Positivity preservation of the free Dirac equation

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MTA-ELTE Theoretical Physics Research Group

Outline

1. Introduction
   - Path integrals and simulation
   - Checkerboard model
   - Persistent random walk in $1+1$ dimensions
   - Higher dimensional walks
2. Positivity preservation of the Dirac equation
   - The equation
   - Positivity preservation and Bochner's theorem
   - Main result and outline of its proof
3. Conlusion

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Feynman's path integral

HUNGARIAN ACADEMY OF SCIENCES

Consider the one-particle time dependent Schrödinger equation:

$$\mathrm{i}\hbar\partial_t \psi(\boldsymbol{x},t) = \left(-(\hbar^2/2m)\Delta + V(\boldsymbol{x},t)\right)\psi(\boldsymbol{x},t)$$

Feynman's deep insight:

$$K(\boldsymbol{x}_2,t_2;\boldsymbol{x}_1,t_1) = \int_{\boldsymbol{q}(t_{1,2})=\boldsymbol{x}_{1,2}} \mathscr{D}\boldsymbol{q}(t)\exp\left(\frac{\mathrm{i}}{\hbar}\int_0^T L(\boldsymbol{q},\dot{\boldsymbol{q}},t)\mathrm{d}t\right)$$

- Extremely powerful tool for quantizing relativistic field theories and
- by a clever sampling of the paths, enables estimation of the propagator.

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Feynman-Kac theorem

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Inspired by the work of Feynman, Kac proved that the parabolic system

$$\partial_t u(x,t) - \frac{\sigma^2}{2}\partial_x^2 u(x,t) - V(x,t)u(x,t) = 0,$$

with $V(x,t)$, σ^2 and the terminal condition $u(x,T) = v(x)$ are given, can be solved by computing the conditional expectation

$$u(x,t) = \mathbb{E}\left[e^{-\int_t^T V(X_\tau,\tau)\,\mathrm{d}\tau} v(X_T)\middle| X_t = x\right]$$

on the space of sample paths of the process $\mathrm{d}X_t = \sigma dW$.

Allows the estimation of $u(x,t)$ by simulation of a Wiener process and calculation of $\int_t^T V(X_\tau,\tau)\mathrm{d}\tau$.

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The checkerboard model

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How can we find a path integral representation of the time evolution of a spin$-1/2$ particle described by the massive Dirac equation?

$$(\mathrm{i}\hbar\gamma^{\mu}\partial_{\mu} - mc)\psi = 0$$

Feynman's idea:

- introduce an inner state based on some finite memory,
- estimate the propagator on discrete spacetime by assigning appropriate complex phases to paths of the spacetime lattice,
- take the formal continuum limit.

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In $1+1$ dimensions:

- assign the inner state $\omega(t) = +1$ (-1) to the particle at time t if it has a positive (negative) instantaneous velocity
- in the next time step the particle moves form the current position $x(t) \in \mathbb{Z}$ to $x(t+1) = x(t) + \omega(t)$, but when it arrives to the desired position, it can switch its inner state
- denote the space of admissable spacetime trajectories connecting l to k in T steps starting at the inner state ω and ending in the inner state τ by $\mathscr{P}_{l\to k}^{\omega\to\tau}(T)$
- if $P \in \mathscr{P}_{l\to k}^{\omega\to\tau}(T)$, denote the number of reversals by $R(P)$

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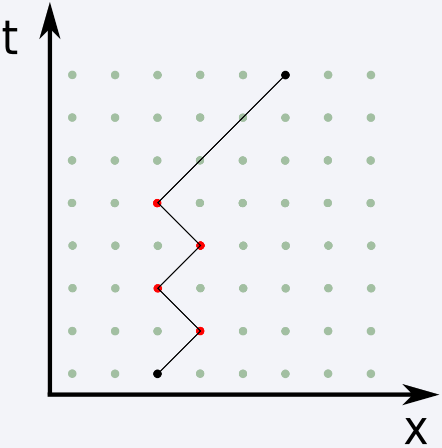

The checkerboard model

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Feynman's proposal is

Checkerboard propagator

$$K_{\tau\omega}(k\Delta x, l\Delta x, T\Delta t) \approx \sum_{P \in \mathscr{P}_{l\to k}^{\omega\to\tau}(T)} \left(\mathrm{i}\frac{mc^2}{\hbar}\Delta t \right)^{R(P)}$$

Writing down a finite difference equation for the r.h.s. in order to express its value corresponding to $T+1$ and applying the scaling limit $\Delta x \to 0$ and $\Delta t \to 0$ such that $\Delta x/\Delta t \to c$. Results in the $1+1$ dimensional Dirac equation for the propagator in the Weyl representation.

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To sum up the result with Feynman's own words:

Feynman's Nobel Lecture (extract)

(...) Another problem on which I struggled very hard, was to represent relativistic electrons with this new quantum mechanics. (...) I was very much encouraged by the fact that in one space dimension, I did find a way of giving an amplitude to every path by limiting myself to paths, which only went back and forth at the speed of light. (...)

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Persistent random walk

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Can we translate the checkerboard model to the language of the stochastic processes also?

A particle has two internal states $+$ and $-$. If it is in the $+$ $(-)$ state, it moves to the right (left) with Δx in time Δt, until it changes its internal state. The probability of such a transition is $\lambda\Delta t$. The resulting Kolmogorov forward equation is

$$p_{\pm}(x,t+\Delta t) = (1-\lambda\Delta t)p_{\pm}(x\mp\Delta x,t) + \lambda\Delta t p_{\pm}(x\pm\Delta x,t)$$

The $\Delta x \to 0$, $\Delta t \to 0$, $\Delta x/\Delta t \to c$ (ballistic) limit is

Dirac equation with real coefficients?

$$\partial_t p = \lambda(\sigma_1 - \mathbb{1}_2)p - c\sigma_3\partial_x p$$

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The walk and the Dirac equation

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Relation to the Dirac equation with complex coefficients:

Let $\lambda \mapsto mc^2/(\mathrm{i}\hbar)$ and introduce $\psi(x,t) = \mathrm{e}^{\lambda t}\sigma_1 p(x,t)$, then

$$\mathrm{i}\hbar(\sigma_1 \partial_t + c\varepsilon \partial_x)\psi = mc^2 \psi,$$

where $\varepsilon = \mathrm{i}^{-1}\sigma_2$.

Since σ_1 and ε generate $C\ell_{1,1}(\mathbb{R})$ and the chiral projections $P_L = \frac{1}{2}(1-\sigma_1\varepsilon)$, $P_R = \frac{1}{2}(1+\sigma_1\varepsilon)$ are diagonal, we see that the previous equation is the massive Dirac equation in $1+1$ dimensions in the Weyl representation.

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The checkerboard model in $1 < d$

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What is the situation in higher dimensions?

Feynman's Nobel Lecture (extract)

(...) I dreamed that if I were clever, I would find a formula for the amplitude of a path that was beautiful and simple for three dimensions of space and one of time, which would be equivalent to the Dirac equation, and for which the four components, matrices, and all those other mathematical funny things would come out as a simple consequence - I have never succeeded in that either. But, I did want to mention some of the unsuccessful things on which I spent almost as much effort, as on the things that did work.

The $d=2$ persistent walk

HUNGARIAN ACADEMY OF SCIENCES

In $d=2$,

- we assign the inner states $++$, $+-$, $-+$ and $--$ to the particle with a transition matrix Q between them
- write down the forward Kolmogorov equation
- take the $\Delta t \to 0$; $\Delta x, \Delta y \to 0$; $\Delta x/\Delta t, \Delta y/\Delta t \to c$ limit.

What we get for the time evolution of the probability is

$$\partial_t p = Lp - ce_1 \partial_x p - ce_2 \partial_y p,$$

where L is the infinitesimal generator of the Markov process with transition matrix Q and

$$e_1 = \mathbb{1}_2 \oplus (-\mathbb{1}_2) \qquad e_2 = \sigma_3 \oplus \sigma_3$$

Apparently not the Dirac equation.

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An alternative strategy

HUNGARIAN ACADEMY OF SCIENCES

Instead of following the instructions

- define a process on the lattice then,
- take the continuum limit

try the following

- choose a representation of the Clifford algebra
- discretize the Dirac equation
- check whether it can define a stochastic process or not

To show a concrete example, take the representation of $C\ell_{3,0}(\mathbb{R})$

$$e_0 = \begin{pmatrix} 0 & \mathbb{1}_2 \\ \mathbb{1}_2 & 0 \end{pmatrix} \quad e_1 = \begin{pmatrix} 0 & -\varepsilon \\ \varepsilon & 0 \end{pmatrix} \quad e_2 = \begin{pmatrix} \mathbb{1}_2 & 0 \\ 0 & -\mathbb{1}_2 \end{pmatrix}$$

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The equation is

$$\partial_t p = \lambda e_0 p - \alpha p - c\beta_1 e_1 \partial_x p - c\beta_2 e_2 \partial_y p$$

with constants λ, α, β_1, β_2 and c. By discretization we can obtain

$$p_1(x,y,t+\Delta t) = q_{11,1}p_1(x,y,t) + q_{11,2}p_1(x,y-\Delta y,t) + q_{13}p_3(x,y,t) + q_{14,1}p_4(x-\Delta x,y+\Delta y,t) + q_{14,2}p_4(x,y,t)$$

with

$$q_{11,1} = 1 - \alpha\Delta t - \frac{\beta_2 c}{\Delta x}\Delta t \quad q_{11,2} = \frac{\beta_2 c}{\Delta x}\Delta t \quad q_{13} = \lambda\Delta t$$

$$q_{14,1} = \frac{\beta_1 c}{\Delta x}\Delta t \quad q_{14,2} = -\frac{\beta_1 c}{\Delta x}\Delta t$$

which clearly cannot define a discrete time stochastic process.

An alternative strategy

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- Path integrals and simulation
- Checkerboard model
- Persistent random walk in $1+1$ dimensions
- Higher dimensional walks

2 Positivity preservation of the Dirac equation
- The equation
- Positivity preservation and Bochner's theorem
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3 Conlusion

The Dirac equation

- The dimensionless Dirac equation with real coefficients:

$$\sum_{\mu=0}^{d} \gamma^{\mu} \partial_{\mu} \psi = \psi,$$

with $\{\gamma^{\mu}, \gamma^{\nu}\} = 2\eta^{\mu\nu} \mathbb{1}_S$ and each γ^{μ} is $S \times S$ and hermitian matrices

- Defining $p(t) = e^{-\alpha t}\gamma^0 \psi(t)$

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Positivity preservation

Definition

We say that

$$\partial_t p = -\alpha p + e_0 p - \sum_{\mu=1}^{d} e_\mu \partial_\mu p,$$

preserves positivity if for all $0 < t$

$$\sum_{q=1}^{S} \int_{\mathbb{R}^d} p_q(\mathbf{x},t) d^d\mathbf{x} = 1 \qquad 0 \leq p(\mathbf{x},t)$$

provided that normalization and non-negativity holds at $t = 0$.

How to prove?

The spatial Fourier transform of $p(t)$ has a much more simple evolution:

$$\partial_t \Phi[p(t)](\boldsymbol{k}) = -\alpha \Phi[p(t)](\boldsymbol{k}) + e_0 \Phi[p(t)](\boldsymbol{k}) - \mathrm{i} \sum_{\mu=1}^{d} k_\mu e_\mu \Phi[p(t)](\boldsymbol{k})$$

But the direct accessability of non-negativity is lost when $\Phi[p(t)]$ is calculated.

What we need is a characterization of Fourier transforms of non-negative functions.

Is there anything such like that?

The answer is - fortunately - yes: Bochner's theorem.

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The function $\Phi : \mathbb{R}^d \to \mathbb{C}$ is positive definite if for all finite subsets $\Lambda = \{\boldsymbol{k}_1, \ldots, \boldsymbol{k}_N\} \subset \mathbb{R}^d$ the $N \times N$ matrix $F^{(\Lambda)}$ defined by $F^{(\Lambda)}_{ab} := \Phi(\mathbf{k}_a - \mathbf{k}_b)$ is positive definite.

Theorem (Bochner)

The function $\Phi : \mathbb{R}^d \to \mathbb{C}$ is a characteristic function of a probability measure over $\mathbb{R}^d$ if and only if

1. *Φ is continuous,*
2. *Φ is positive definite,*
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Example

The diffusion equation

$$\partial_t p = \Delta p$$

preserves positivity in all dimensions.

The time evolution of the Fourier transform

$$\partial_t \Phi[p(t)](\boldsymbol{k}) = -\boldsymbol{k}^2 \Phi[p(t)]$$

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If $\zeta \in \mathbb{C}^N$ is an arbitrary non-zero vector, then we have to show:

$$0 < (\zeta, F^{(\Lambda)}(t)\zeta)$$

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Which can be shown by the application of the Hubbard-Stratonovich transformation:

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Usually, showing the positive definiteness of a function is an awkward task, but showing the possible breakdown of the conditions can be much simpler

Test cases:

- $|\Lambda| = 1$ we have $0 < \Phi(\mathbf{0}) = \varphi(\mathbf{0})$
- $|\Lambda| = 2$, say $\Lambda = \{\boldsymbol{K}, \boldsymbol{K}+\boldsymbol{k},\}$ and we test on $\mathbf{1}_2 = (1,1)^T$:

$$0 < \varphi(\mathbf{0}) + \varphi(\boldsymbol{k})$$

It turns out that the examination of two conditions above are enough to prove the main result.

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Result

Theorem

The massive free Dirac equation with real coefficients

$$\partial_t p = -\alpha p + e_0 p - \sum_{\mu=1}^{d} e_\mu \partial_\mu p,$$

preserves positivity for all $0 \leq t$ *if and only if*

1. $d = 1$,
2. *there is an integer* $0 < m$ *and a permutation matrix* Π *such that*
$$\Pi e_0 \Pi^{-1} = \sigma_1^{\oplus m} \qquad \Pi e_1 \Pi^{-1} = \sigma_3^{\oplus m},$$
3. $\alpha = 1$.

Proof in the forward direction

There are two main cases depending on whether e_0 is irreducible or not.

- When e_0 is irreducible the examination of the time evolution of
$$\varphi(\mathbf{0},t)=\int_{\mathbb{R}^d} p(\mathbf{x},t)\mathrm{d}^d\boldsymbol{x}$$
and some linear algebra is enough to prove that $S=2$, so $d=1$ such that $e_0=\sigma_1$, $e_1=\pm\sigma_3$ and $\alpha=1$.
- When e_0 is reducible the examination of the time evolution of $\varphi(\mathbf{0},t)$ leads only to the conclusion $\Pi e_0 \Pi^{-1}=\sigma_1^{\oplus m}$ with some $1<m$ and permutation matrix Π. Then, the close examination of the second condition $0<\varphi(\mathbf{0},t)+\varphi(\boldsymbol{k},t)$ leads to the desired result.

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Proof in the backward direction

HUNGARIAN ACADEMY OF SCIENCES

It is enough to consider only the $m = 1$ case, when the equation has the form

$$\partial_t p = -p + \sigma_1 p - \sigma_3 \partial_x p$$

which has the formal solution

$$p(t) = \exp\left(t(-\mathbb{1}_2 + \sigma_1) - t\sigma_3\partial_x\right) p(0)$$

Without dwelling on the technical details, the exponential on the r.h.s can be approximated with the Lie-Trotter-Kato product formula:

$$\lim_{N\to\infty} \left(\exp(tN^{-1}(-\mathbb{1}_2 + \sigma_1))\exp(-tN^{-1}\sigma_3\partial_x)\right)^N$$

Since all the factors of these products preserves positivity, then must so the original equation.

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At last but not least: my motivation

HUNGARIAN ACADEMY OF SCIENCES

Given a representation of $C\ell_{d+1,0}(\mathbb{R})$, it is remarkable that every hermitian generator is unitary and also hermitian.

Consider again the Dirac equation with complex coefficients. The dimension of the spinor is S.

$$\partial_t \psi = \frac{mc^2}{i\hbar} e_0 \psi - c \sum_{\mu=1}^{d} e_\mu \partial_\mu \psi$$

Let U_μ be unitary matrices that intertwine between e_μ and $\sigma_3^{\oplus S/2}$, i.e. $e_\mu = U_\mu \sigma_3^{\oplus S/2} U_\mu^*$.

At last but not least: my motivation

Application of the Lie-Trotter-Kato product formula gives

$$\psi(t+\Delta t) \approx U_0 e^{-i\frac{mc^2\Delta t}{\hbar}e_0} U_0^* U_1 e^{-c\Delta t\sigma_3\partial_1} U_1^* \cdots U_d e^{-c\Delta t\sigma_3\partial_d} U_d^* \psi(t).$$

All the terms in the product are unitary.

Furthermore, it describes a unitary Quantum Walk with an S dimensional coin space:

- the operators U_μ and $\exp(-i\frac{mc^2\Delta t}{\hbar}e_0)$ belongs to $U(S)$ and act only on the coin space
- the operators $\exp(-c\Delta t\sigma_3\partial_\mu)$ define spin-dependent shifts.

This was a particular example of a new concept of simulation: *the unitary one*.

At last but not least: my motivation

Lamata, Lucas, et al. *Dirac equation and quantum relativistic effects in a single trapped ion*. PRL **98** 253005 (2007)
Massive Dirac equation in the Dirac representation

$$i\hbar\partial_t\psi = -i\hbar c\sigma_1\partial_x\psi + mc^2\sigma_z\psi$$

- Confine an ion in a linear Paul trap
- Two internal levels are coupled by a resonant laser field: $\hbar\Omega \leftrightarrow mc^2$
- Red-sideband and blue-sideband Jaynes-Cummings interaction can result in the partial shift of the CM and (de-)excitation $2\eta\Delta_x\tilde{\Omega}_x \leftrightarrow c$, $\Delta_x = \sqrt{\hbar/2M\nu_x}$

At last but not least: my motivation

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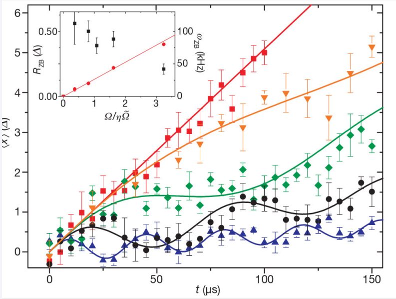
Gerritsma, R., Kirchmair, G., Zähringer, F., Solano, E., Blatt, R. and Roos, C.F., 2010. *Quantum simulation of the Dirac equation.* Nature, **463**, pp. 68-71.

- Ca^+ ion with internal states $|S_{1/2}, m_J = 1/2\rangle$ and $|D_{5/2}, m_J = 3/2\rangle$
- initial state: nearly zero momentum and $|S_{1/2}, m_J = 1/2\rangle$.



Conclusion

1. The Dirac equation cannot be simulated directly by a $\{1,\ldots,S\} \times \mathbb{R}^d$ valued stochastic process
2. Quantum simulators can compute the solutions of the Dirac equation
3. The Dirac equation is not the only example of the super capabilities of quantum simulators: recent post on arXiv (1609.04408) claims that there are stochastic processes such that the memory usage of the corresponding quantum simulation with precision 2^{-n} remains bounded when $n \to \infty$.

Thank You for your attention!