New Mathematical View on Quantum Mechanics

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"Dirichlet Forms and Related Topics"
In Honor of Masatoshi Fukushima's Beiju

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Outline

I. Two typical new results:
Schrödinger operator,
Hermitizable matrix and its isospectral one.

II. Hermitizable matrix. Framework, spectral, and algorithm of quantum mechanics (QM).

III. Hermitizable differential operator and isospectral operator.

I. Two new results. Schrödinger operator

1) The most popular approach to study the Schrödinger operator

96 years old

$$L = \frac{1}{2}\Delta + V$$

unbounded, spectrum

is the Feynman-Kac semigroup $\{T_t\}_{t\geqslant 0}$:

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

where (w_t) is the standard Brownian motion.

Wave mechanics: Schrödinger operator

2) New method to study the spectrum of Schrödinger operator. Replacing L by

$$\tilde{L} = \frac{1}{2}\Delta + \tilde{b}^h \nabla,$$

standard spectrum

where h is harmonic: $Lh = 0$, $h \neq 0$ (a.e.). Then, the operator L on $L^2(\mathrm{d}x)$ is isospectral to the one $\tilde{L}$ on $L^2(\tilde{\mu})$, where $\mathrm{d}\tilde{\mu} := |h|^2 \mathrm{d}x$.

Remark g is eigenfunction: $Lg = \lambda g$, $g \neq 0$.
If dim$=1$, V, g oscillated; $\tilde{L}\tilde{g} = \lambda\tilde{g}$, $\tilde{g}$ is monotone.
10 years may not be enough for a new theory!

Matrix mechanics. Hermitizable matrix

Definition

A complex matrix $A = (a_{ij})$ on a countable set E is called Hermitizable if there exists a positive measure $(\mu_k : k \in E)$ such that

$$\mu_i a_{ij} = \mu_j \bar{a}_{ji}, \qquad i, j \in E,$$

where $\bar{a}$ is the conjugate of a.

Claim: A is Hermitizable (w.r.t. μ) iff A is self-adjoint on complex $L^2(\mu)$. Real Sp! $\exists \mu?$

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

Profs M.L. Silverstein+M.P. Qian+2

Dirichlet Forms and
Markov Processes

著者校

1979 再校

by

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部分の中 ご確認ください。

Spectrum of Hermitizable matrix

Theorem (C. 2018)

The spectrum of a finite Hermitizable matrix A is equal to the union of the spectrums of m birth-death (BD) matrices, where m is the largest multiplicity of eigenvalues of A. 3 string

To play a music = spectrum of QM

By a Shanxian's Music Score

II. Matrix Mechanics. Tridiagonal/BD matrix

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

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

[T] $(a_k), (b_k), (c_k)$: complex sequences. $N \leqslant \infty$

[Q] 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

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

- The diagonals (c_k) are real.
- Either $a_{i+1} \& b_i = 0$ [Separated into blocks] or $a_{i+1} b_i > 0$ $(\Leftrightarrow b_i / \bar{a}_{i+1} > 0)$.

Then

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

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 $\widetilde{Q} \sim (\tilde{a}_k, -\tilde{c}_k, \tilde{b}_k)$ such that T is isospectral to $\widetilde{Q}$.

In general, we have $\tilde{c}_N \geqslant \tilde{a}_N$. We assume that $\tilde{c}_N > \tilde{a}_N$ in what follows.

The case $\tilde{c}_N = \tilde{a}_N$ was also treated in the published papers (C. 2018, 2019).

Explicit $u_k := a_k b_{k-1} > 0$ & $c_k =: \tilde{c}_k$

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

$$\boxed{\tilde{b}_0 = c_0, \ \tilde{b}_k = c_k - u_k / \tilde{b}_{k-1}}$$

$$\tilde{a}_k = c_k - \tilde{b}_k, \ k < N; \quad \tilde{a}_N = u_N / \tilde{b}_{N-1}.$$

Exercise: $Q \sim (1, -3, 2) \to \tilde{Q} = ?$ 2018/2/1-2

Theorem

Every irreducible$^+$ Hermitizable tridiagonal matrix T on complex $L^2(\mu)$ is isospectral to a birth-death (BD) Q-matrix $\tilde{Q}$ on real $L^2(\tilde{\mu})$: $\tilde{\mu} = |h|^2\mu$, where $Th = 0$ on $[0, N)$. Explicit h

$$h_0 = 1, \quad h_n = h_{n-1}\frac{\tilde{b}_{n-1}}{b_{n-1}}, \quad 1 \leqslant n \leqslant N.$$

$\tilde{Q} = D_h^{-1}\, T\, D_h$. Unknown immortal help 未知的仙人相助

$$h_0 = 1, \; h_n = \prod_{k=0}^{n-1} \tilde{b}_k \Big/ \prod_{k=0}^{n-1} b_k, \quad 1 \leqslant n \leqslant N.$$

General Hermitizable A and $\hat{A}$ [a_{ii} real, $\forall i$]

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

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

$$\mathrm{D}_\mu A = A^H \mathrm{D}_\mu \quad \boxed{A^H := (\bar{A})^*}$$

$$\Leftrightarrow \mathrm{D}_\mu A\, \mathrm{D}_\mu^{-1} = A^H$$

$$\Leftrightarrow [\hat{A} :=] \mathrm{D}_\mu^{1/2} A \mathrm{D}_\mu^{-1/2} = \mathrm{D}_\mu^{-1/2} A^H \mathrm{D}_\mu^{1/2}.$$

A is Hermitizable $\Leftrightarrow$ $\hat{A}$ is Hermitian.

$\hat{A}$: Hermitizing of A

Theory/algorithm of Hermitian matrix
$\longrightarrow$ Hermitizable one

Spectrum of Hermitizable matrix

Hermitizable $A \to$ Hermite $\hat{A}$

$\xrightarrow{U}$ tridiagonal, Hermite T

$\to$ BD (by our result) [Blocks]   [5; §4]

In 2000, two journals selected

"Top 10 algorithms in 20th century". $\mathbf{1/3}$ matrix:

Householder transformation

Eigenproblem: C.G.J. Jacobi in 1846, 176 years.

Meaning of Hermite→Hermitizable:

Homogeneous medium → Inhomogeneous medium

dx, $N = \infty$. No Equil. Phys. Gibbs; Prob: dies out

Criterion for Hermitizability of general A

Theorem (C. 2018)

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

- Co-zero property. 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.

A.N. Kolmogorov (1936), finite time-discrete MC.

Hou & C. (1979)|1982↑. The ignorant are fearless!

Schrödinger, 1931	2018↑

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Kolmogorov's Circle & Conservative Field

Closed Path: $i_0 \to i_1 \to \cdots \to i_n = i_0 \ [a_{i_k i_{k+1}} \neq 0]$

$\Longrightarrow a_{i_0 i_1} \cdots a_{i_{n-1} i_n} = \bar{a}_{i_n i_{n-1}} \cdots \bar{a}_{i_1 i_0}$ Circle condition

$$\Longleftrightarrow \frac{a_{i_0 i_1}}{\bar{a}_{i_1 i_0}} \cdots \frac{a_{i_{n-1} i_n}}{\bar{a}_{i_n i_{n-1}}} = 1$$

$$\Longleftrightarrow \log \frac{a_{i_0 i_1}}{\bar{a}_{i_1 i_0}} + \cdots + \log \frac{a_{i_{n-1} i_n}}{\bar{a}_{i_n i_{n-1}}} = 0$$

$$\Longleftrightarrow w(i_0 \to i_1) + \cdots + w(i_{n-1} \to i_n) = 0$$

$$\Longleftrightarrow w(i_0 \to i_1 \to \cdots \to i_{n-1} \to i_n) = 0$$

$\Longleftrightarrow w(\text{each closed path}) = 0$ Conservative field

Claim: Hermitizable A with work w consists a conservative field. $w(2 \to 0 \to 2) = \log \frac{a_{20}}{\bar{a}_{02}} + \log \frac{a_{02}}{\bar{a}_{20}} = 0.$

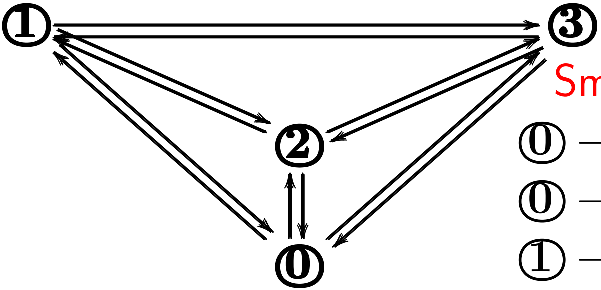
复可配称矩阵之例

$$A = \begin{bmatrix} -6 & \frac{8-6i}{5} & \frac{8+14i}{13} & \frac{18+4i}{17} \\ 3+\frac{9i}{4} & -\frac{55}{4} & \frac{-5+40i}{13} & \frac{30+35i}{17} \\ \frac{12-21i}{5} & \frac{-4-32i}{5} & -13 & \frac{60-66i}{17} \\ \frac{63-14i}{10} & \frac{84-98i}{15} & \frac{70+77i}{13} & -16 \end{bmatrix}$$

$$\mu = \left(1, \frac{8}{15}, \frac{10}{39}, \frac{20}{119}\right)$$ Hermitizing measure.

3 method for computing μ: [5; Algorithm 1]

复可配称矩阵之例 $\mu_k = r_{0k}$, $\mu_k = \mu_{k-1} r_{k-1,k}$



$C_3^1 + C_3^2 + C_3^3 = 7$

Smallest closed paths

⓪ → ① → ② → ⓪

⓪ → ③ → ② → ⓪

① → ③ → ② → ①

$$r_{ij} = \frac{a_{ij}}{\bar{a}_{ji}}, \qquad r_{01} = \frac{8}{15}, \quad r_{12} = \frac{25}{52}, \quad r_{20} = \frac{39}{10},$$

$$r_{ji} = \frac{1}{r_{ij}}, \qquad r_{03} = \frac{20}{119}, \quad r_{32} = \frac{119}{78}, \quad r_{31} = \frac{238}{75}.$$

⓪ → ① → ② → ⓪: $r_{01} r_{12} r_{20} = 1.$

Hermitizing $\hat{A} = D_{\mu^{1/2}} A D_{\mu^{-1/2}}$

$$\begin{pmatrix} -6 & (4-3i)\sqrt{\frac{3}{10}} & (4+7i)\sqrt{\frac{6}{65}} & (9+2i)\sqrt{\frac{7}{85}} \\ (4+3i)\sqrt{\frac{3}{10}} & -\frac{55}{4} & -\frac{2-16i}{\sqrt{13}} & (6+7i)\sqrt{\frac{14}{51}} \\ (4-7i)\sqrt{\frac{6}{65}} & -\frac{2+16i}{\sqrt{13}} & -13 & (10-11i)\sqrt{\frac{42}{221}} \\ (9-2i)\sqrt{\frac{7}{85}} & (6-7i)\sqrt{\frac{14}{51}} & (10+11i)\sqrt{\frac{42}{221}} & -16 \end{pmatrix}$$

Tridiagonalizing $\hat{A}$ using Householder transformation

Refer to [1; Example 7] and [6; §2]. The transformation in terms of a unitary matrix U_j is $\hat{A} \to A_1$:

$$A_1 = U_1 \hat{A} U_1^H, \quad A_1 \to A_2: \quad A_2 = U_2 A_1 U_2^H.$$

Tridiagonalizing Step 1: A_1 Hermitian

$$A_1 = \begin{pmatrix} -6 & \sqrt{\frac{41}{2}} & 0 & 0 \\ \sqrt{\frac{41}{2}} & -\frac{633}{164} & * & * \\ 0 & * & -\frac{2\left(23488+21\sqrt{615}\right)}{2501} & * \\ 0 & * & * & \frac{-100577+84\sqrt{615}}{5002} \end{pmatrix}$$

Algebraic expression.

$$A_1 = \begin{pmatrix} -6 & 4.52769 & 0 & 0 \\ 4.52769 & -3.85976 & .146245+1.47229i & -.998788+.445783i \\ 0 & .146245-1.47229i & -19.1993 & 1.81102-.278314i \\ 0 & -.998788-.445783i & 1.81102+.278314i & -19.6909 \end{pmatrix}$$

Numerical expression.

Tridiagonalizing Step 2: A_2 Hermitian

$$A_2 = \begin{pmatrix} -6 & \sqrt{41/2} & 0 & 0 \\ \sqrt{41/2} & -633/164 & * & 0 \\ 0 & * & -30525529/1599902 & * \\ 0 & 0 & * & -386525/19511 \end{pmatrix}$$

$$A_2 = \begin{pmatrix} -6 & 4.52769 & 0 & 0 \\ 4.52769 & -3.85976 & 1.83992 & 0 \\ 0 & 1.83992 & -19.0796 & 1.21995+1.34007i \\ 0 & 0 & 1.21995-1.34007i & -19.8106 \end{pmatrix}$$

A_3: real, symmetric!

For tridiagonal Hermitizable matrix, optimal algorithm: O(N):

C. & Y.S. Li (2019). Development of powerful algorithm for maximal eigenpair. Front. Math. China 14(3): 493-519.

Tridiagonalizing the next symmetric matrix, using Householder transformation. 5 steps

$$A=\begin{bmatrix}
\frac{8074}{2601} & \frac{271}{5202} & \frac{373}{1734} & \frac{746}{2601} & \frac{1355}{5202} & \frac{169}{867} & \frac{676}{2601} & -\frac{959}{5202}\\
\frac{271}{5202} & \frac{31483}{10404} & \frac{373}{3468} & \frac{373}{2601} & \frac{1355}{10404} & \frac{169}{1734} & \frac{338}{2601} & -\frac{959}{10404}\\
\frac{373}{1734} & \frac{373}{3468} & \frac{2787}{1156} & \frac{475}{867} & \frac{1865}{3468} & \frac{271}{578} & \frac{542}{867} & -\frac{245}{3468}\\
\frac{746}{2601} & \frac{373}{2601} & \frac{475}{867} & \frac{7102}{2601} & \frac{1865}{2601} & \frac{542}{867} & \frac{2168}{2601} & -\frac{245}{2601}\\
\frac{1355}{5202} & \frac{1355}{10404} & \frac{1865}{3468} & \frac{1865}{2601} & \frac{37987}{10404} & \frac{845}{1734} & \frac{1690}{2601} & -\frac{4795}{10404}\\
\frac{169}{867} & \frac{169}{1734} & \frac{271}{578} & \frac{542}{867} & \frac{845}{1734} & \frac{1223}{289} & \frac{268}{867} & -\frac{1673}{1734}\\
\frac{676}{2601} & \frac{338}{2601} & \frac{542}{867} & \frac{2168}{2601} & \frac{1690}{2601} & \frac{268}{867} & \frac{11476}{2601} & -\frac{3346}{2601}\\
-\frac{959}{5202} & -\frac{959}{10404} & -\frac{245}{3468} & -\frac{245}{2601} & -\frac{4795}{10404} & -\frac{1673}{1734} & -\frac{3346}{2601} & \frac{46123}{10404}
\end{bmatrix}$$

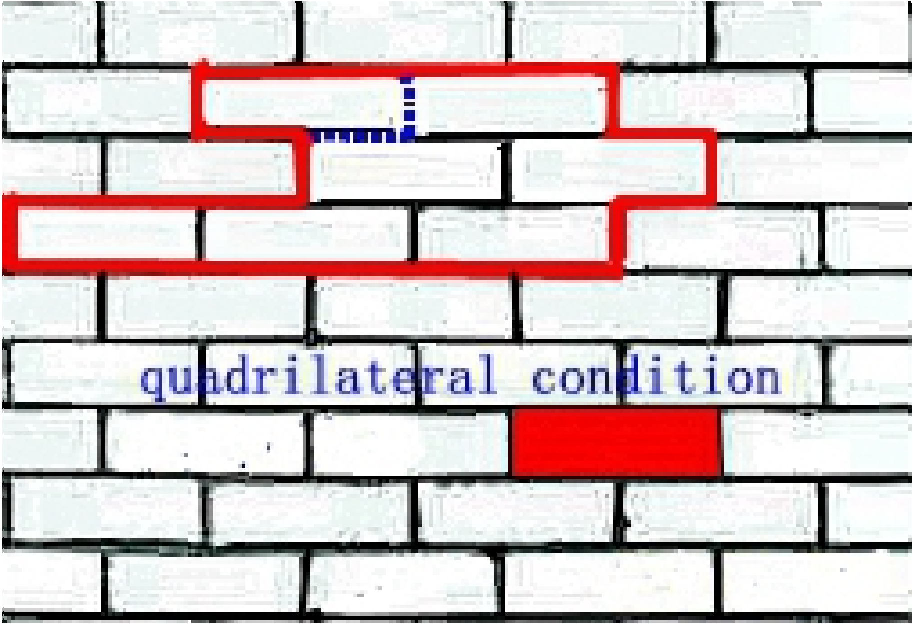
Actually, use 4 steps only, since one step can be ignored. Refer to [5; Example 9].

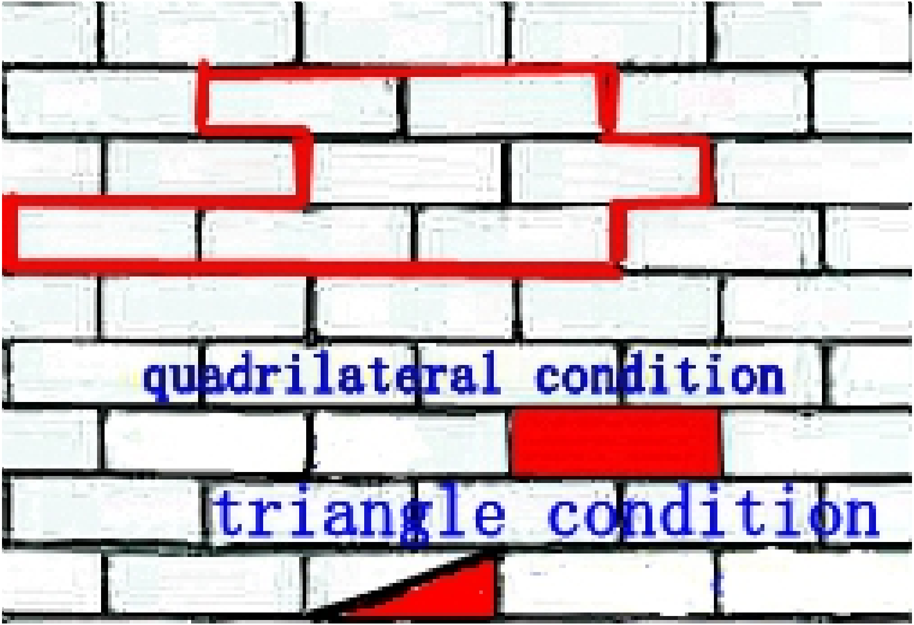
Resulting tridiagonal matrix, symmetric

$$T=\begin{bmatrix} 3.10419 & .581915 & & & & & & \\ .581915 & 6.43398 & 1.2267 & & & & & \\ & 1.2267 & 3.6022 & 1.03145 & & & & \\ & & 1.03145 & 2.85964 & 0 & & & \\ & & & 0 & 2.72146 & .448281 & & \\ & & & & .448281 & 2.27854 & 0 & \\ & & & & & 0 & 3.88097 & .323827 \\ & & & & & & .323827 & 3.11903 \end{bmatrix}.$$

The eigenvalues of the blocks are $\{7, 4, 3, 2\}$, $\{3, 2\}$ and $\{4, 3\}$ respectively. Here $m = 3$.

In genral, there are infinite many closed paths (infinite systems for instance). However, we often need only two types of smallest closed paths. We have seen the triangle one as above.


quadrilateral condition


quadrilateral condition
triangle condition

Symmetrizable (1979)→Hermitizable (2018)

Symmetrizable: real case. Z.T. Hou & C.(1979): "Markov Processes and Field Theory"

→ Statistical Physics.

C.(04) "From Markov Chains to Non-equilibrium..."

Chapter 7: Field Theory

Chapter 11: Reversible Spin Processes and ...

Section 14.3: Reversible RD-processes

Hermitizable (C. 2018) → Quantum Mechanics.

2 characteristics: wave(complex)+meas.(discrete spectrum) ↔ Hermitizable A+spectrum of BD.

"Hundred year war in QM": ∃ randomness?

Einstein: "God doesn't roll dice!"

III. Hermitizable differential operators

Let $\boldsymbol{a} = (\boldsymbol{a}_{ij})_{i,j=1}^{d}$, $\boldsymbol{b} = (\boldsymbol{b}_i)_{i=1}^{d}$ and $\boldsymbol{c}$ are complex but $\boldsymbol{V}$ is real on $\mathbb{R}^d$. Define $\mathrm{d}\boldsymbol{\mu} = \boldsymbol{e}^{\boldsymbol{V}}\mathrm{d}\boldsymbol{x}$ and $\boldsymbol{L} = \nabla(\boldsymbol{a}\nabla) + \boldsymbol{b}\cdot\nabla - \boldsymbol{c}$.

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

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

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

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

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 $\big(\tilde{L},\ \mathscr{D}(\tilde{L})\big)$:

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

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

New framework, new spectral theory, and new algorithm of QM.

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The end!

Thank you, everybody!

谢谢大家!

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