# Klein-Gordon equation on discrete lattice

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# Outline

1. Klein-Gordon equation

2. Crypto-Hermiticity

3. Discrete model in 1D

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# Klein-Gordon differential equation

- 1926 - Klein, Gordon, Kudar, Fock and de Donder and Van Dungen

$$\left(\Box + \frac{m^2 c^2}{\hbar^2}\right) \psi(t, \vec{x}) = 0$$

d'Alembert operator $\Box = \frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \Delta$

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- Problems
  - Negative energies $E = \pm\sqrt{p^2 + m^2}$
  - Extra degree of freedom: we need to know both $\psi$ and $\partial_t \psi$ at $t = 0$
  - Probability interpretation: conserved quantity $Q$ is indefinite

$$Q = \frac{i}{2m} \int_{\mathbb{R}^3} d\vec{x} (\psi^* \partial_t \psi - \psi \partial_t \psi^*)$$

    therefore cannot be identified with probability

# Indefinite inner product approach

- Indefinite Klein-Gordon inner product

$$\langle\psi|\phi\rangle_{KG} = \frac{i}{2m}\int_{\mathbb{R}^3} d\vec{x}(\psi^*\partial_t\phi - \psi\partial_t\phi^*) , \quad Q = \langle\psi|\psi\rangle_{KG}$$

- Charge density describing a Klein-Gordon field of charged particles

$$\rho_Q = \frac{ie}{2m}(\psi^*\partial_t\psi - \psi\partial_t\psi^*)$$

- Physical space - subspace of positive-energy solutions

# Quasi-Hermitian approach

- Feshbach, Villars 58', Mostafazadeh 03', Znojil 04', Kleefeld 06' etc.
- Let $c = \hbar = 1$

$$(i\partial_t)^2\psi = (-\Delta + m^2)\psi$$

- $K = -\Delta + m^2$

$$(i\partial_t)^2\psi = K\psi$$

- Denote

$$\Psi = \begin{pmatrix} \Psi^{(1)} \\ \Psi^{(2)} \end{pmatrix} , \quad H = \begin{pmatrix} 0 & K \\ 1 & 0 \end{pmatrix}$$

$$\Psi^{(1)} = i\partial_t\psi , \quad \Psi^{(2)} = \psi$$

**Schrödinger form**

$$i\partial_t\Psi = H\Psi$$

# Mostafazadeh 03'-06'

- Defined a positive-definite, relativistically invariant and conserved inner product on the solution space of KG equation

$$\langle\psi|\phi\rangle_{AM} = \frac{\kappa}{2\mu}\left[\langle\psi|K^{1/2}|\phi\rangle + \langle\partial_t\psi|K^{-1/2}|\partial_t\phi\rangle + ia(\langle\psi|\partial_t\phi\rangle - \langle\partial_t\psi|\phi\rangle)\right]$$

where $\mu = \frac{mc}{\hbar}$, $a \in (-1,1)$, $\kappa \in \mathbb{R}^+$

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## Relationship between inner products

Two Hilbert spaces $\mathcal{H}^{(F)} = (V, \langle\cdot|\cdot\rangle)$, $\mathcal{H}^{(S)} = (V, \langle\langle\cdot|\cdot\rangle)$

$$\langle\langle\varphi|\psi\rangle = \langle\varphi|\Theta|\psi\rangle \ .$$

$\Theta$ ... *Metric operator* = Hermitian, positive definite, bounded, bounded inverse

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## Crypto-Hermitian operators

Bounded linear operator $H : \mathcal{H} \mapsto \mathcal{H}$ is called *crypto-Hermitian* if and only if there exists metric operator $\Theta$ defining inner product, i.e. representation space $\mathcal{H}^{(S)}$, under which $H$ is Hermitian.

# Properties

- Satisfy Dieudonné equation

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- Similar to Hermitian operators

$$h = \Omega H \Omega^{-1} = h^\dagger \ ,$$

where $\Omega$ is an invertible similarity operator, often called the *Dyson's map*, satisfying

$$\Theta = \Omega^\dagger \Omega \ .$$

$h$ acts in its own "physical" Hilbert space $\mathcal{H}^{(P)}$

# Three Hilbert space formulation of QM - Znojil 09'

| Hilbert space | ket | bra | inner product |
|---|---|---|---|
| $\mathcal{H}^{(F)}$ | $\vert\psi\rangle$ | $\langle\psi\vert$ | $\langle\psi\vert\psi\rangle$ |
| $\mathcal{H}^{(S)}$ | $\vert\psi\rangle$ | $\langle\langle\psi\vert = \langle\psi\vert\Theta$ | $\langle\langle\psi\vert\psi\rangle = \langle\psi\vert\Theta\vert\psi\rangle$ |
| $\mathcal{H}^{(P)}$ | $\vert\psi\succ = \Omega\vert\psi\rangle$ | $\prec\psi\vert = \langle\psi\vert\Omega^\dagger$ | $\prec\psi\vert\psi\succ = \langle\psi\vert\Theta\vert\psi\rangle$ |

Table : Three-Hilbert-space formulation notation

# Outline

# Finding metric for KG equation

- KG equation in Schrödinger form

$$i\partial_t \Psi(t,x) = H\Psi(t,x)$$

- Non-Hermitian Hamiltonian

$$H = \begin{pmatrix} 0 & K \\ 1 & 0 \end{pmatrix} \,, \quad K = -\Delta + m^2$$

- Dieudonné equation

$$H^\dagger \Theta = \Theta H$$

# Finite difference method

- Discretization of the spatial coordinate

$$x_k = kh \ , \quad k = 0, \pm 1, \pm 2 \dots$$

- Laplacian in 1D can be expressed as

$$\Delta\psi(x_k) = \frac{\partial^2\psi}{\partial x^2}(x_k) \approx -\frac{\psi(x_{k+1}) - 2\psi(x_k) + \psi(x_{k-1})}{h^2}$$

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- Laplace operator approximated as discrete matrix $n \times n$ acting on $\mathbb{R}^n$

$$-\Delta^{(n)} = \frac{1}{h^2}\begin{pmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & -1 & 2 & \ddots & \\ & & \ddots & \ddots & -1 \\ & & & -1 & 2 \end{pmatrix}$$

# Discrete model of 1D KG equation

- Operator $K$ in discrete approximation has a form of tridiagonal Toëplitz matrix $n \times n$

$$K = \begin{pmatrix} z & -1 & \cdots & 0 \\ -1 & z & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & -1 & z \end{pmatrix}$$

where $z = 2 + m^2$, $h = 1$

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- $K$ is similar to a diagonal matrix $n \times n$

$$\widetilde{K} = \begin{pmatrix} a_1 & 0 & \cdots & 0 \\ 0 & a_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & a_n \end{pmatrix}$$

where $a_k = 2 + m^2 + 2cos\left(\frac{k\pi}{n+1}\right)$, $k = 1, 2 \ldots n$

# Family of metrics

- $H = \begin{pmatrix} 0 & \tilde{K} \\ I & 0 \end{pmatrix}$ , $H^\dagger \Theta = \Theta H$

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- $H = \begin{pmatrix} 0 & \tilde{K} \\ I & 0 \end{pmatrix} \ , \quad H^\dagger \Theta = \Theta H$
- Metric depending on parameters $\alpha = (\alpha_1, \ldots, \alpha_n)$, $\beta = (\beta_1, \ldots, \beta_n)$

$$\Theta(\alpha, \beta) = \begin{pmatrix} \alpha_1 & \cdots & 0 & \beta_1 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & \alpha_n & 0 & \cdots & \beta_n \\ \beta_1 & \cdots & 0 & a_1\alpha_1 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & \beta_n & 0 & \cdots & a_n\alpha_n \end{pmatrix}$$

- Conditions on $2n$ real parameters $\alpha_i$, $\beta_i$

$$\alpha_i > 0 \ , \quad a_i\alpha_i^2 > \beta_i^2 \ , \quad i = 1, 2, \ldots, n$$

# Construction of $\mathcal{H}^{(S)} = (\mathbb{R}^{2n}, \langle\langle\cdot|\cdot\rangle)$

- New positive definite inner product

$$\langle\langle\psi|\varphi\rangle = \langle\psi|\Theta(\alpha,\beta)|\phi\rangle = \sum_{i=1}^{n} \alpha_i\psi_i\varphi_i +$$

$$+ \sum_{i=1}^{n} \beta_i(\psi_i\varphi_{n+i} + \psi_{n+i}\varphi_i) + \sum_{i=1}^{n} a_i\alpha_i\psi_{n+i}\varphi_{n+i}$$

where $\psi = (\psi_1, \psi_2, \ldots \psi_{2n})^T$, $\varphi = (\varphi_1, \varphi_2 \ldots, \varphi_{2n})^T$ are real vectors

# Hamiltonian in $\mathcal{H}^{(P)} = (\mathbb{R}^{2n}, \langle\cdot|\cdot\rangle)$ I

- Dyson's map $\Omega$, $\Theta = \Omega^\dagger\Omega$

$$\Omega(\alpha,\beta) = \begin{pmatrix} \sqrt{\alpha_1} & \cdots & 0 & \frac{\beta_1}{\sqrt{\alpha_1}} & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & \sqrt{\alpha_n} & 0 & \cdots & \frac{\beta_n}{\sqrt{\alpha_n}} \\ 0 & \cdots & 0 & \sqrt{\frac{a_1\alpha_1^2-\beta_1^2}{\alpha_1}} & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 0 & 0 & \cdots & \sqrt{\frac{a_n\alpha_n^2-\beta_n^2}{\alpha_n}} \end{pmatrix}$$

# Hamiltonian in $\mathcal{H}^{(P)} = (\mathbb{R}^{2n}, \langle\cdot|\cdot\rangle)$ II

- Hermitian Hamiltonian $h = \Omega H \Omega^{-1} = h^\dagger$, acting in $\mathcal{H}^{(P)}$, isospectral with original Hamiltonian $H$.

$$h(\alpha,\beta) = \begin{pmatrix} \frac{\beta_1}{\alpha_1} & \cdots & 0 & \frac{\sqrt{a_1\alpha_1^2-\beta_1^2}}{\alpha_1} & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & \frac{\beta_n}{\alpha_n} & 0 & \cdots & \frac{\sqrt{a_n\alpha_n^2-\beta_n^2}}{\alpha_n} \\ \frac{\sqrt{a_1\alpha_1^2-\beta_1^2}}{\alpha_1} & \cdots & 0 & -\frac{\beta_1}{\alpha_1} & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & \frac{\sqrt{a_n\alpha_n^2-\beta_n^2}}{\alpha_n} & 0 & \cdots & -\frac{\beta_n}{\alpha_n} \end{pmatrix}$$

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