Title: Quantum Spin Simulations (PHYS 7380) - Lecture 8

Date: Apr 14, 2010 11:00 AM

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Abstract:

Reflection symmetry (parity)

Define a reflection (parity) operator

$$P|S_1^z, S_2^z, \ldots, S_N^z\rangle = |S_N^z, \ldots, S_2^z, S_1^z\rangle$$

Consider a hamiltonian for which [H,P]=0 and [H,T]=0; but note that [P,T]≠0

Can we still exploit both P and T at the same time? Consider the state

$$|a(k,p)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^r (1 + pP)|a\rangle, \quad p = \pm 1$$

This state has momentum k, but does it have parity p? Act with P

$$P|a(k,p)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^{-r} (P + p)|a\rangle$$

$$= p\frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{ikr} T^r (1 + pP)|a\rangle \ = p|a(k,p)\rangle \text{ if } k = 0 \text{ or } k = \pi$$

k=0,π momentum blocks are split into p=+1 and p=–1 sub-blocks

- [T,P]=0 in the k=0,π blocks
- physically clear because -k=k on the lattice for k=0,π

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Semi-momentum states

Mix momenta +k and –k for k≠0,π. Introduce function

$$C_k^{\sigma}(r) = \begin{cases} \cos(kr), & \sigma = +1 \\ \sin(kr), & \sigma = -1. \end{cases}$$

Useful trigonometric relationships

$$\begin{aligned} C_k^{\pm}(-r) &= \pm C_k^{\pm}(r), \\ C_k^{\pm}(r+d) &= C_k^{\pm}(r)C_k^{+}(d) \mp C_k^{\mp}(r)C_k^{-}(d). \end{aligned}$$

Semi-momentum state

$$|a^{\sigma}(k)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} C_k^{\sigma}(r) T^r |a\rangle$$

$$k = m\frac{2\pi}{N}, \quad m = 1, \ldots, N/2-1, \quad \sigma = \pm 1$$

States with same k, different σ are orthogonal

$$\langle a^{-\sigma}(k)|a^{\sigma}(k)\rangle = \frac{1}{\;} \sum^{R_a} \sin(kr)\cos(kr) = 0$$

Normalization of semi-momentum states

$$N_a = \left(\frac{N}{R_a}\right)^2 \sum_{r=1}^{R_a} [C_k^\sigma(r)]^2 = \frac{N^2}{2R_a}$$

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Hamiltonian: ac with H

$$H|a^\pm(k)\rangle = \sum_{j=0}^{N} h_a^j \sqrt{\frac{R_a}{R_{b_j}}} \Big(C_k^+(l_j)|b_j^\pm(k)\rangle \mp C_k^-(l_j)|b_j^\mp(k)\rangle \Big),$$

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The matrix elements are

$$\langle b^\tau(k)|H_j|a^\sigma(k)\rangle = \tau^{(\sigma-\tau)/2} h_a^j \sqrt{\frac{N_{b_j}}{N_a}} C_k^{\sigma\tau}(l_j)$$

σ is mot a conserved quantum number

- H and T mix σ=+1 and σ=−1 states
- the H matrix is twice as large as for momentum states

Why are the semi-momentum states useful then?

Because we can construct a real-valued basis:

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This state has definite parity with p=+1 or p=–1

$$|a^\sigma(k,p)\rangle = \frac{1}{\sqrt{N_a^\sigma}} \sum_{r=0}^{N-1} C_k^\sigma(r) T^r (1+pP)|a\rangle$$

- (k,–1) and (k,+1) blocks
- roughly of the same size as original k blocks
- but these states are real, not complex!
- For k≠0,π, the p=-1 and p=+1 states are degenerate

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r	T^r		$T^r P$	
0	27	0 0 0 1 1 0 1 1	216	1 1 0 1 1 0 0 0
1	54	0 0 1 1 0 1 1 0	177	1 0 1 1 0 0 0 1
2	108	0 1 1 0 1 1 0 0	99	0 1 1 0 0 0 1 1
3	216	1 1 0 1 1 0 0 0	198	1 1 0 0 0 1 1 0
4	177	1 0 1 1 0 0 0 1	141	1 0 0 0 1 1 0 1
5	99	0 1 1 0 0 0 1 1	27	0 0 0 1 1 0 1 1
6	198	1 1 0 0 0 1 1 0	54	0 0 1 1 0 1 1 0

P,T transformations

example: N=8;note that

- $T^5 P|a\rangle = |a\rangle$

such P,T relationships will affect normalization

Normalization: We have to check whether or not

$$T^m P|a\rangle = |a\rangle \quad \text{for some } m \in \{1, \ldots, N-1\}$$

Simple algebra gives

$$N_a^\sigma = \frac{N^2}{R_a} \times \begin{cases} 1, & T^m P|a\rangle \neq |a\rangle \\ 1 + \sigma p \cos(km), & T^m P|a\rangle = |a\rangle \end{cases}$$

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In the latter case the σ=-1 and σ=+1 states are not orthogonal

Then only one of them should be included in the basis
- convention: **use σ=+1 if 1+*σp*cos(*km*)≠0, else σ=-1**

If both σ=+1 and σ=–1 are present:
- **we store 2 copies of the same representative**
- we will store the σ value along with the periodicity of the representative

Pseudocode: semi-momentum, parity basis construction

```
do s = 0, 2^N − 1
    call checkstate(s, R, m)
    do σ = ±1 (do only σ = +1 if k = 0 or k = N/2)
        if (m ≠ −1) then
            if  (1 + σp cos(ikm2π/N) = 0)  R = −1
            if  (σ = −1 and 1 − σp cos(ikm2π/N) ≠ 0);  R = −1
        endif
        if R > 0 then a = a + 1; s_a = s; R_a = σR; m_a = m endif
    enddo
enddo
```

In the subroutine **checkstate**(), we now find whether

$$T^m P|a\rangle = |a\rangle \;\; \text{for some } m \in \{1,\ldots,N-1\}$$

m=–1 if there is no such transformation

if m≠-1, then the σ=+1 and σ=-1 states are not orthogonal

- use only the σ=+1 state if it has non-zero normalization
- use the σ=-1 state if σ=+1 has normalization=0
- R=–1 for not including in the basis

the subroutine **checkstate**()
is modified to gives us:

- periodicity R (R=–1 if incompatible)
- m>0 if $T^m P|s\rangle = |s\rangle$
- m=–1 if no such relationship

check all translations of |s>

construct reflected state P|s>

check all translations of P|s>

subroutine checkstate(s, R, m)
$R = -1$
if $(\sum_i s[i] \neq n_\uparrow)$ **return**
$t = s$
do $i = 1, N$
    $t =$ **cyclebits**(t, N)
    if $(t < s)$ **then**
        return
    elseif $(t = s)$ **then**
        if (**mod**$(k, N/i) \neq 0)$ **return**
        $R = i$; **exit**
    endif
enddo
$t =$ **reflectbits**(s, N); $m = -1$
do $i = 0, R - 1$
    if $(t < s)$ **then**
        $R = -1$; **return**
    elseif $(t = s)$ **then**
        $m = i$; **return**
    endif
    $t =$ **cyclebits**(t, N)

Hamiltonian : Act with an operator H_j on a representative state:

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We can write H acting on a basis state as

$$H|a^\sigma(k,p)\rangle = \sum_{j=0}^{N} \frac{h_a^j (\sigma p)^{q_j}}{\sqrt{N_a^\sigma}} \sum_{r=0}^{N-1} C_k^\sigma(r+l_j)(1+pP)T^r|b_j\rangle$$

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Using the properties (trigonometry) of the C-functions:

$$H|a^\sigma(k,p)\rangle = \sum_{j=0}^{N} h_a^j(\sigma p)^{q_j} \sqrt{\frac{N_{b_j}^\sigma}{N_a^\sigma}} \times$$

$$\left(\cos(kl_j)|b_j^\sigma(k,p)\rangle - \sigma\sqrt{\frac{N_{b_j}^{-\sigma}}{N_{b_j}^\sigma}} \sin(kl_j)|b^{-\sigma}(k,p)\rangle\rangle\right)$$

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$$\left(\cos(kl_j)|b_j^\sigma(k,p)\rangle - \sigma\sqrt{\frac{N_{b_j}^{-\sigma}}{N_{b_j}^\sigma}}\sin(kl_j)|b^{-\sigma}(k,p)\rangle\rangle\right)$$

If, for some m, $T^m P|b_j\rangle = |b_j\rangle$ then

$$\sqrt{\frac{N_{b_j}^{-\sigma}}{N_{b_j}^\sigma}} = \sqrt{\frac{1-\sigma p\cos(km)}{1+\sigma p\cos(km)}} = \frac{|\sin(km)|}{1+\sigma p\cos(km)}$$

$$\langle b^\mp(k,p)|b^\pm(k,p)\rangle = -p$$

The matrix elements are

diagonal in σ

$$\langle b_j^\sigma(k,p)|H_j|a^\sigma(k,p)\rangle = h_a^j(\sigma p)^{q_j}\sqrt{\frac{N_{b_j}^\sigma}{N_a^\sigma}} \times$$

$$\begin{cases} \cos(kl_j), & P|b_j\rangle \neq T^m|b_j\rangle \\ \frac{\cos(kl_j)+\sigma p\cos(k[l_j-m])}{1+\sigma p\cos(km)}, & P|b_j\rangle = T^m|b_j\rangle \end{cases}$$

off-diagonal in σ

$$\langle b_j^{-\sigma}(k,p)|H_j|a^\sigma(k,p)\rangle = h_a^j(\sigma p)^{q_j}\sqrt{\frac{N_{b_j}^{-\sigma}}{N_a^\sigma}} \times$$

$$\begin{cases} -\sigma\sin(kl_j), & P|b_j\rangle \neq T^m|b_j\rangle, \\ \frac{-\sigma\sin(kl_j)+p\sin(k[l_j-m])|}{1-\sigma p\cos(km)}, & P|b_j\rangle = T^m|b_j\rangle, \end{cases}$$

Pseudocode: semi-momentum, parity hamiltonian

If 2 copies of the same representative, σ=−1 and σ=+1:

- do both in the same loop iteration
- examine the previous and next element
- carry out the loop iteration only if representative found for the first time

do $a = 1, M$
    if $(a > 1$ **and** $s_a = s_{a-1})$ **then**
        cycle
    elseif $(a < M$ **and** $s_a = s_{a+1})$ **then**
        $n = 2$
    else
        $n = 1$
    endif
    ...
enddo

n is the number of copies of the representative

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```

n is the number of copies of the representative

```
do i = a, a + n - 1
    H(a, a) = H(a, a) + E_z
enddo
```

diagonal matrix elements

- E_z = diagonal energy

```
s = flip(s_a, i, j)
call representative(s, r, l, q)
call findstate(r, b)
if (b ≥ 0) then
    if (b > 1 and s_b = s_{b-1}) then
        m = 2; b = b - 1
    elseif (b < M and s_b = s_{b+1}) then
        m = 2
    else
        m = 1
    endif
    do j = b, b + m - 1
    do i = a, a + n - 1
        H(i, j) = H(i, j) + helement(i, j, l, q)
    enddo
    enddo
endif
```

construct off-diagonal matrix elements

helement() computes the values based on

- stored info
- and l,q

Using spin-inversion symmetry

Spin inversion operator: $Z|S_1^z, S_2^z, \ldots, S_N^z\rangle = |-S_1^z, -S_2^z, \ldots, -S_N^z\rangle$

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In the magnetization block m^z=0 we can use eigenstates of Z

$$|a^\sigma(k,p,z)\rangle = \frac{1}{\sqrt{N_a^\sigma}} \sum_{r=0}^{N-1} C_k^\sigma(r) T^r (1+pP)(1+zZ)|a\rangle$$

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Normalization: must check how a representative transforms under Z,P,T

$$\begin{array}{llll}
1) & T^m P|a\rangle \neq |a\rangle, & T^m Z|a\rangle \neq |a\rangle & T^m PZ|a\rangle \neq |a\rangle \\
2) & T^m P|a\rangle = |a\rangle, & T^m Z|a\rangle \neq |a\rangle & T^m PZ|a\rangle \neq |a\rangle \\
3) & T^m P|a\rangle \neq |a\rangle, & T^m Z|a\rangle = |a\rangle & T^m PZ|a\rangle \neq |a\rangle \\
4) & T^m P|a\rangle \neq |a\rangle, & T^m Z|a\rangle \neq |a\rangle & T^m PZ|a\rangle = |a\rangle \\
5) & T^m P|a\rangle = |a\rangle, & T^n Z|a\rangle = |a\rangle & \Rightarrow T^{m+n} PZ|a\rangle = |a\rangle
\end{array}$$

For cases 2,4,5 only σ=+1 or σ=−1 included

lamiltonian: acting on a state gives a transformed representative

$$H_j|a\rangle = h_a^j P^{q_j} Z^{g_j} T^{-l_j}|b_j\rangle$$

$$q_j \in \{0,1\}, \quad g_j =\in \{0,1\}, \quad l_j = \{0,1,\ldots,N-1\}$$

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ıfter some algebra .... we can obtain the matrix elements

diagonal in σ

$$\langle b_j^\sigma(k,p)|H_j|a^\sigma(k,p)\rangle = h_a^j(\sigma p)^{q_j} z^{g_j} \sqrt{\frac{N_{b_j}^\tau}{N_a^\sigma}} \times$$

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Example: block sizes

k=0, m_z=0 (largest block)

		$(p=\pm1, z=\pm1)$		
N	$(+1,+1)$	$(+1,-1)$	$(-1,+1)$	$(-1,-1)$
8	7	1	0	2
12	35	15	9	21
16	257	183	158	212
20	2518	2234	2136	2364
24	28968	27854	27482	28416
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Total spin S conservation

- more difficult to exploit
- complicated basis states
- calculate S using **S^2=S(S+1)**

$$\mathbf{S}^2 = \sum_{i=1}^{N}\sum_{j=1}^{N}\mathbf{S}_i \cdot \mathbf{S}_j$$

$$= 2\sum_{i<j}\mathbf{S}_i \cdot \mathbf{S}_j + \frac{3}{4}N$$

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Full diagonalization; expectation values

shorthand block label: **j=(m_z,k,p)** or **j=(m_z=0,k,p,z)**

$$D_j^{-1} H_j D_j = E_j, \quad \langle n_j | A | n_j \rangle = [D_j^{-1} A D_j]_{nn}$$

T>0: sum over all blocks j and states in block n=0,M_j–1

$$\langle A \rangle = \frac{1}{Z} \sum_j \sum_{n=0}^{M_j-1} \mathrm{e}^{-\beta E_{j,n}} [D_j^{-1} A_j U_j]_{nn}, \quad Z = \sum_j \sum_{n=0}^{M_j-1} \mathrm{e}^{-\beta E_{j,n}}$$

E_j = diagonal (energy) matrix, $E_{j,n}$ = energies, n=0,...,M_j–1

Example: Thermodynamics

some quantities can be computed using only the magnetization m_z=0 sector

- spin-inversion symmetry can be used, smallest blocks
- spin-S state is **(2S+1)**-fold degenerate (no magnetix field) → weight factor
- possible spin dependence of expectation value → average over **m_z=–S,...,S**

$$C = \frac{d\langle H\rangle}{dt} = \frac{1}{T^2}\left(\langle H^2\rangle - \langle H\rangle^2\right)$$

$$\chi^z = \frac{d\langle m_z\rangle}{dh_z} = \frac{1}{T}\left(\langle m_z^2\rangle - \langle m_z\rangle^2\right)$$

$$\langle m_z\rangle = 0, \qquad \langle m_z^2\rangle = \frac{\langle m_x^2 + m_y^2 + m_z^2\rangle}{3} = \frac{\langle S^2\rangle}{3} = \frac{S(S+1)}{3}$$

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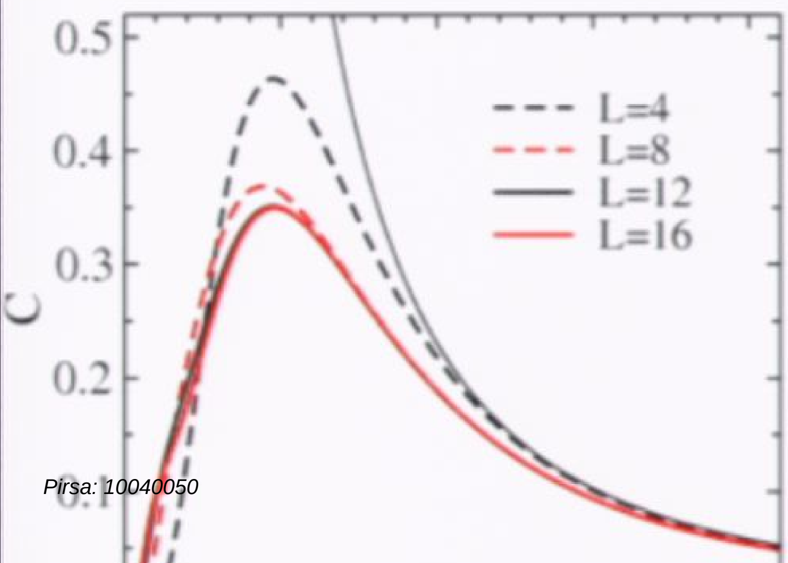

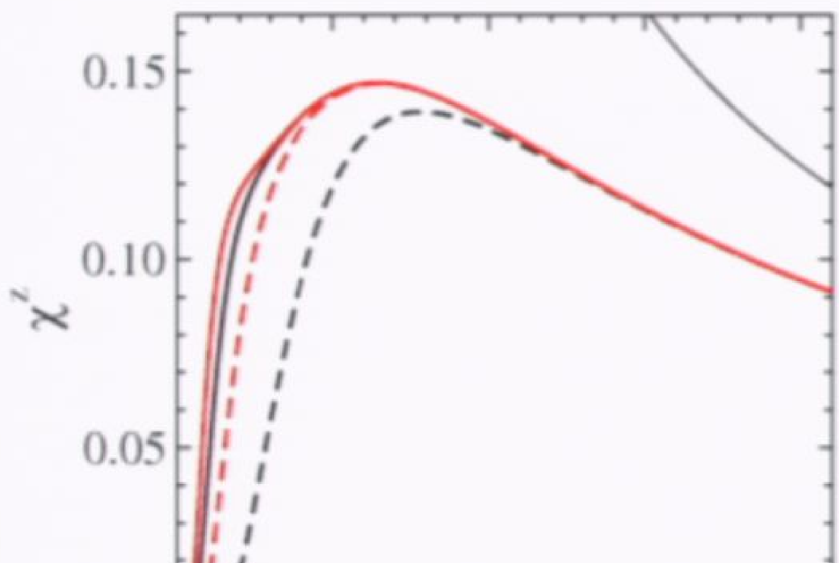

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k=0, m_z=0 (largest block)

N	$(+1,+1)$	$(+1,-1)$	$(-1,+1)$	$(-1,-1)$
	$(p=\pm1, z=\pm1)$			
8	7	1	0	2
12	35	15	9	21
16	257	183	158	212
20	2518	2234	2136	2364
24	28968	27854	27482	28416
28	361270	356876	355458	359256
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Total spin S conservation

- more difficult to exploit
- complicated basis states
- calculate S using **S^2=S(S+1)**

$$\mathbf{S}^2 = \sum_{i=1}^{N}\sum_{j=1}^{N}\mathbf{S}_i\cdot\mathbf{S}_j$$

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Full diagonalization; expectation values

shorthand block label: **j=(m_z,k,p)** or **j=(m_z=0,k,p,z)**

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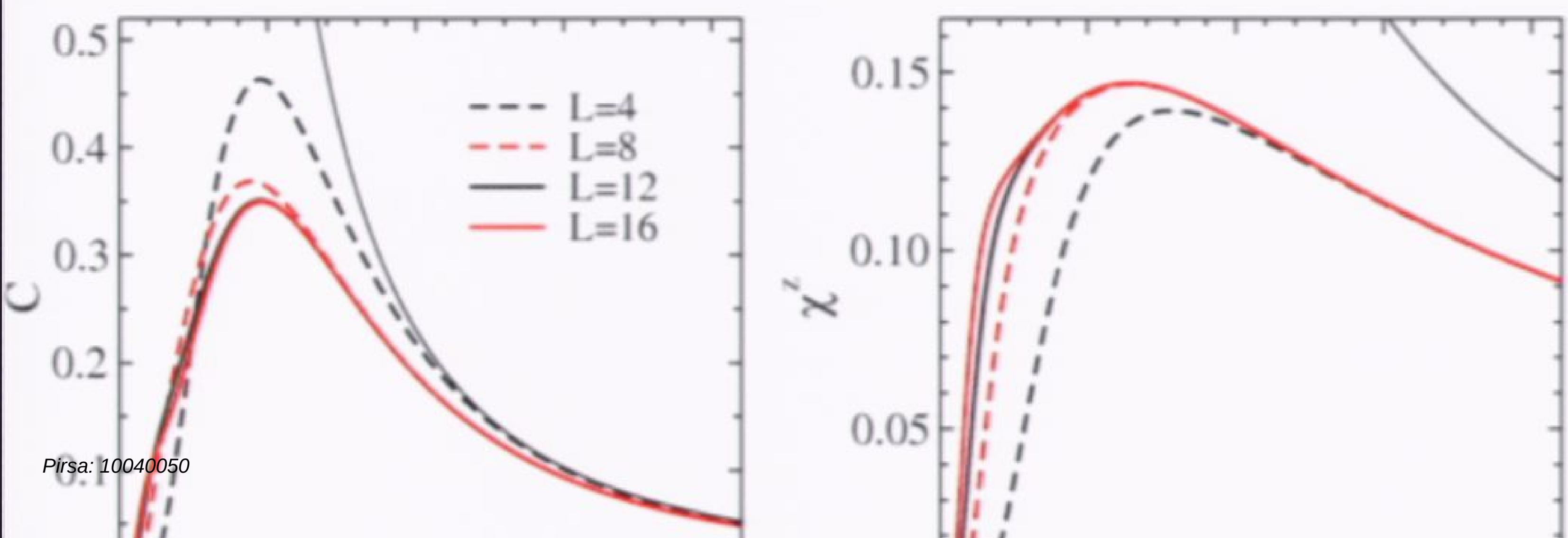

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If we need only the ground state and a small number of excitations

- can use “Krylov space” methods, which work for much larger matrices
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Start with an arbitrary state $|\psi\rangle$

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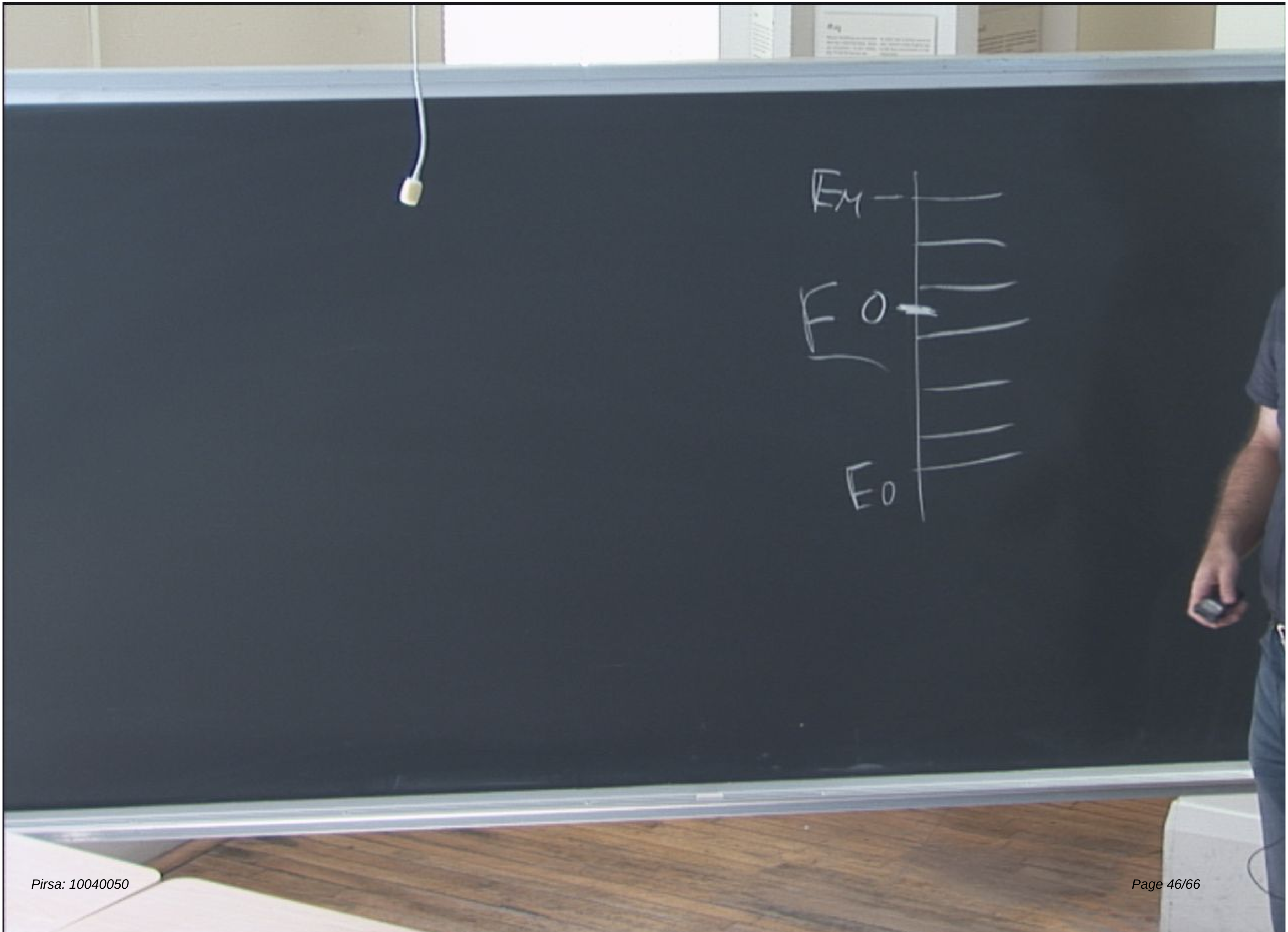
- diagonalize H in this basis


E0


EM
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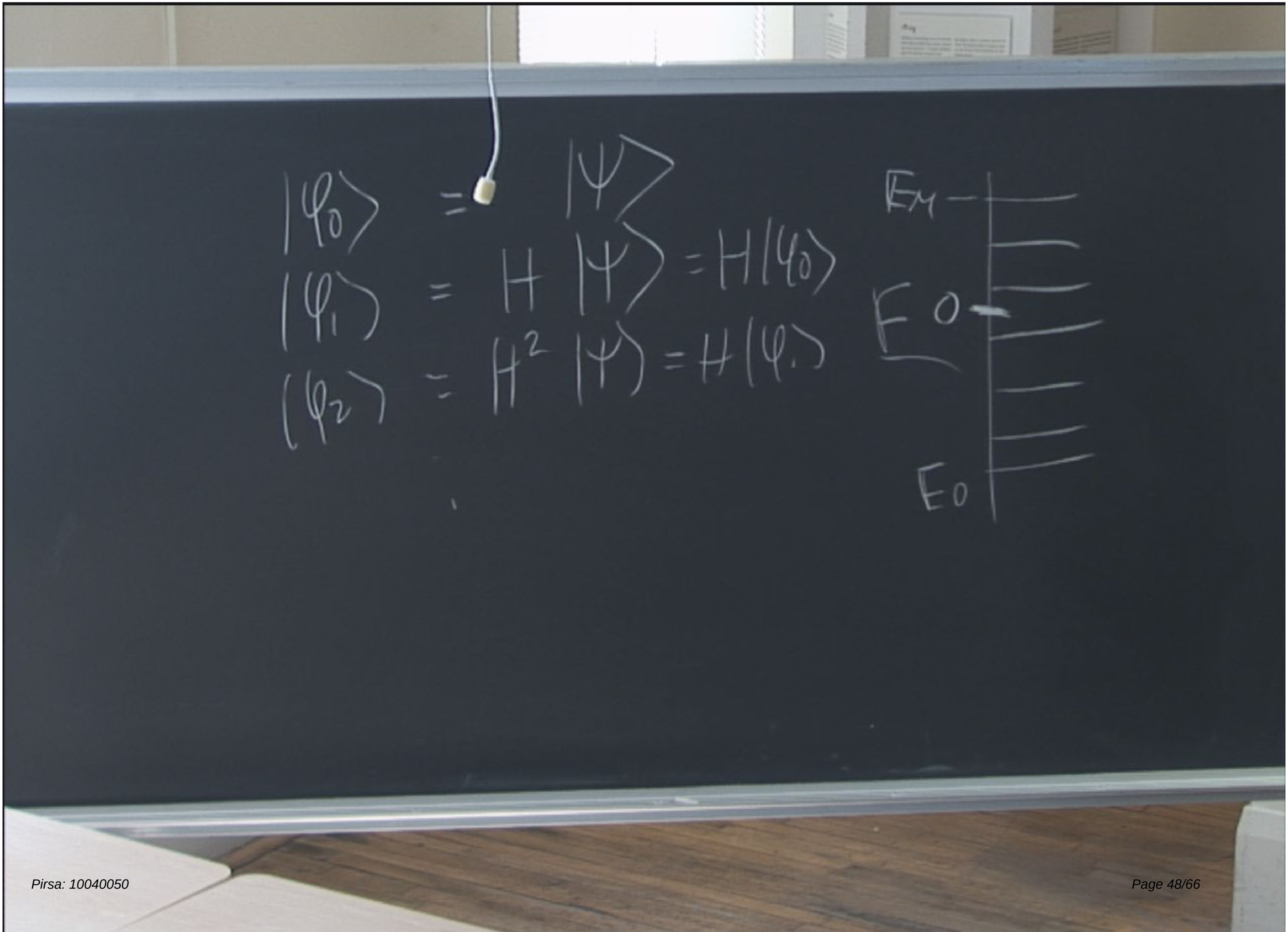

|φ0> = |ψ>
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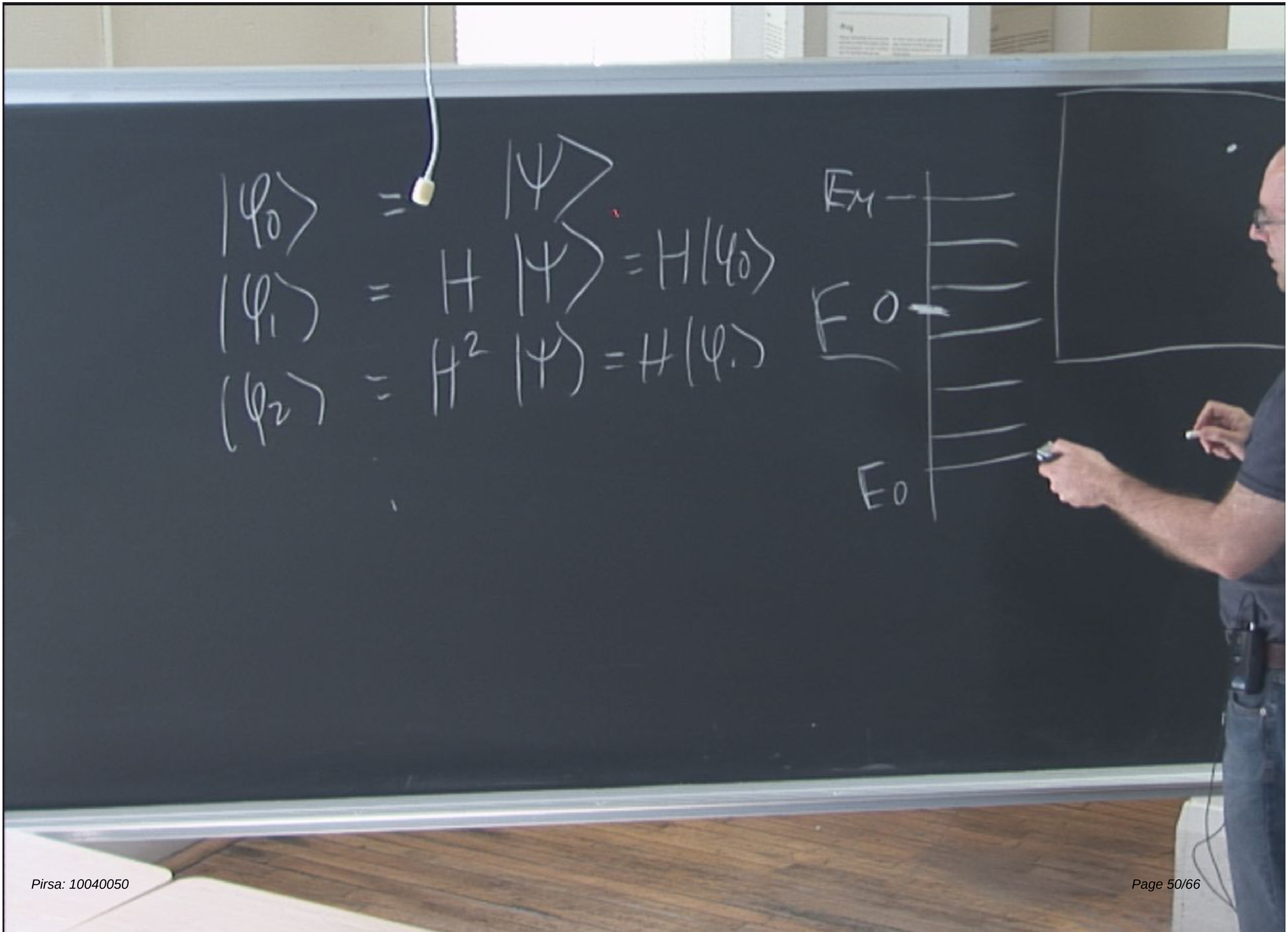

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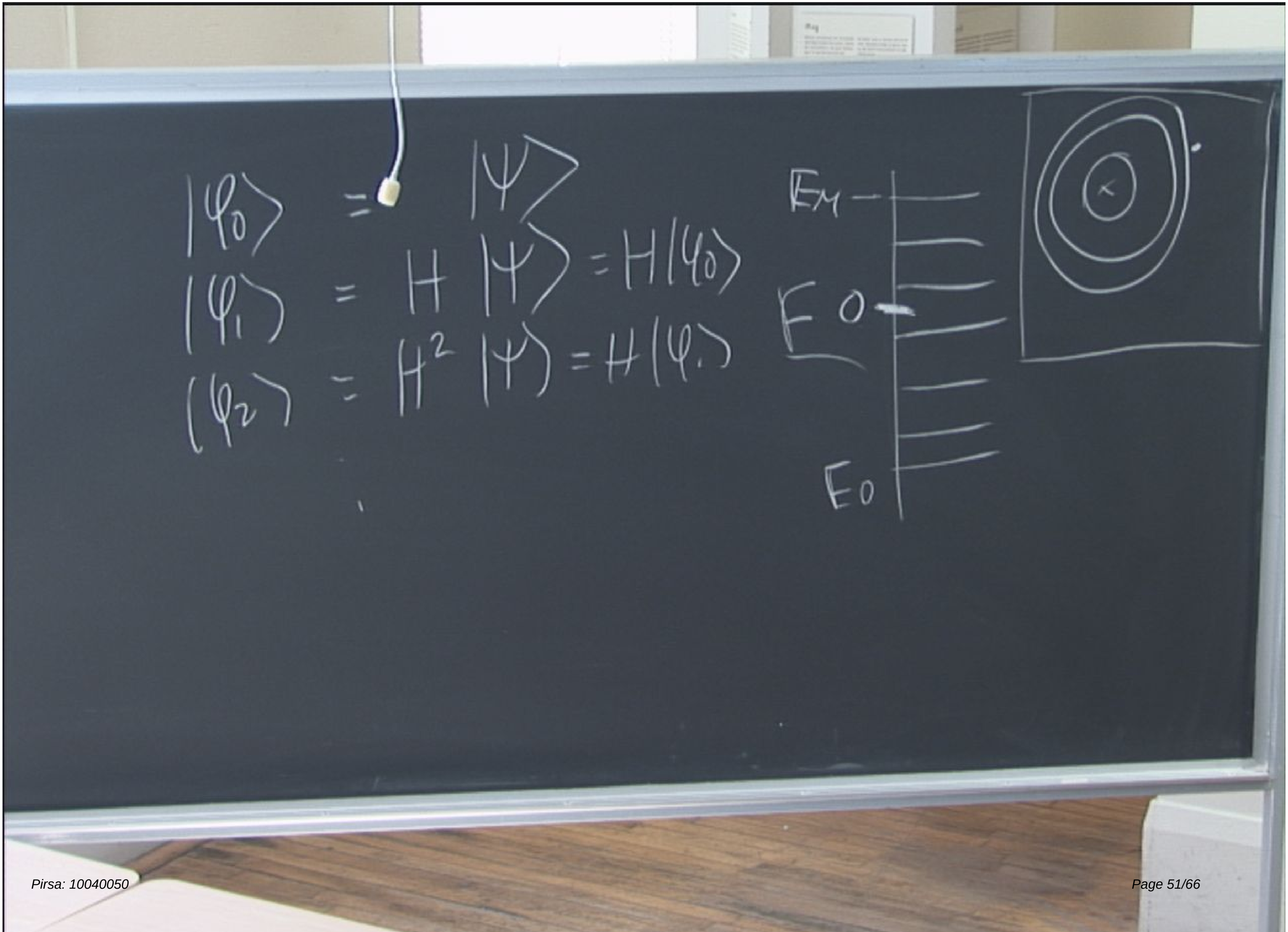
E_M
E 0
E_0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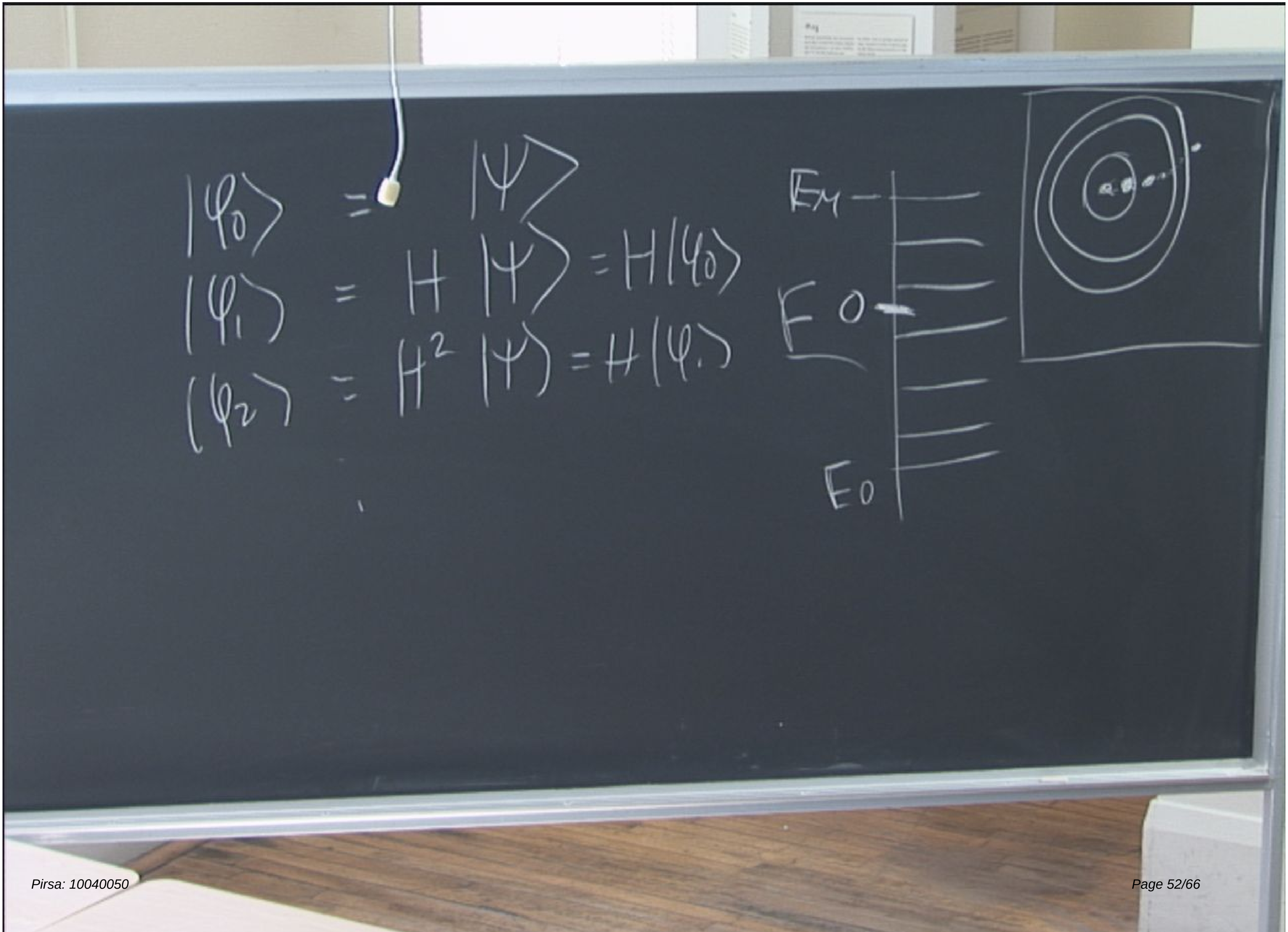
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In this basis the H-matrix is

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