

Unveiling arithmetic triangular structures in the Kronig–Penney model

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Joint work with

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1. Finite Kronig–Penney model

Transfer matrix and scattering coefficients

2. Powers of the transfer matrix

Coefficient patterns and emerging triangular arrays

3. Combinatorial structure

Closed-form representation via Chebyshev polynomials and combinatorial coefficients

4. Hypercomplex Appell structure

HAGN and the underlying combinatorial identity

5. Conclusions and perspectives

The physical model

- Formulated back in 1931, the **Kronig–Penney model** is a simple quantum-mechanical model for describing *the motion of electrons in a crystalline structure*.
- The central idea is to replace the complicated potential generated by the atoms in a real crystal with a one-dimensional periodic potential, typically represented by a sequence of barriers.
- Despite this idealisation, the model captures a fundamental feature of crystalline materials: the spectrum separates into allowed energy bands and forbidden gaps.
- This band structure is central to the electronic properties of materials and provides the basic physical picture underlying semiconductor devices, from transistors and microprocessors to LEDs and photovoltaic cells.

Mathematical formulation

- We consider a one-dimensional quantum particle with energy $E > 0$ interacting with N equally spaced point barriers:

$$V(x) = \lambda \sum_{n=1}^N \delta(x - nL), \quad \lambda > 0.$$

- The stationary states are governed by the **time-independent Schrödinger equation**

$$-\frac{\hbar^2}{2m} \psi''(x) + \lambda \sum_{n=1}^N \delta(x - nL) \psi(x) = E \psi(x)$$

- This equation together with boundary conditions defines the one-dimensional *scattering problem*.

The piecewise general solution

Since $V(x) = 0$ between consecutive δ -barriers, the Schrödinger equation reduces to the free-particle equation in each region. Thus, the wave function has the form

$$\psi(x) = \begin{cases} A_1 e^{ikx} + B_1 e^{-ikx}, & \text{Region } R_1 : \quad x \leq L, \\ A_n e^{ikx} + B_n e^{-ikx}, & \text{Region } R_n : \quad (n-1)L \leq x \leq nL, \\ A_{N+1} e^{ikx}, & \text{Region } R_{N+1} : \quad x \geq NL, \end{cases}$$

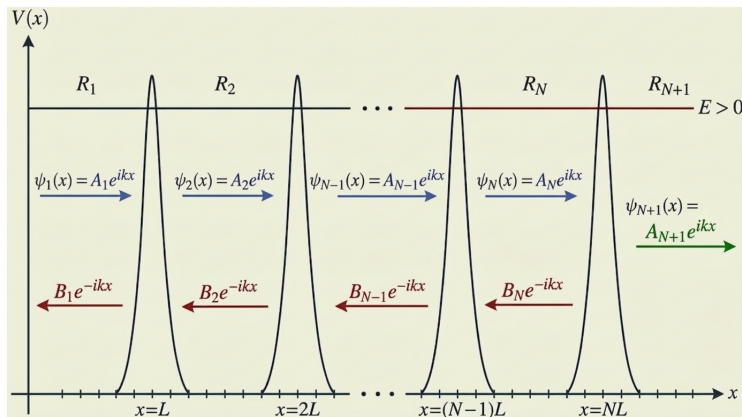
where

$$k = \frac{\sqrt{2mE}}{\hbar}$$

is the wave number.

- A_j and $B_j, j = 1, 2, \dots, N+1$, are the amplitudes of the **right-moving** and **left-moving** waves, respectively.
- In the rightmost region, $B_{N+1} = 0$: since the wave is incident from the left, there is **no incoming wave from the right**.

Wave function in the different regions



Scattering configuration for a particle with energy E traversing an array of N Dirac delta barriers located at $x = L, 2L, \dots, NL$. Each delta potential is represented by a narrow normalized Gaussian function with a width of ϵ , which approximates $\delta(\cdot)$ as $\epsilon \rightarrow 0$.

Matching conditions

- At each barrier $x = nL$, the wave function remains continuous, while its derivative has a finite jump induced by the δ -potential:

$$\psi_R(nL) = \psi_L(nL), \quad \psi'_R(nL) - \psi'_L(nL) = \frac{2m\lambda}{\hbar^2} \psi_L(nL)$$

where the R, L index corresponds to the left and right wave functions with respect to $x = nL$.

- Introducing the parameter $c = (i\hbar^2 k)/(2m\lambda)$, the matching conditions can be written directly in terms of the wave amplitudes:

$$\begin{aligned} A_n e^{iknL} + B_n e^{-iknL} &= A_{n+1} e^{iknL} + B_{n+1} e^{-iknL} \\ (1 + c) A_n e^{iknL} + (1 - c) B_n e^{-iknL} &= c A_{n+1} e^{iknL} - c B_{n+1} e^{-iknL} \end{aligned}$$

Matching conditions in matrix form

For convenience, set

$$K = e^{ikL}.$$

Then, the matching conditions at $x = nL$ take the matrix form

$$\begin{pmatrix} K^n & K^{-n} \\ (1+c)K^n & (1-c)K^{-n} \end{pmatrix} \begin{pmatrix} A_n \\ B_n \end{pmatrix} = \begin{pmatrix} K^n & K^{-n} \\ cK^n & -cK^{-n} \end{pmatrix} \begin{pmatrix} A_{n+1} \\ B_{n+1} \end{pmatrix}.$$

To remove the explicit dependence on n , we introduce the normalized amplitudes

$$\tilde{A}_n = A_n K^n, \quad \tilde{B}_n = B_n K^{-n}.$$

The matching conditions then become

$$\begin{pmatrix} 1 & 1 \\ 1+c & 1-c \end{pmatrix} \begin{pmatrix} \tilde{A}_n \\ \tilde{B}_n \end{pmatrix} = \begin{pmatrix} K^{-1} & K \\ cK^{-1} & -cK \end{pmatrix} \begin{pmatrix} \tilde{A}_{n+1} \\ \tilde{B}_{n+1} \end{pmatrix}$$

Principal transfer matrix

From the previous relation, we obtain

$$\begin{pmatrix} \tilde{A}_n \\ \tilde{B}_n \end{pmatrix} = \frac{1}{2c} T \begin{pmatrix} \tilde{A}_{n+1} \\ \tilde{B}_{n+1} \end{pmatrix},$$

where

$$T = \begin{pmatrix} (2c - 1)K^{-1} & -K \\ K^{-1} & (2c + 1)K \end{pmatrix}.$$

Iterating this relation across the N barriers gives

$$\begin{pmatrix} \tilde{A}_1 \\ \tilde{B}_1 \end{pmatrix} = \frac{1}{(2c)^N} T^N \begin{pmatrix} \tilde{A}_{N+1} \\ 0 \end{pmatrix}.$$

We refer to T^N as the **principal transfer matrix** of the finite array.

Transmission coefficient

From the first row of the transfer-matrix relation,

$$\tilde{A}_1 = \frac{(T^N)_{11}}{(2c)^N} \tilde{A}_{N+1}$$

we obtain

$$A_1 K = \frac{(T^N)_{11}}{(2c)^N} A_{N+1} K^{-N-1}, \quad K = e^{ikL}, \quad c = \frac{i\hbar^2 k}{2m\lambda}.$$

Hence, the **transmission coefficient** is

$$\mathcal{T}_N \equiv \frac{|A_{N+1}|^2}{|A_1|^2} = \left(\frac{\hbar^2 k}{m\lambda} \right)^{2N} \frac{1}{|(\mathbf{T}^N)_{11}|^2}$$

A regular pattern in the entry $(T^N)_{11}$

$$T^N = \begin{pmatrix} \alpha & -K \\ K^{-1} & \beta \end{pmatrix}^N$$

$$\alpha = (2c - 1)K^{-1}$$

$$\beta = (2c + 1)K$$

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Letter

A novel transfer matrix framework for multiple Dirac delta potentials

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N	$(T^N)_{11}$
1	α
2	$\alpha^2 - \boxed{1}$
3	$\alpha^3 - \boxed{(2\alpha + \beta)}$
4	$\alpha^4 - \boxed{(3\alpha^2 + 2\alpha\beta + \beta^2)} + \boxed{1}$
5	$\alpha^5 - \boxed{(4\alpha^3 + 3\alpha^2\beta + 2\alpha\beta^2 + \beta^3)} + \boxed{(3\alpha + 2\beta)}$
6	$\alpha^6 - \boxed{(5\alpha^4 + 4\alpha^3\beta + 3\alpha^2\beta^2 + 2\alpha\beta^3 + \beta^4)} + \boxed{(6\alpha^2 + 6\alpha\beta + 3\beta^2)} - 1$
7	$\alpha^7 - \boxed{(6\alpha^5 + 5\alpha^4\beta + 4\alpha^3\beta^2 + 3\alpha^2\beta^3 + 2\alpha\beta^4 + \beta^5)} + \boxed{(10\alpha^3 + 12\alpha^2\beta + 9\alpha\beta^2 + 4\beta^3)} - (4\alpha + 3\beta)$

Triangular arrays

These coefficients coincide with known integer triangular arrays.

Triangular arrays	OEIS link
$\begin{array}{cccccc} 1 & & & & & \\ 2 & 1 & & & & \\ 3 & 2 & 1 & & & \\ 4 & 3 & 2 & 1 & & \\ 5 & 4 & 3 & 2 & 1 & \\ 6 & 5 & 4 & 3 & 2 & 1 \end{array}$	A004736
$\begin{array}{cccc} 1 & & & \\ 3 & 2 & & \\ 6 & 6 & 3 & \\ 10 & 12 & 9 & 4 \end{array}$	A104633

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Why do these triangular arrays appear in the matrix-power problem?

The Cayley–Hamilton theorem

$$T = \begin{pmatrix} \alpha & -K \\ K^{-1} & \beta \end{pmatrix}, \quad \text{with } \begin{cases} \alpha = (2c - 1)K^{-1} \\ \beta = (2c + 1)K \end{cases}$$

Theorem

Every square matrix satisfies its own characteristic equation.

- For T , the characteristic polynomial is

$$\det(T - \mu I) = \mu^2 - \operatorname{Tr}(T)\mu + \det(T)$$

Since

$$\operatorname{Tr}(T) = \alpha + \beta \quad \det(T) = \alpha\beta + 1$$

$$T^2 - (\alpha + \beta)T + (\alpha\beta + 1)I = O$$

The recurrence relation

- Multiplying the characteristic equation by T^{n-1} , for $n \geq 1$, yields the second-order matrix recurrence

$$T^{n+1} = (\alpha + \beta)T^n - (\alpha\beta + 1)T^{n-1}$$

- Since matrix addition and scalar multiplication act entrywise, each matrix entry satisfies the same recurrence. Defining

$$M_{11}^{(n)} := (T^n)_{11}$$

we obtain

$$M_{11}^{(n+1)} = (\alpha + \beta)M_{11}^{(n)} - (\alpha\beta + 1)M_{11}^{(n-1)}$$

with initial conditions

$$M_{11}^{(0)} = 1, \quad M_{11}^{(1)} = \alpha$$

Mapping to Chebyshev polynomials

- Introduce the rescaling

$$M_{11}^{(n)} = (\alpha\beta + 1)^{n/2} z_n$$

Substituting this expression into the recurrence yields

$$z_{n+1} = 2x z_n - z_{n-1}, \quad x := \frac{\alpha + \beta}{2\sqrt{\alpha\beta + 1}}$$

with initial conditions

$$z_0 = 1, \quad z_1 = \frac{\alpha}{\sqrt{\alpha\beta + 1}}$$

- This is the standard three-term recurrence relation for the *Chebyshev polynomials of the second kind*, U_n .

Determination of the coefficients

- The general solution of the recurrence can be written as a linear combination

$$z_n = \mathbf{c}_1 U_n(x) + \mathbf{c}_2 U_{n-1}(x)$$

- Recalling that the Chebyshev polynomials of the second kind satisfy

$$U_{-1}(x) = 0, \quad U_0(x) = 1, \quad U_1(x) = 2x,$$

using the initial conditions z_0 and z_1 , we obtain

$$z_0 = \mathbf{c}_1 U_0(x) + \mathbf{c}_2 U_{-1}(x) \implies \mathbf{c}_1 = z_0 = 1,$$

$$z_1 = \mathbf{c}_1 U_1(x) + \mathbf{c}_2 U_0(x) \implies \mathbf{c}_2 = z_1 - 2xz_0 = -\frac{\beta}{\sqrt{\alpha\beta + 1}}.$$

Therefore,

$$z_n = U_n(x) - \frac{\beta}{\sqrt{\alpha\beta + 1}} U_{n-1}(x)$$

Chebyshev closed-form for $M_{11}^{(N)}$

Recalling

$$M_{11}^{(n)} = (\alpha\beta + 1)^{n/2} z_n, \quad x = \frac{\alpha + \beta}{2\sqrt{\alpha\beta + 1}}$$

we obtain

$$M_{11}^{(N)} = (\alpha\beta + 1)^{N/2} \left[\frac{\alpha}{\sqrt{\alpha\beta + 1}} U_{N-1}(x) - U_{N-2}(x) \right]$$

- The $(1, 1)$ entry of T^N is expressed entirely in terms of $U_n(x)$.
- **Closed-form expression:** no recursive matrix multiplications are required.

Combinatorial closed-form for $M_{11}^{(N)}$

Using the standard series expansion

$$U_m(x) = \sum_{j=0}^{\lfloor m/2 \rfloor} (-1)^j \binom{m-j}{j} (2x)^{m-2j}$$

substitution of

$$x = \frac{\alpha + \beta}{2\sqrt{\alpha\beta + 1}}$$

and combination of the resulting sums yield the following combinatorial formula

$$M_{11}^{(N)} = \sum_{n=0}^{\lfloor N/2 \rfloor} (-1)^n (\alpha\beta + 1)^n \left[\alpha \binom{N-1-n}{n} (\alpha + \beta)^{N-1-2n} + \binom{N-1-n}{n-1} (\alpha + \beta)^{N-2n} \right]$$

The combinatorial structure behind the triangles

Starting from the generating function

$$G(t) := \sum_{N=0}^{\infty} M_{11}^{(N)} t^N = \frac{1 - \beta t}{1 - (\alpha + \beta)t + (\alpha\beta + 1)t^2}$$

we obtain the following bivariate polynomial expansion, making the powers of α and β explicit:

$$M_{11}^{(N)} = \alpha^N + \sum_{n=1}^{\lfloor N/2 \rfloor} (-1)^n \sum_{s=0}^{N-2n} \binom{N-n-s}{n} \binom{n+s-1}{n-1} \alpha^{N-2n-s} \beta^s$$

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The triangular arrays above naturally emerge from this expansion.

The identity

$$\binom{N-n-s}{n} \binom{n+s-1}{n-1} = \binom{N}{2n} T_s^{N-2n}(2n+1)$$

where $T_s^{N-2n}(2n+1)$ denotes the *Hypercomplex Appell Generated Numbers* (HAGN), was established in [I. Cação, H. R. Malonek, M. I. Falcão, G. Tomaz, *J. Integer Sequences* 26 (2023)].

- The identity links the observed **triangular arrays** to **hypercomplex Appell polynomials**, previously studied in the context of hypergeometric function theory [M. I. Falcão and H. R. Malonek, *Opuscula Math.* 32(4) (2012), 661–673].

Conclusions and perspectives

- ▶ We established a **closed-form representation of $M_{11}^{(N)}$** for finite one-dimensional Kronig–Penney arrays of Dirac delta potentials, providing a rigorous resolution of the open question in [J. Figueroa, I. Gonzalez, D. Salinas-Arizmendi, *Phys. Lett. A*, 555 (2025)].

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- ▶ The explicit representation reveals a rich interplay between quantum scattering, matrix combinatorics, and hypercomplex analysis, with the emergence of characteristic **integer triangular arrays**.

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The triangular structures suggest a deeper connection between scattering theory and hypercomplex analysis.

- L. A., P. A. Grassi, H. R. Malonek, *Arithmetic triangular structures in the transfer-matrix of finite Kronig–Penney models*, **arXiv:2609.08523** (2026).

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