Computation of extremal eigenvalues of large Hermitian and Hamiltonian matrices in quantum and classical physics

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SCS Colloquium, George Mason University
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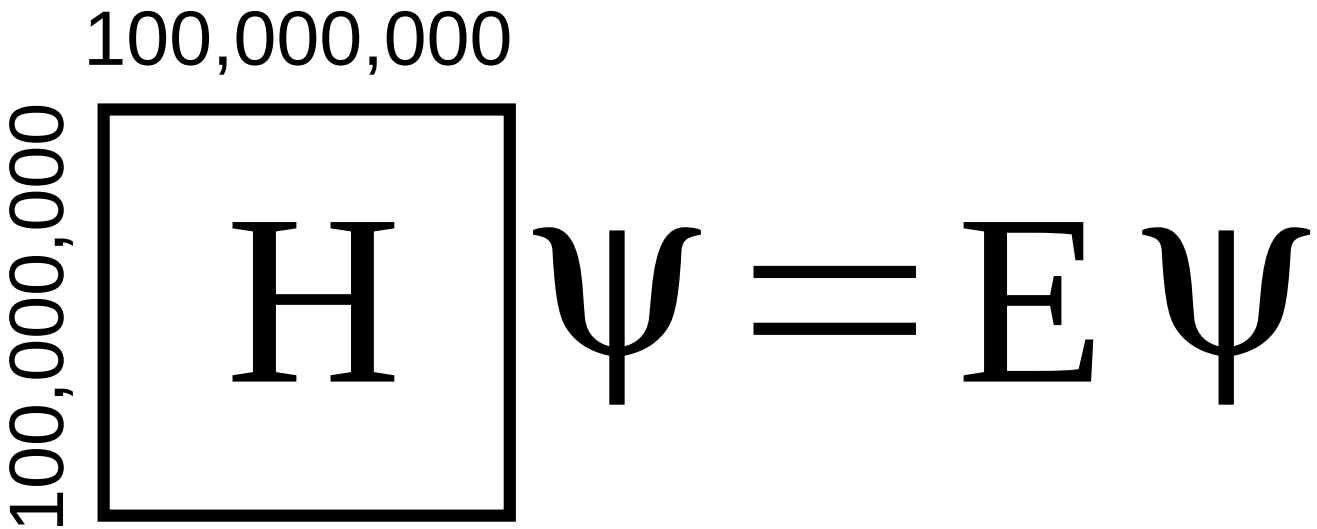
Quantum Mechanics:
a Hermitian Eigenvalue Problem



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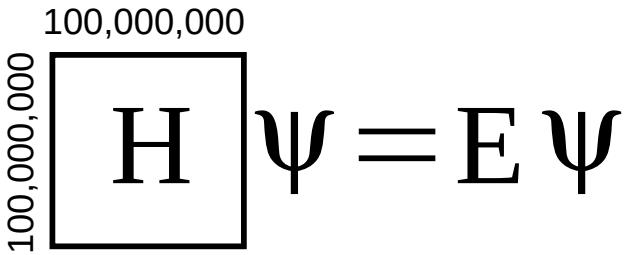

$$\mathcal{H}\psi = \epsilon\psi \quad \longrightarrow \quad \begin{matrix} \epsilon^{(1)},\ \epsilon^{(2)},\ \ldots,\ \epsilon^{(M)} \\ \psi^{(1)}, \psi^{(2)}, \ldots, \psi^{(M)} \end{matrix}$$

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Rayleigh-Ritz Minimum Principle

$$\epsilon^{(1)} = \min_{(\psi\psi)=1} (\psi\mathcal{H}\psi)$$

Classical Mechanics: a Hamiltonian Eigenvalue Problem

Newton's eqs:

$$\mathcal{M}\ddot{x} = -\mathcal{K}x$$

$$\downarrow$$

$$\omega^2 \mathcal{M}x = \mathcal{K}x$$

$\longrightarrow$ normal frequencies $\omega^{(1)}, \omega^{(2)}, \ldots, \omega^{(\mathrm{M})}$

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• **all real!**

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Generalized Minimum Principle

$$\omega^{(1)} = \min_{(px)=1} \frac{(p\mathcal{T}p)}{2} + \frac{(x\mathcal{K}x)}{2}$$

[E.V. Tsiper, JETP Letters 70, 11, 751 (1999)]

Two Problems in Linear Algebra

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- **Diagonalization of a Hermitian matrix**
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  by similarity transformations (rotations + rescaling):

  Recipe:

  1. Rotate the basis to diagonalize one matrix
  2. Rescale coordinates to make it a unit matrix
  3. Rotate space to diagonalize the other matrix
  (the unit matrix does not change)

Origin of Large Matrices in Quantum Mechanics

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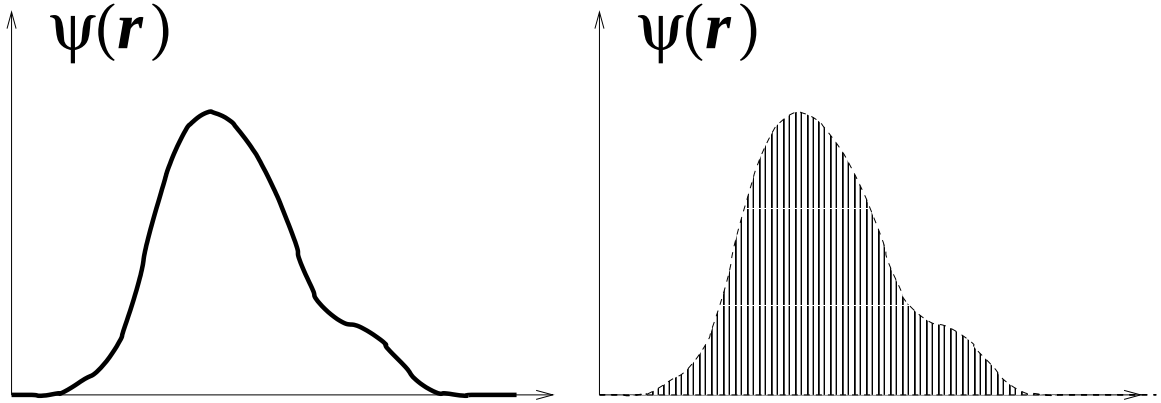
A. Ordinary Quantum Mechanics

- The wave function $\psi(r)$ *is* an infinite vector:



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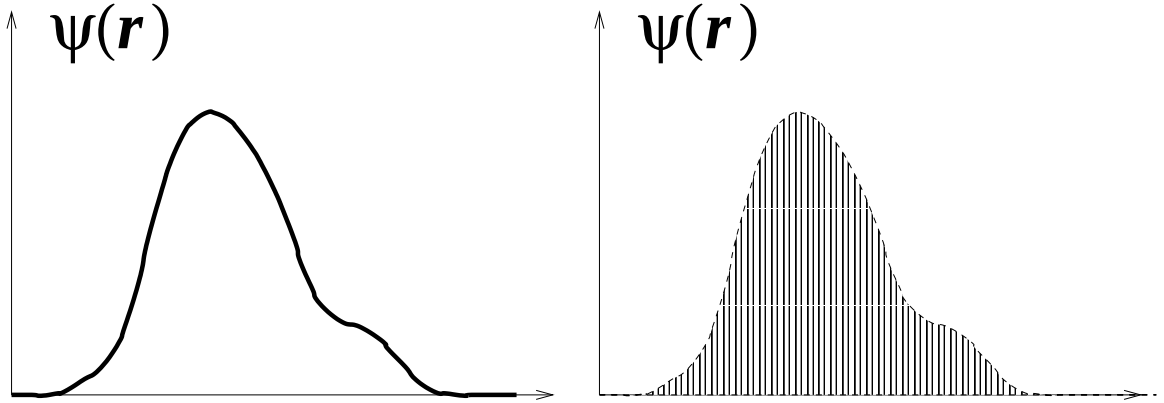
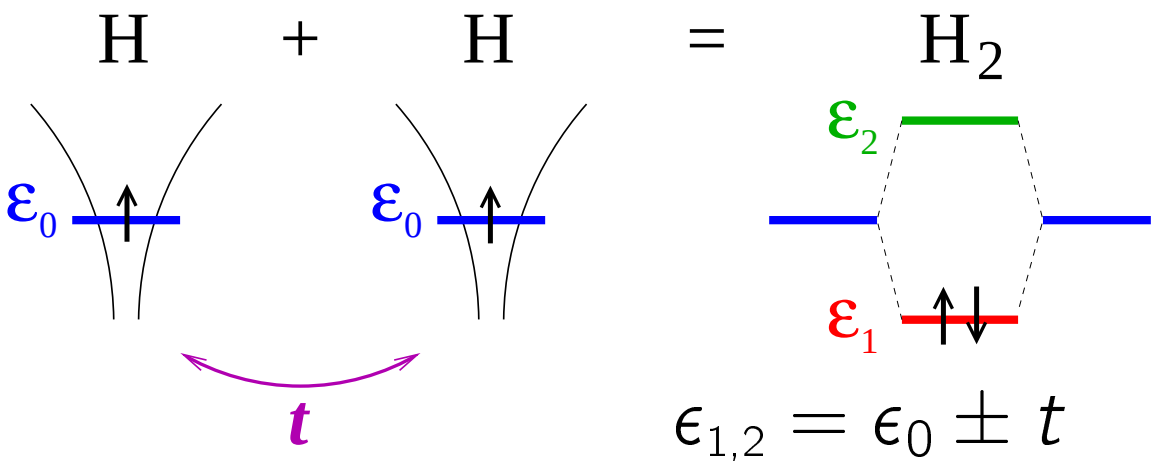


- Simplest chemical bond:

2×2 matrix

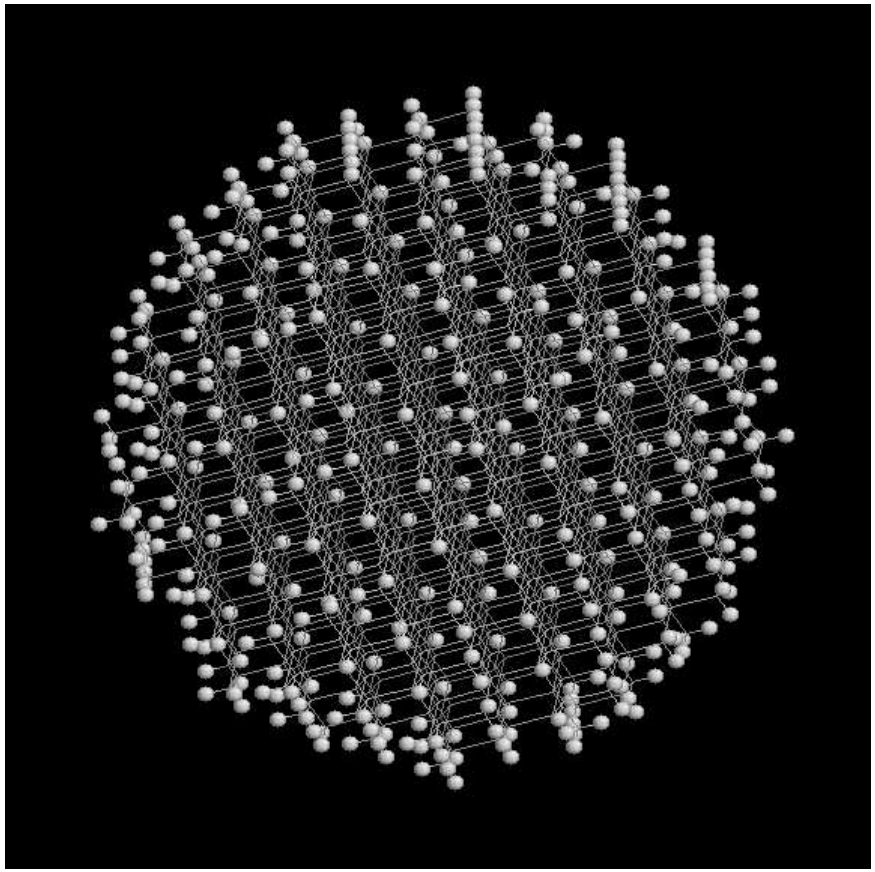
$$\mathcal{H} = \begin{pmatrix} \epsilon_0 & t \\ t & \epsilon_0 \end{pmatrix}$$



Origin of Large Matrices in Quantum Mechanics

B. Realistic electronic structure calculations

- Many states per atom:
  $(1s + 3p + 5d) \times 2$ spins $= 20$
- 10^{23} atoms per cm^3
- A typical ~ 10 nm nanocrystal contains about 50,000 atoms



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For N particles

$$\psi(\mathbf{r}) \overset{\text{becomes}}{\longrightarrow} \psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \ldots, \mathbf{r}_N) \quad \Rightarrow \text{matrix size } M = L^N$$

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Fermion symmetry reduces it to N particles in L boxes:

$$M = \binom{L}{N} \approx \frac{1}{\sqrt{2\pi N(1-f)}} \left[\frac{1}{f^f (1-f)^{(1-f)}}\right]^L,$$

$f = N/L =$ *filling factor* (< 1)

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— still a huge number:

$$\binom{36}{1} = 36, \quad \binom{36}{2} = \frac{36 \times 35}{2} = 630, \quad \ldots \quad \binom{36}{12} = \mathbf{1{,}251{,}677{,}700}, \quad \ldots$$

$$\ldots, \binom{36}{18} = \mathbf{9{,}075{,}135{,}300}, \quad \ldots \quad \binom{36}{34} = 630, \quad \binom{36}{35} = 36, \quad \binom{36}{36} = 1$$

An Example of Strongly-Correlated Quantum Many-Body System:

2D electon gas in strong magnetic field

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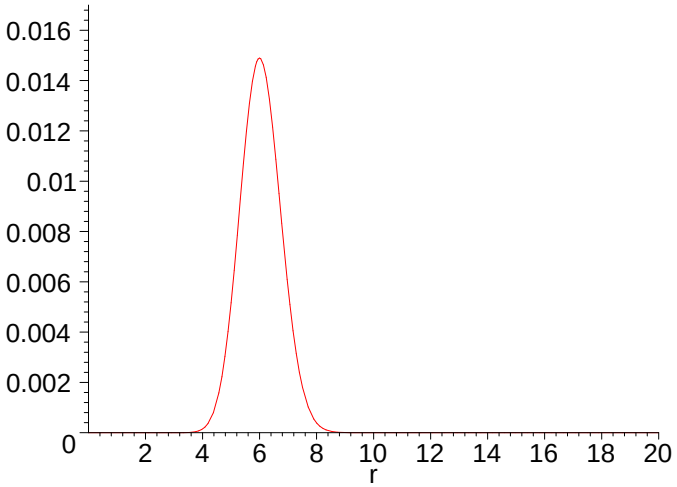
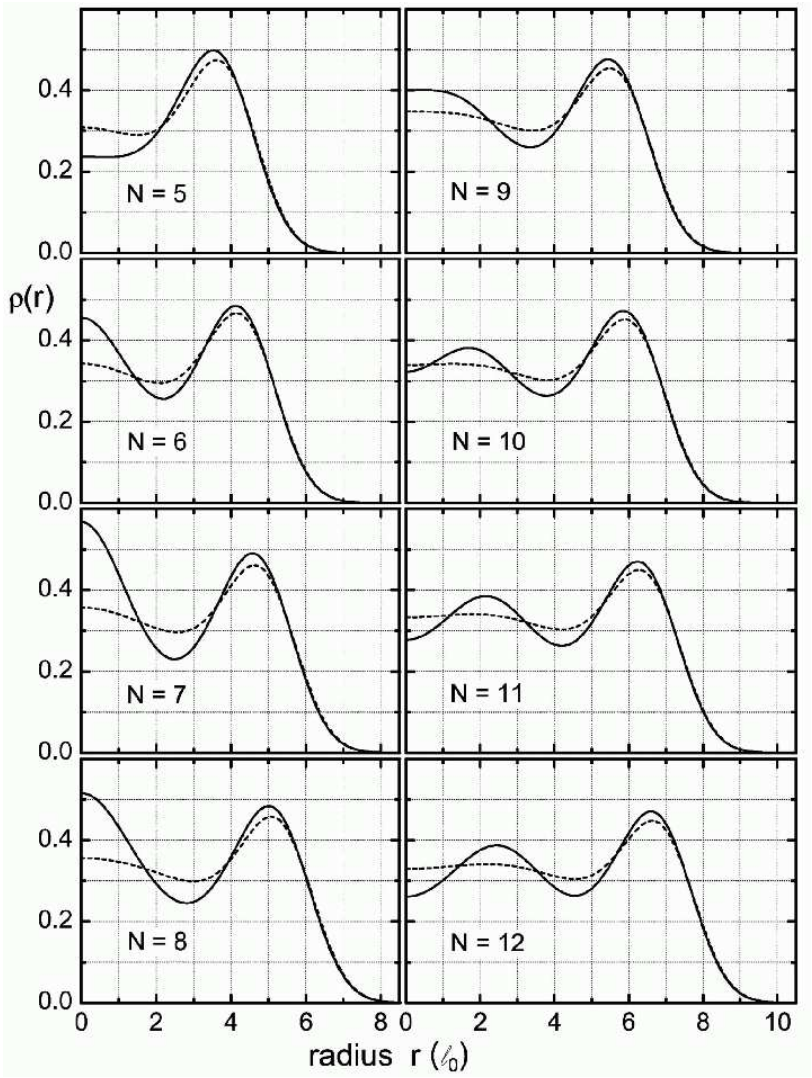
Lowest Landau Level:

$$\psi_m(\mathbf{r}) = \frac{1}{\sqrt{2\pi 2^m m!}}\, r^m\, e^{im\phi}\, e^{-r^2/4}$$

$m = 0, 1, 2, \ldots, 36, \ldots$



$$\mathcal{H} = \sum_{mnl} V^l_{mn}\; c^\dagger_{m+l} c^\dagger_n c_{n+l} c_m$$



[E.V. Tsiper and V.J. Goldman, Phys. Rev. B64, 165311 (2001)]

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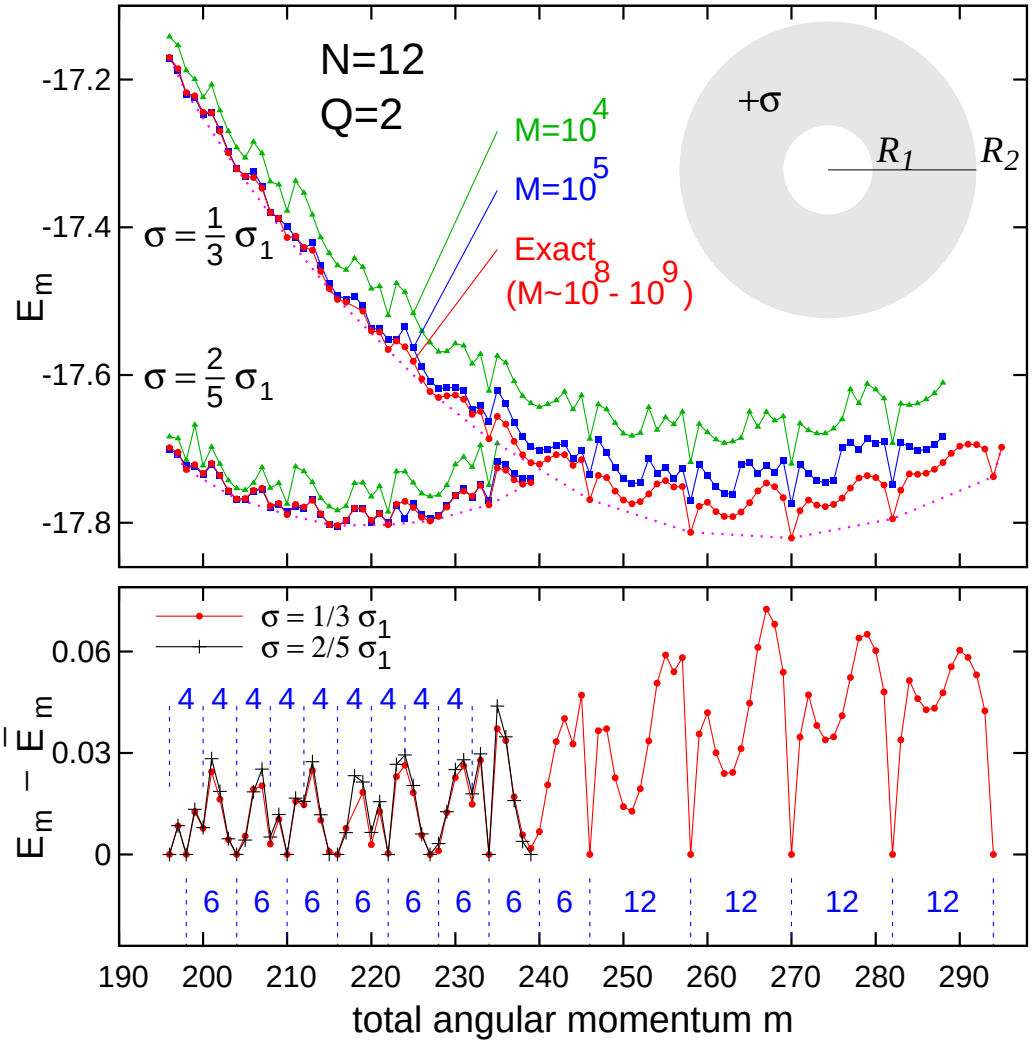
FQHE: Fractional Quantum Hall Effect

Fractionalization of elemental charge

$$e^* = \frac{e}{3}, \quad \frac{2e}{5}, \quad \frac{3e}{7} \quad \ldots?$$



[E.V. Tsiper (2005), to be published]

How was this done ?

Extremal Eigenvalue of a Hermitian Matrix

Consider Typical Computer Limitations

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- **CPU** Limitations: 3 GHz $= 3 \times 10^9$ ops/second $= 10^{14}$ ops/hour
  Can be overcome by multiple parallel CPUs or by patience

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- **Full diagonalization** (all eigenvalues and eigenvectors)
  Need to store the $M \times M$ dense matrix
  (an answer — the set of M eigenvectors — *is* a dense matrix)

$$M \lesssim \sqrt{2.5 \times 10^8} = 16,300$$

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- **Only the ground state** $\epsilon^{(1)}$, $\psi^{(1)}$
  Suppose we do not need to store $\mathcal{H}$ (re-compute as needed)

$$M \lesssim \frac{1}{2}\left(2.5 \times 10^8\right) \sim 100,000,000$$

Extremal Eigenvalue of a Hermitian Matrix

Concept: Power Method

- All bases are equivalent:
  Pretend that we know the basis where $\mathcal{H}$ is diagonal.
  An arbitrary vector

$$\psi = c_1\psi^{(1)} + c_2\psi^{(2)} + \ldots + c_M\psi^{(M)}$$

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Upon doing

$$\mathcal{H}^k\psi = \mathcal{H}\mathcal{H}\mathcal{H}\mathcal{H}\mathcal{H}\ldots\psi$$

all components of ψ die away exponentially with k except the one with the largest $\left|\epsilon^{(i)}\right|$, either $\epsilon^{(1)}$ or $\epsilon^{(M)}$.

- We can choose $\epsilon^{(1)}$ or $\epsilon^{(M)}$ by shifting the matrix $\mathcal{H} \pm \lambda$.
- Convergence is usually slow: the exponent is $1 - \epsilon^{(2)}/\epsilon^{(1)}$.

Extremal Eigenvalue of a Hermitian Matrix

Krylov Subspace

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  But only "slightly."
  $\Rightarrow$ ψ turns towards $\psi^{(1)}$ upon action of $\mathcal{H}$.

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- Try to extrapolate: draw a plane through ψ and $\mathcal{H}\psi$;
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- Generalize: build a subspace of ψ, $\mathcal{H}\psi$, $\mathcal{H}^2\psi$, ..., $\mathcal{H}^k\psi$;
  find the best approximation to $\psi^{(1)}$ in this *Krylov subspace*.

$=$ **Lanczos method**

Krylov subspace is an "almost invariant" subspace of $\mathcal{H}$.

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Lanczos Recursion

- ψ, $\mathcal{H}\psi$, $\mathcal{H}^2\psi$, ..., $\mathcal{H}^k\psi$ are not orthogonal
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- Remarkable discovery [C. Lanczos, 1950]:
  A recursion builds an orthonormal basis in the Krylov subspace

$$\psi_{i+1} = \frac{1}{\beta_{i+1}}(\mathcal{H}\psi_i - \alpha_i\psi_i - \beta_i\psi_{i-1})$$

  α_i and β_i are chosen to orthogonalize ψ_{i+1} to **two previous vectors**.

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  α_i and β_i are chosen to orthogonalize ψ_{i+1} to **two previous vectors**.

- Miraculously, ψ_{i+1} is orthogonal to **all** ψ_1, ψ_2, ...: $(\psi_i\psi_j) = \delta_{ij}$
  Moreover, $\mathcal{H}$ is **tridiagonal** in the new basis:

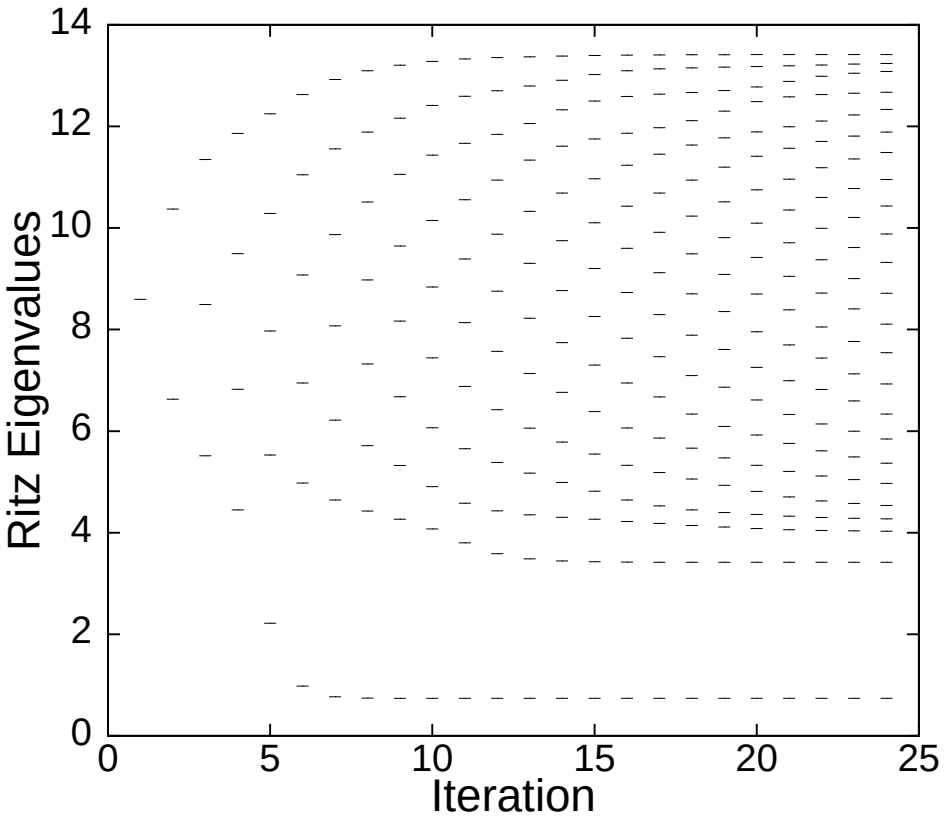
$$(\psi_i\mathcal{H}\psi_i) = \alpha_i \quad (\psi_i\mathcal{H}\psi_{i-1}) = \beta_i \quad (\psi_i\mathcal{H}\psi_j) = 0 \quad \text{otherwise.}$$

  $\Longrightarrow$ All we need to find $\min(\psi\mathcal{H}\psi)$.

Extremal Eigenvalue of a Hermitian Matrix

Typical Lanczos Convergence

- Start with an arbitrary ψ_1
- At every step k we have a $k \times k$ tridiagonal matrix $(\psi_i \mathcal{H} \psi_j)$.
- Extremal eigenvalues of $(\psi_i \mathcal{H} \psi_j)$ give best *variational* approximation to $\epsilon^{(1)}$ and $\epsilon^{(M)}$.
- Corresponding eigenvectors of length k are the expansion coefficients for ψ_{approx} in terms of ψ_i



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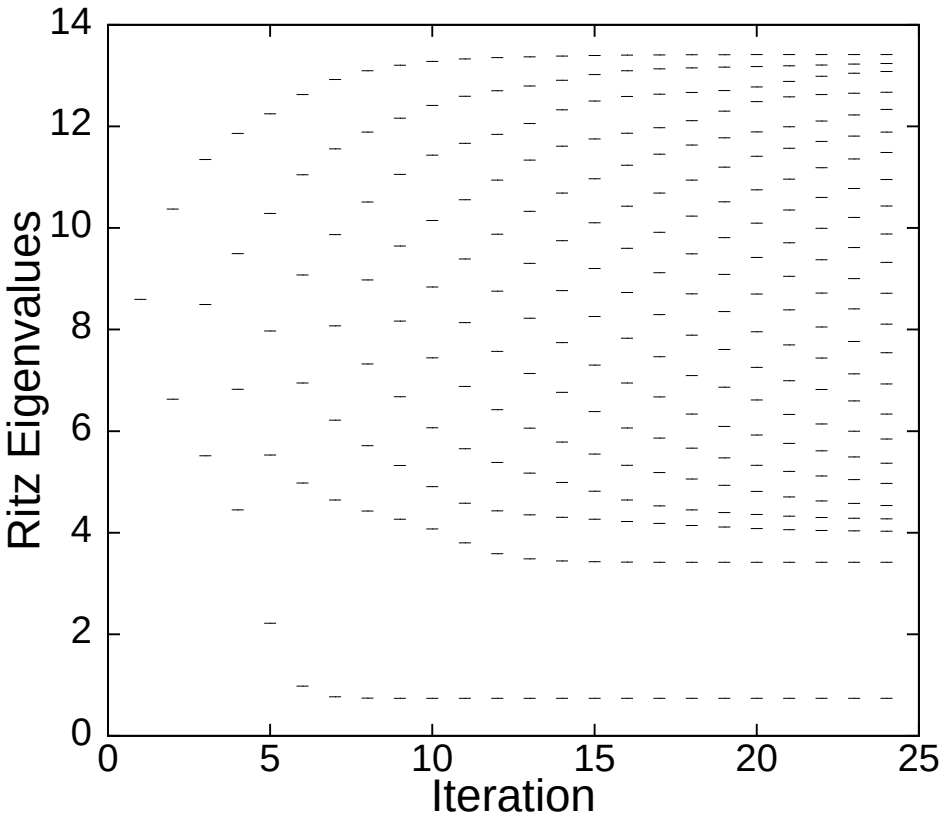

- Convergence is usually exponential
- Worst-case convergence: number of iterations $\sim \sqrt{M}$ (vary rare)
  Usually need 50 — 200 iterations to get all 14 digits.

Lowest Eigenvalue of a Hamiltonian Matrix

Generalized Variational Procedure

Apply the same idea:

1. Build Krylov subspace of $\mathcal{L}$: ξ, $\mathcal{L}\xi$, $\mathcal{L}^2\xi$, ..., $\mathcal{L}^k\xi$:

$$\mathcal{L} = \begin{bmatrix} 0 & \mathcal{T} \\ \mathcal{K} & 0 \end{bmatrix}; \quad \xi = \begin{bmatrix} x \\ p \end{bmatrix}, \; \mathcal{L}\xi = \begin{bmatrix} \mathcal{T}p \\ \mathcal{K}x \end{bmatrix}, \; \mathcal{L}^2\xi = \begin{bmatrix} \mathcal{T}\mathcal{K}x \\ \mathcal{K}\mathcal{T}p \end{bmatrix}, \ldots$$

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2. Find the **best** approximation to $\omega^{(1)}$, $\xi^{(1)}$ within this subspace using the **minimum principle**

$$\min_{(px)=1} \frac{(p\mathcal{T}p)}{2} + \frac{(x\mathcal{K}x)}{2}$$

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$$\min_{(px)=1} \frac{(p\mathcal{T}p)}{2} + \frac{(x\mathcal{K}x)}{2}$$

$$\underrightarrow{\text{leads to}} \qquad \begin{bmatrix} 0 & \widetilde{\mathcal{T}} \\ \widetilde{\mathcal{K}} & 0 \end{bmatrix} \begin{bmatrix} c \\ d \end{bmatrix} = \widetilde{\omega} \begin{bmatrix} c \\ d \end{bmatrix}$$

$\widetilde{\omega}$ gives a *variational* approximation to $\omega^{(1)}$, and
c and d are the expansion coefficients for $x^{(1)}$ and $p^{(1)}$
in terms of x_i and p_i, respectively

Lowest Eigenvalue of a Hamiltonian Matrix

Generalized Lanczos Recursion

The following recursion

$$x_{i+1} = \frac{1}{\beta_{i+1}}(\mathcal{T} p_i - \alpha_i x_i - \beta_i x_{i-1})$$
$$p_{i+1} = \frac{1}{\delta_{i+1}}(\mathcal{K} x_i - \gamma_i p_i - \delta_i p_{i-1})$$

retains all the nice properties of the Hermitian Lanczos recursion and yields

- A globally bi-orthogonal basis $\{x_i, p_i\}$ $\quad (x_i p_j) = \delta_{ij}$
- Both matrices $\widetilde{\mathcal{T}}$ and $\widetilde{\mathcal{K}}$

$$(p_i \mathcal{T} p_i) = \alpha_i, \ (p_i \mathcal{T} p_{i-1}) = \beta_i \quad (p_i \mathcal{T} p_j) = (x_i \mathcal{K} x_j) =$$
$$(x_i \mathcal{K} x_i) = \gamma_i, \ (x_i \mathcal{K} x_{i-1}) = \delta_i \quad = 0 \text{ otherwise.}$$

Lowest Eigenvalue of a Hamiltonian Matrix

Typical Generalized Lanczos Convergence

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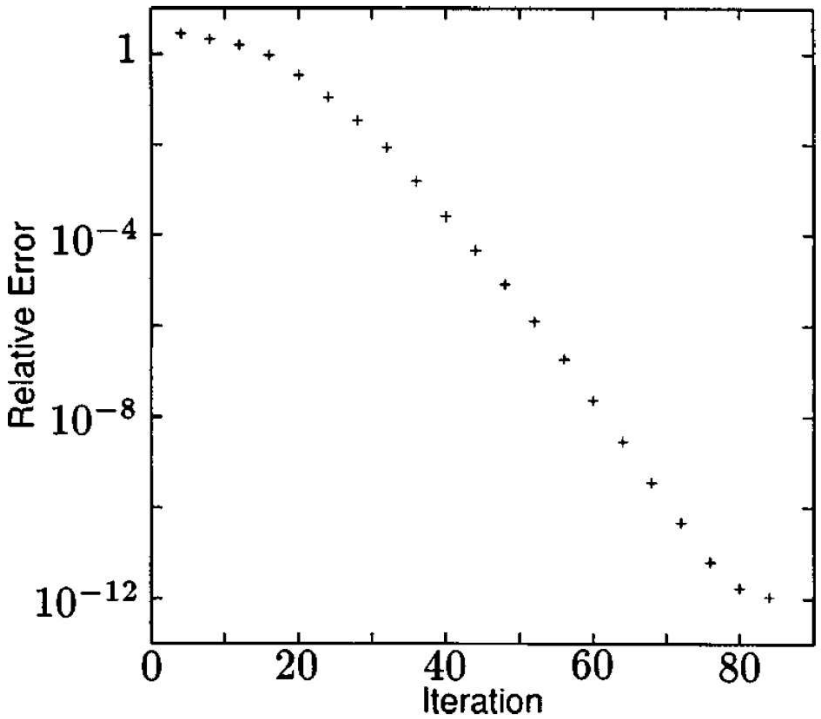
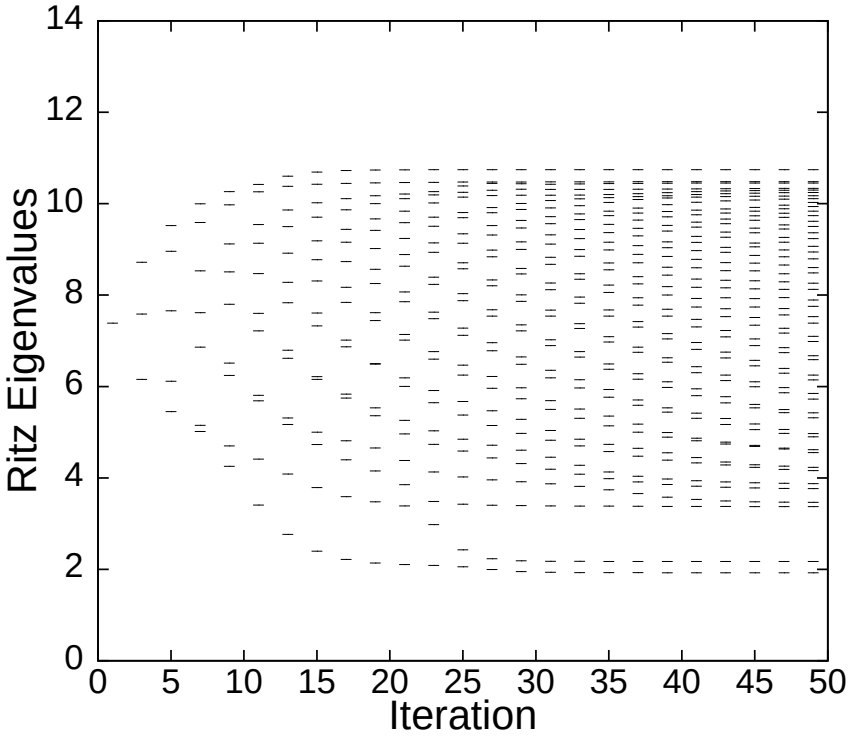


200,000×200,000
random test matrix



smaller test matrix

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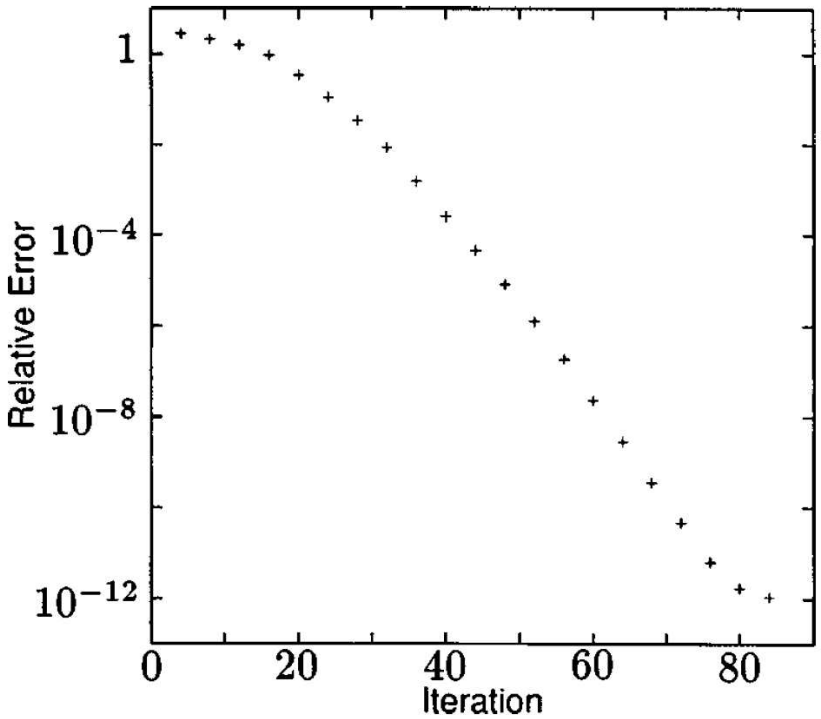
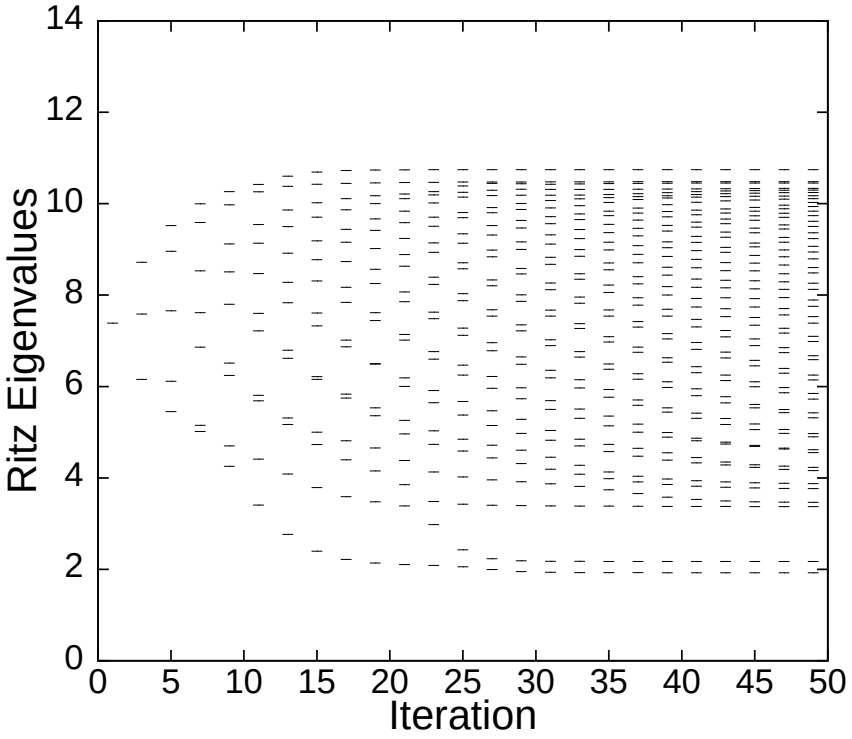


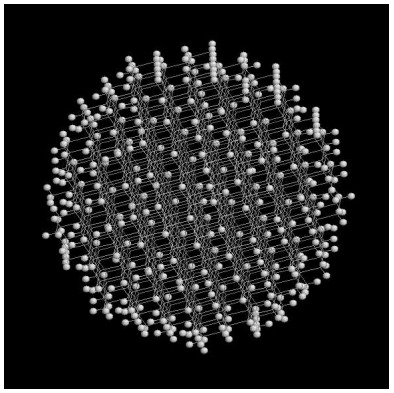
200,000×200,000
random test matrix

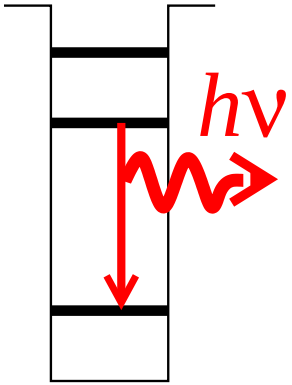


smaller test matrix

Why are we interested in this ?

Excitations of a Quantum System as Classical Oscillations of ψ



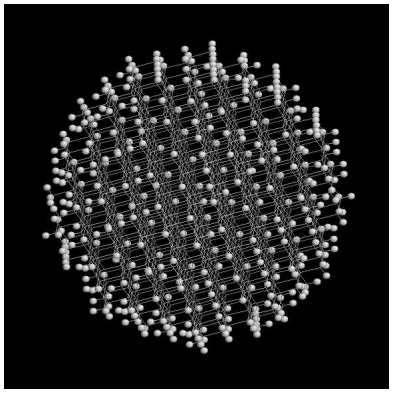


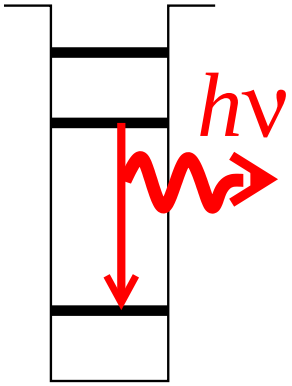
Consider a system driven out of equilibrium. Excitation energies

$$\Omega_{21} = \epsilon^{(2)} - \epsilon^{(1)} \text{ etc.}$$

are resonance frequencies for the evolution of the wave function $\psi(t)$ about the ground-state equlibirum $\psi^{(1)}$

Excitations of a Quantum System as Classical Oscillations of ψ





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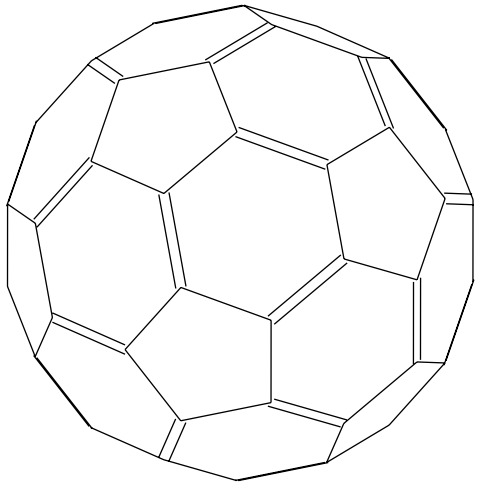
Time Dependent quantum methods

- TDHF = Time-Dependent Hartree-Fock
- TDDFT = Time-Dependent Density Functional Theory etc.
  target Ω_{i1} directly by solving *equations of motion for* $\psi(t)$.
- These equations of motion are technically classical Hamiltonian equation for small oscillations with **many** degrees of freedom.

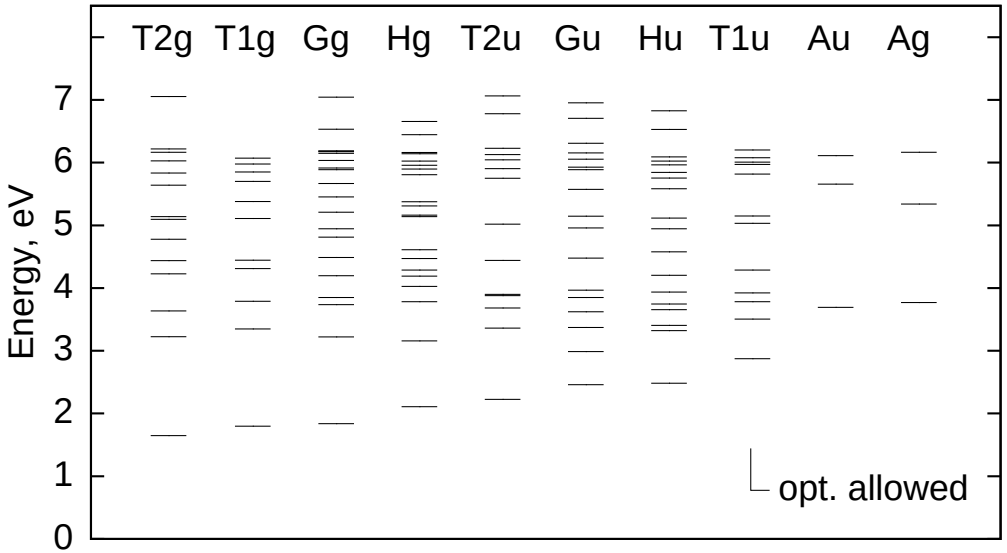
Excitations of a Quantum System as Classical Oscillations of ψ

Proof of Concept: Excitation spectrum of C_{60}



$N_e = 240$

TDHF:
$M = 28,800$



Absorption Experiment $\hbar\Omega$, eV	TDHF Calculation $\hbar\Omega$, eV
3.04	2.874 (5%)
3.30	3.505 (6%)
3.78	3.782 (0%)
4.06	3.924 (3%)
4.35	4.287 (1%)
4.84	5.031 (4%)
5.46	5.150 (6%)
5.88	5.816 (1%)
	6.008
	6.078
6.36	6.202 (2%)

[E.V. Tsiper, J. Phys. B (Letter) 34, L401 (2001)]

Conclusions

- Full diagonalization of a matrix is limited to

$$\sim 16,600 \times 16,000$$

- Lanczos recursion allows to find the ground state and a few lowest-energy excited states of large Hermitian matrices up to

$$\sim 10^8 \times 10^8$$

- Lanczos method can be extended to the problem of small classical oscillations in Hamiltonian form with large number of degrees of freedom

- The latter problem appears in time-dependent quantum qnsatze that target directly the excitation energies of quantum system.