New Mathematical View on Quantum Mechanics

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Inst Adv Study in Math HIT

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Outline

- Background
  Computational mathematics
- From Hermite to Hermitizable
  Criteria for Hermitizability
  Isospectral matrices
  Discrete spectrum
- Isospectral differential operators.
  Schrödinger operator
  Second order differential operator
  Isospectral operators

Example. Maximal real part of λ's

Semigroup $\{e^{tA}\}_{t\geqslant 0}$. Let $A = P^{-1}BP$,

$B = \text{Diag}(4 \pm 3i,\ 3 \pm 2i,\ 2 \pm i,\ 5 + i)$,

$$P = \begin{bmatrix} 3 & 5 & 3+i & 2 & 3 & 1 & 3+i \\ 5 & 4 & 2+i & 4 & 5 & 1 & i \\ 3-i & 2-i & 5 & 1+i & 2 & 1 & 3+i \\ 2 & 4 & 1-i & 2 & i & 1 & 2 \\ 3 & 5 & 2 & -i & 1 & 1 & 2 \\ 1 & 2 & 3 & 4 & 5 & 2 & 3 \\ 7 & 6 & 5 & 4 & 3 & 2 & 1 \end{bmatrix}.$$

Use shift inverse iteration: Initial (v_0, z_0).

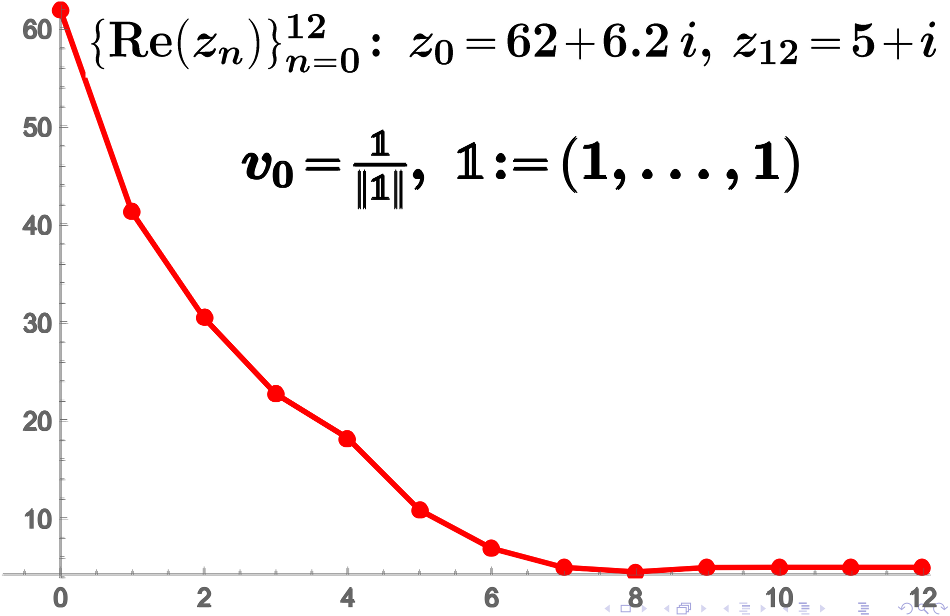
$$v_n = (z_{n-1}I - A)^{-1}v_{n-1}, \qquad z_k = z_0, k \leqslant 4$$

Output (v_n, z_n). 由 v_n 算出 z_n.

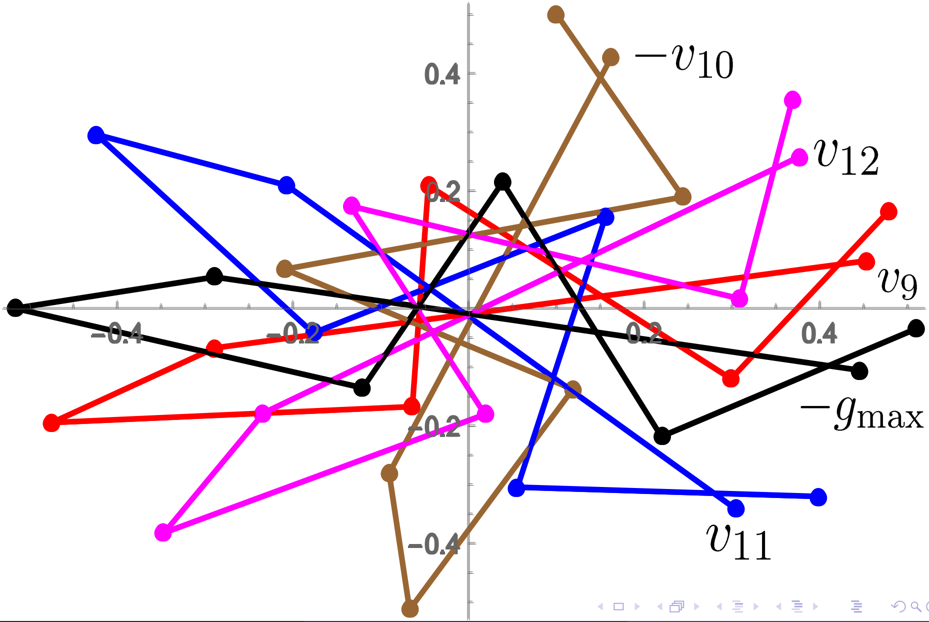
$v_n \to g_{\max}$, $\mathrm{Re}(z_n) \to \max_j \mathrm{Re}(\lambda_j)$.

$$\{\mathrm{Re}(z_n)\}_{n=0}^{12}:\ z_0 = 62 + 6.2\,i,\ z_{12} = 5 + i$$

$$v_0 = \frac{\mathbb{1}}{\|\mathbb{1}\|},\ \mathbb{1} := (1, \ldots, 1)$$



Do vectors $\{v_n\}_{n=9}^{12}$ converge?



What operator has real spectrum?

Selfadjoint A on $L^2(\mu)$ has real spectrum.

Known μ, find A? Gibbsian in Equilibrium.

Matrix, diff operators. Finite/infinite dim.

Known A, find μ? Quantum mechanics

Hermitian matrix $\rightarrow \mu =$ constant.

几乎非负 Given complex A, $\exists \mu$? find μ?

Definition

Complex matrix $A = (a_{ij})$ Hermitizable if $\exists \mu = (\mu_k) > 0$ such that $\mu_i a_{ij} = \mu_j \bar{a}_{ji}$.

Hermitizable $\Rightarrow a_{ii}$ 实

$A = (a_{ij})$ is Hermitizable [可厄米] if

$\exists(\mu_k > 0)$ s.t. $\mu_i a_{ij} = \mu_j \bar{a}_{ji}$. co-zero

A: symmetric/selfadjoint on complex $L^2(\mu)$

$\text{Diag}(\mu)A$ [A 可厄米 $\Leftrightarrow A^{-1}$ 可厄米]

$= A^H \text{Diag}(\mu)$ $\quad A^H := (\bar{A})^*$

$\Leftrightarrow \text{Diag}(\mu)^{1/2} A \text{Diag}(\mu)^{-1/2}$ Hermitizing

$= \text{Diag}(\mu)^{-1/2} A^H \text{Diag}(\mu)^{1/2}$. 实谱

厄米阵的理论和算法 $\to$ 可厄米阵

Criterion and representation

Path: $i_0 \to i_1 \to \cdots \to i_n, \quad a_{i_k i_{k+1}} \neq 0$

$$\mu_{i_0} \frac{a_{i_0 i_1}}{\bar{a}_{i_1 i_0}} = \mu_{i_1} \qquad \frac{a_{i_0 i_1}}{\bar{a}_{i_1 i_0}} > 0$$

$$\mu_{i_0} \frac{a_{i_0 i_1}}{\bar{a}_{i_1 i_0}} \cdot \frac{a_{i_1 i_2}}{\bar{a}_{i_2 i_1}} = \mu_{i_1} \frac{a_{i_1 i_2}}{\bar{a}_{i_2 i_1}} = \mu_{i_2}$$

$$\frac{a_{i_0 i_1}}{\bar{a}_{i_1 i_0}} \frac{a_{i_1 i_2}}{\bar{a}_{i_2 i_1}} \cdots \frac{a_{i_{n-1} i_n}}{\bar{a}_{i_n i_{n-1}}} = \frac{\mu_{i_n}}{\mu_{i_0}} \qquad (\star)$$

$i_n = i_0$: Kolmogorov (1936) circle theorem.
Time-discrete finite Markov chains. QM

Path: $i_0 \to i_1 \to \cdots \to i_n$, $a_{i_k i_{k+1}} \neq 0$

$$\frac{a_{i_0 i_1}}{\bar{a}_{i_1 i_0}} \frac{a_{i_1 i_2}}{\bar{a}_{i_2 i_1}} \cdots \frac{a_{i_{n-1} i_n}}{\bar{a}_{i_n i_{n-1}}} = \frac{\mu_{i_n}}{\mu_{i_0}} \qquad (\star)$$

Path independence! Conservative field Th.

Set $\mu_0 = 1$, μ_n defined by $(\star)$, using shortest path.

Circle Th: smallest closed path without round-trip.

Criterion for Hermitizability

Theorem (C. 2018)

Complex $A = (a_{ij})$ is Hermitizable iff two conditions hold simultaneously.

- For each pair i, j, either $a_{ij} \& a_{ji} = 0$ or $a_{ij}a_{ji} > 0$ ($\Leftrightarrow a_{ij}/\bar{a}_{ji} > 0$).
- The circle condition holds for each smallest closed path without round-trip.

Comparison of symmetric and symmetrizable

Hermitian → symmetric.

Hermitizable → symmetrizable.

Symmetrizable: Z.T. Hou & C. (1979).

Only the case $a_{ij} \geqslant 0, \ i \neq j$ until 2018.

Symmetric case: no Equilibrium Phys.

Gibbs distribution.

System dies out in Probability Theory.
Symmetrizable case: Quadrilateral or Triangle Condition. Book: Chapters 7, 11. Section 14.3. 判定可厄米的算法

Tridiagonal/Jacobi/Birth-death matrix

$T \sim (a_k, -c_k, b_k), \quad E = \{k \in \mathbb{Z}_+ : 0 \leqslant k < N+1\}$

$$\begin{matrix} T \\ Q \end{matrix} = \begin{pmatrix} -c_0 & b_0 & & & 0 \\ a_1 & -c_1 & b_1 & & \\ & a_2 & -c_2 & b_2 & \\ & & \ddots & \ddots & b_{N-1} \\ 0 & & & a_N & -c_N \end{pmatrix},$$

$(a_k), (b_k), (c_k)$: complex sequences.

BD: $a_k > 0$, $b_k > 0$, $c_k = a_k + b_k$, $c_N \geqslant a_N$.

Tridiagonal matrix: $T \sim (a_k, -c_k, b_k)$

Theorem (C. 2018)

The tridiagonal T is Hermitizable iff the following two conditions hold simultaneously.

$N \leqslant \infty$

- The diagonals (c_k) are real.
- Either $a_{i+1} \& b_i = 0$ or $a_{i+1} b_i > 0$

分块 $(\Leftrightarrow b_i / \bar{a}_{i+1} > 0)$.

Then
$$\mu_0 = 1, \; \mu_k = \mu_{k-1} \frac{b_{k-1}}{\bar{a}_k}.$$

Isospectral to birth–death Q-matrix

Theorem/Algorithm

Given Hermitizable $T \sim (a_k, -c_k, b_k)$ with $c_k \geqslant |a_k| + |b_k|$ (or $\tilde{c}_k = c_k + m$) Then $\exists$ an explicit birth–death matrix $\tilde{Q} \sim (\tilde{a}_k, -\tilde{c}_k, \tilde{b}_k)$ such that T is isospectral to $\tilde{Q}$.

Comparison. 5:1 sequences, $\tilde{a}_k,\ \tilde{b}_k > 0$.

Explicit $u_k := a_k b_{k-1} = |a_k b_{k-1}|$ & c_k

$N \leqslant \infty$

$$\begin{cases} \tilde{c}_k \equiv c_k; \\ \tilde{b}_k = c_k - u_k/\tilde{b}_{k-1}, \ \tilde{b}_0 = c_0; \\ \tilde{a}_k = c_k - \tilde{b}_k, \ k < N; \quad \tilde{a}_N = u_N/\tilde{b}_{N-1}. \end{cases}$$

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h-transform. h: nearly harmonic $Th = 0$.

$$h_0 = 1, \quad h_n = h_{n-1}\tilde{b}_{n-1}/b_{n-1}, \quad n \geqslant 1.$$

$$h_0 = 1, \quad h_n = \prod_{j=0}^{n-1} \tilde{b}_j \Big/ \prod_{j=0}^{n-1} b_j, \quad n \geqslant 1.$$

Explicit $u_k := a_k b_{k-1} = |a_k b_{k-1}|$ & c_k

$$\tilde{b}_k = c_k - \cfrac{u_k}{c_{k-1} - \cfrac{u_{k-1}}{c_{k-2} - \cfrac{u_{k-2}}{\ddots\, c_2 - \cfrac{u_2}{c_1 - \cfrac{u_1}{c_0}}}}}$$

Invariant. 3 Proofs: 2018, 2020∼2.

Discrete spectrum. $\mathbb{Z}_+ = \{0, 1, 2, \cdots\}$

Let $\widetilde{Q} \sim (\tilde{a}_k, -\tilde{c}_k, \tilde{b}_k)$. Define

$$\tilde{\mu}_0 = 1, \ \tilde{\mu}_k = \frac{\tilde{b}_0 \cdots \tilde{b}_{k-1}}{\tilde{a}_1 \cdots \tilde{a}_k}, \ \tilde{\nu}_k = \frac{1}{\tilde{\mu}_k \tilde{b}_k} \qquad k \geqslant 1;$$

$$\tilde{\mu}[0, n] = \sum_{j=0}^{n} \tilde{\mu}_j, \quad \tilde{\nu}[0, n] = \sum_{j=0}^{n} \tilde{\nu}_j.$$

Theorem (C. 2014. $\widetilde{Q} \to T$)

(1) Let $\tilde{\nu}[0, \infty) < \infty$. Then Spec$(T_{\min})$ is discrete iff $\lim_{n\to\infty} \tilde{\mu}[0, n]\tilde{\nu}[n, \infty) = 0$.

Discrete spectrum. $\mathbb{Z}_+ = \{0, 1, 2, \cdots\}$

Theorem (Continued)

(2) Let $\tilde{\mu}[0,\infty) < \infty$. Then Spec$(T_{\max})$ is discrete iff $\lim_{n\to\infty} \tilde{\nu}[0,n]\tilde{\mu}[n+1,\infty) = 0$

(3) Let $\tilde{\nu}[0,\infty) = \infty = \tilde{\mu}[0,\infty)$. Then Spec$(T_{\min})$ = Spec$(T_{\max})$ is not discrete.

In particular, if $\sum_{k=0}^{\infty} \tilde{\nu}_k \tilde{\mu}[0,k] = \infty$, then $T_{\min} = T_{\max}$.

Remove condition "tridiagonal"

Theorem (Householder transformation)

For each Hermite $\boldsymbol{H}$, ∃ a sequence of extended reflection matrices $\{\boldsymbol{U}_j\}_{j=0}^{N-1}$:

$$\boldsymbol{U}_j = \boldsymbol{I} + (\boldsymbol{\kappa} - 1)\boldsymbol{u}\boldsymbol{u}^{\boldsymbol{H}}$$

$\boldsymbol{\kappa}$: constant with $|\boldsymbol{\kappa}| = 1$, $\boldsymbol{u}$: unit vector, such that $\boldsymbol{U} := \prod_{j=0}^{N-1} \boldsymbol{U}_j$ is unitary and $\boldsymbol{T} := \boldsymbol{U}\boldsymbol{H}\boldsymbol{U}^{\boldsymbol{H}}$ becomes a real, symmetric tridiagonal matrix. ★

⇒Hermitizable

Blocked, BD

Remove condition “tridiagonal”

Eigenproblem: started by C.G.J. Jacobi in 1846. 175 years. In 2000, two academic organizations selected

“Top 10 algorithms in 20th century”

Three of them are on matrix eigenproblem, one is Householder transformation.

On this topic, any progress is unusual.

Remove condition "tridiagonal"

Theorem (C. 2018)

Each Hermitizable matrix is isospectral to a birth–death Q-matrix.

$\boldsymbol{A}$: complex $L^2(\mu) \to \widetilde{Q}$: real $L^2(|h|^2 \mathrm{d}x)$

New mathematical view.

New framework: common frame for observ.

New spectral theory: ignoring the potential

New algorithm: allow general diagonals, starting point to study algorithm.

Centennial Debate

Born's Probability amplitude^{1926}: $|\psi_m|^2$.

Bohr^{1927}: "the principle of complementarity".

"Electrons are both waves and particles, when you observe them, it exists in the form of particles; without observation, it exists in the form of waves. The so-called wave-particle duality, just depends on the way we observe it. "

Centennial Debate

Schrödinger: never accepted the orthodox interpretation of 'almost psychical' advocated by the Copenhagen School.

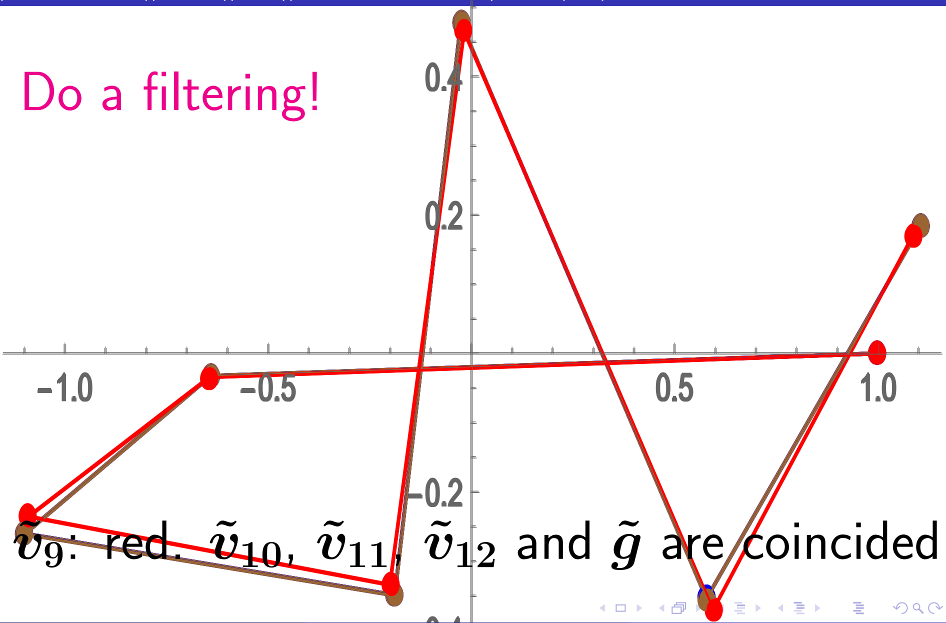
Einstein: "God does not play dice!"

$\boldsymbol{A}$: complex $\boldsymbol{L^2(\mu)} \to \widetilde{\boldsymbol{Q}}$: real $\boldsymbol{L^2(|h|^2 \mathrm{d}x)}$

No randomness. Common frame for observ.
薛猫、扩散. 寻波动方程解概率模型. 柯氏解～平衡态统计物理, 无波动. 可厄米含波动. 生灭阵源于概率, 给出矩阵/波动力学的谱刻画. 长文,137 页

$\|e^{i\theta_n}x\| = \|x\|$. $\tilde{v} := v/v(0)$. Conformal

Do a filtering!



$\tilde{v}_9$: red. $\tilde{v}_{10}$, $\tilde{v}_{11}$, $\tilde{v}_{12}$ and $\tilde{g}$ are coincided

New spectral theory for T

$\boldsymbol{Q}\mathbb{1} = \mathbb{0} \Rightarrow$ potential/keeling $= \mathbf{0}$,
Discrete spectrum.
Principle eigenvalues in 4 cases [C. 2010+]:
DD, NN, DN, ND
Essential point: eigenfunctions are good:
concave, increasing, increasing, decreasing.
If potential/keeling $\neq \mathbf{0}$, no the properties.
Using isospectral theorem $\Rightarrow$ results for $\boldsymbol{T}$.
One-dim diffusions, in parallel !? 谢颖超团队

Mathematical methods. real $L = \frac{1}{2}\Delta + V$

- Feynman-Kac semigroup:

$$T_t f(x) = \mathbb{E}_x \left\{ f(w_t) \exp\left[\int_0^t V(w_s) \mathrm{d}s \right] \right\}.$$

- h-transform [C. & Xu Zhang, 2014]:

$L = \Delta + V \to \widetilde{L} = \Delta + \tilde{b}^h \nabla, \quad Lh = 0,$

L on $L^2(\mathrm{d}x)$ is isospectral to $\widetilde{L}$ on $L^2(\tilde{\mu}) := L^2(|h|^2 \mathrm{d}x)$.

Differential operators

Let $\boldsymbol{a} = (a_{ij})_{i,j=1}^d$, $\boldsymbol{b} = (b_i)_{i=1}^d$, a_{ij}, b_i, c, $[V] : \mathbb{R}^d \to \mathbb{C}/[\mathbb{R}]$. Define $\mathrm{d}\boldsymbol{\mu} = e^V \mathrm{d}\boldsymbol{x}$, $\boldsymbol{L} = \nabla(\boldsymbol{a}\nabla) + \boldsymbol{b} \cdot \nabla - \boldsymbol{c}$.

Theorem (C.&J.Y. Li 2020)

Dirichlet boundary. Operator $\boldsymbol{L}$ is Hermitizable w.r.t. $\boldsymbol{\mu}$ iff $\bar{\boldsymbol{a}}^* = \boldsymbol{a}$ and

$$\mathrm{Re}\,\boldsymbol{b} = (\mathrm{Re}\,\boldsymbol{a})(\nabla V),$$

$$2\,\mathrm{Im}\,\boldsymbol{c} = -\big((\nabla V)^* + \nabla^*\big)\big((\mathrm{Im}\,\boldsymbol{a})(\nabla V) + \mathrm{Im}\,\boldsymbol{b}\big).$$

Isospectral differential operators

Theorem (C.&J.Y. Li 2020)

Denote $\mathscr{D}(L)$ be the domain of the Hermitizable L as above in $L^2(\mu)$ and let h: $Lh = 0$, $h \neq 0$ (a.e.). Then L is isospectral to $\big(\tilde{L},\ \mathscr{D}(\tilde{L})\big)$:

$$\begin{cases} \tilde{L} = \nabla(a\nabla) + \tilde{b}\cdot\nabla - 0, \\ \mathscr{D}(\tilde{L}) = \{\tilde{f} \in L^2(\tilde{\mu}) : \tilde{f}h \in \mathscr{D}(L)\}; \end{cases}$$

where

$$\tilde{b} = b + 2\,\mathrm{Re}(a)\mathbb{1}_{[h\neq 0]}\frac{\nabla h}{h}, \quad \tilde{\mu} := |h|^2\mu.$$

New spectral theory for Schrödinger operator

Matrix mechanics: Heisenberg 1925.

Wave mechanics: Schrödinger 1926.

Equivalence of two mechanics 1926.

Schrödinger operator is now 95 years old.

A huge number of publications for it.
Five years are not enough to develop a new spectral theory for the operator.

http://math0.bnu.edu.cn/~chenmf

Collection of papers: volumes 1–4

The end!

Thank you, everybody!

谢谢大家!

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