Feynman propagators for tight-binding regular lattices

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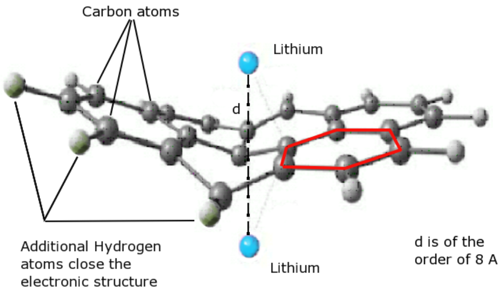
Outline

Introduction

Graphene



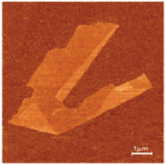


Fig. 2 Atomic force microscopy image of a graphene crystal on top of an oxidized Si substrate. Folding of the flake can be seen. The measured thickness of graphene corresponds to the interlayer distance in graphite. Scale bar = 1 μm. (Reprinted with permission from[13]. © 2005 National Academy of Sciences.)

Comparison

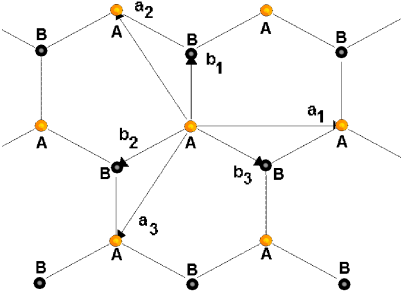
Relativistic Quantum Mechanics

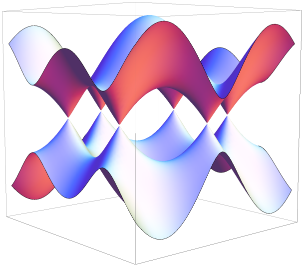
- $\boldsymbol{\sigma}$: $*$-spin, big and small components of spinors.
- c: Speed of light.
- mc^2: Rest mass of the particle.

Hexagonal and dimeric lattices

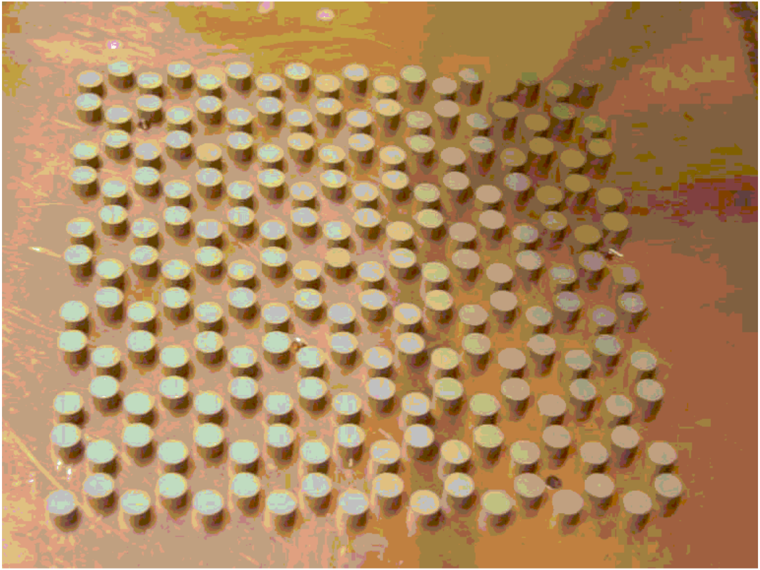
- $\boldsymbol{\sigma}$: spin $\pm$ for sublattices A and B.
- $\Delta \sim c$: Hopping energy or Fermi velocity (nearest neighbors).
- $E_2 - E_1 \sim mc^2$: Spectral gap (semiconductors).

Graphene

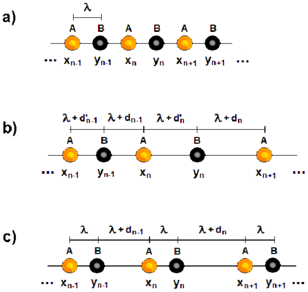


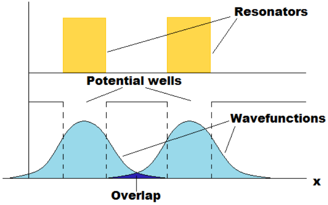


Microwave resonators



Linear chains (polymers)





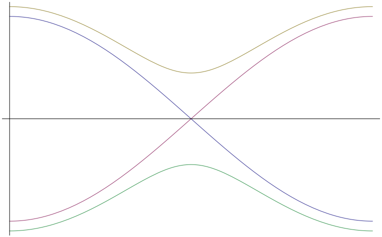
- $1+1$ Dirac equation.
- $1+1$ Dirac oscillator.
- Spin-orbit terms (gyroscope).

Spectrum

Expansion around $k = \pi/2$

$$E_k = E_0 \pm \sqrt{\Delta^2 \cos^2 k + (\delta E)^2} \quad (1)$$

$$E_k^{rel} = \pm\sqrt{c^2 p^2 + m^2 c^4} \quad (2)$$



Discrete propagators in 1d

Space discretization

Introducing the constants Δ (with units of energy $\times$ length^2) and a (lattice spacing), the Schrödinger dynamical problem is described by the equation

$$-\frac{\Delta}{2a^2}\left[\phi_{n+1}(\tau) - 2\phi_n(\tau) + \phi_{n-1}(\tau)\right] = i\hbar\frac{\partial \phi_n(\tau)}{\partial \tau} \qquad (3)$$

or, more concisely

$$-\frac{1}{2}\left[\psi_{n+1}(t) + \psi_{n-1}(t)\right] = i\frac{\partial \psi_n(t)}{\partial t}, \qquad (4)$$

Spectral decomposition

Tight-binding homogeneous models are solved by Bloch waves, therefore

$$K(n, m; t) = \int_0^{2\pi} dk \quad e^{i(n-m)k} e^{it \cos k} \tag{5}$$

It is also possible to describe the system with canonical variables

$$P = \frac{\sin(ap)}{a}, \qquad X = \frac{1}{2}\{\sec(ap), x\} \tag{6}$$

Properties

Bessel representation

$$K(n, m; t) = \theta(t) i^{n-m} J_{n-m}(t), \tag{7}$$

Green's function

$$\frac{1}{2}\left[K(n+1, m; t) + K(n-1, m; t)\right] - i\frac{\partial K(n, m; t)}{\partial t} = -i\delta(t)\delta_{n,m}. \tag{8}$$

Continuous limit $n - n' = a(x - x')$

$$K(n, n'; t) \to \left[ae^{it}\right] \times \sqrt{\frac{m}{2\pi i\hbar\tau}} \exp\left(i\frac{m(x-x')^2}{2\hbar\tau}\right) \tag{9}$$

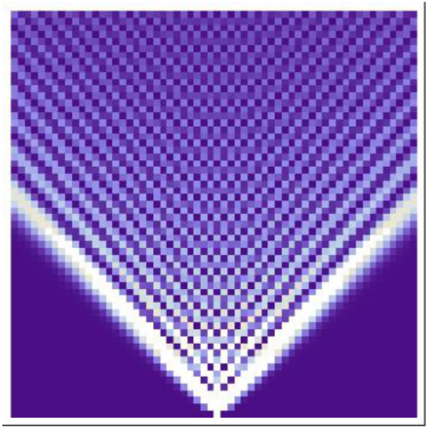


Figure 2. Probability density in the plane n (abscissa) and t (ordinate) of a point-like source. We can see an expansion of the density at a constant velocity (set as unity). The expansion is accompanied by oscillations between the fronts $n \pm t$. These features cannot be found in the propagation of a point-like source in continuous variables.

Diffractive effects

Moshinsky shutter in discrete space = Diffraction in periodic media

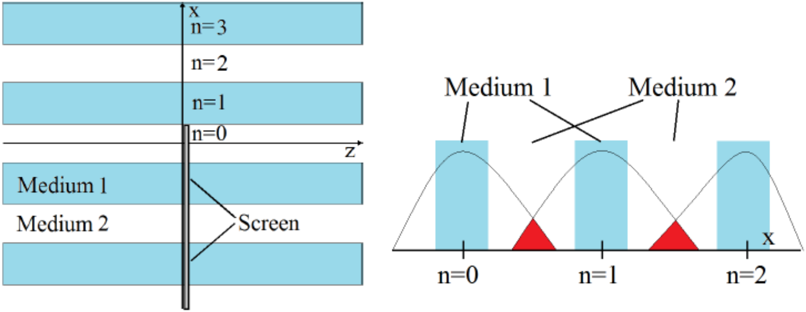
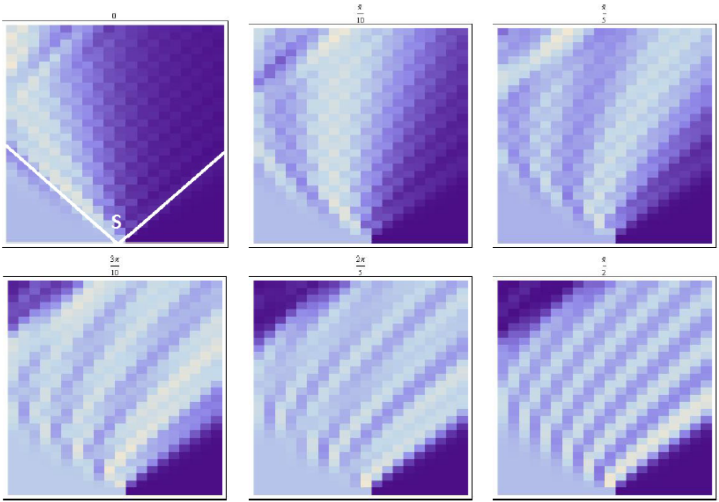
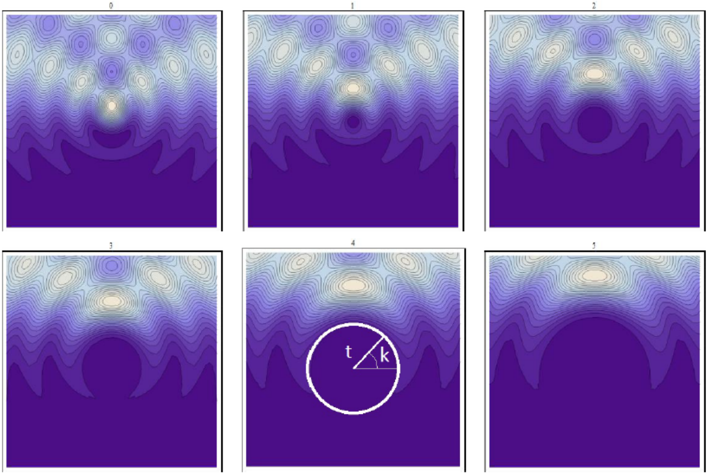


Figure 5. Left panel: A periodic background realized through the alternation of two materials (solid state) or two potentials (quantum case). A screen blocks a wave propagating along z. Right panel: The two media represented as potential barriers along the x variable. A sketch of the profile for localized states is shown, with coloured areas indicating the overlaps and nearest-neighbour interactions.

Moshinsky shutter in discrete space = Diffraction in periodic media



Moshinsky shutter in discrete space = Diffraction in periodic media



Limits

Relevant limits

In general lattices (1 or 2d) we find the following cases

- 0. Continuous non-relativistic kernel (square lattice and linear chain). In this regime $a \to 0$.
- 1. Gapless limit $\mu \to 0$ (Graphene vs Boron Nitride)
- 2. Strong gap limit $\mu \to \infty$ (time rescaling).
- 3. Klein-Gordon propagator (triangular lattice) $\Delta \to \infty$, x, t near light cones.
- 4. Dirac propagator (hexagonal lattice) $\Delta \to \infty$, x, t near light cones.

Feynman paths

Action and weights

$$K(n,m;t) = \sum_{\text{Paths}} w(t) F[\{\nu\}] \exp\left(i\frac{\pi}{2} S_{N+1,0}\right) \tag{10}$$

$$S_{N+1,0} = \sum_{j=0}^{N} |\nu_{j+1} - \nu_j| \tag{11}$$

$$W = \left(\frac{t}{2(N+1)}\right)^{S_{N+1,0}} \times \prod_{j=0}^{N} \frac{1}{(S_{j+1,j})!} \equiv w(t) \times F[\{\nu\}]. \tag{12}$$

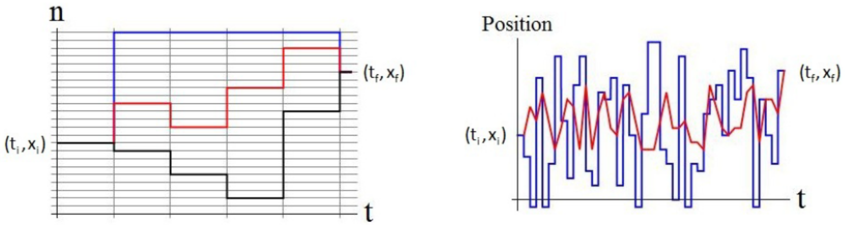


Figure 1. Left panel: Three discontinuous paths of equal length joining $(t_i, x_i) - (t_f, x_f)$. The blue path contains only one change in direction. Right panel: Comparison of a typical continuous path in Feynman's integrals (Red curve) and a discontinuous trajectory in our path formulation (Blue curve)

Many bodies

Field quantization

For any type of lattice described by $\mathbf{n}, \mathbf{m}$, we have
Bosons:

$$\left[a_{\mathbf{n}}(t), a_{\mathbf{m}}^{\dagger}(t')\right] = K(\mathbf{n}, \mathbf{m}; t - t') \tag{13}$$

Fermions:

$$\{f_{\mathbf{n}}(t), f_{\mathbf{m}}^{\dagger}(t')\} = K(\mathbf{n}, \mathbf{m}; t - t') \tag{14}$$

with the possibility of finding the evolution of Fock states in closed form

$$\langle N(\mathbf{n}, t = 0) | N(\mathbf{m}, t = t') \rangle = \mathrm{Products\, of\ K's} \tag{15}$$

Summary of propagators

1d and 2d

- (2) $\circ -$: Homogeneous chain
- (2) $\circ - \bullet$: Chain with two species
- (4) $\square$: Square lattices with one and two species
- (6) $\triangledown$: Homogeneous triangular lattice
- (3) $\circledast$: Hexagonal lattice with one a two species

Linear chain

Homogeneous chain Hamiltonian

$$H_{\circ -} f_n = E_0 f_n + \Delta(f_{n+1} + f_{n-1}) \tag{16}$$

Propagator

$$K_{\circ -}(n, m; t) = i^{m-n} J_{n-m}(2\Delta t)\, e^{-iE_0 t} \tag{17}$$

Dimer chain Hamiltonian

$$H_{\circ-\bullet} f_n = (E_0 + (-1)^n \mu)\, f_n + \Delta\,(f_{n+1} + f_{n-1}) \tag{18}$$

Propagator

$$\begin{aligned} K_{\circ-\bullet}(n,m;t) &= e^{-iE_0 t}\left[H_{\circ-\bullet} - E_0 + i\frac{\partial}{\partial t}\right] G(n,m;t) \\ G(n,m;t) &= \begin{cases} K_{\circ-}\left(n,m;\frac{2i\Delta^2}{\mu}\frac{\partial}{\partial\mu}\right)\frac{\cos\left(t\sqrt{\mu^2+2\Delta^2}\right)}{\sqrt{\mu^2+2\Delta^2}} & \text{for } n-m \text{ even} \\ 0 & \text{for } n-m \text{ odd} \end{cases} \end{aligned} \tag{19}$$

Spherical wave expansion

$$G(n,m;t) = \begin{cases} -4i\Delta t \sum_{l=0}^{\infty} j_l(\mu_- t) j_l(\mu_+ t) \left[P_l^{\frac{n-m}{2}}(0) \right]^2 & \text{for } n-m \text{ even} \\ 0 & \text{for } n-m \text{ odd} \end{cases} \quad (20$$

where $\mu_\pm \equiv \frac{1}{2}(\sqrt{4\Delta^2+\mu^2} \pm \mu)$.
Descending series in μ

$$\begin{aligned} G(n,m;t) &= \left[\frac{1+(-1)^{n-m}}{4} \right] \\ &\times \left[K_{\circ -}\left(n,m;\frac{2\Delta^2 t}{\sqrt{\mu^2+2\Delta^2}}\right) + K_{\circ -}\left(n,m;\frac{-2\Delta^2 t}{\sqrt{\mu^2+2\Delta^2}}\right) \right] \\ &+ O(\Delta^3/\mu^3). \end{aligned} \quad (21)$$

Square lattice

The hamiltonian for a homogeneous square lattice reads

$$H_{\square} = H^{\mathbf{i}}_{\circ -} + H^{\mathbf{j}}_{\circ -} - E_0 \tag{22}$$

with propagator

$$K_{\square}(\mathbf{A}, \mathbf{A}'; t) = K_{\circ -}(n, n'; t) K_{\circ -}(m, m'; t). \tag{23}$$

This product can be extended to all homogeneous cubic lattices in arbitrary dimensions. Two species:

$$K_{\square}(\mathbf{A}, \mathbf{A}'; t) = K_{\circ -}(n, n'; t) K_{\circ - \bullet}(m, m'; t). \tag{24}$$

Triangular lattice

Hamiltonian

$$H_{\bigtriangledown} = \Delta \sum_{\mathbf{A}, i=1,\ldots,6} \{|\mathbf{A}\rangle\langle\mathbf{A}+\boldsymbol{\alpha}_i| + |\mathbf{A}+\boldsymbol{\alpha}_i\rangle\langle\mathbf{A}|\} + E_0 \tag{25}$$

Propagator

$$\begin{aligned} K_{\bigtriangledown}(\mathbf{A},\mathbf{A}';t) &= i^{n_1'+n_2'-n_1-n_2} J^{(+)}_{n_1-n_1',n_2-n_2'}(2\Delta t;-i)\, e^{-itE_0} \\ &= I^{(+)}_{n_1-n_1',n_2-n_2'}(2i\Delta t)\, e^{-itE_0} \end{aligned} \tag{26}$$

where $J^{(+)}_{n,m}$ is the two-index Bessel function and $I^{(+)}_{n,m}$ is the modified two-index Bessel function.

$$K_{\bigtriangledown}(\mathbf{A},\mathbf{A}';t) = \sum_{s\in\mathbf{Z}} K_{\circ-}(n_1, n_1'+s;t) K_{\circ-}(n_2, n_2'+s;t) K_{\circ-}(s,0;t) \tag{27}$$

Hexagonal lattice

Hamiltonian

$$H_{\circledast} = \Delta \sum_{\mathbf{A}, i=1,\dots,3} \{|\mathbf{A}\rangle\langle\mathbf{A}+\mathbf{b}_i| + |\mathbf{A}+\mathbf{b}_i\rangle\langle\mathbf{A}|\} + \mu \sum_{\mathbf{A}} \{|\mathbf{A}\rangle\langle\mathbf{A}| + |\mathbf{A}-\mathbf{b}_1\rangle\langle\mathbf{A}+\mathbf{b}_1|\} + E_0, \tag{28}$$

This operator is related to a triangular hamiltonian in the form $(H_{\circledast} - E_0)^2 = \Delta H_{\triangledown} + \mu^2$. For any spinorial function with components $f^{\pm}$ and triangular lattice variables n_1, n_2, we write the action of $H_{\circledast}$ as

$$\begin{aligned} H_{\circledast} f^{+}_{n_1,n_2} &= \Delta \left(f^{-}_{n_1,n_2} + f^{-}_{n_1-1,n_2} + f^{-}_{n_1-1,n_2+1} \right) + (E_0 + \mu) f^{+}_{n_1,n_2} \\ H_{\circledast} f^{-}_{n_1,n_2} &= \Delta \left(f^{+}_{n_1,n_2} + f^{+}_{n_1-1,n_2} + f^{+}_{n_1-1,n_2+1} \right) + (E_0 - \mu) f^{-}_{n_1,n_2} \end{aligned} \tag{29}$$

Propagator: The hexagonal kernel can be written in terms of the triangular propagator (26). We have the 2×2 kernel

$$K_{\circledast}(\mathbf{A}, \mathbf{A}'; t) = e^{-iE_0 t} \left[H_{\circledast} - E_0 + i\frac{\partial}{\partial t} \right] G_{\triangledown}(\mathbf{A}, \mathbf{A}'; t) \tag{30}$$

with the entries of the 2×2 auxiliary $G_{\triangledown}$ given by

$$\begin{aligned} G_{\triangledown}^{+,+}(\mathbf{A}, \mathbf{A}'; t) &= K_{\triangledown}\left(\mathbf{A}, \mathbf{A}'; \frac{2i\Delta^2}{\mu}\frac{\partial}{\partial \mu}\right) \frac{\cos\left(t\sqrt{\mu^2 + 3\Delta^2}\right)}{\sqrt{\mu^2 + 3\Delta^2}} \\ G_{\triangledown}^{+,+}(\mathbf{A}, \mathbf{A}'; t) &= G_{\triangledown}^{-,-}(\mathbf{A}, \mathbf{A}'; t) \\ G_{\triangledown}^{+,-}(n, m; t) &= G_{\triangledown}^{-,+}(n, m; t) = 0. \end{aligned} \tag{31}$$

Conclusion

- We have calculated propagators in discrete variables, apparently for the first time.
- In order to understand such novel objects, we have studied their properties and extended the Feynman path sums to discrete variables.
- We discussed some relevant examples, including the diffraction by edges and the effects emerging from a minimal spacing.
- We established the mathematical form of the solutions and gave a detailed comparison with a problem in two dimensional space in a periodic background.
- A possible realization has been proposed in tight-binding arrays.
- The wide interest in photonic structures suggests applications of our results in this area, as well as solid state physics in time domain.

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Thanks