,t)
x(t)
Goal: find x(t)
→ compute v = dx/dt
p = mv
T = ½ mv²


Classical Description
m
F(x,t)
x(t)
Goal: find x(t)
→ compute v = dx/dt
p = mv
T = ½ mv²
Use F = ma to get x(t)
m d²x/dt² = − ∂V/∂x
Solve → x(t)
Quantum Mecha


x(t)
Quantum Mechanics
In QM, we have a wave function Ψ(x,t)

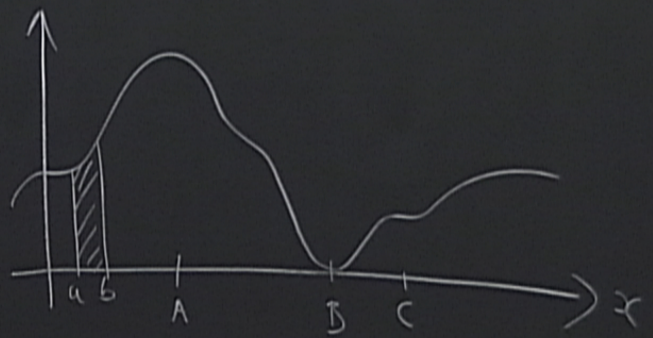
Use $F = ma$ to get $x(t)$

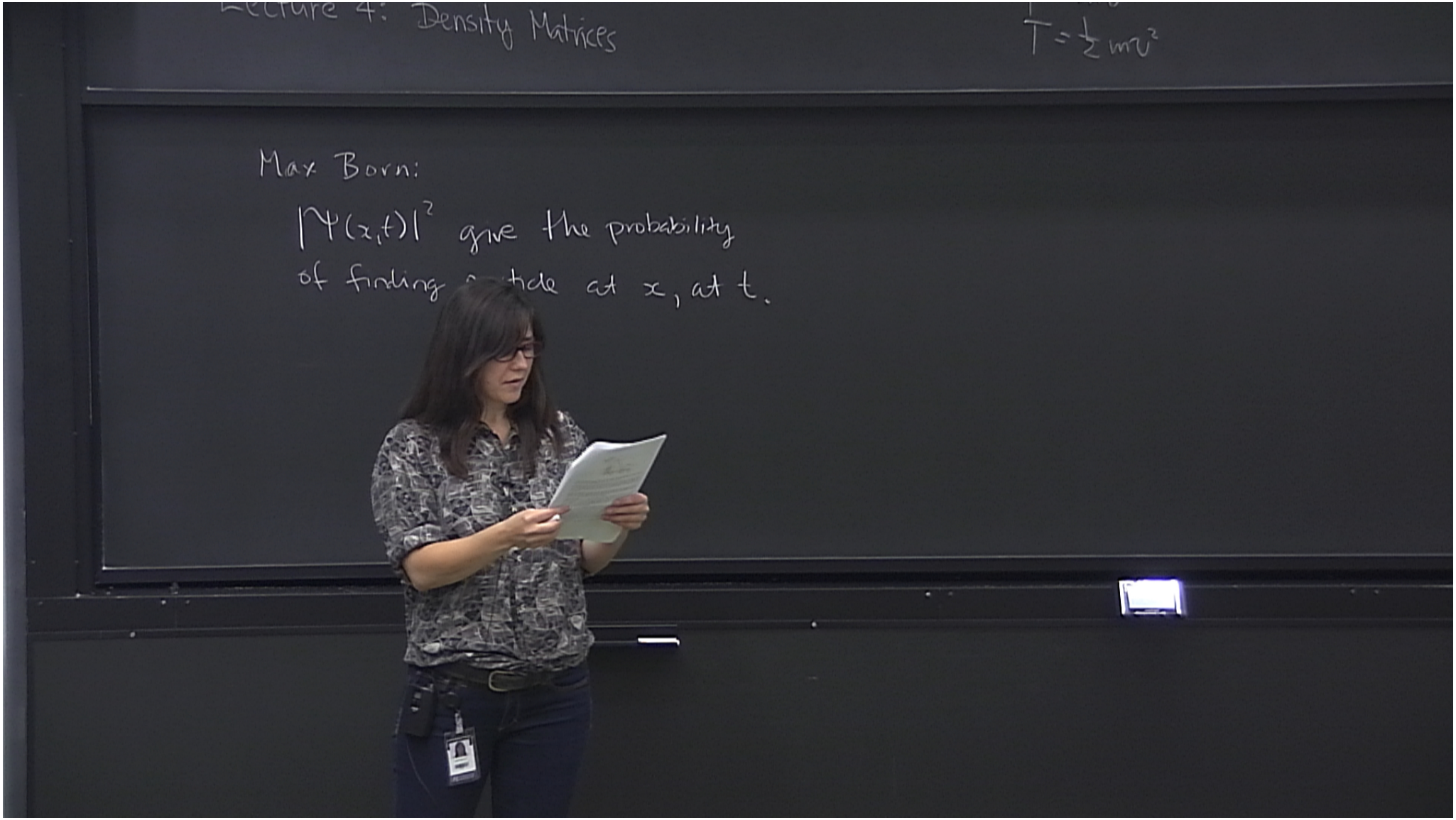
$$m\frac{d^2x}{dt^2} = -\frac{\partial V}{\partial x}$$

Solve → $x(t)$

Quantum Mechanics

In QM, we have a wave function $\Psi(x,t)$




Lecture 4: Density Matrices
$T = \frac{1}{2}mv^2$
Max Born:
$|\Psi(x,t)|^2$ give the probability
of finding a tide at x, at t.

Lecture 4: Density Matrices

$T = \frac{1}{2} m v^2$

Max Born:

$|\Psi(x,t)|^2$ give the probability of finding particle at x, at t.

More precisely:

$$\int_a^b |\Psi(x,t)|^2 \, dx$$

Lecture 4: Density Matrices

$T = \frac{1}{2} m v^2$

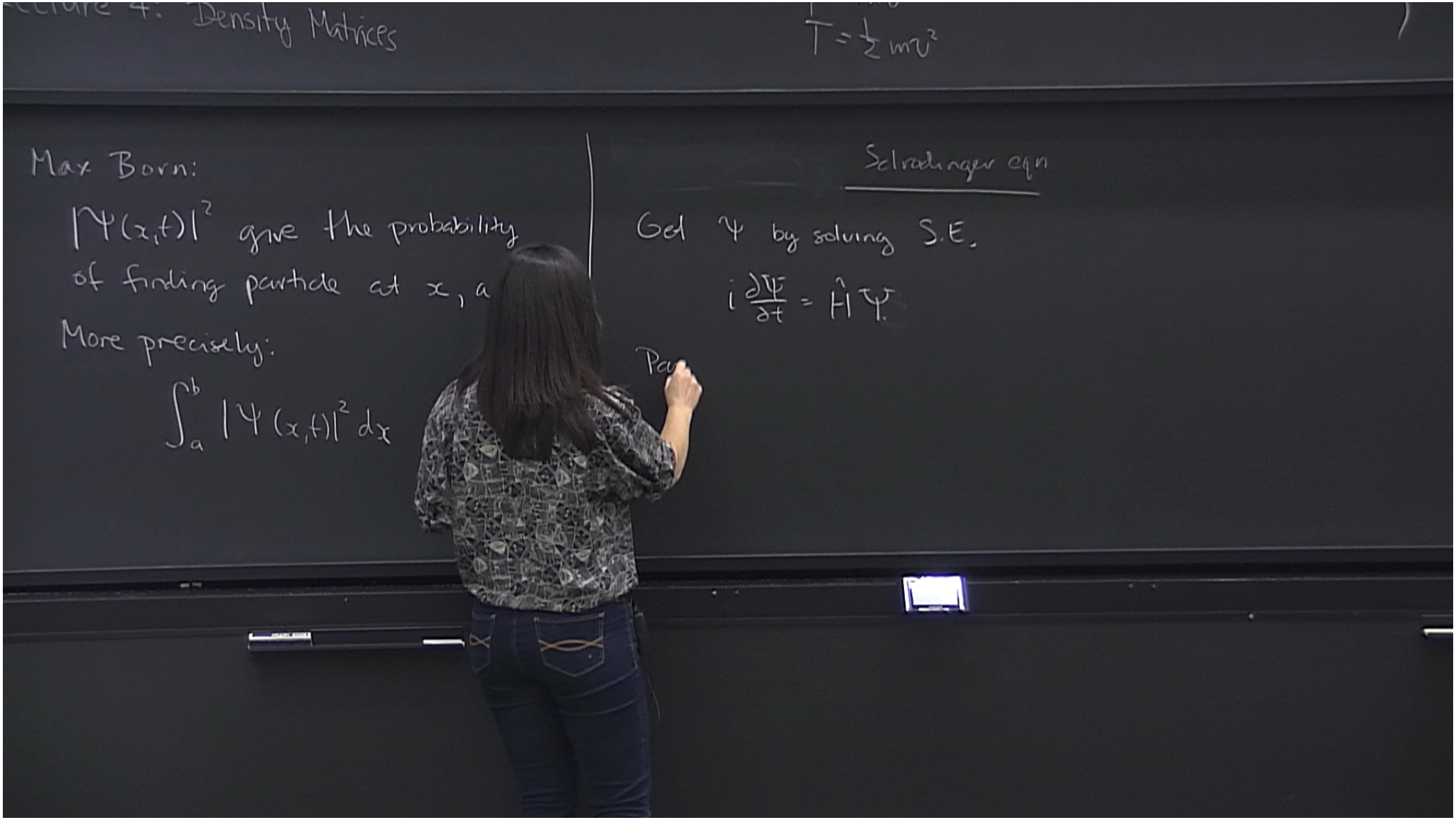
Max Born:

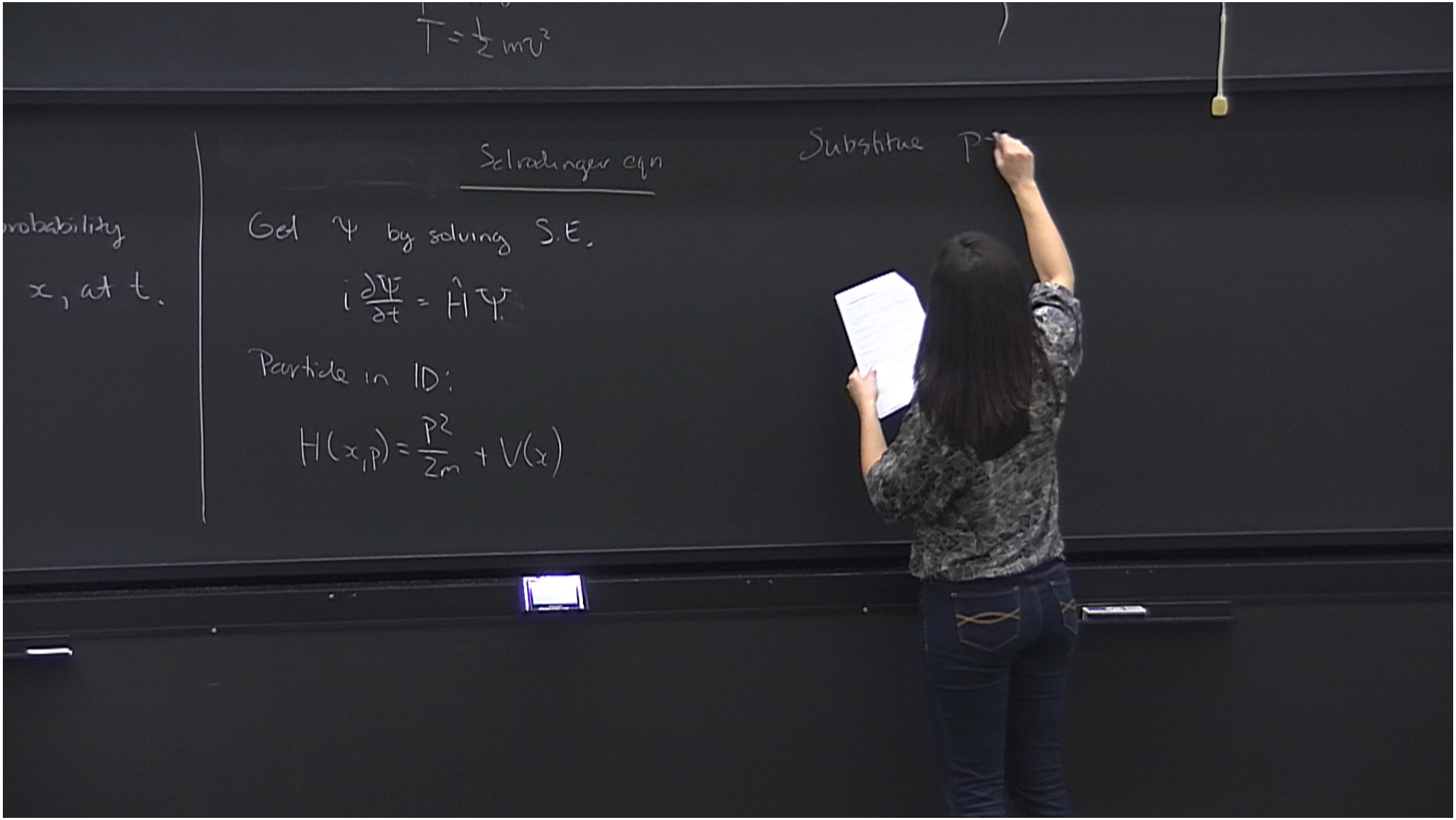
$|\Psi(x,t)|^2$ give the probability of finding particle at x, at t.

More precisely:

$$\int_a^b |\Psi(x,t)|^2 \, dx$$

Time-Independent Schrodinger eqn


ecture 4: Density Matrices
$T = \frac{1}{2} m v^2$
Max Born:
$|\Psi(x,t)|^2$ give the probability
of finding particle at x, a
More precisely:
$\int_a^b |\Psi(x,t)|^2 dx$
Schrodinger eqn
Get Ψ by solving S.E.
$i \frac{\partial \Psi}{\partial t} = \hat{H} \Psi$
Pa


$T = \frac{1}{2}mv^2$
Schrodinger eqn
Substitue
robability
x, at t.
Get Ψ by solving S.E.
$i\frac{\partial\Psi}{\partial t} = \hat{H}\Psi$
Particle in 1D:
$H(x,p) = \frac{p^2}{2m} + V(x)$

$T = \frac{1}{2} m v^2$

robability

at t.

Schrodinger eqn

Get Ψ by solving S.E.

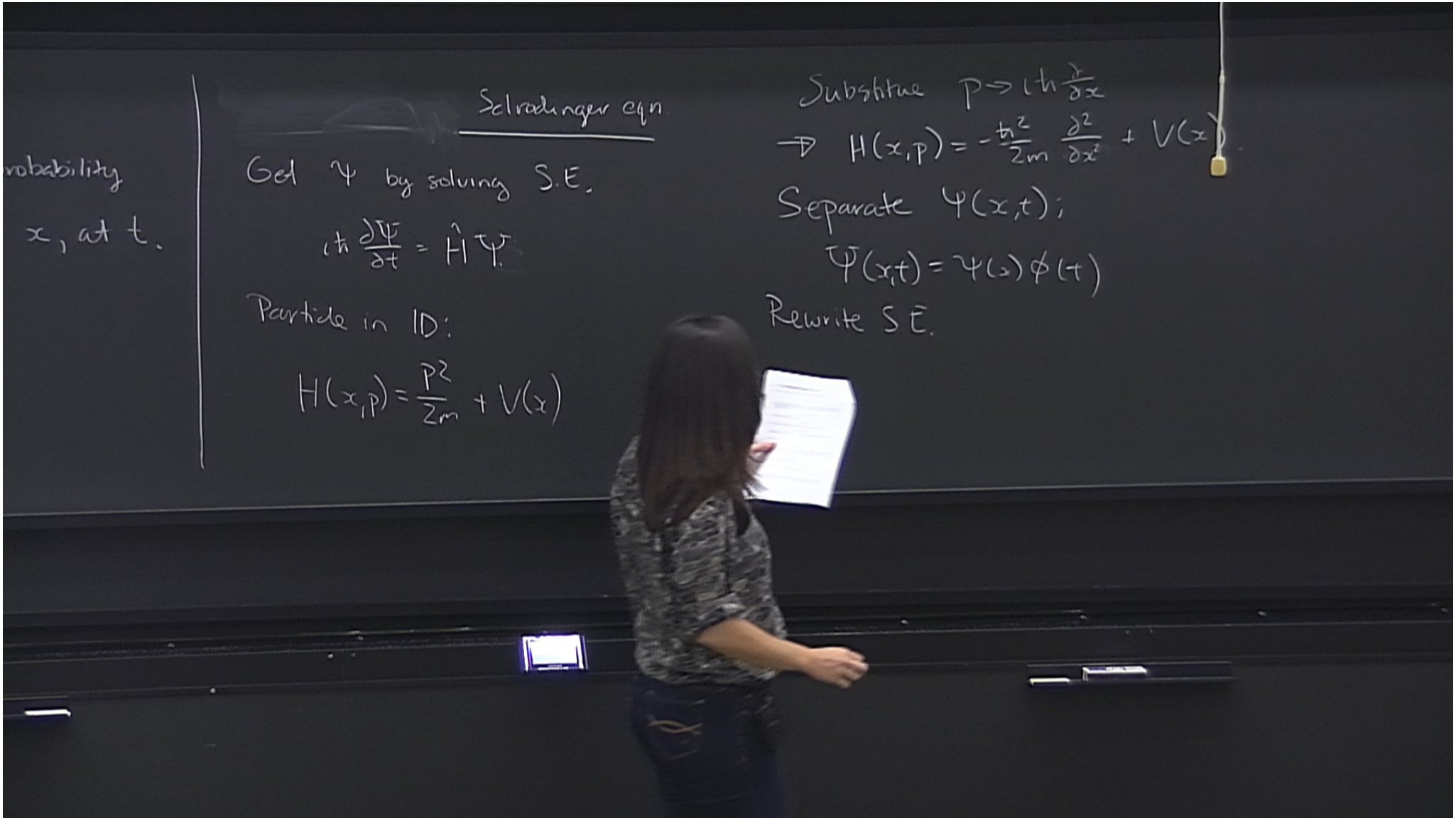
$$i \frac{\partial \Psi}{\partial t} = \hat{H} \Psi$$

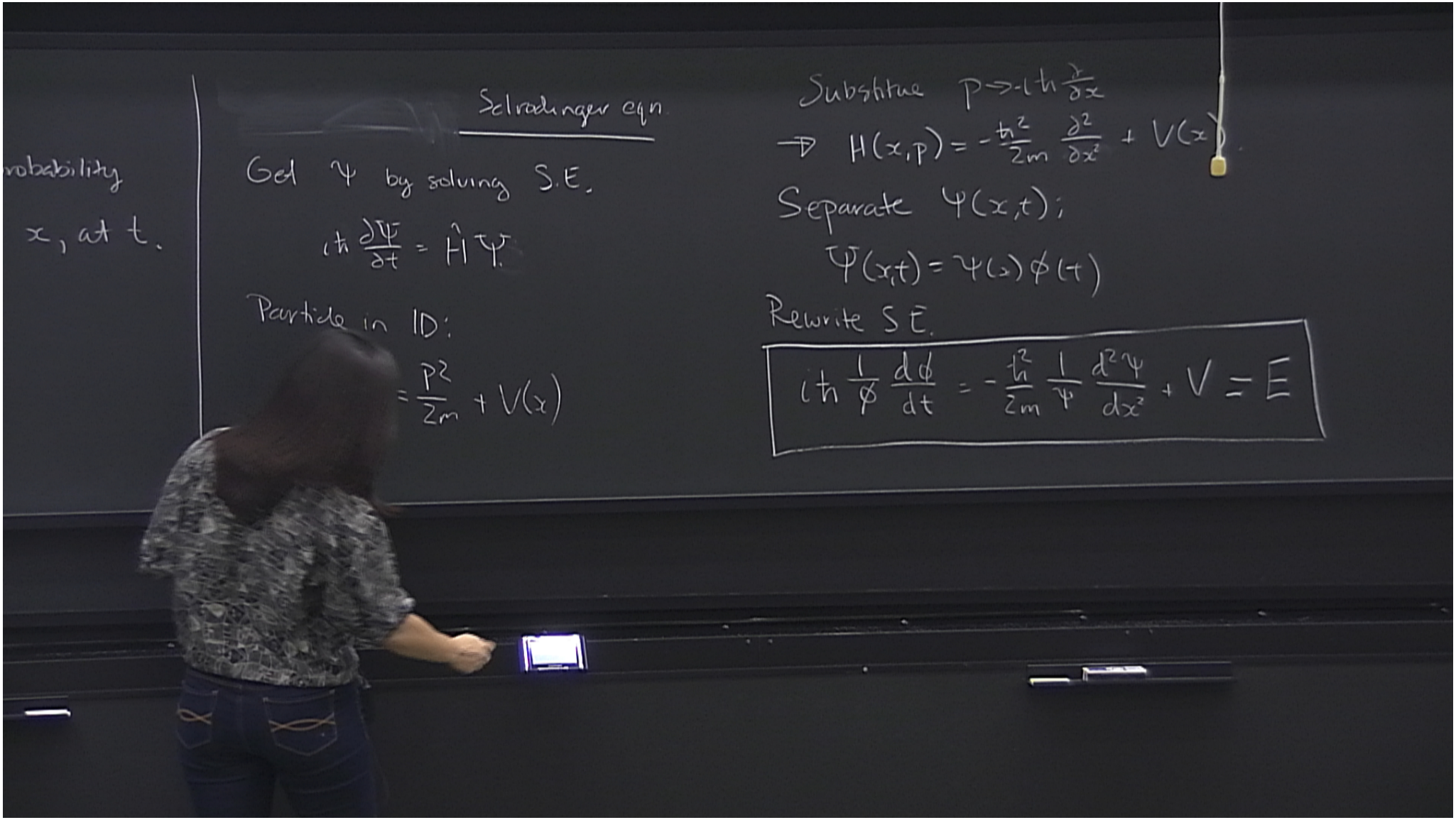
Particle in 1D:

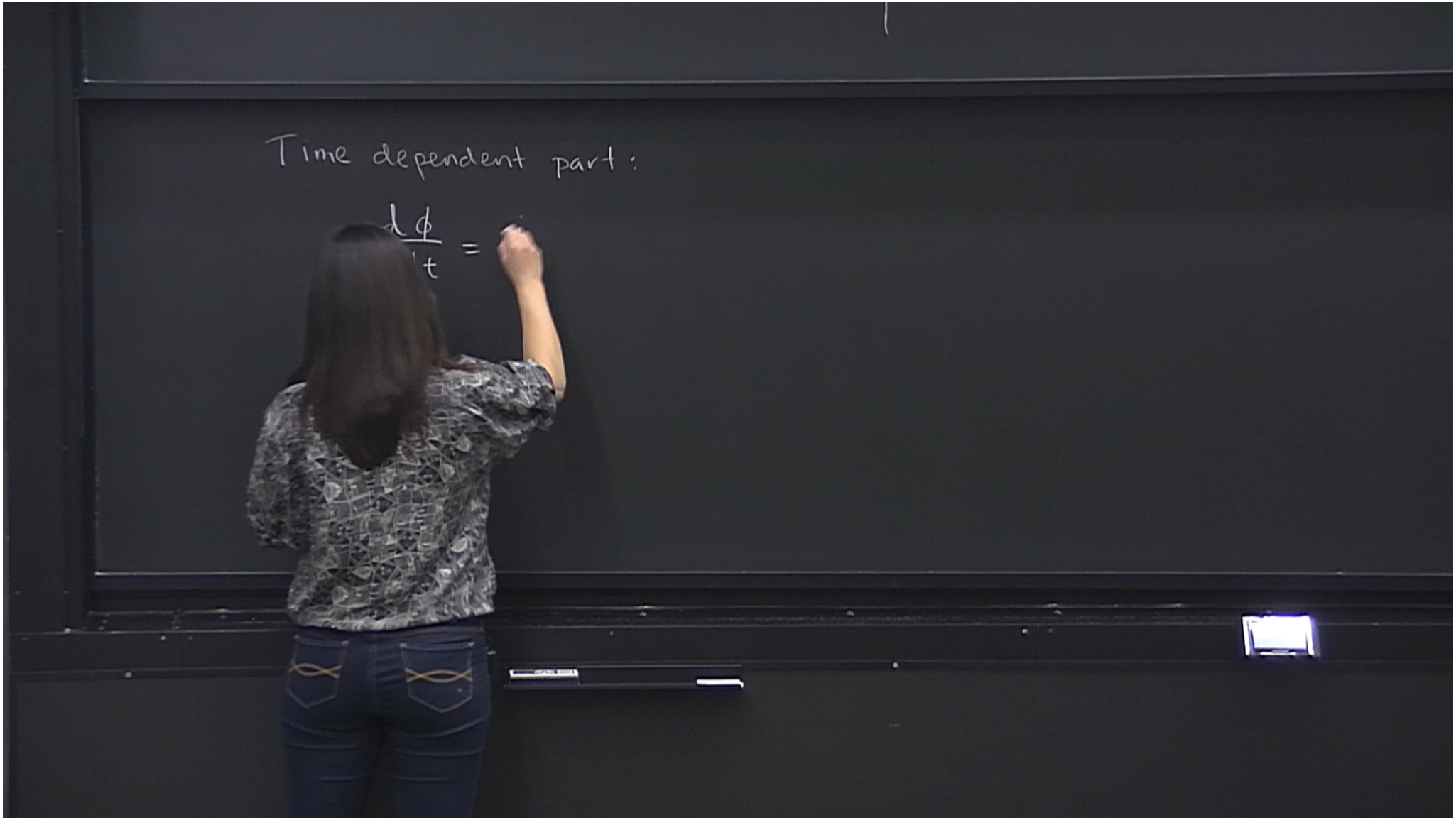
$$H(x,p) = \frac{p^2}{2m} + V(x)$$

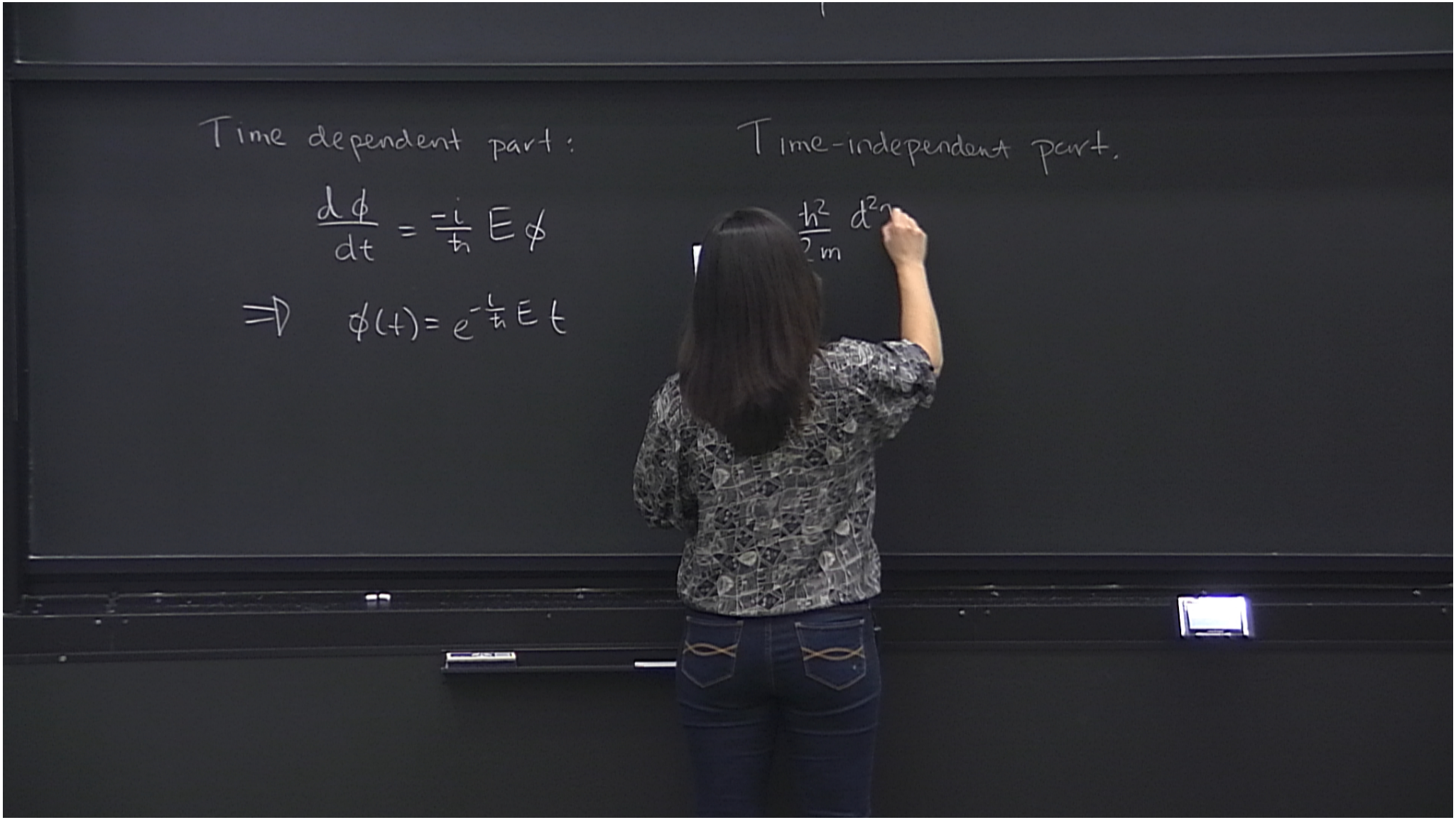
Substitue $p \Rightarrow -i\hbar \frac{\partial}{\partial x}$

$$\Rightarrow H(x,p) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x)$$


robability
x, at t.
Schrodinger eqn
Get Ψ by solving S.E.
$ih\frac{\partial\Psi}{\partial t} = \hat{H}\Psi$
Particle in 1D:
$H(x,p) = \frac{p^2}{2m} + V(x)$
Substitue $p \to ih\frac{\partial}{\partial x}$
$\Rightarrow H(x,p) = -\frac{h^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$
Separate Ψ(x,t);
$\Psi(x,t) = \psi(x)\phi(t)$
Rewrite SE.


robability
x, at t.
Schrodinger eqn
Get Ψ by solving S.E.
$ih\frac{\partial\Psi}{\partial t} = \hat{H}\Psi$
Particle in 1D:
$= \frac{p^2}{2m} + V(x)$
Substitue $p \to -ih\frac{\partial}{\partial x}$
$\Rightarrow H(x,p) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$
Separate $\Psi(x,t)$;
$\Psi(x,t) = \psi(x)\phi(t)$
Rewrite S.E.
$ih\frac{1}{\phi}\frac{d\phi}{dt} = -\frac{\hbar^2}{2m}\frac{1}{\psi}\frac{d^2\psi}{dx^2} + V = E$


Time dependent part:
$\frac{\partial \phi}{\partial t} =$


Time dependent part:
$\frac{d\phi}{dt} = \frac{-i}{\hbar} E \phi$
$\Rightarrow \quad \phi(t) = e^{-\frac{i}{\hbar} E t}$
Time-independent part.
$\frac{\hbar^2}{2m} d^2$

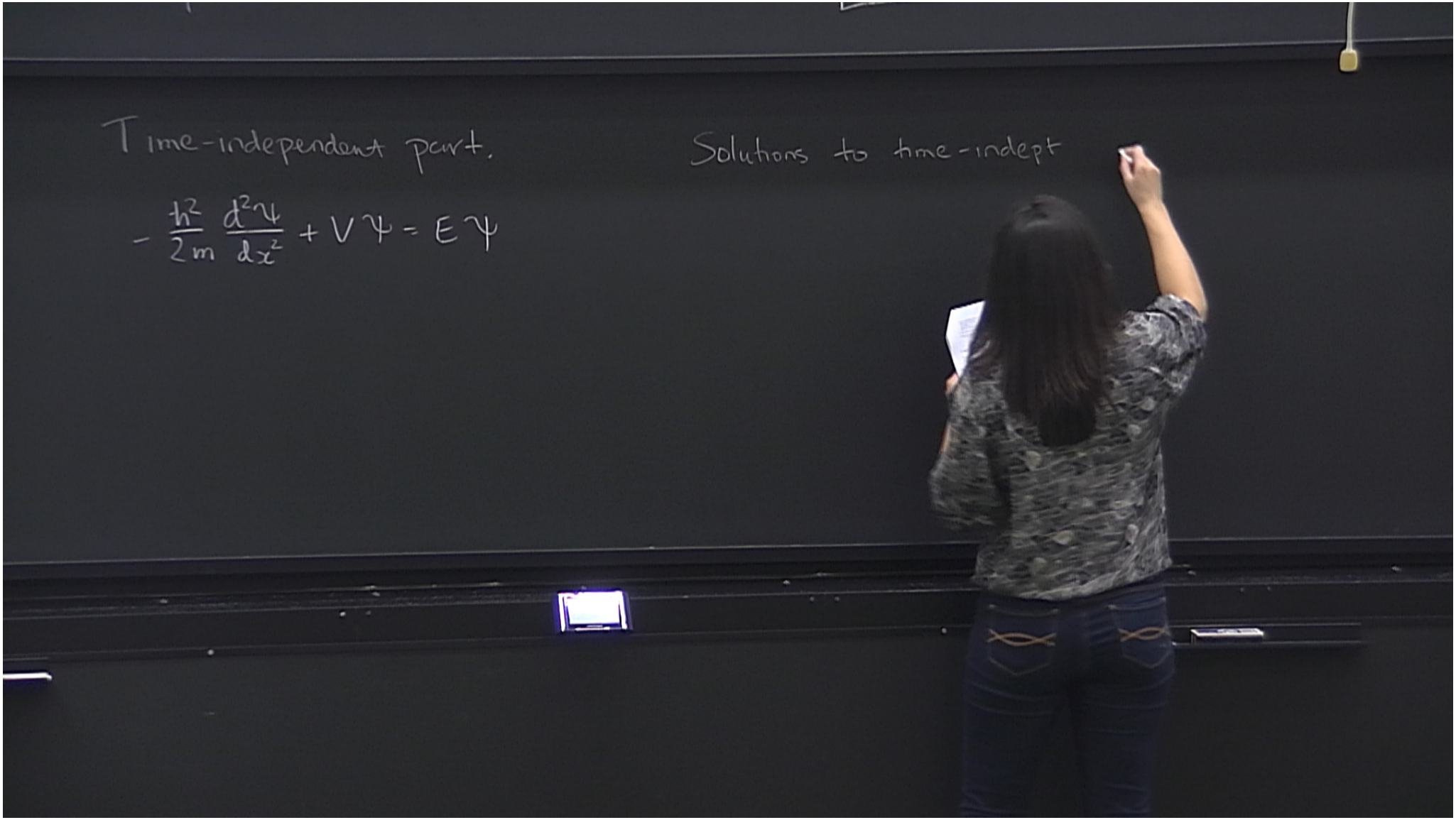
Time dependent part:

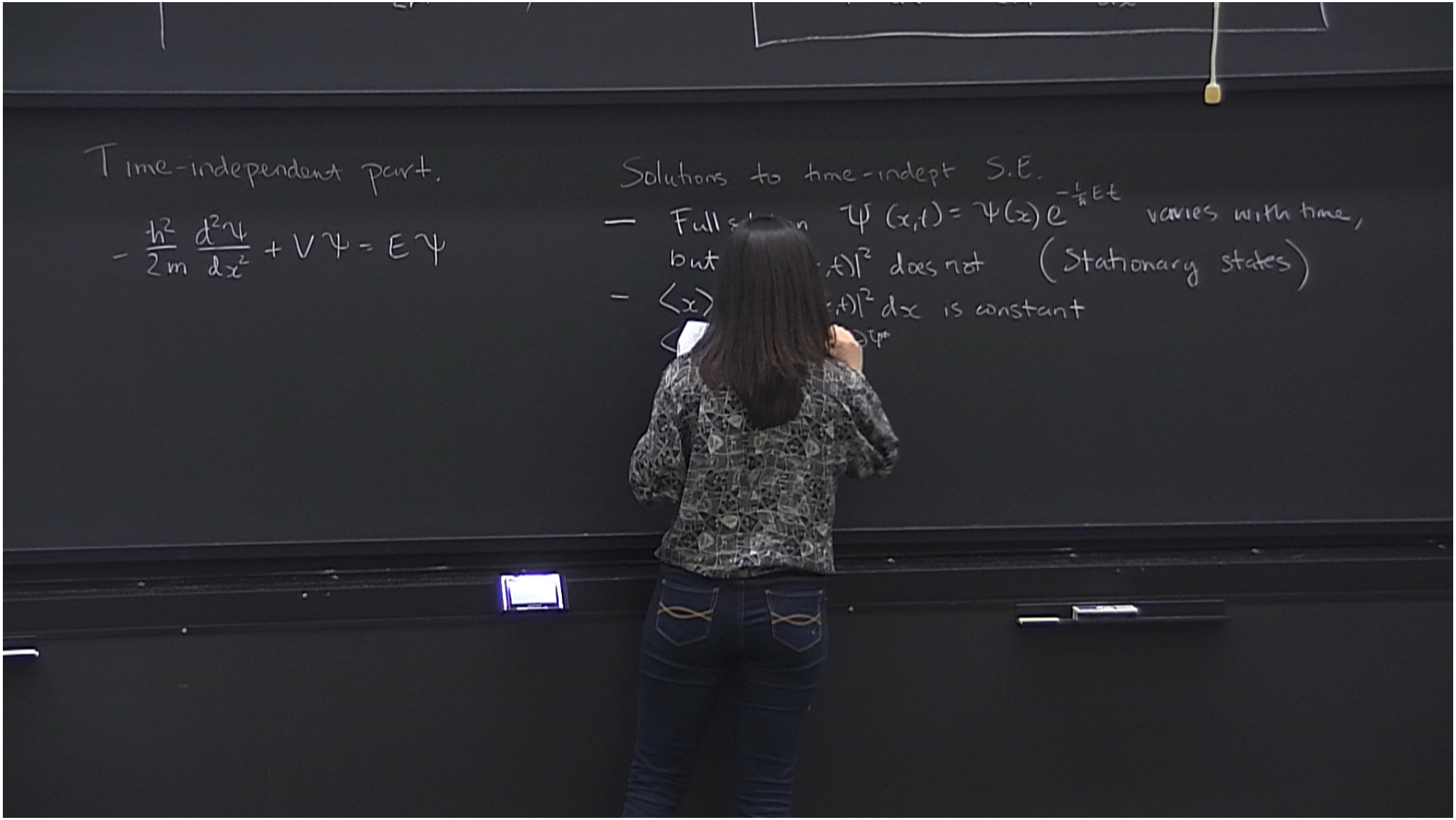
$$\frac{d\phi}{dt} = \frac{-i}{\hbar} E \phi$$

$$\Rightarrow \quad \phi(t) = e^{-\frac{i}{\hbar} E t}$$

Time-independent part.

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = E\psi$$


Time-independent part.
$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = E\psi$
Solutions to time-indept


Time-independent part.
$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = E\psi$
Solutions to time-indept S.E.
– Full solution $\Psi(x,t) = \psi(x)e^{-\frac{i}{\hbar}Et}$ varies with time,
but $|\Psi(x,t)|^2$ does not (Stationary states)
– $\langle x \rangle$ $|\Psi(x,t)|^2 dx$ is constant

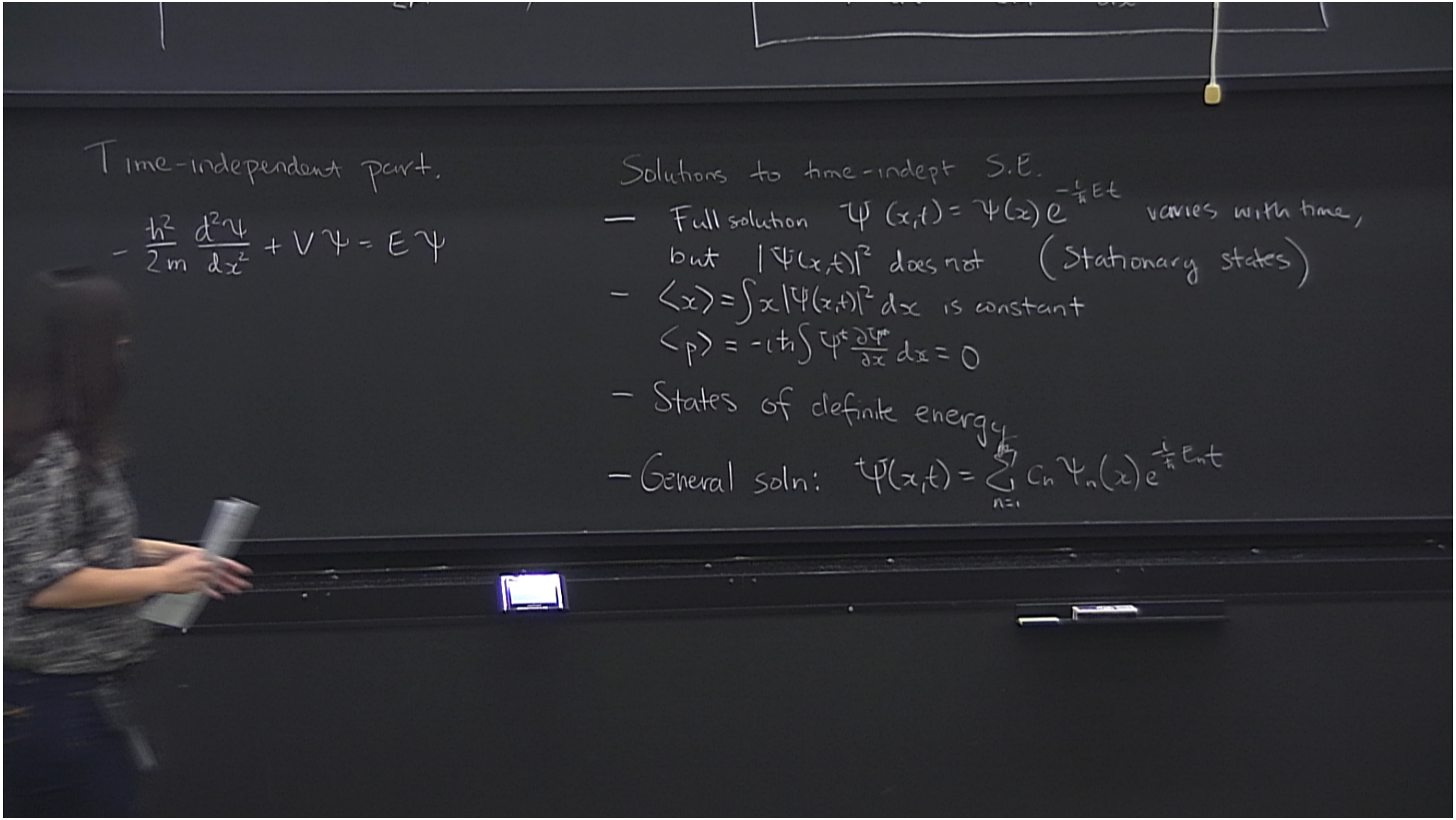
Time-independent part.

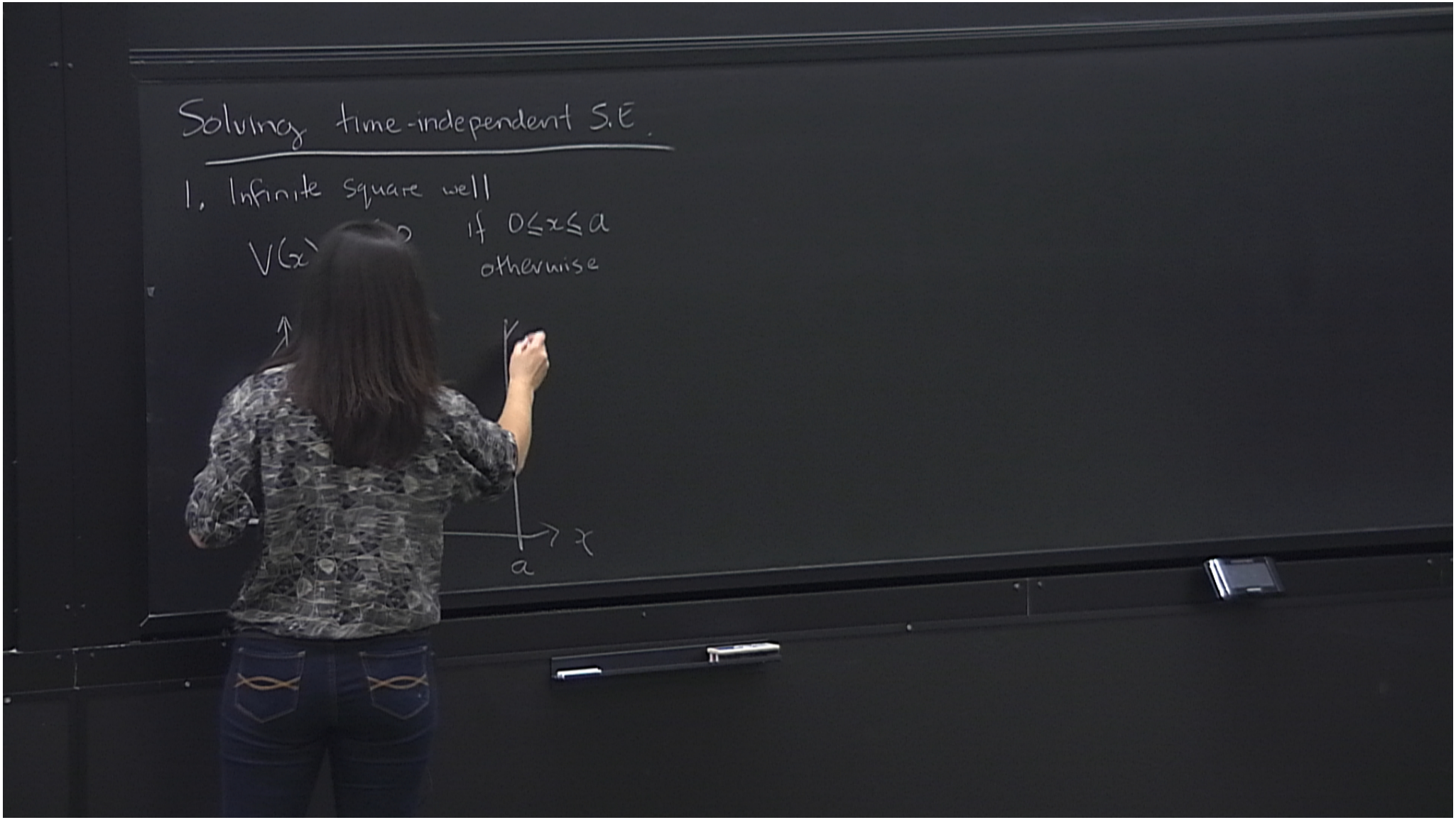
$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = E\psi$$

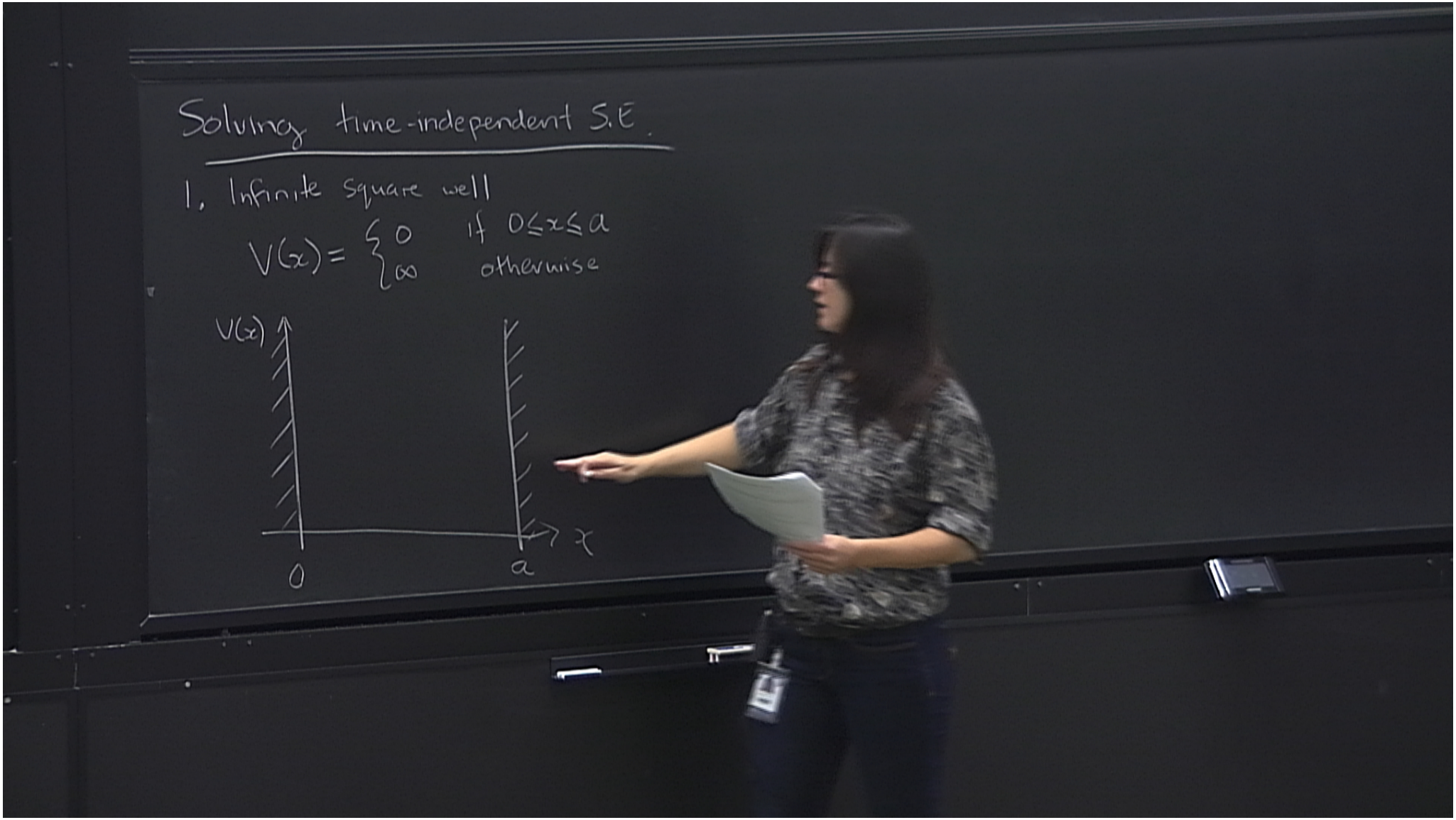
Solutions to time-indept S.E.

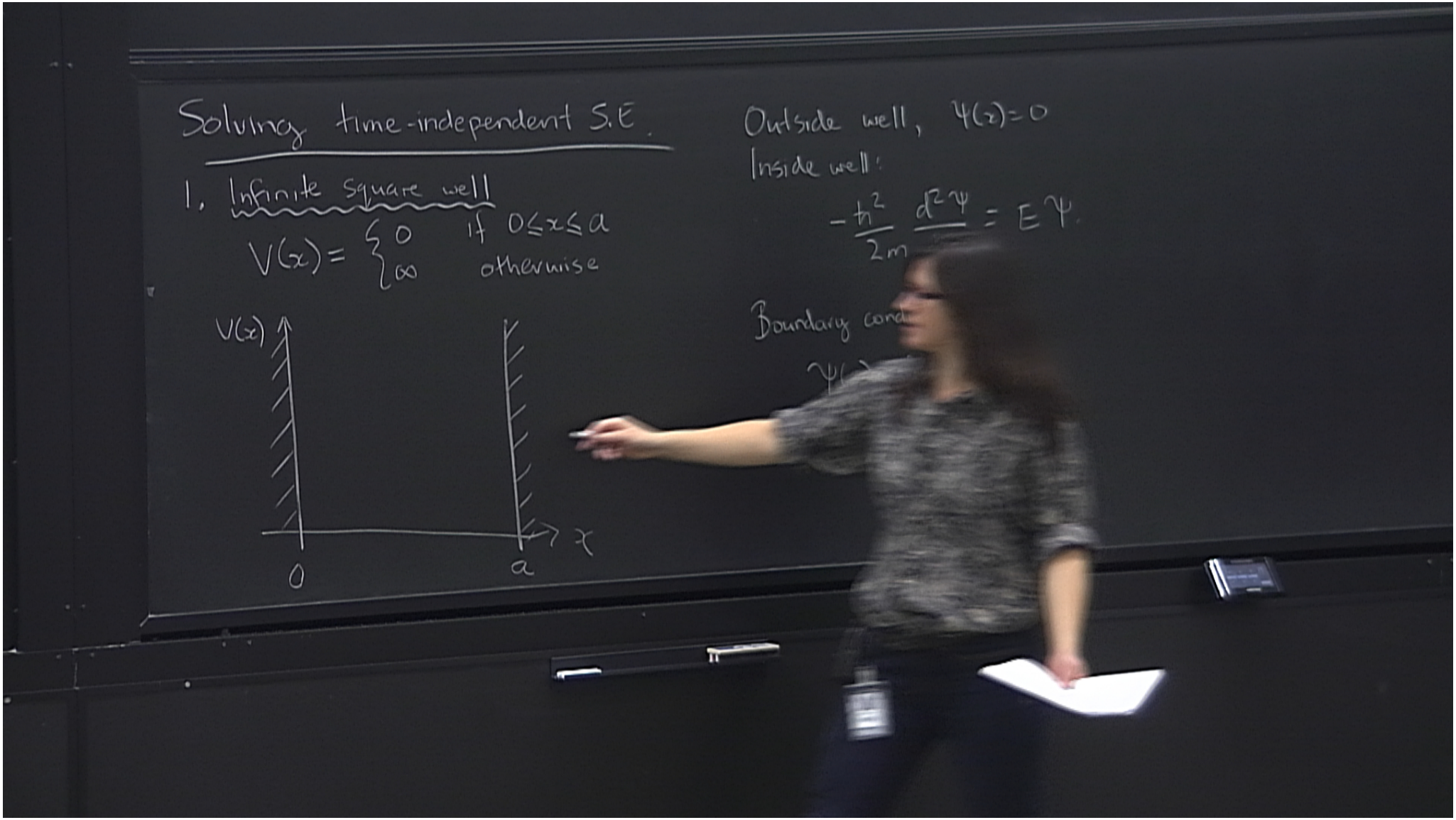
- Full solution $\Psi(x,t) = \psi(x)e^{-\frac{i}{\hbar}Et}$ varies with time, but $|\Psi(x,t)|^2$ does not (Stationary states)
- $\langle x \rangle = \int x|\Psi(x,t)|^2 dx$ is constant

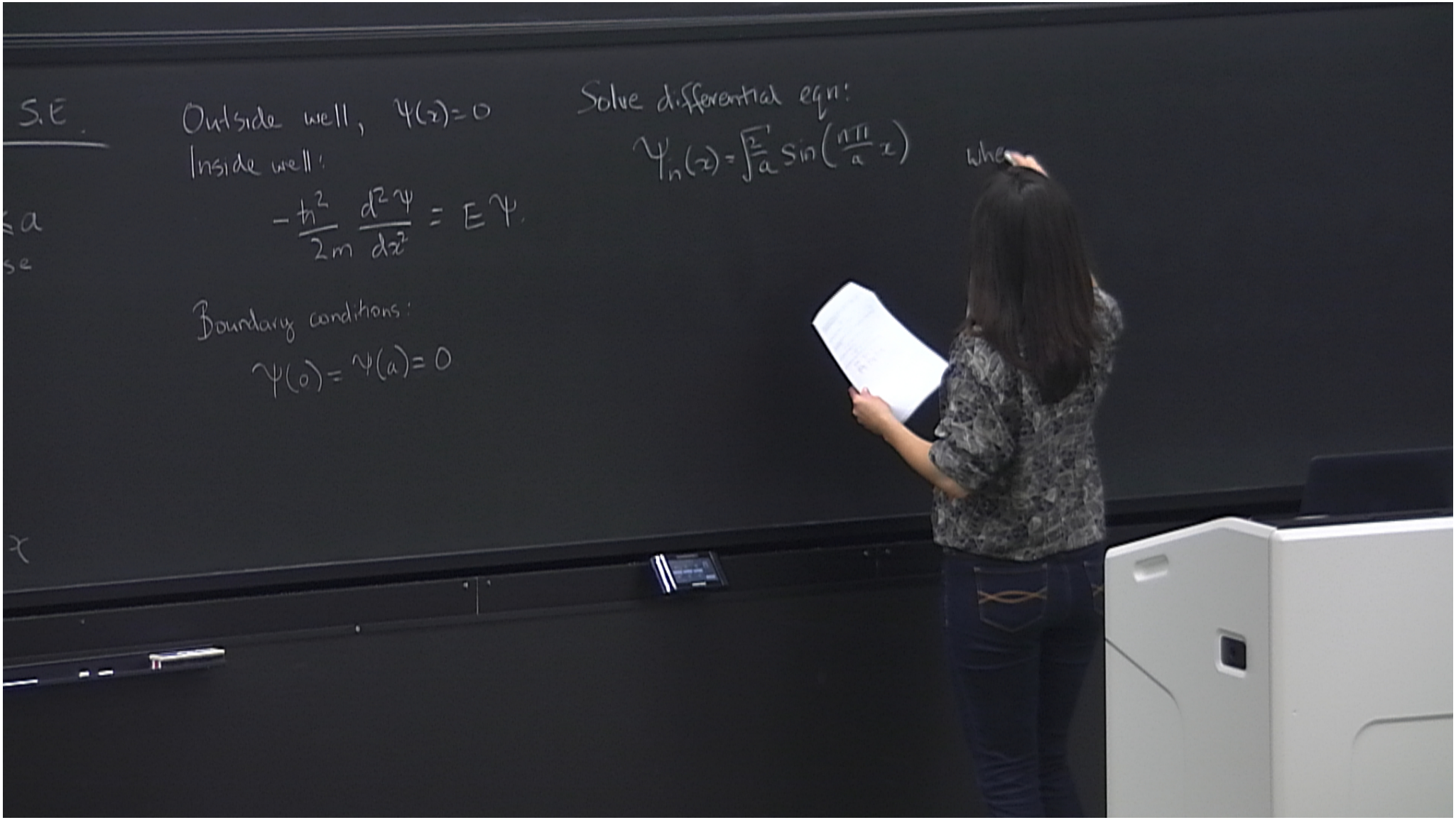
  $\langle p \rangle = -i\hbar\int \Psi^* \frac{\partial \Psi^*}{\partial x} dx = 0$

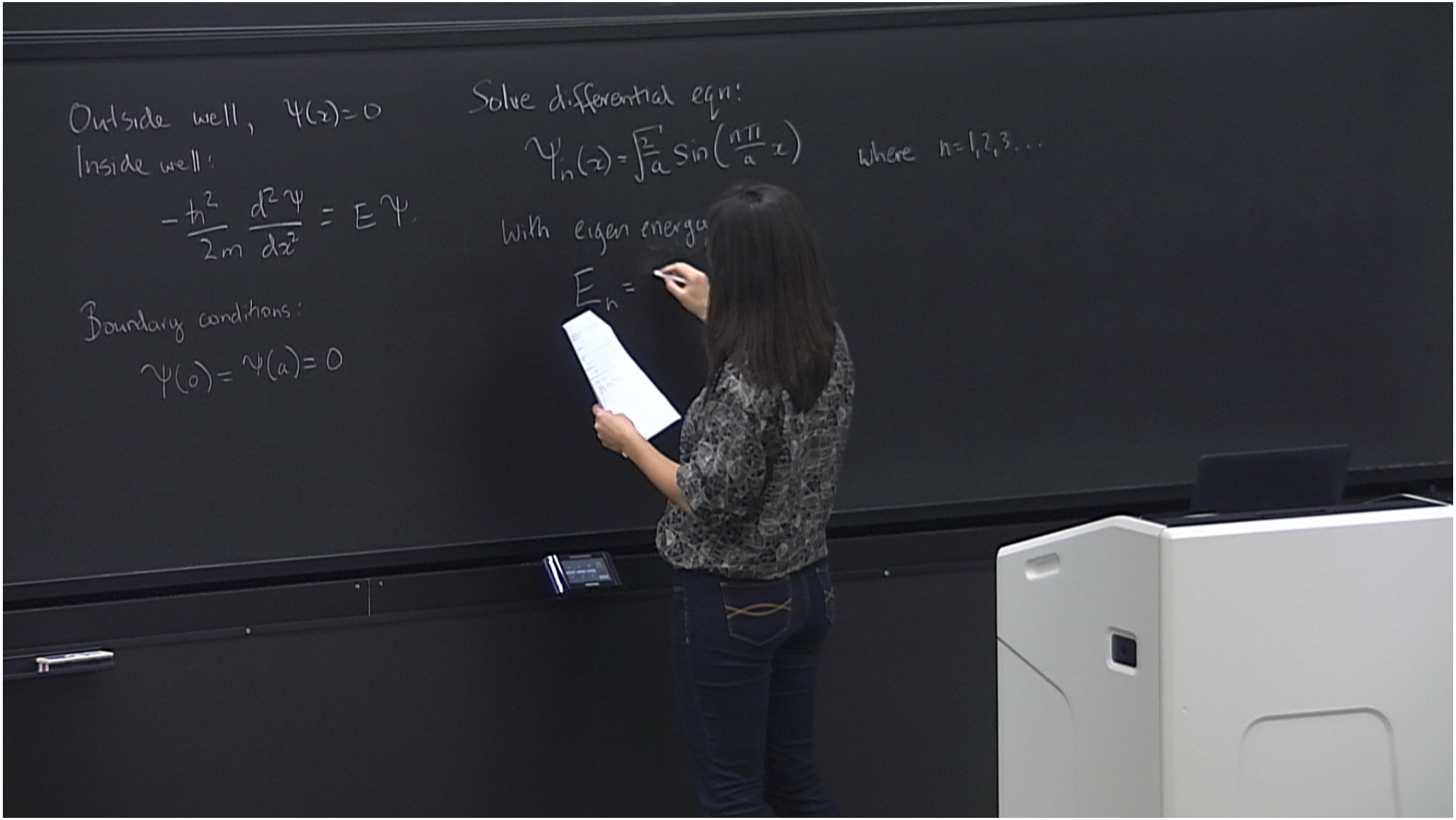

Time-independent part.
$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = E\psi$
Solutions to time-indept S.E.
– Full solution $\Psi(x,t) = \psi(x)e^{-\frac{i}{\hbar}Et}$ varies with time, but $|\Psi(x,t)|^2$ does not (Stationary states)
– $\langle x\rangle = \int x|\Psi(x,t)|^2 dx$ is constant
$\langle p\rangle = -i\hbar\int \Psi^* \frac{\partial \Psi}{\partial x} dx = 0$
– States of definite energy
– General soln: $\Psi(x,t) = \sum_{n=1}^{\infty} c_n \psi_n(x) e^{\frac{i}{\hbar}E_n t}$

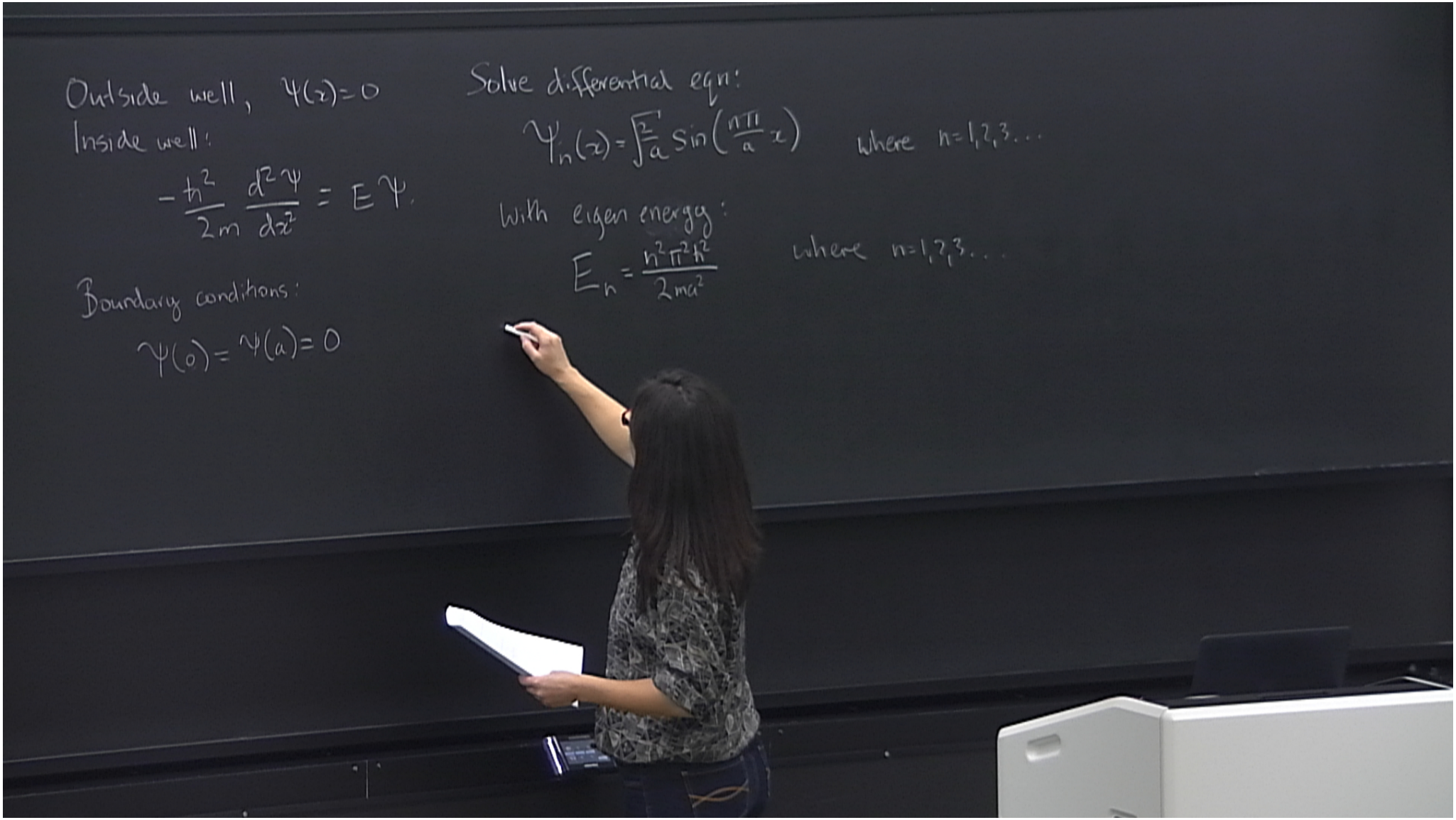

Solving time-independent S.E.
1. Infinite square well
if 0≤x≤a
otherwise
a
x


Solving time-independent S.E.
1. Infinite square well
$V(x) = \begin{cases} 0 & \text{if } 0 \le x \le a \\ \infty & \text{otherwise} \end{cases}$
V(x)
0
a
x


Solving time-independent S.E.
1. Infinite square well
$V(x) = \begin{cases} 0 & \text{if } 0 \le x \le a \\ \infty & \text{otherwise} \end{cases}$
V(x)
0
a
x
Outside well, $\psi(x) = 0$
Inside well:
$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi$
Boundary cond


S.E
Outside well, $\psi(x)=0$
Inside well:
$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}=E\psi$
Boundary conditions:
$\psi(0)=\psi(a)=0$
Solve differential eqn:
$\psi_n(x)=\sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right)$


Outside well, $\psi(x)=0$
Inside well:
$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}=E\psi$
Boundary conditions:
$\psi(0)=\psi(a)=0$
Solve differential eqn:
$\psi_n(x)=\sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right)$ where $n=1,2,3\ldots$
With eigen energy
$E_n=$


Outside well, $\psi(x)=0$
Inside well:
$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}=E\psi$
Boundary conditions:
$\psi(0)=\psi(a)=0$
Solve differential eqn:
$\psi_n(x)=\sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right)$ where $n=1,2,3\ldots$
With eigen energy:
$E_n=\frac{n^2\pi^2\hbar^2}{2ma^2}$ where $n=1,2,3\ldots$

Outside well, $\psi(x) = 0$

Inside well:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi$$

Boundary conditions:

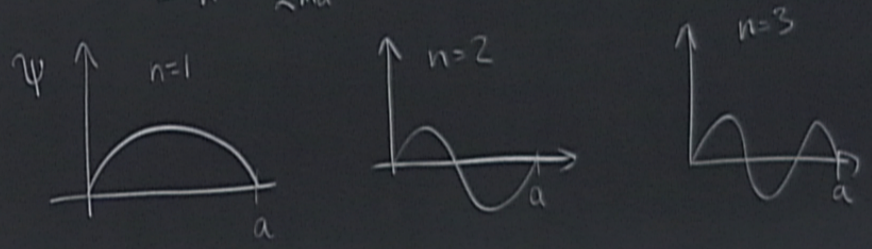
$$\psi(0) = \psi(a) = 0$$

Solve differential eqn:

$$\psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right) \quad \text{where } n = 1, 2, 3\ldots$$

With eigen energy:

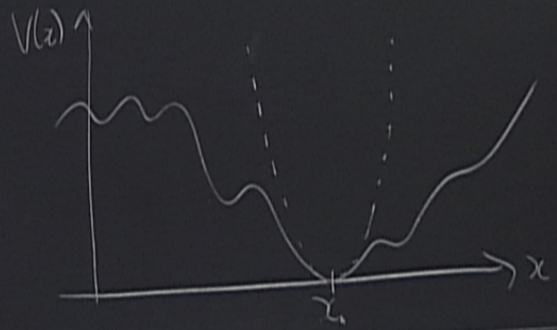
$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2} \quad \text{where } n = 1, 2, 3\ldots$$



General solution:

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a} x\right) e^{-iE_n t}$$

2. Harmonic Oscillator



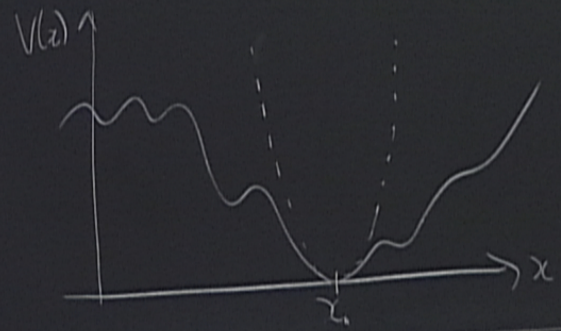
General solution:

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) e^{-\frac{i}{\hbar}E_n t}$$

Potential energy:

$$V(x) = \frac{1}{2}m(\omega x)^2$$

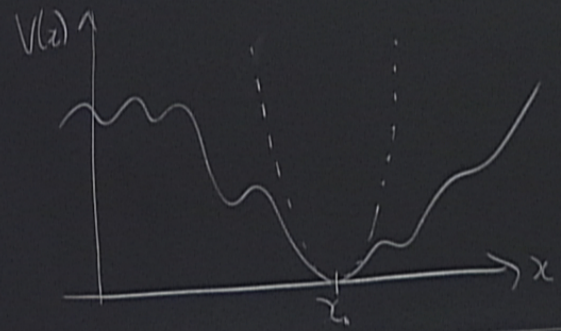
2. Harmonic Oscillator



General solution:

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a} x\right) e^{-\frac{i}{\hbar} E_n t}$$

2. Harmonic Oscillator



Potential energy:

$$V(x) = \frac{1}{2} m (\omega x)^2$$

Schrödinger eqn:

$$-\frac{\hbar^2}{2m} \frac{d^2\Psi}{dx^2} + \frac{1}{2} m(\omega$$

$= E\Psi$

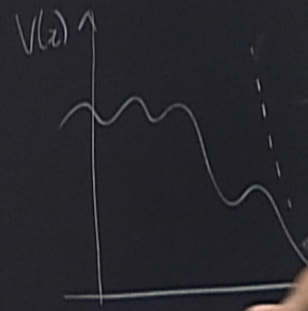
Rewrite Hamiltonian

$$H = \frac{1}{2m}$$

General solution:

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) e^{-\frac{i}{\hbar}E_n t}$$

2. Harmonic Osci



Potential energy:

$$V(x) = \frac{1}{2}m(\omega x)^2$$

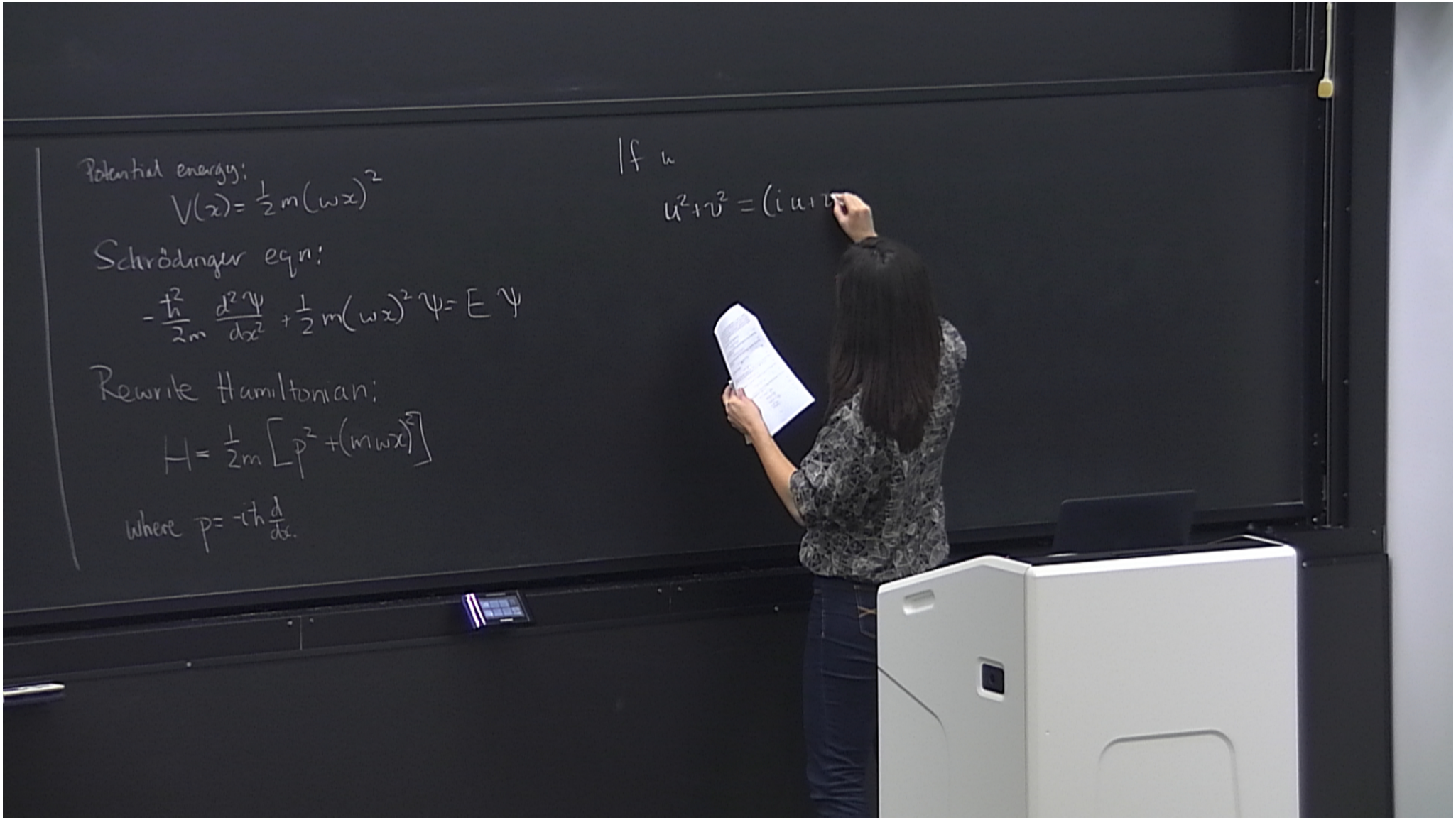
Schrödinger eqn:

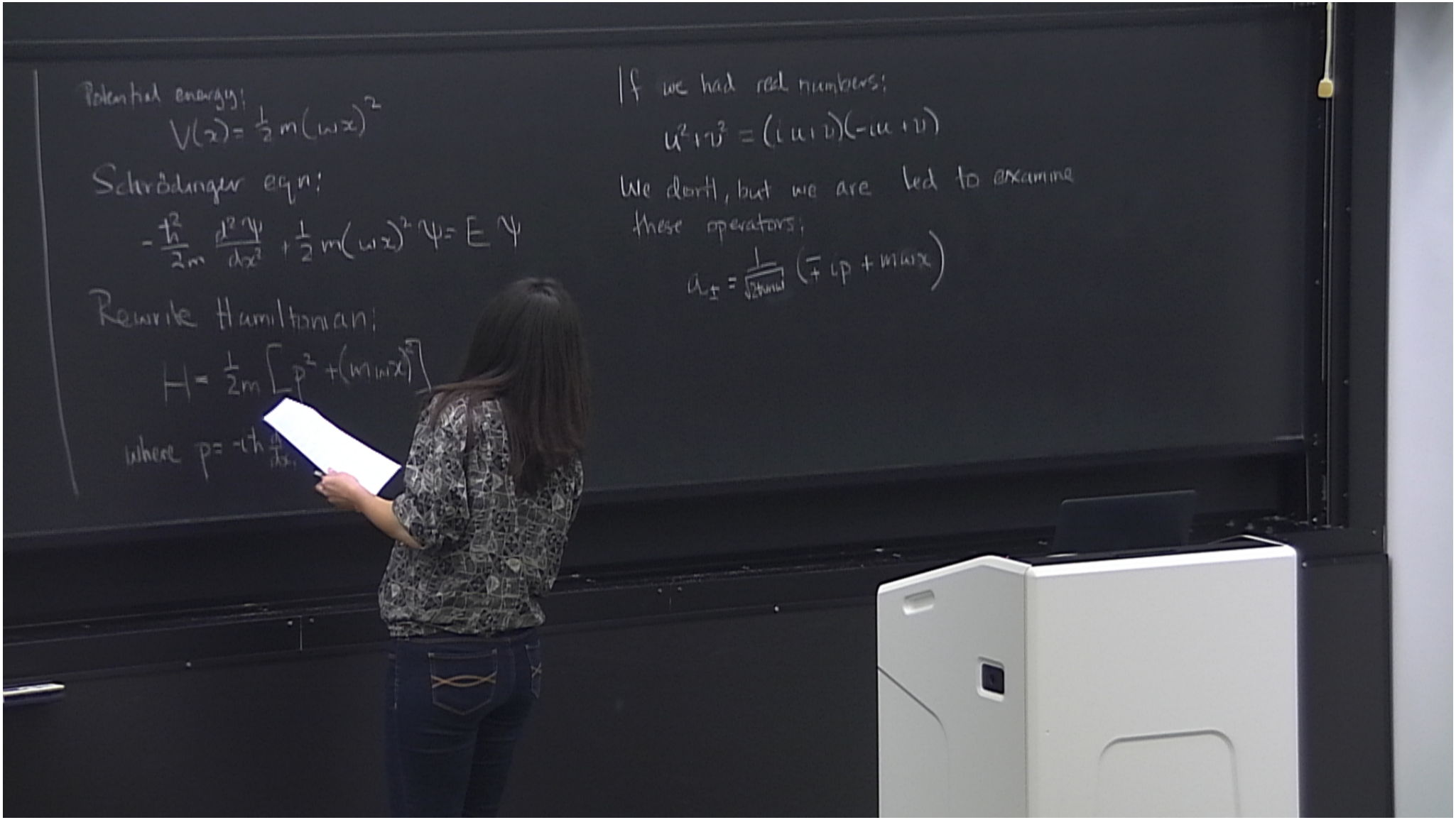
$$-\frac{\hbar^2}{2m}\frac{d^2\Psi}{dx^2} + \frac{1}{2}m(\omega x)^2\Psi = E\Psi$$

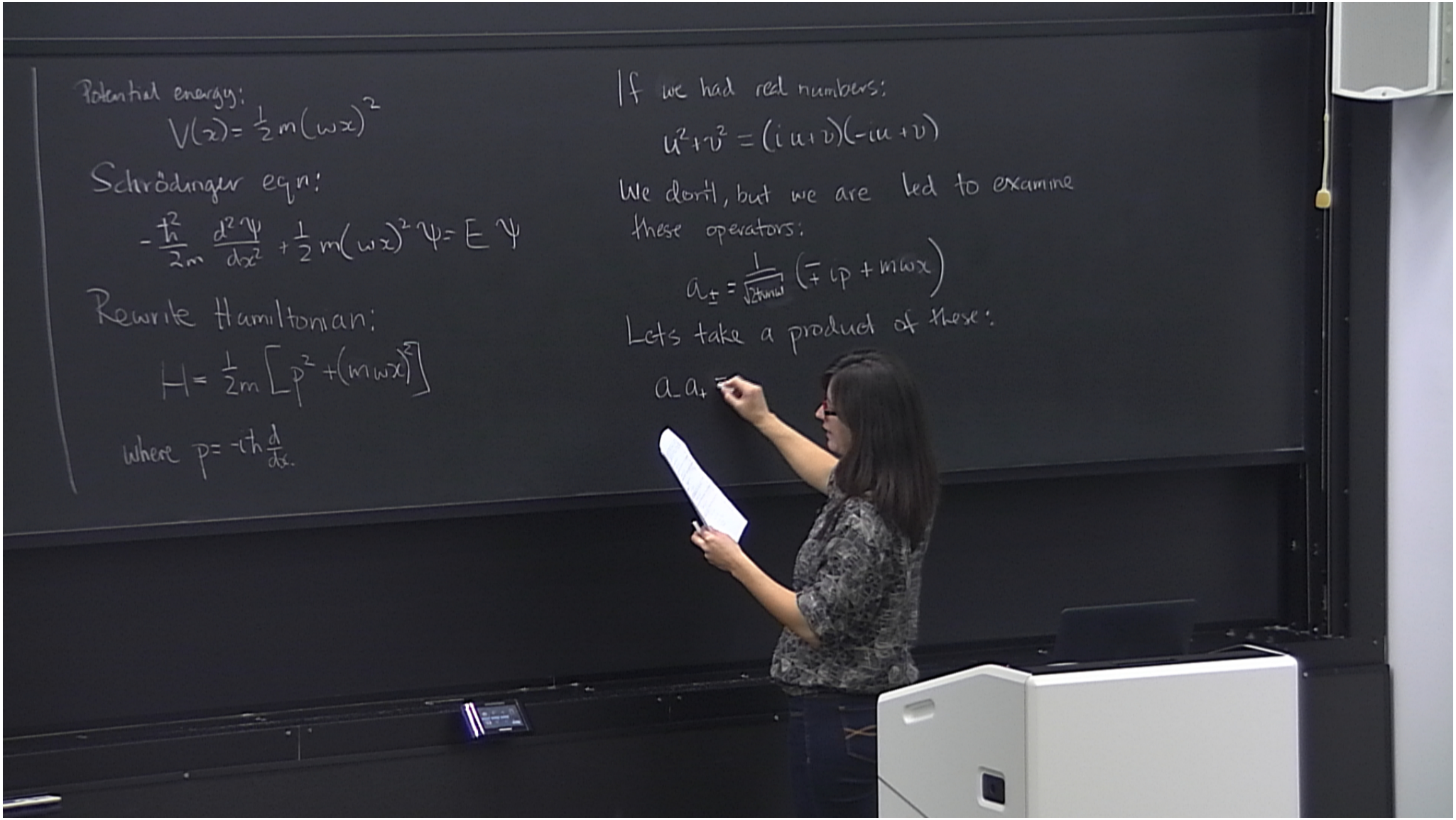
Rewrite Hamiltonian:

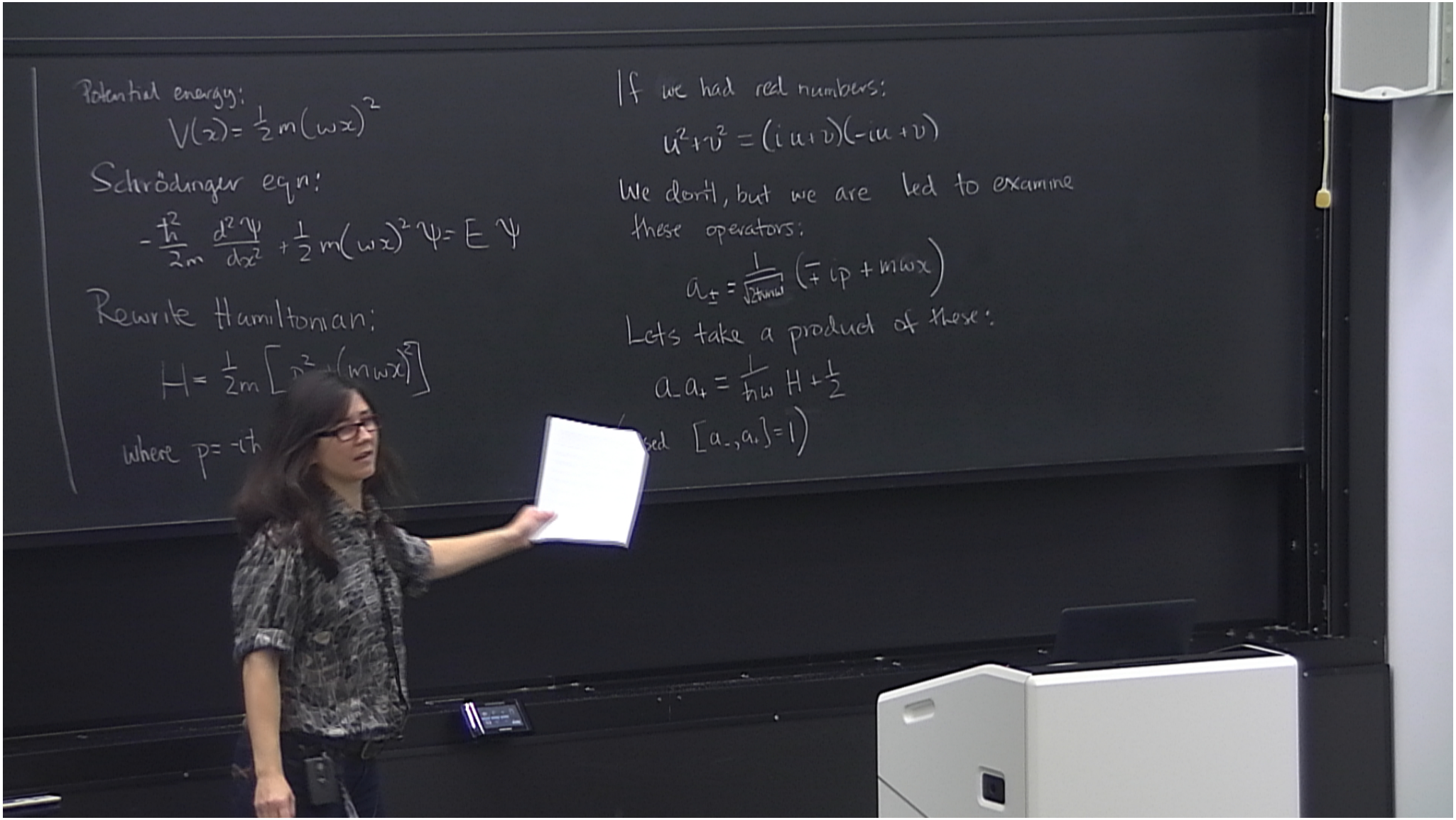
$$H = \frac{1}{2m}\left[p^2 + (m\omega x)\right]$$

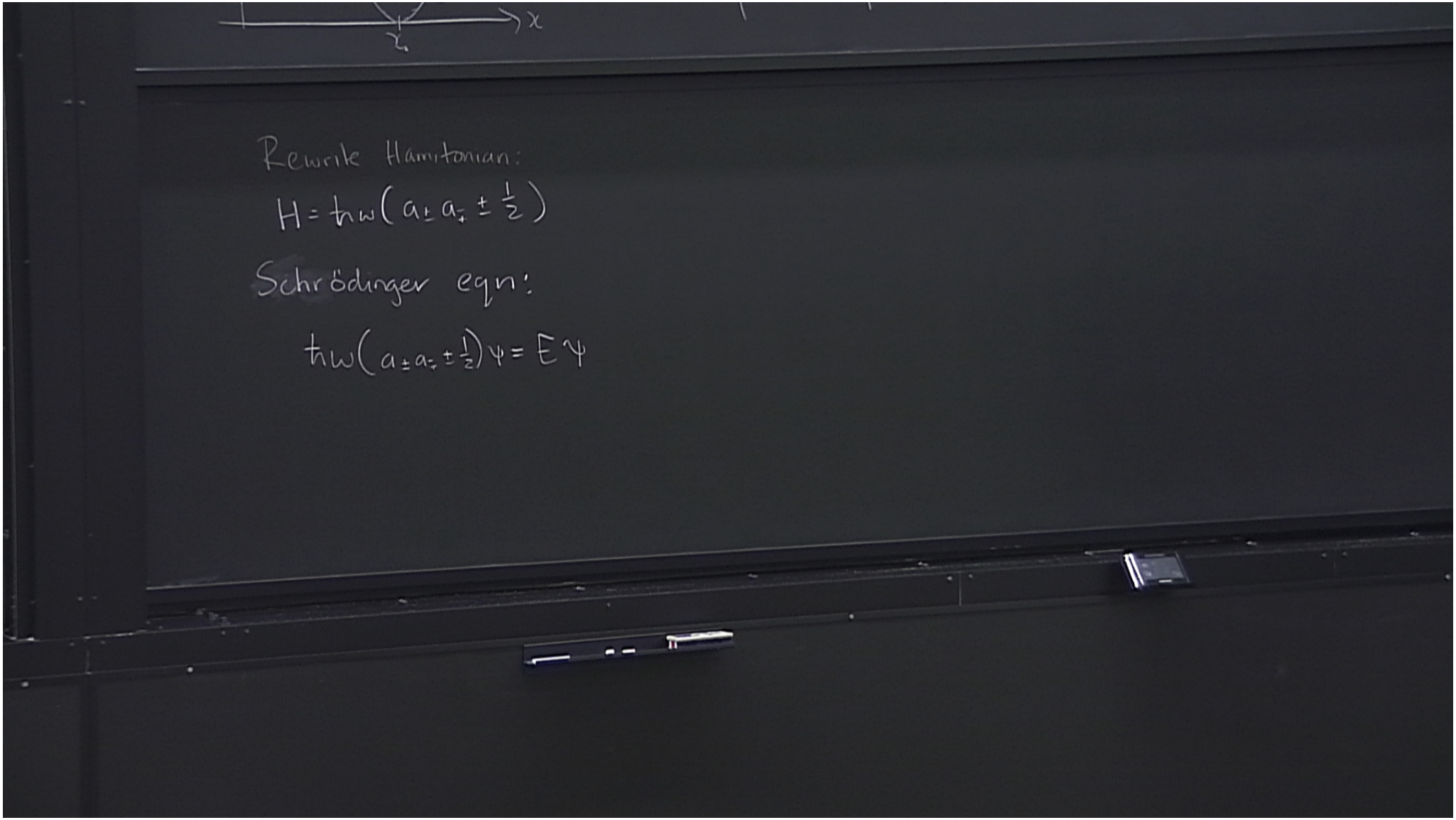
where $p = -i\hbar\frac{d}{dx}$.

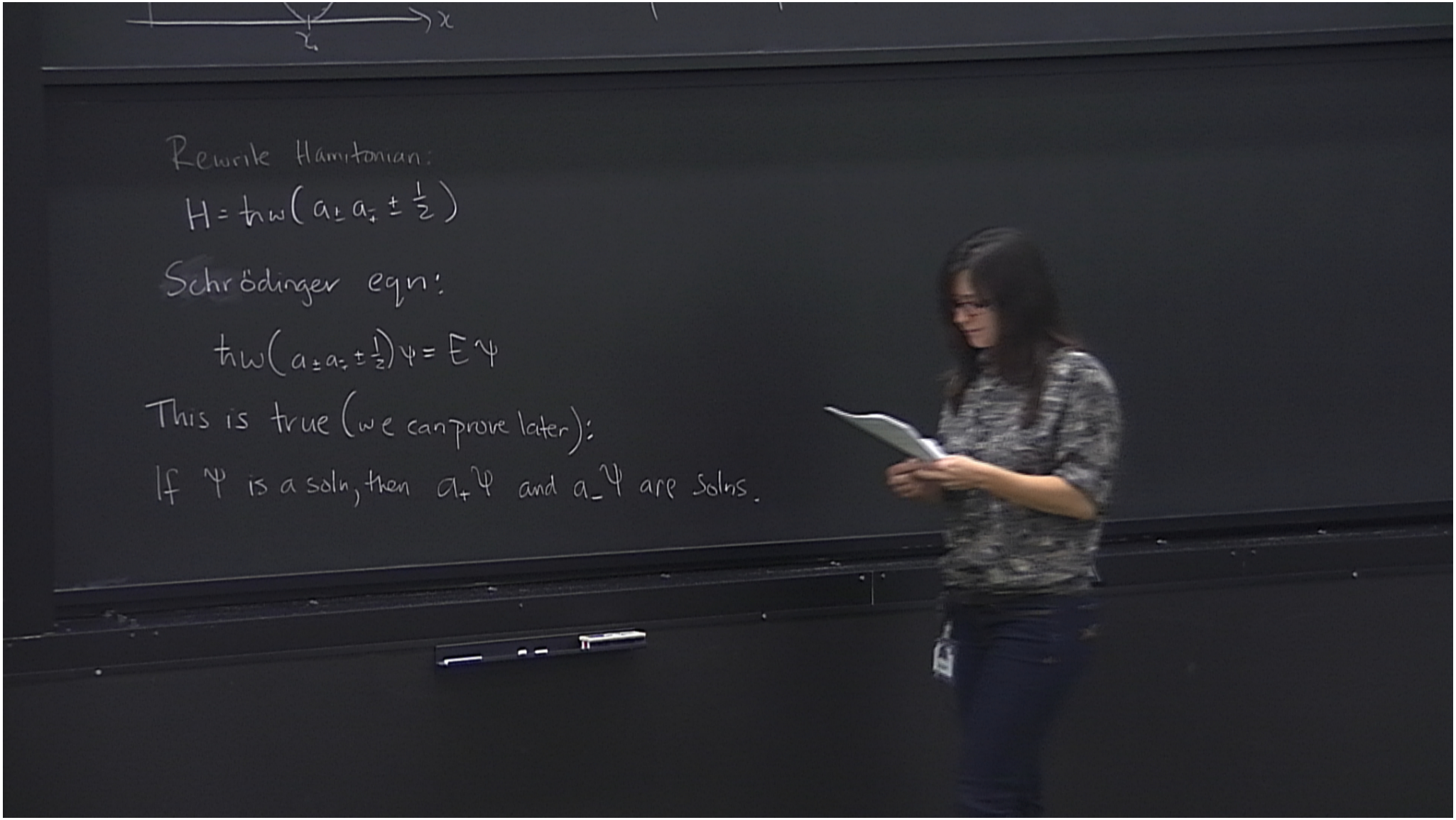

Potential energy:
$V(x) = \frac{1}{2} m(\omega x)^2$
Schrödinger eqn:
$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2} m(\omega x)^2 \psi = E\psi$
Rewrite Hamiltonian:
$H = \frac{1}{2m}\left[p^2 + (m\omega x)^2\right]$
where $p = -i\hbar\frac{d}{dx}$.
If u
$u^2 + v^2 = (iu + v$

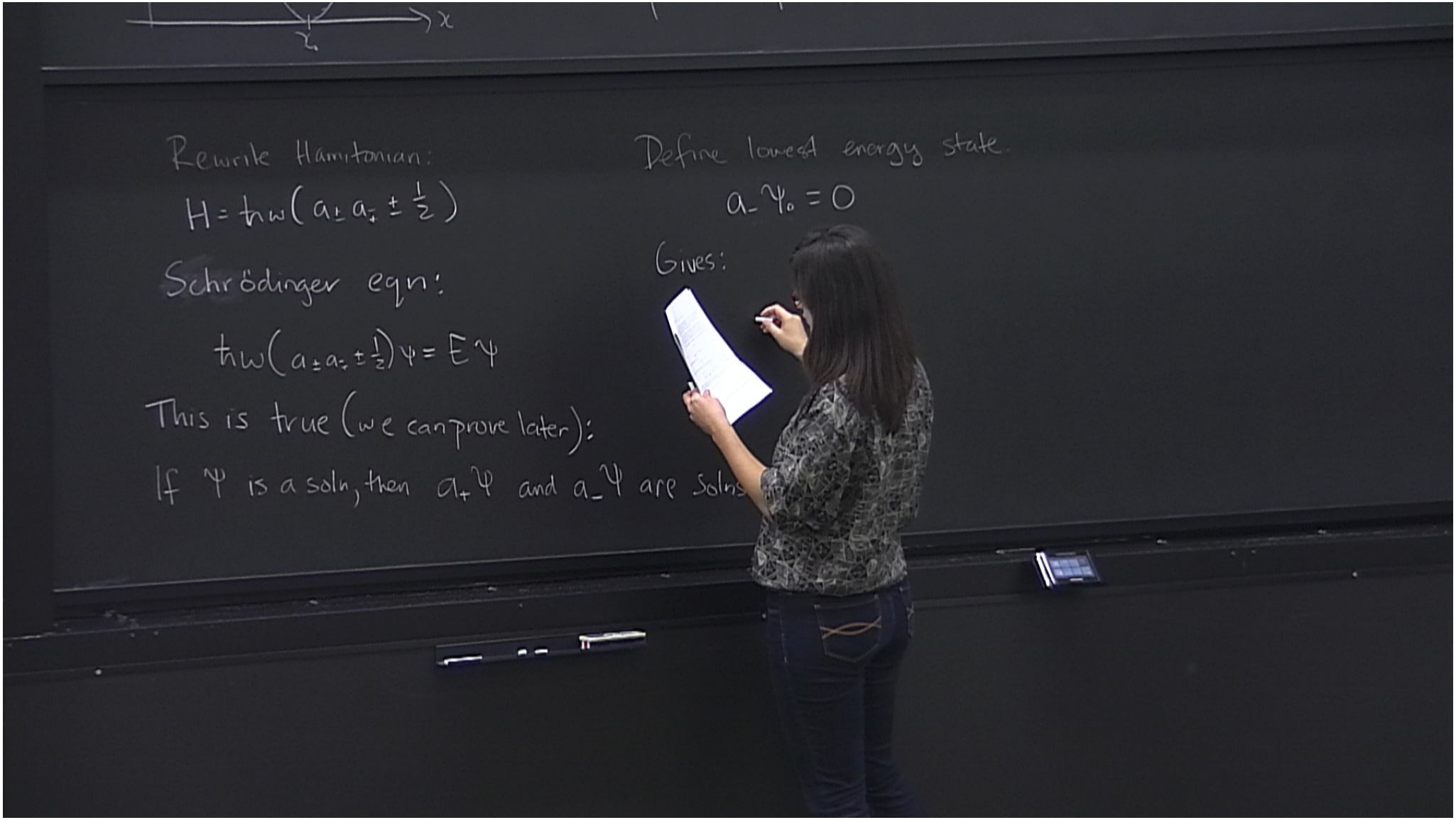

Potential energy:
$V(x) = \frac{1}{2} m(\omega x)^2$
Schrödinger eqn:
$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2} m(\omega x)^2 \psi = E\psi$
Rewrite Hamiltonian:
$H = \frac{1}{2m}\left[p^2 + (m\omega x)^2\right]$
where $p = -i\hbar\frac{d}{dx}$
If we had real numbers:
$u^2 + v^2 = (iu + v)(-iu + v)$
We don't, but we are led to examine these operators:
$a_\pm = \frac{1}{\sqrt{2\hbar m\omega}}(\mp ip + m\omega x)$

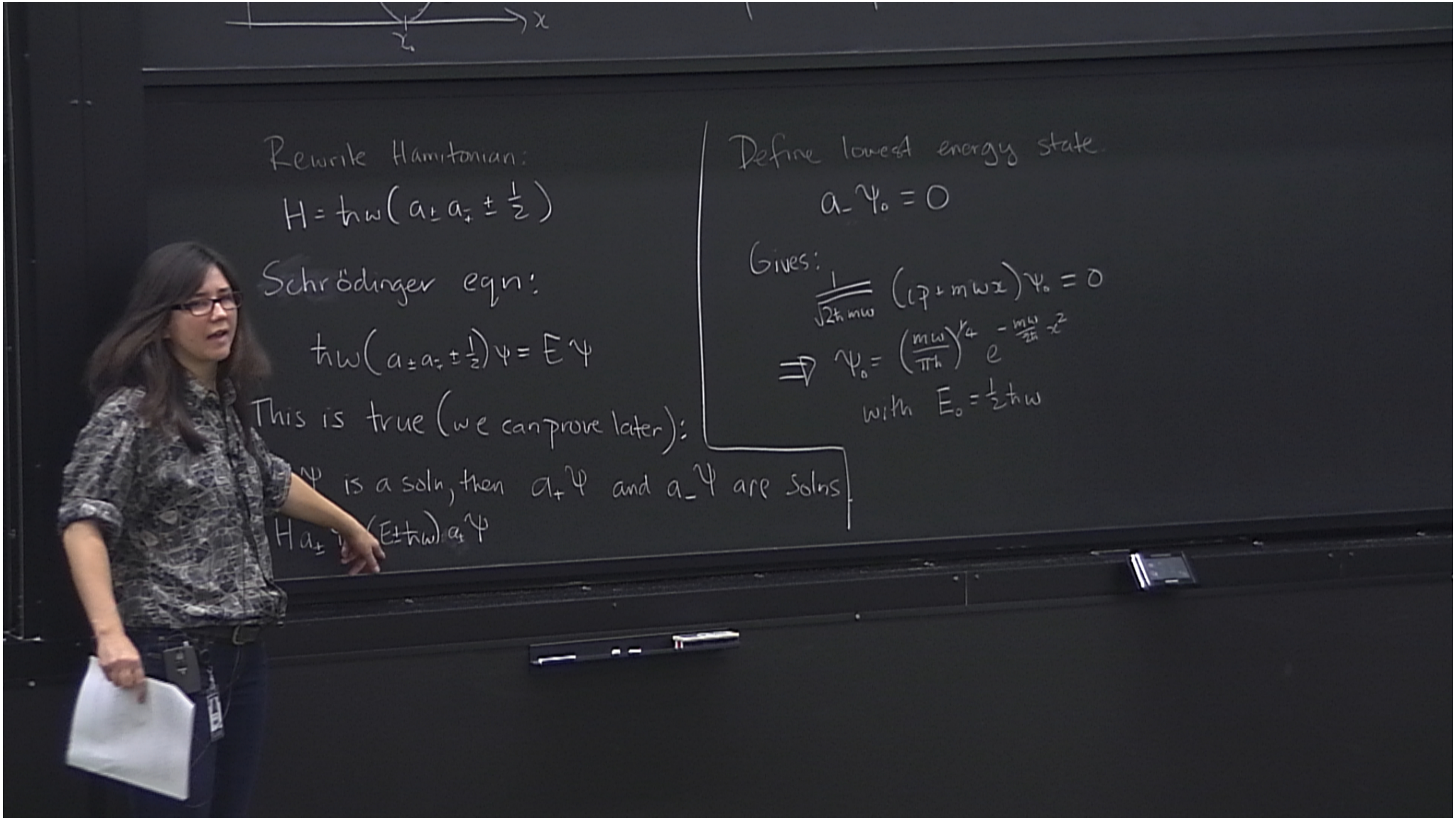

Potential energy:
$V(x) = \frac{1}{2} m(\omega x)^2$
Schrödinger eqn:
$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2} m(\omega x)^2 \psi = E\psi$
Rewrite Hamiltonian:
$H = \frac{1}{2m}\left[p^2 + (m\omega x)^2\right]$
where $p = -i\hbar\frac{d}{dx}$.
If we had real numbers:
$u^2 + v^2 = (iu + v)(-iu + v)$
We don't, but we are led to examine these operators:
$a_\pm = \frac{1}{\sqrt{2\hbar m\omega}}\left(\mp ip + m\omega x\right)$
Lets take a product of these:
$a_- a_+$

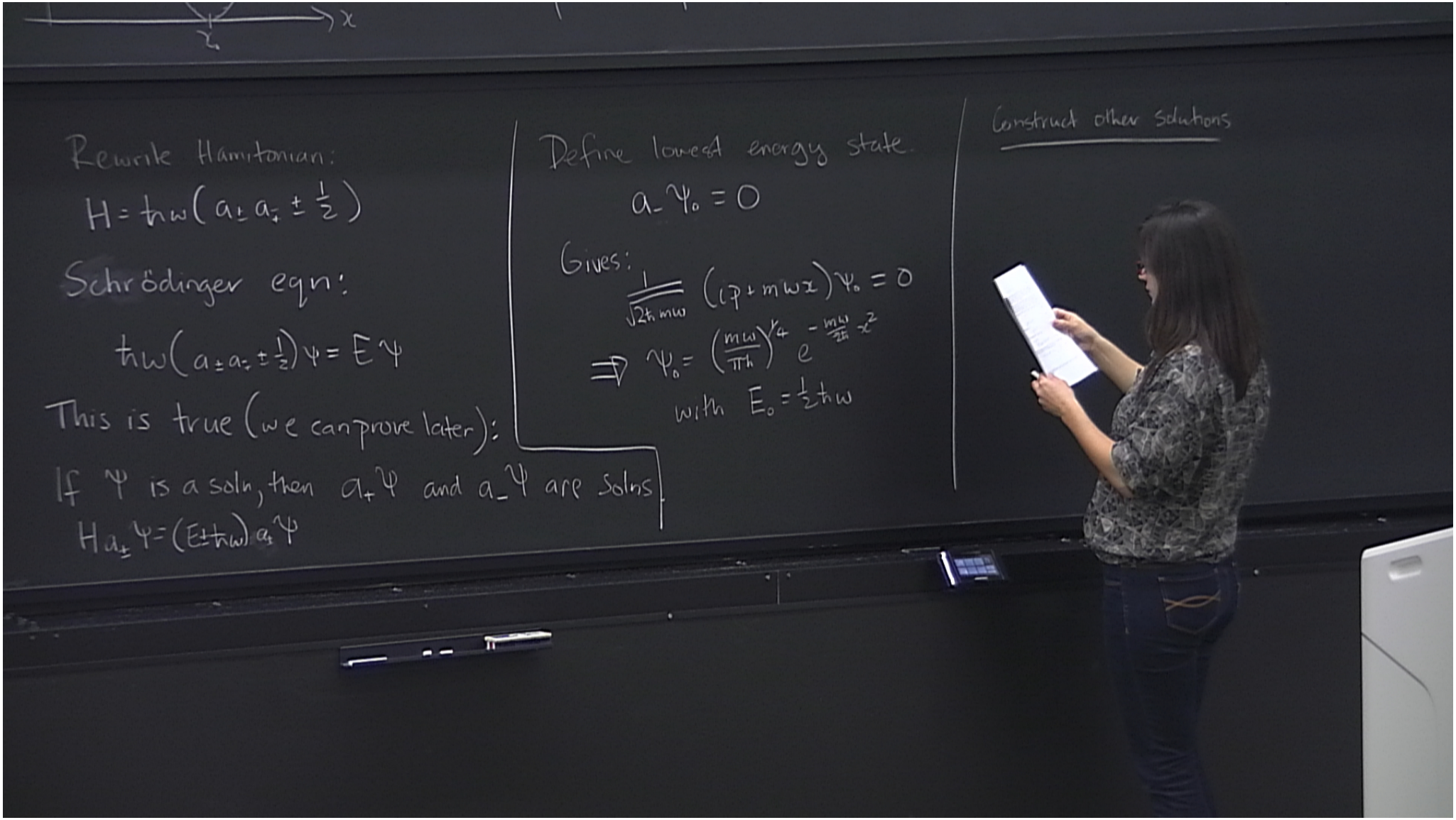

Potential energy:
$V(x) = \frac{1}{2} m(\omega x)^2$
Schrödinger eqn:
$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2} m(\omega x)^2 \psi = E\psi$
Rewrite Hamiltonian:
$H = \frac{1}{2m}\left[p^2 + (m\omega x)^2 \right]$
where $p = -i\hbar$
If we had real numbers:
$u^2 + v^2 = (iu + v)(-iu + v)$
We don't, but we are led to examine these operators:
$a_\pm = \frac{1}{\sqrt{2\hbar m\omega}} (\mp ip + m\omega x)$
Lets take a product of these:
$a_- a_+ = \frac{1}{\hbar\omega} H + \frac{1}{2}$
sed $[a_-, a_+] = 1$)

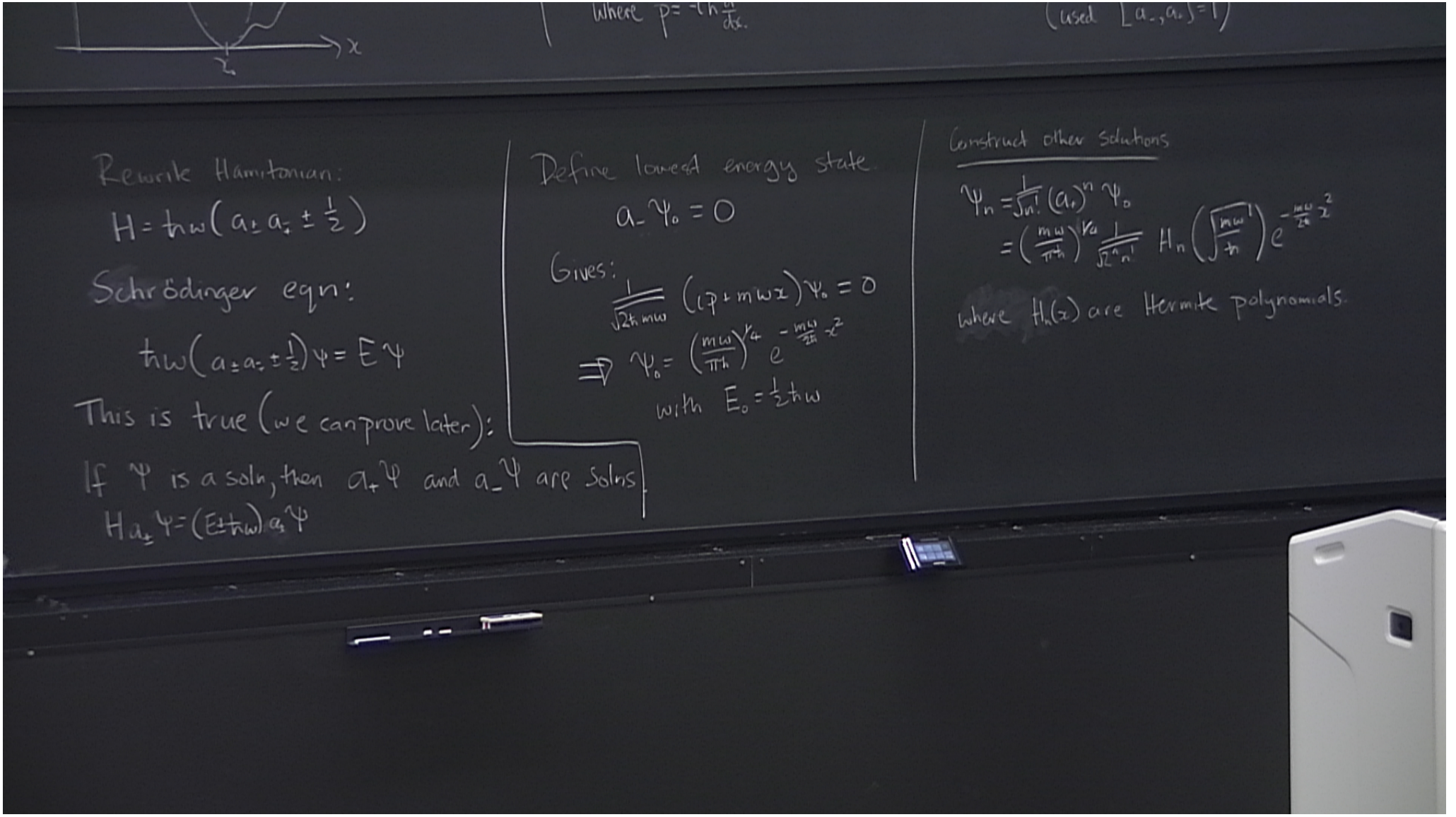

x
Rewrite Hamiltonian:
$H = \hbar\omega\left(a_+ a_- \pm \frac{1}{2}\right)$
Schrödinger eqn:
$\hbar\omega\left(a_+ a_- \pm \frac{1}{2}\right)\psi = E\psi$

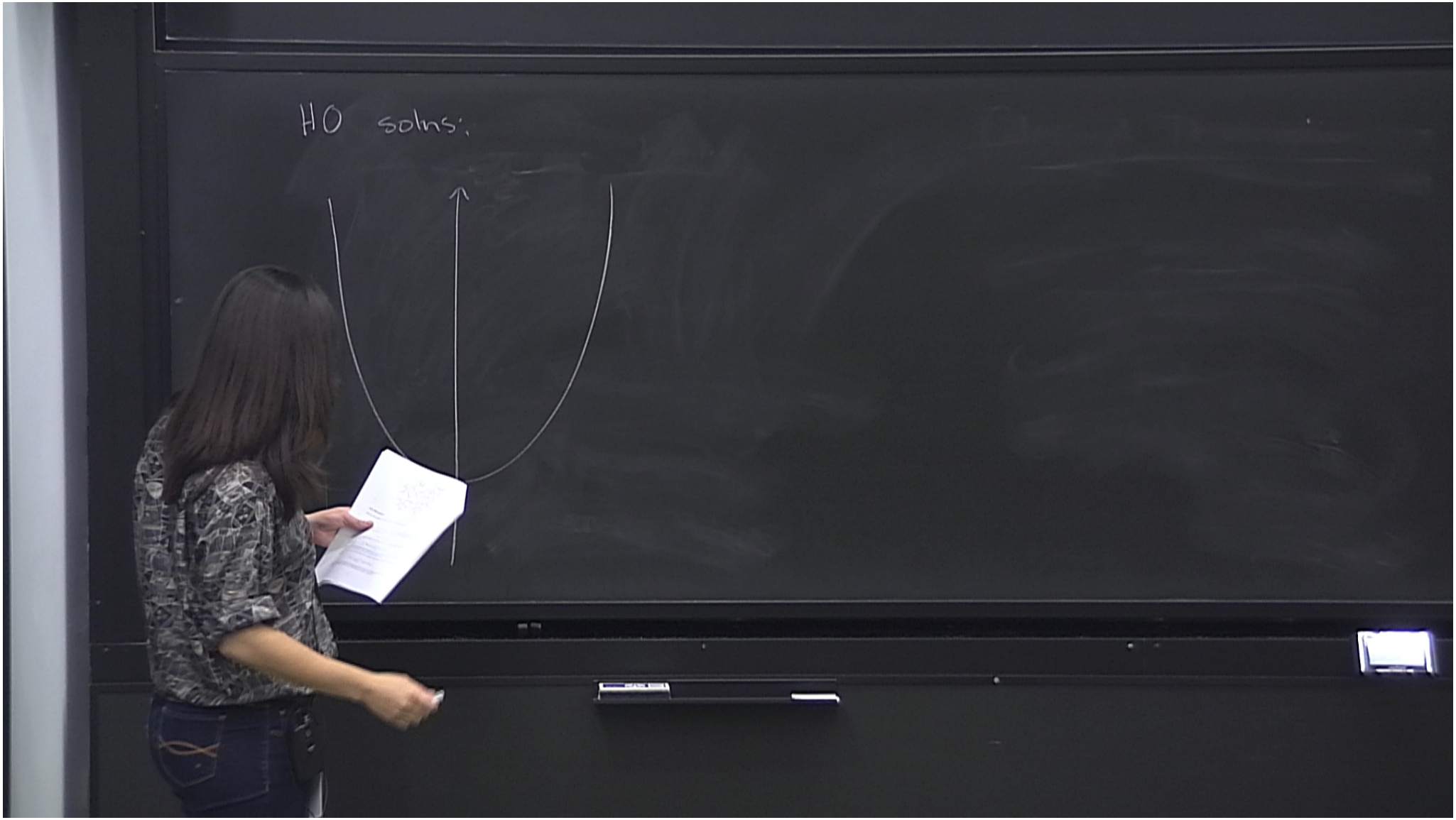

x
Rewrite Hamiltonian:
$H = \hbar\omega(a_\pm a_\mp \pm \frac{1}{2})$
Schrödinger eqn:
$\hbar\omega(a_\pm a_\mp \pm \frac{1}{2})\psi = E\psi$
This is true (we can prove later):
If ψ is a soln, then $a_+\psi$ and $a_-\psi$ are solns.

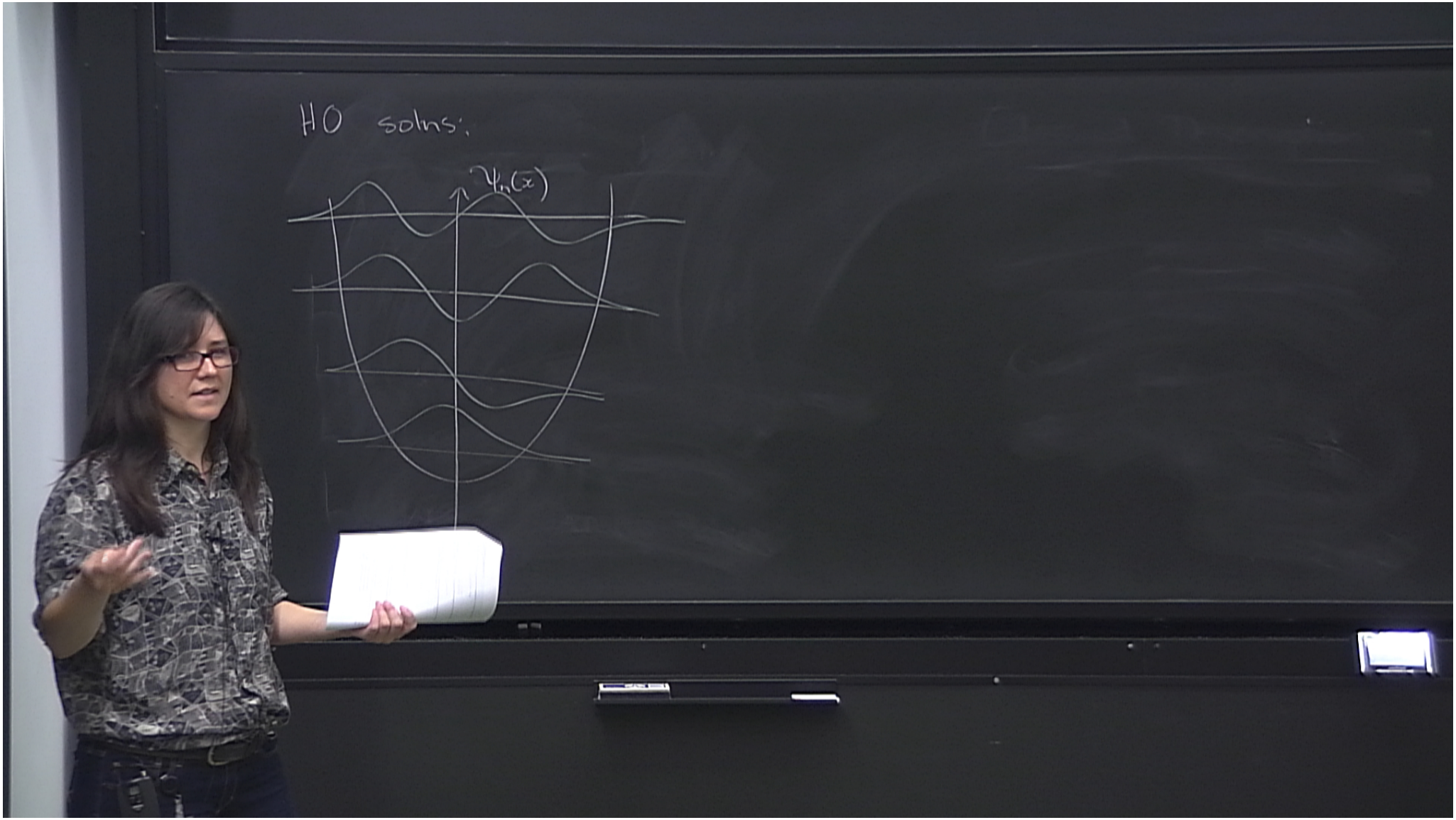

x
Rewrite Hamiltonian:
$H = \hbar\omega(a_\pm a_\mp \pm \frac{1}{2})$
Schrödinger eqn:
$\hbar\omega(a_\pm a_\mp \pm \frac{1}{2})\psi = E\psi$
This is true (we can prove later):
If ψ is a soln, then $a_+\psi$ and $a_-\psi$ are solns
Define lowest energy state.
$a_-\psi_0 = 0$
Gives:


x
Rewrite Hamiltonian:
$H = \hbar\omega(a_\pm a_\mp \pm \frac{1}{2})$
Schrödinger eqn:
$\hbar\omega(a_\pm a_\mp \pm \frac{1}{2})\psi = E\psi$
This is true (we can prove later):
ψ is a soln, then $a_+\psi$ and $a_-\psi$ are solns
$H a_\pm \psi = (E \pm \hbar\omega) a_\pm \psi$
Define lowest energy state
$a_- \psi_0 = 0$
Gives:
$\frac{1}{\sqrt{2\hbar m\omega}}(\hat{p} + im\omega x)\psi_0 = 0$
$\Rightarrow \psi_0 = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2}$
with $E_0 = \frac{1}{2}\hbar\omega$


x
Rewrite Hamiltonian:
$H = \hbar\omega(a_\pm a_\mp \pm \frac{1}{2})$
Schrödinger eqn:
$\hbar\omega(a_\pm a_\mp \pm \frac{1}{2})\psi = E\psi$
This is true (we can prove later):
If ψ is a soln, then $a_+\psi$ and $a_-\psi$ are solns
$Ha_\pm\psi = (E \pm \hbar\omega)a_\pm\psi$
Define lowest energy state
$a_-\psi_0 = 0$
Gives:
$\frac{1}{\sqrt{2\hbar m\omega}}(ip + m\omega x)\psi_0 = 0$
$\Rightarrow \psi_0 = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2}$
with $E_0 = \frac{1}{2}\hbar\omega$
Construct other solutions

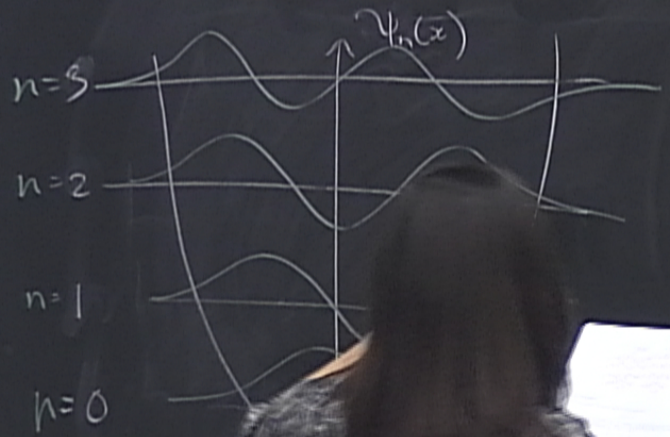

x
z_+
where $p = -i\hbar \frac{d}{dx}$.
(used $[a_-, a_+] = 1$)
Rewrite Hamiltonian:
$H = \hbar\omega(a_\pm a_\mp \pm \frac{1}{2})$
Schrödinger eqn:
$\hbar\omega(a_\pm a_\mp \pm \frac{1}{2})\psi = E\psi$
This is true (we can prove later):
If ψ is a soln, then $a_+\psi$ and $a_-\psi$ are solns.
$Ha_\pm\psi = (E \pm \hbar\omega)a_\pm\psi$
Define lowest energy state
$a_-\psi_0 = 0$
Gives:
$\frac{1}{\sqrt{2\hbar m\omega}}(ip + m\omega x)\psi_0 = 0$
$\Rightarrow \psi_0 = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2}$
with $E_0 = \frac{1}{2}\hbar\omega$
Construct other solutions
$\psi_n = \frac{1}{\sqrt{n!}}(a_+)^n\psi_0$
$= \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\frac{1}{\sqrt{2^n n!}} H_n\left(\sqrt{\frac{m\omega}{\hbar}}\right) e^{-\frac{m\omega}{2\hbar}z^2}$
where $H_n(z)$ are Hermite polynomials.


HO solns:


HO solns:
$\psi_n(x)$

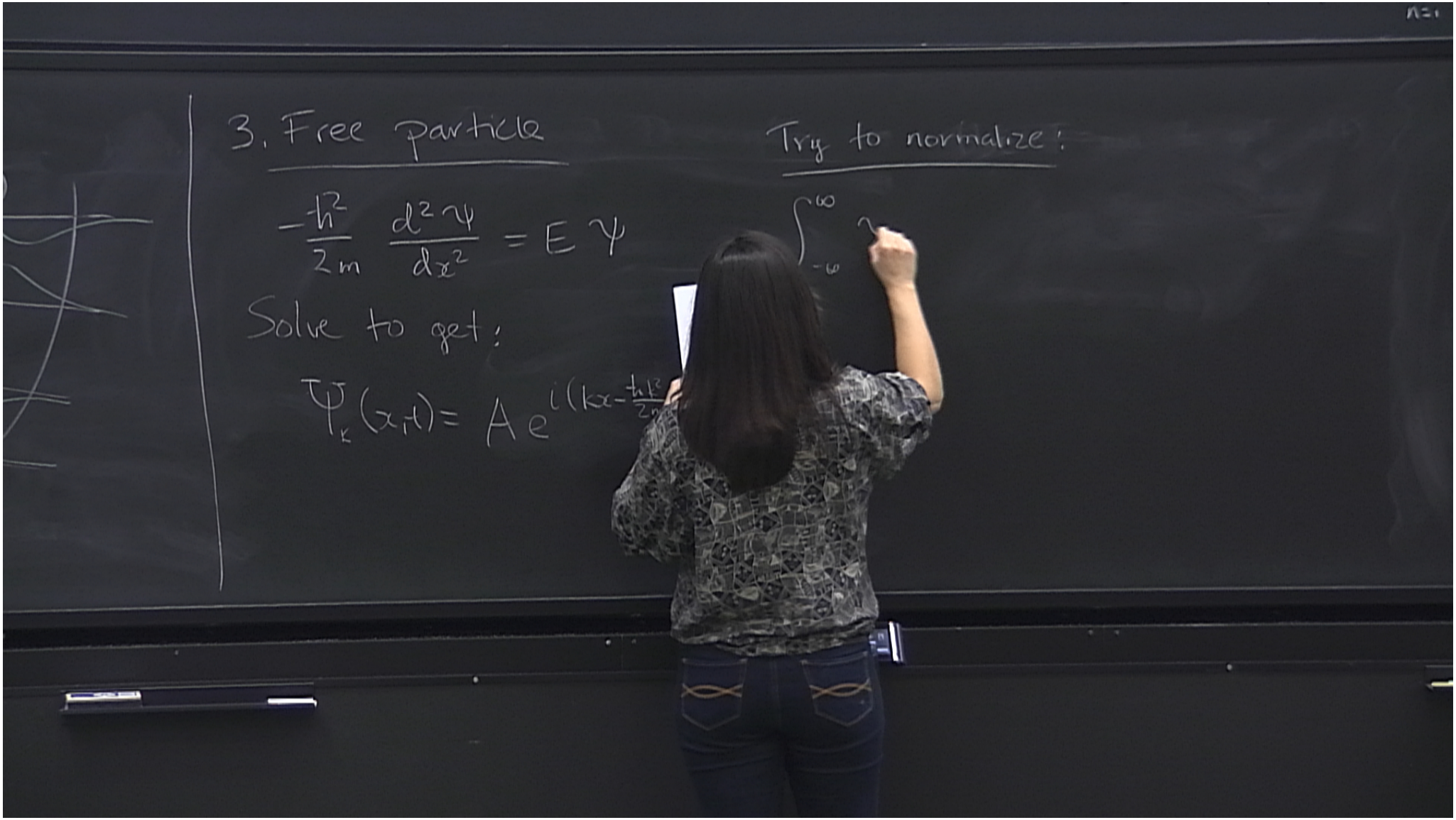

HO solns:
$\psi_n(x)$
n=3
n=2
n=1
n=0
3. Free particle

HO solns:



3. Free particle

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi$$


3. Free particle
$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi$
Solve to get:
$\Psi_k(x,t) = Ae^{i(kx-\frac{\hbar k^2}{2m}t)}$
Try to normalize:
$\int_{-\infty}^{\infty}$

n=1

3. Free particle

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi$$

Solve to get:

$$\Psi_k(x,t) = Ae^{i\left(kx-\frac{\hbar k^2}{2m}t\right)}$$

Try to normalize:

$$\int_{-\infty}^{+\infty} \psi_E^* \psi_k \, dx = |A|^2 \int_{-\infty}^{+\infty} dx = |A|^2 \times \infty$$

n=1

3. Free particle

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi$$

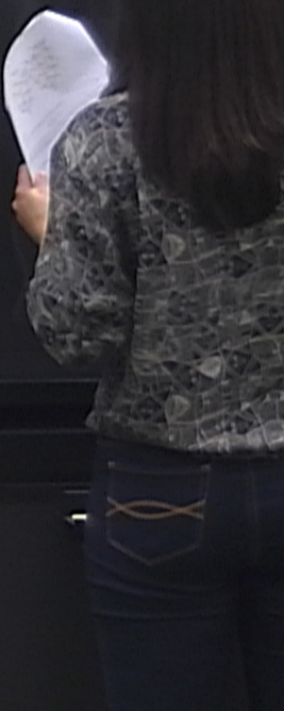
Solve to get:

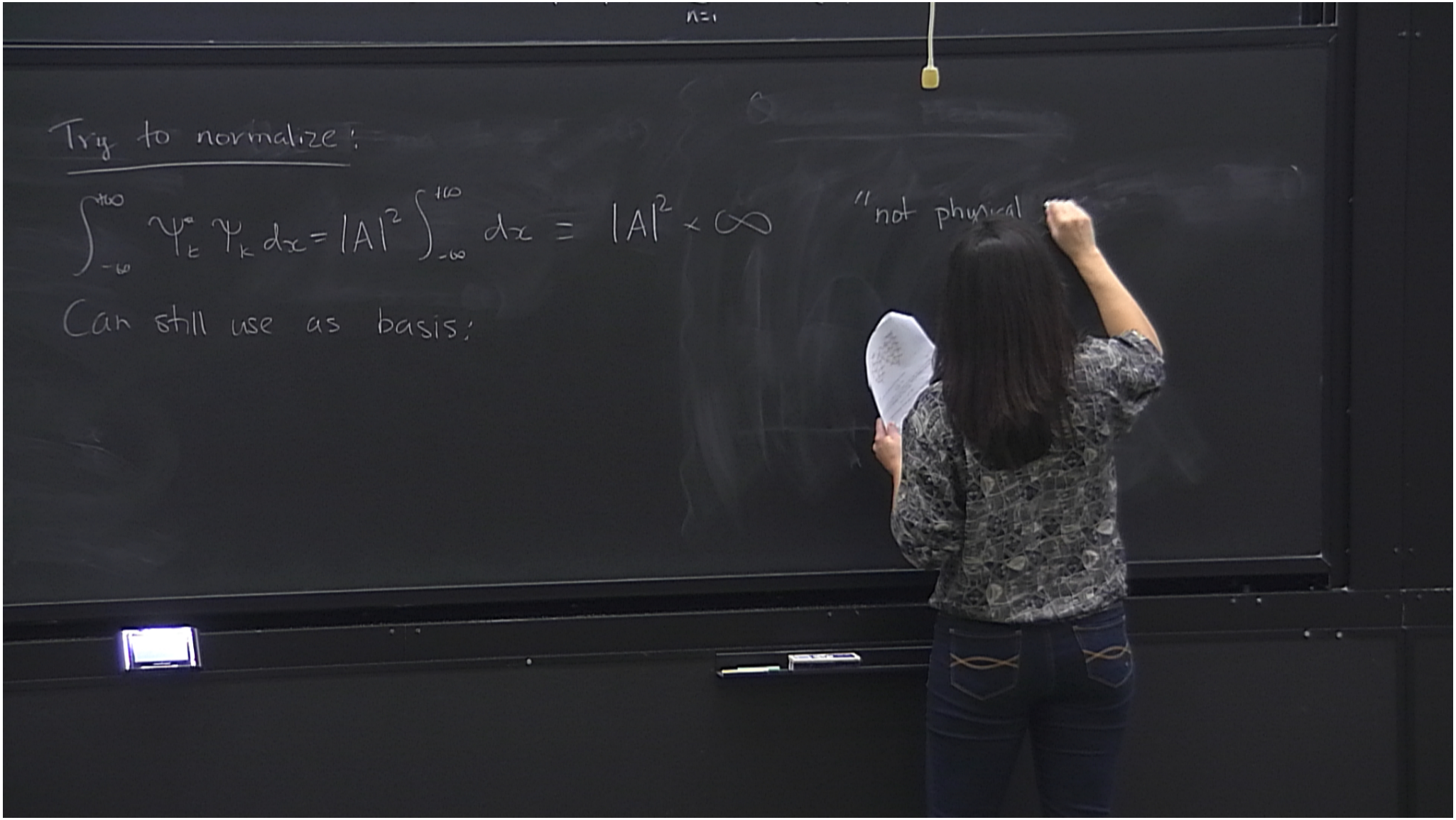
$$\Psi_k(x,t) = Ae^{i\left(kx-\frac{\hbar k^2}{2m}t\right)}$$

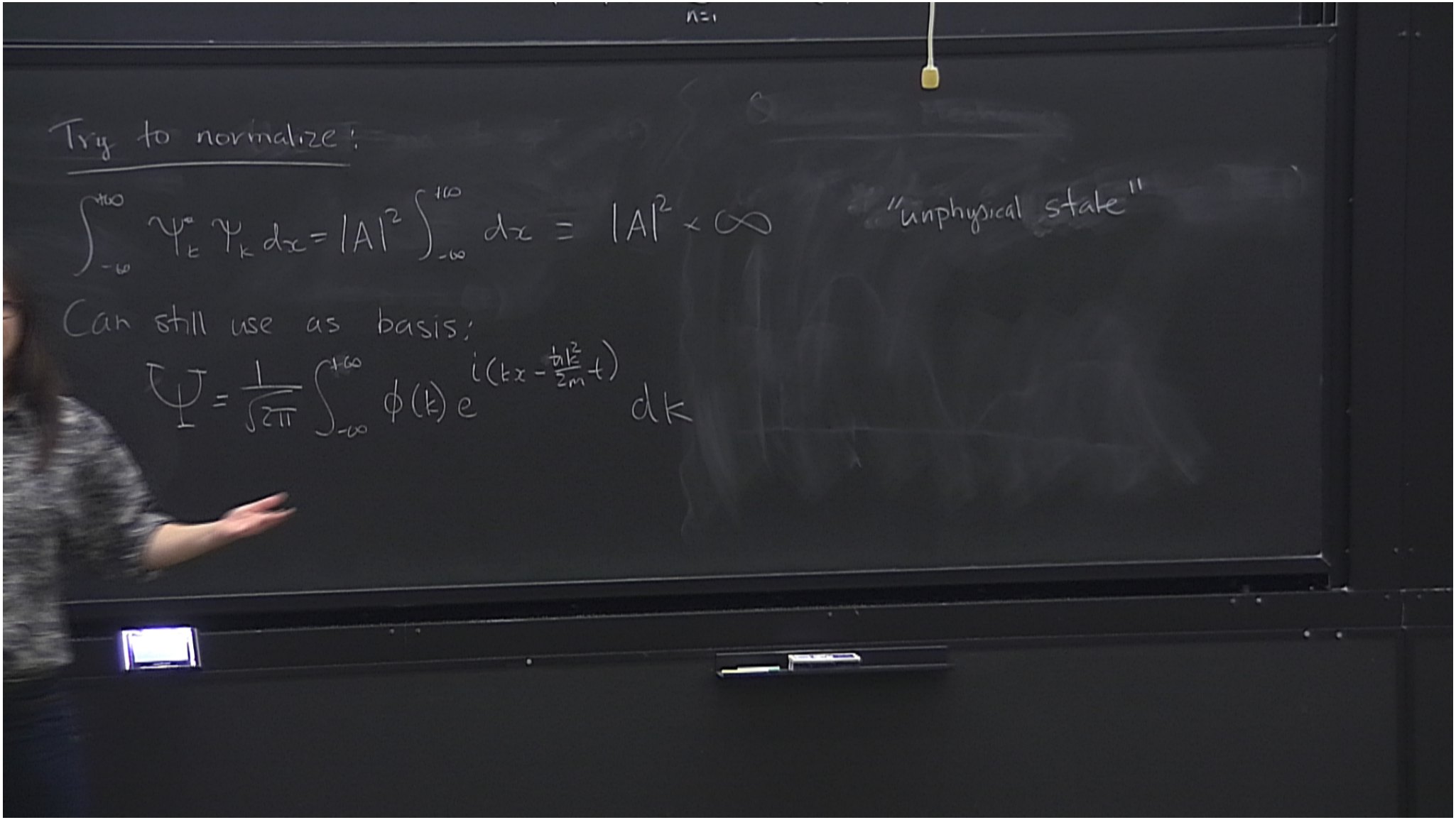
Try to normalize:

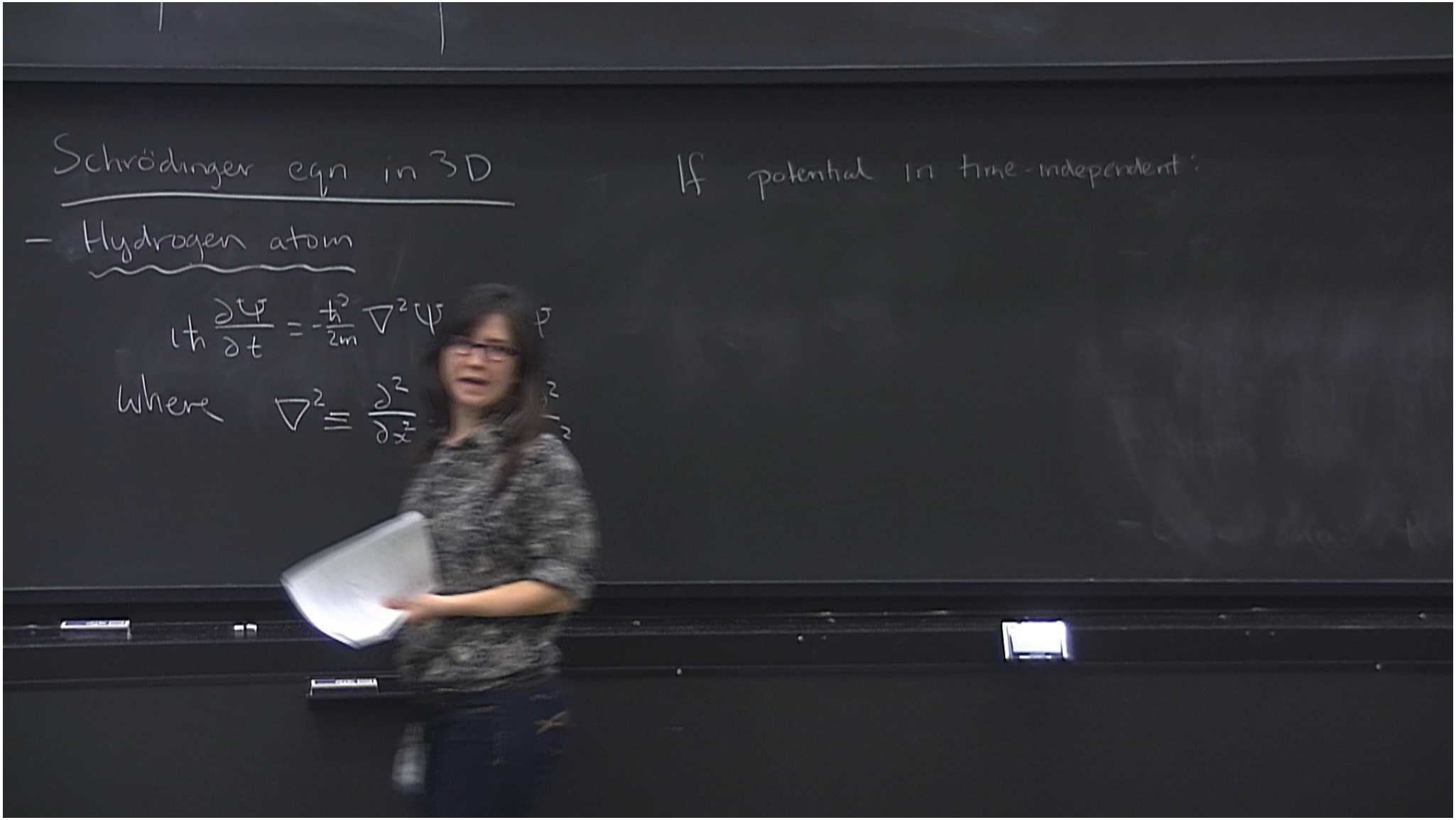
$$\int_{-\infty}^{+\infty} \psi_E^* \psi_k \, dx = |A|^2 \int_{-\infty}^{+\infty} dx = |A|^2 \times \infty$$

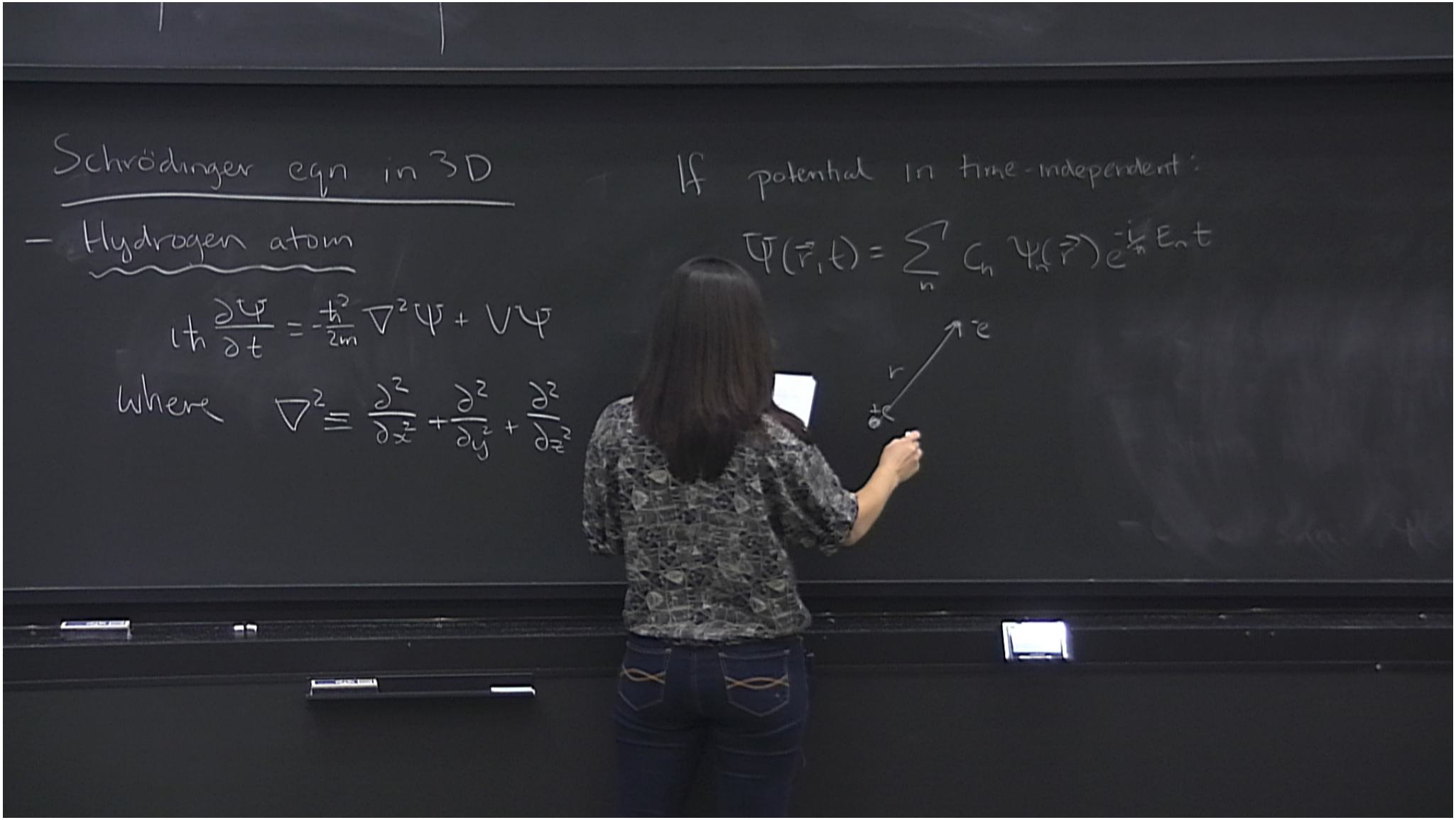
Can still use as basis:




Try to normalize:
$\int_{-\infty}^{+\infty} \psi_k^* \psi_k \, dx = |A|^2 \int_{-\infty}^{+\infty} dx = |A|^2 \times \infty$
"not physical
Can still use as basis:


Try to normalize:
$\int_{-\infty}^{+\infty} \psi_k^* \psi_k \, dx = |A|^2 \int_{-\infty}^{+\infty} dx = |A|^2 \times \infty$
"unphysical state"
Can still use as basis:
$\Psi = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k) \, e^{i(kx - \frac{\hbar k^2}{2m} t)} \, dk$


Schrödinger eqn in 3D
- Hydrogen atom
$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi$
where $\nabla^2 \equiv \frac{\partial^2}{\partial x^2}$
If potential in time-independent:


Schrödinger eqn in 3D
- Hydrogen atom
$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi + V\Psi$
where $\nabla^2 \equiv \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$
If potential in time-independent:
$\Psi(\vec{r},t) = \sum_n c_n \psi_n(\vec{r}) e^{-\frac{i}{\hbar}E_n t}$
r
e

Schrödinger eqn in 3D

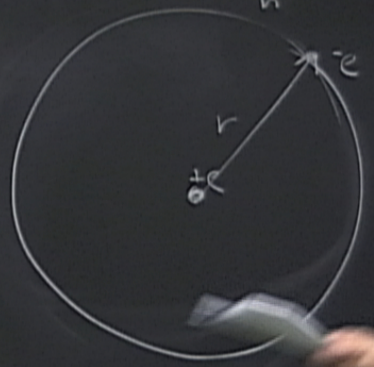
- Hydrogen atom

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi + V\Psi$$

where $\nabla^2 \equiv \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$

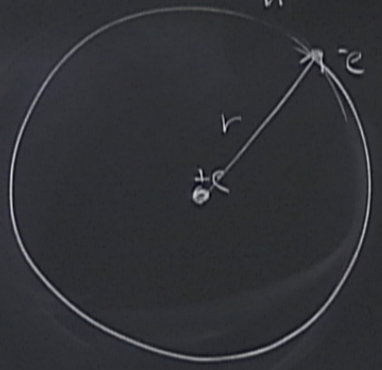
If potential in time-independent:

$$\Psi(\vec{r},t) = \sum_n c_n \psi_n(\vec{r}) e^{-\frac{i}{\hbar}E_n t}$$



If potential in time-independent:

$$\Psi(\vec{r},t) = \sum_n c_n \psi_n(\vec{r}) e^{-\frac{i}{\hbar} E_n t}$$

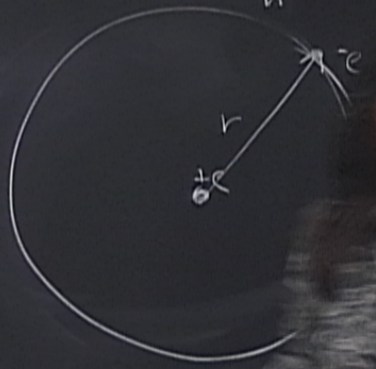


Coulomb's Law:

$$V(r) = -\frac{e^2}{4\pi\epsilon_0}\frac{1}{r}$$

If potential in time-independent:

$$\Psi(\vec{r},t) = \sum_n c_n \psi_n(\vec{r}) e^{-\frac{i}{\hbar} E_n t}$$



Coulomb's Law:

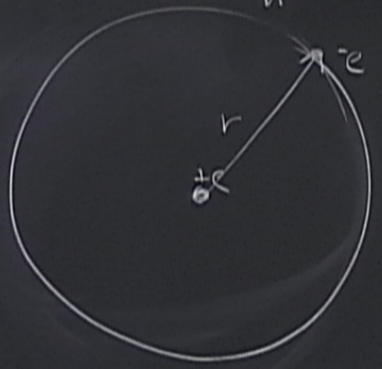
$$V(r) = -\frac{e^2}{4\pi\epsilon_0}\frac{1}{r}$$

Solution to S.E.

$$\psi_{n\ell m} = \sqrt{\left(\frac{2}{na}\right)^3 \frac{(n-\ell-1)!}{2n[(n+\ell)!]^3}}\, e^{-r/na} \left(\frac{2r}{na}\right)^{\ell} L_{n-\ell-1}^{2\ell+1}\left(\frac{2r}{na}\right) Y_\ell^m(\theta,\phi)$$

If potential in time-independent:

$$\Psi(\vec{r},t) = \sum_n C_n \psi_n(\vec{r}) e^{-\frac{i}{\hbar} E_n t}$$

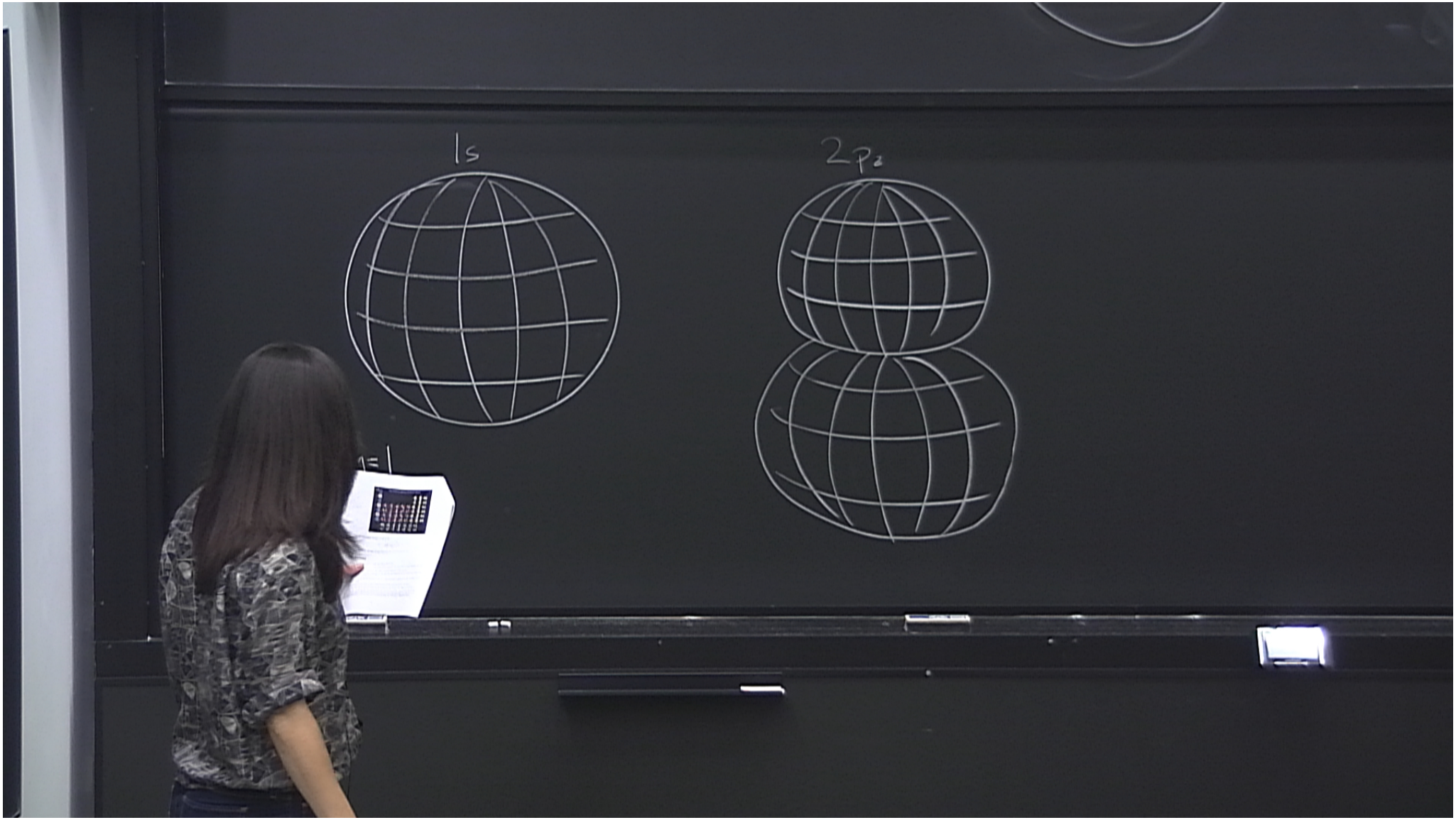


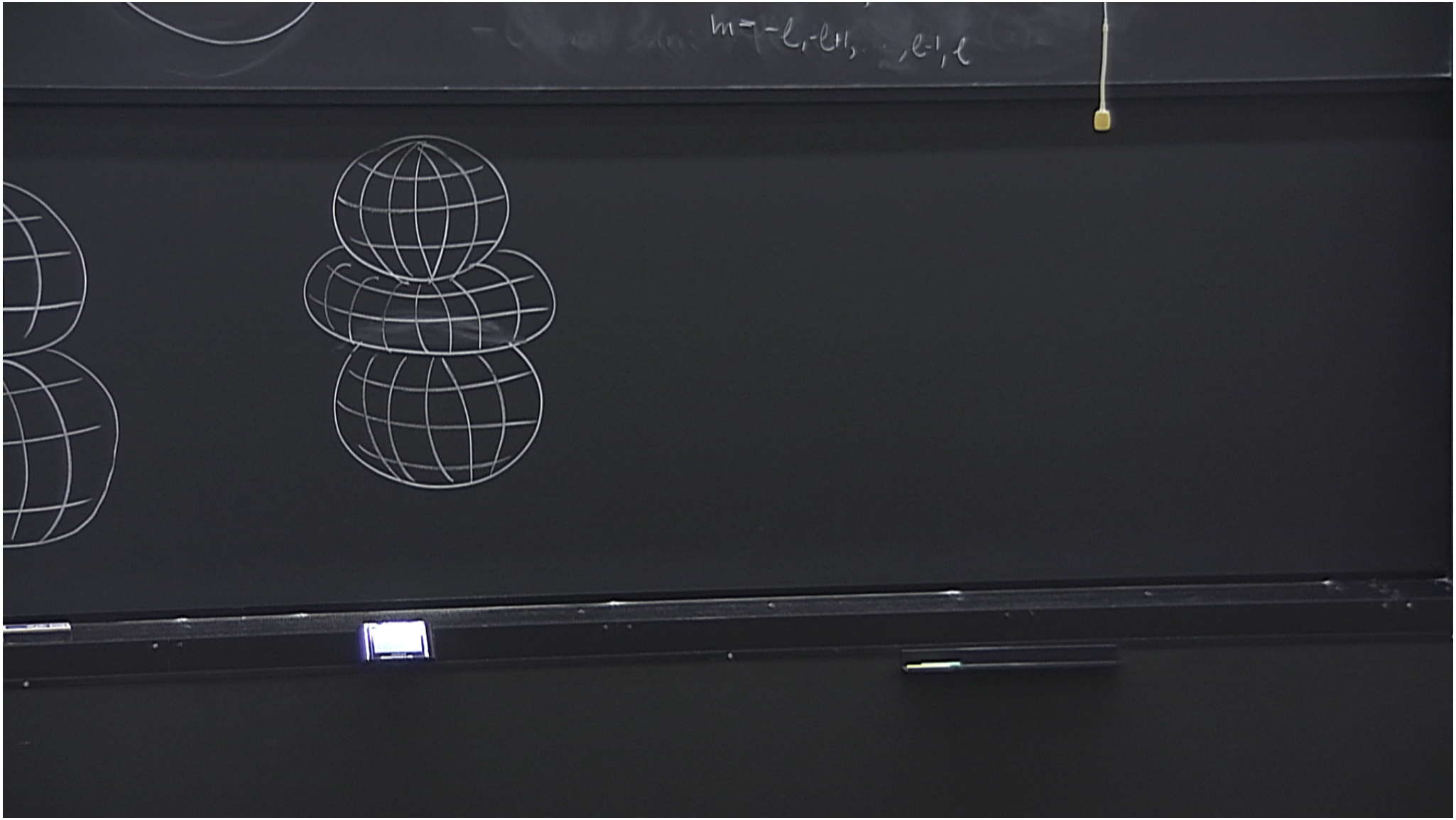
Coulomb's Law:

$$V(r) = -\frac{e^2}{4\pi\epsilon_0}\frac{1}{r}$$

Solution to S.E.

$$\psi_{n\ell m} = \sqrt{\left(\frac{2}{na}\right)^3 \frac{(n-\ell-1)!}{2n[(n+\ell)!]^3}}\, e^{-r/na} \left(\frac{2r}{na}\right)^{\ell} L_{n-\ell-1}^{2\ell+1}\left(\frac{2r}{na}\right) Y_\ell^m(\theta,\phi)$$


1s
2pz


m = -l, -l+1, ..., l-1, l