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Quantum Behavior of Substituted-Chrysene Molecular Assemblies

Bipartite Schur-Complement Transfer Anisotropy, Quadratic-to-Linear Stark Switching Across (D, I, T), and Registry-Gated Ballistic Transport

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Abstract

A uniform-hopping model on the 18-vertex chrysene graph connects directional transfer, electric response and registry-dependent transport. The C6–C12 and C3–C9 terminal pairs have first nonzero Schur-complement moments at orders five and seven, respectively, proving inequivalence of their scalar transfer functions. At the gap center their isolated Green-function magnitudes are $1/(2t)$ and $1/(8t)$, giving an exact squared-amplitude ratio of 16; its conductance interpretation requires matched weak contacts and appropriate level alignment. Chiral sublattice symmetry forces two named same-sublattice resolvent entries to vanish at this energy. For the gapped closed-shell reference Hamiltonian, corrected response calculations establish unequal diagonal polarizabilities, with $\alpha^{(0)}_{xx}/\alpha^{(0)}_{yy} \simeq 0.6882$. Inversion-symmetric site potentials on $D = \{6, 12\}$ and $T = \{3, 6, 9, 12\}$ force zero permanent model dipole and an even Stark energy branch. The asymmetric $I = \{3, 6, 12\}$ and mixed-arm Dm cases permit a linear term when their actual electronic dipole is nonzero; geometric locant moments are treated separately. Finally, a coherent $2N$-site chain with $2N - 1$ registry bits and matched leads has exact zero-energy transmission $T(0; \eta) = \mathrm{sech}^2(\Delta m(\eta) \ln \tau)$. Reversal and global orientation complement preserve this transmission. At six sites, the 32 fields split into counts $(10, 15, 6, 1)$ by $|\Delta m|$, while the uniform-ensemble mean scales as $\Theta(N^{-1/2})$ for fixed $0 < \tau < 1$. The results supply explicit operator realizations and identify the additional molecular and experimental conditions needed to apply them.

Keywords: Chrysene Formalism; quantum molecular electronics; Schur-complement transfer; directional anisotropy; Kekulé resolvent; Coulson–Rushbrooke pairing; Stark effect; exciton dissociation; ballistic transport.

1 Introduction

1.1 Molecular electronics across the foundational and source arcs

In Volume 1, Issue 1 of this journal, Article 15 [Sch26a] introduced a quantum molecular-electronics model on the 3,6,9,12-tetrasubstituted chrysene core built around four proposed model mechanisms. Their physical implications are re-examined under the explicit realization conditions below:

(i) a longitudinal *Data Channel* anchored at the C6 and C12 coordinates ($v_y^+ = v_6, v_y^- = v_{12}$) and a transverse *Control Channel* anchored at the C3 and C9 coordinates ($v_x^- = v_3, v_x^+ = v_9$) [Sch26a, Def. 4];

(ii) bipartite sublattice charge isolation on the 18-carbon skeleton and a *Zero Divisor* crosstalk node decoupling the two channels [Sch26a, Thms. 2, 7];

(iii) a *Stark Tuning Operator* $\hat{S}_E$ that acts as a purely quadratic perturbation $\Delta E = -\frac{1}{2}\mathbf{F}^T \boldsymbol{\alpha} \mathbf{F}$ in the C_{2h}-symmetric interior ([Sch26a, Lem. 3]), but switches to a first-order linear dipole coupling at the boundary $\partial\mathcal{M}$ via $C_{2h} \to C_s$ symmetry breaking to dissociate a Frenkel exciton and inject a ballistic carrier ([Sch26a, Thm. 6]); and

(iv) *reflectionless transmission* ($T(E) = 1$ at resonance vs. $T(E) \to 0$ at destructive interference) across the discrete $\mathbb{Z}^3$ lattice [Sch26a, Thm. 4].

In Issue 2, Article 40 [Sch26c] reconstructed the Chrysene Formalism on twelve axioms, carefully separating molecular geometry (Axioms A_1–A_3) from the physical motif Hamiltonian and Schur-complement transfer operator $\mathcal{T}_\alpha^{(N)}(z)$ (Ax-

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iom A_{10}) and from the causal Kubo polarizability tensor $\alpha_{ij}(z)$ (Axiom A_{11}). Article 40 recorded that geometric inequivalence of the x- and y-axes ($\hat{\mathcal{D}}_x \nsim \hat{\mathcal{D}}_y$) does not automatically prove transfer anisotropy or optical anisotropy [Sch26c, Rems. 32, 34, eq. (581)], and posed both as explicit deferred targets: the *Directional Transfer Anisotropy Theorem* ($\mathcal{T}_x \neq_u \mathcal{T}_y$ via unequal Laurent moments $M_{k,x} \neq M_{k,y}$, [Sch26c, Thm. 42]) and the *Polarization Anisotropy Theorem* ($\alpha_{xx} \not\equiv \alpha_{yy}$ via unequal transition-dipole measures, [Sch26c, Thm. 43]), to be proved under the Conjugated π-Framework Hypothesis $H_{\partial\pi}$ [Sch26c, Def. 4].

In the source and registry sequence, Articles 79, 84, 90, 91, and 92 [Sch26g, Sch26e, Sch26f, Sch26b, Sch26d] established the chemical and informational supply of the assembly. The source models provide the locant sets $D = \{6, 12\}$, $I = \{3, 6, 12\}$ and $T = \{3, 6, 9, 12\}$, and distinguish a prescribed registry field from a specified endogenous ensemble. Their stream fractions and preparation routes are model inputs rather than experimental measurements in this paper. We use the corrected separation of preparation, persistence, decorated geometry and physical realization in Articles 90–92. An endogenous uniform registry law is an explicit statistical hypothesis; exogenous placement prescribes an initial field but does not alone establish its lifetime.

1.2 Contributions and realization scope

We establish three connected results in explicit models. First, the uniform-hopping chrysene graph has inequivalent scalar transfer functions along its two contact pairs: their first nonzero Laurent moments occur at different orders, their band-center squared amplitude ratio is 16, and two named same-sublattice resolvent entries vanish. Second, the unperturbed closed-shell response is anisotropic, while inversion-symmetric site potentials force zero permanent model dipole. An asymmetric cap permits a linear Stark term when its actual occupied-state dipole is nonzero. Third, an ideal matched-lead chain has an exact registry-dependent zero-energy transmission, with reflectionless balanced fields and an explicit finite-ensemble distribution.

The finite graph, model-response and scattering conclusions are proved below without importing the earlier articles' theorem proofs. Earlier theorem numbers identify the program to which these realizations respond, not a certification of every earlier formulation. Physical application requires the stated Hamiltonian, contact, conformational and statistical premises. Molecular geometry, spectroscopy and reaction kinetics remain distinct levels of evidence.

2 Conventions, nomenclature, and non-implications

Convention 2.1 (Status labels and documentary marks)**.** Every numbered statement carries one of four labels: **[A]** finite, algebraic, or axiom-free; **[D]** derived under hypotheses named and registered in Appendix A; **[C]** imported from a cited source; **[E]** a molecular or physical reading, entering no proof. Scholia are unlabelled and enter no proof. All quantitative macros are generated from the corrected calculations in `verify_a93.py` (blocks T1–T6, Appendix B).

Notation 2.2 (Graph, Hamiltonian, and response objects)**.** $G_{\mathrm{chr}} = (V_{\mathfrak{C}}, E_{\mathfrak{C}})$ the 18-vertex, 21-edge reference chrysene graph of [Sch26c, eq. (645)] with bipartition $V_{\mathfrak{C}} = V_A \sqcup V_B$ ($|V_A| = |V_B| = 9$, [Sch26c, eqs. (647)–(648)]); A_{chr} its 18×18 adjacency matrix; $H_{\mathrm{chr}} = -tA_{\mathrm{chr}}$ the Hückel π-Hamiltonian under $H_{\partial\pi}$ ([Sch26c, Def. 4]); $\mathcal{T}_\alpha(z) = \mathcal{J}_\alpha + W_{L,\alpha}^\dagger (zI - H_B)^{-1} W_{R,\alpha}$ the effective directional transfer operator and $M_{k,\alpha} = W_{L,\alpha}^\dagger H_B^k W_{R,\alpha}$ its transfer moments ([Sch26c, eqs. (370), (392)]); $\alpha_{ij}(z)$ the causal polarizability tensor ([Sch26c, eqs. (401)–(404)]).

Proposition 2.3 (Non-implications)**. [A]** *None of the following is asserted:*

(i) No automatic transfer anisotropy from geometry alone. *In accordance with [Sch26c, Rem. 32, eq. (581)], $\mathcal{T}_x \neq_u \mathcal{T}_y$ is not inferred from $\hat{\mathcal{D}}_x \nsim \hat{\mathcal{D}}_y$; it is proved in Theorem 3.3 from the explicit bridge Hamiltonian H_{chr} under $H_{\partial\pi}$.*

(ii) No perimeter ring-current claim. *Invoking $H_{\partial\pi}$ asserts standard sp^2 benzenoid π-conjugation across G_{chr} ([Sch26c, Def. 4, Rem. 1]), not an autonomous superconducting perimeter loop.*

(iii) No vanishing of opposite-sublattice cross-channel coupling at all energies. *Bipartite pairing forces the same-sublattice Green's functions $G_{3,12}(z)$ and $G_{6,9}(z)$ to vanish at the band center $z = 0$ (and to be purely odd in z), whereas opposite-sublattice elements such as $G_{3,6}(0)$ are non-zero (Theorem 3.4, Remark D.1).*

(iv) No finite-fragment-to-bulk dielectric relabeling. *Theorem 4.2 establishes reference-model polarizability anisotropy $\alpha_{xx}^{(0)} \neq \alpha_{yy}^{(0)}$ on G_{chr}; extending it to a bulk susceptibility $\chi_{ij}(\omega)$ requires the thermodynamic limit of [Sch26c, Def. 62, Rem. 35].*

3 Bipartite Schur-complement transfer anisotropy (Theorem 42 of Article 40)

We first instantiate Axiom A_{10} of Article 40 [Sch26c, §8.2] on the reference chrysene carbon skeleton G_{chr} under the Conjugated π-Framework Hypothesis $H_{\partial\pi}$ ([Sch26c, Def. 4]).

Definition 3.1 (The bipartite chrysene bridge Hamiltonian)**. [D]** Under $H_{\partial\pi}$, let $\mathcal{H}_B := \ell^2(V_{\mathbb{C}}) \cong \mathbb{C}^{18}$ carry the tight-binding π-electron Hamiltonian $H_{\mathrm{chr}} := -tA_{\mathrm{chr}}$ $(t > 0)$, where A_{chr} is the adjacency matrix of [Sch26c, eq. (645)]. For $\alpha \in \{x, y\}$, let $\mathcal{H}_{L,\alpha} = \mathcal{H}_{R,\alpha} = \mathbb{C}$ be one-dimensional terminal spaces coupled strictly through the primary attachment vertices of [Sch26c, eqs. (50)–(51)] ($\mathcal{J}_\alpha = 0$):

$$\begin{aligned} W_{R,x}(1) &= \gamma_c|v_3\rangle, \quad W_{L,x}(1) = \gamma_c|v_9\rangle \quad \text{(Control } x\text{)}, \\ W_{R,y}(1) &= \gamma_c|v_{12}\rangle, \quad W_{L,y}(1) = \gamma_c|v_6\rangle \quad \text{(Data } y\text{)}, \end{aligned} \tag{1}$$

with contact coupling $\gamma_c > 0$. By [Sch26c, eq. (370)], the effective directional transfer operator $\mathcal{T}_\alpha(z) : \mathbb{C} \to \mathbb{C}$ at $z \in \rho(H_{\mathrm{chr}})$ is the scalar Green's function entry

$$\mathcal{T}_\alpha(z) = \gamma_c^2 G_\alpha(z) := \gamma_c^2 \langle v_\alpha^+ \,|\, (zI - H_{\mathrm{chr}})^{-1} \,|\, v_\alpha^- \rangle. \tag{2}$$

Lemma 3.2 (Kekulé count, non-singular Fermi center, and sublattice block structure of G_{chr})**. [A]** *For the reference chrysene graph $G_{\mathrm{chr}} = (V_{\mathbb{C}}, E_{\mathbb{C}})$ of [Sch26c, eq. (645)]:*

(a) Under the balanced bipartition $V_{\mathbb{C}} = V_A \sqcup V_B$ of [Sch26c, eqs. (647)–(648)], where

$$\begin{aligned} V_A &= \{v_1, v_3, v_5, v_8, v_{10}, v_{12}, w_2, w_3, w_6\}, \\ V_B &= \{v_2, v_4, v_6, v_7, v_9, v_{11}, w_1, w_4, w_5\}, \end{aligned} \tag{3}$$

both negative terminals lie in V_A ($v_3, v_{12} \in V_A$) and both positive terminals lie in V_B ($v_6, v_9 \in V_B$).

(b) G_{chr} possesses exactly $K(G_{\mathrm{chr}}) = 8$ Kekulé structures (perfect matchings), and its adjacency determinant is

$$\det(A_{\mathrm{chr}}) = (-1)^9 K(G_{\mathrm{chr}})^2 = -64 \neq 0. \tag{4}$$

Consequently, $0 \in \rho(H_{\mathrm{chr}})$ (the bipartite band center $z = 0$ lies strictly inside the HOMO–LUMO gap $\Delta_{\mathrm{HL}} = 1.0403\,t > 0$; T1).

Proof. Part (a) is read directly from [Sch26c, eqs. (647)–(648)]. In this basis $A_{\mathrm{chr}} = \left(\begin{smallmatrix} 0 & B \\ B^T & 0 \end{smallmatrix}\right)$ where B is the 9×9 biadjacency matrix. For this specified 9×9 matrix, enumeration of the nonzero permutation products gives eight matchings, all with the same determinant sign. Thus $|\det B| = 8$ and $\det A_{\mathrm{chr}} = -\det(B)^2 = -64$. This is a finite matrix calculation, not a general assertion that benzenoids have no $4m$-cycles. The exact permutation enumeration and determinant are independently checked in block T1. □

Theorem 3.3 (Directional Transfer Anisotropy Theorem; Discharge of Article 40, Theorem 42)**. [A], [D]** *For the chrysene realization of Definition 3.1, identify the one-dimensional terminal spaces by $U_L = U_R = 1$. Then:*

(a) Shortest-path and transfer-moment inequality: *In G_{chr}, the graph distance along the C6–C12 Data Channel (y) is $d_{G_{\mathrm{chr}}}(v_{12}, v_6) = 5$ with 3 shortest paths, whereas along the C3–C9 Control Channel (x) it is $d_{G_{\mathrm{chr}}}(v_3, v_9) = 7$ with 1 shortest path. The directional transfer moments $M_{k,\alpha} = \gamma_c^2(-t)^k(A_{\mathrm{chr}}^k)_{v_\alpha^+, v_\alpha^-}$ of [Sch26c, Def. 59, eq. (392)] therefore satisfy*

$$\begin{aligned} M_{k,y} &= 0 \ \ (0 \le k \le 4), \quad M_{5,y} = -3\,\gamma_c^2 t^5 \neq 0, \\ M_{k,x} &= 0 \ \ (0 \le k \le 6), \quad M_{7,x} = -1\,\gamma_c^2 t^7 \neq 0. \end{aligned} \tag{5}$$

In particular, $M_{5,x} = 0 \neq M_{5,y}$, so by [Sch26c, Thm. 42, eq. (524)] the analytic transfer functions are unitarily inequivalent:

$$\mathcal{T}_x(\cdot) \not\simeq_u \mathcal{T}_y(\cdot). \tag{6}$$

(b) Exact Fermi-center resolvent ratio: *At $z = 0$, the exact Green's function amplitudes $|G_\alpha(0)| = t^{-1}|(A_{\mathrm{chr}}^{-1})_{v_\alpha^+, v_\alpha^-}| = t^{-1}\frac{K(G_{\mathrm{chr}} \setminus \{v_\alpha^+, v_\alpha^-\})}{K(G_{\mathrm{chr}})}$ are determined by the residual Kekulé counts $K(G_{\mathrm{chr}} \setminus \{v_6, v_{12}\}) = 4$ and $K(G_{\mathrm{chr}} \setminus \{v_9, v_3\}) = 1$:*

$$\begin{aligned} |\mathcal{T}_y(0)| &= \frac{\gamma_c^2}{t} \cdot \frac{4}{8} = \frac{\gamma_c^2}{2t}, \\ |\mathcal{T}_x(0)| &= \frac{\gamma_c^2}{t} \cdot \frac{1}{8} = \frac{\gamma_c^2}{8t}, \end{aligned} \tag{7}$$

giving the exact squared isolated-bridge amplitude ratio $|\mathcal{T}_y(0)/\mathcal{T}_x(0)|^2 = (4/1)^2 = 16$ for the C6–C12 Data Channel (T2). In the weak-contact, off-resonant Landauer regime with matched electrode couplings and Fermi energy at the model band center, this is the leading conductance ratio; finite lead self-energies or shifted level alignment need not preserve it.

Proof. (a) Raising A_{chr} to integer powers in block T2 gives $(A_{\mathrm{chr}}^k)_{v_6,v_{12}} = 0$ for $k < 5$ and $(A_{\mathrm{chr}}^5)_{v_6,v_{12}} = 3$ (via the three paths $v_{12} \to v_{11} \to w_2 \to w_4 \to w_6 \to v_6$, $v_{12} \to v_{11} \to w_2 \to w_5 \to v_5 \to v_6$, and $v_{12} \to w_1 \to w_3 \to w_5 \to v_5 \to v_6$), while $(A_{\mathrm{chr}}^k)_{v_9,v_3} = 0$ for $k < 7$ and $(A_{\mathrm{chr}}^7)_{v_9,v_3} = 1$ (via the unique path $v_3 \to v_4 \to w_3 \to w_5 \to w_2 \to w_4 \to v_{10} \to v_9$). Since $|U_L \mathcal{T}_x(z) U_R^\dagger| = |\mathcal{T}_x(z)|$ for any unitaries $U_L, U_R \in U(1)$, the distinct leading Laurent powers z^{-6} vs. z^{-8} as $|z| \to \infty$ exclude $\mathcal{T}_x \simeq_u \mathcal{T}_y$ for any terminal phase choice. (b) Exact inversion of the displayed graph adjacency matrix gives

$|(A_{\mathrm{chr}}^{-1})_{v_6,v_{12}}| = 1/2$ and $|(A_{\mathrm{chr}}^{-1})_{v_9,v_3}| = 1/8$. Independently enumerating the two vertex-deleted graphs gives four and one perfect matchings, respectively, so the stated ratios agree with these residual counts. The exact inverse identity $A_{\mathrm{chr}}A_{\mathrm{chr}}^{-1} = I$ verifies the cofactor values directly, without a general unsigned-cofactor assumption (T2). □

Theorem 3.4 (Bipartite Coulson–Rushbrooke pairing and the Fermi-center crosstalk node)**. [A]** *Let* $S_{\mathrm{sub}} = \mathrm{diag}(+I_{V_A}, -I_{V_B})$ *be the chiral sublattice grading operator on* $\mathcal{H}_B = \ell^2(V_A) \oplus \ell^2(V_B)$*, which anticommutes with* $H_{\mathrm{chr}} = -tA_{\mathrm{chr}}$ *(*$S_{\mathrm{sub}}H_{\mathrm{chr}}S_{\mathrm{sub}} = -H_{\mathrm{chr}}$*). Then for every* $z \in \rho(H_{\mathrm{chr}})$ *and every pair of vertices* u, v *belonging to the same sublattice (in particular, for the cross-channel pairs* $(v_3, v_{12}) \in V_A \times V_A$ *and* $(v_6, v_9) \in V_B \times V_B$*):*

$$\begin{aligned} G_{u,v}(-z) &= -G_{u,v}(z) \quad (u, v \in V_A \text{ or } u, v \in V_B), \\ G_{3,12}(0) &= \langle v_3 \,|\, (-H_{\mathrm{chr}})^{-1} \,|\, v_{12}\rangle = 0, \\ G_{6,9}(0) &= \langle v_6 \,|\, (-H_{\mathrm{chr}})^{-1} \,|\, v_9\rangle = 0. \end{aligned} \tag{8}$$

Consequently, at the Fermi center $z = 0$*, the Schur-complement transfer amplitude between the x- and y-channel same-sublattice terminals vanishes identically (T2).*

Proof. Since $S_{\mathrm{sub}}H_{\mathrm{chr}}S_{\mathrm{sub}} = -H_{\mathrm{chr}}$ and $S_{\mathrm{sub}}^2 = I$, we have $S_{\mathrm{sub}}(zI - H_{\mathrm{chr}})^{-1}S_{\mathrm{sub}} = (zI + H_{\mathrm{chr}})^{-1} = -(-zI - H_{\mathrm{chr}})^{-1}$. Taking matrix elements between u and v with $S_{\mathrm{sub}}|u\rangle = \sigma_u|u\rangle$ and $S_{\mathrm{sub}}|v\rangle = \sigma_v|v\rangle$ gives $\sigma_u\sigma_v G_{u,v}(z) = -G_{u,v}(-z)$. When u, v lie in the same sublattice, $\sigma_u\sigma_v = +1$, so $G_{u,v}(-z) = -G_{u,v}(z)$. Since $0 \in \rho(H_{\mathrm{chr}})$ by Lemma 3.2(b), $G_{u,v}$ is analytic at $z = 0$, forcing $G_{u,v}(0) = 0$ (T2). □

Remark 3.5 (Reference-core zero and decorated response)**.** The zero entries concern the isolated chiral Hamiltonian $-tA_{\mathrm{chr}}$ at its band center. Diagonal substitution potentials in H_S generally destroy the anticommutation used in the proof, and lead self-energies modify the transport Green function. Other cross-terminal entries need not vanish even in the reference core. The two exact zeros therefore do not imply complete isolation of two physical channels.

Remark 3.6 (Finite-contact conductance correction)**.** With equal local broadenings Γ, isolated same-terminal diagonal entries zero and off-diagonal magnitude g, Dyson dressing gives

$$T_\Gamma(0) = \frac{\Gamma^2 g^2}{(1 + \Gamma^2 g^2/4)^2}. \tag{9}$$

For $g_y = 1/(2t)$ and $g_x = 1/(8t)$, the conductance ratio is

$$\frac{T_{\Gamma,y}}{T_{\Gamma,x}} = 16\left(\frac{1 + \Gamma^2/(256t^2)}{1 + \Gamma^2/(16t^2)}\right)^2. \tag{10}$$

It tends to 16 only as $\Gamma/t \to 0$. This gives a concrete contact-aware interpretation of the isolated ratio [FL81, G+15].

Scholium 3.7 (Graph response and chemical selectivity). The contact labels retain Article 15's Data and Control terminology. The resolvent calculation establishes a property of the specified neutral-core graph with equal hopping. Residual perfect-matchings counts explain this graph identity; they do not constitute a reaction-path calculation or prove bromination regioselectivity, catalytic activity, or an exported-stock yield. Those chemical questions require the corresponding substituted structures, reaction conditions and kinetic evidence.

4 Quadratic-to-linear Stark switching across (D, I, T) and polarization anisotropy (Theorem 43 of Article 40)

We now instantiate Axiom A_{11} of Article 40 [Sch26c, §§8.9–8.11] across the three substituted families $D = \{6, 12\}$, $I = \{3, 6, 12\}$, and $T = \{3, 6, 9, 12\}$ of Article 79, reconciling Article 15's Lemma 3 (quadratic Stark shift) and Theorem 6 (C_s boundary linear dipole splitting) with Article 40's Proposition 29 and Theorem 43.

Definition 4.1 (Substituent-decorated response realization)**. [D]** For a substitution family $S \subseteq \Lambda = \{3, 6, 9, 12\}$ carrying arms at $l \in S$ with inductive site-potential shifts $\delta\varepsilon_l \in \mathbb{R}$ ($\delta\varepsilon_l = \delta\varepsilon$ for identical arms), let the single-particle Hamiltonian on $\mathcal{H}_{\mathrm{resp}} = \mathbb{C}^{18}$ be

$$H_S := -tA_{\mathrm{chr}} + \sum_{l \in S} \delta\varepsilon_l |v_l\rangle\langle v_l|. \tag{11}$$

Using the centered canonical coordinates $\hat{r}_v - c_{\mathrm{mol}} = (x_v, y_v, 0)$, let $X = \mathrm{diag}(x_v)$ and $Y = \mathrm{diag}(y_v)$. The many-electron reference is the closed-shell Slater determinant with nine doubly occupied one-particle orbitals, hence 18 π electrons. A positive gap between orbitals 9 and 10 is assumed where a smooth ground-state response is invoked. In model units, the field perturbation is $-F_xX - F_yY$ per electron. Dipole expectations below refer to the occupied projector P_S: $\boldsymbol{\mu}_S = 2\,\mathrm{Tr}(P_S(X, Y))$ in this sign convention. A physical charge factor, nuclear/ionic contribution and the chosen length scale must be restored for a molecular dipole. Polarizabilities are reported in units e^2a^2/t, where a is the

coordinate length unit. The response-model Cartesian x, y axes are fixed by these coordinates; the C3–C9 and C6–C12 contact vectors are not an orthogonal Cartesian basis.

Theorem 4.2 (Polarization anisotropy in the reference realization)**. [D]** *For the unperturbed closed-shell model $H_0 = -tA_{\mathrm{chr}}$ with the specified coordinates and $t = 1$, the static independent-particle tensor is*

$$\alpha_{ij}^{(0)} = 4 \sum_{o=1}^{9} \sum_{u=10}^{18} \frac{\mathrm{Re}(\langle o|X_i|u\rangle\langle u|X_j|o\rangle)}{E_u - E_o}, \tag{12}$$

where $X_x = X$, $X_y = Y$. Its numerical values are

$$\begin{aligned} \alpha_{xx}^{(0)} &\simeq 4.3658, & \alpha_{yy}^{(0)} &\simeq 6.3438, \\ \alpha_{xy}^{(0)} &\simeq -1.1212, & \alpha_{xx}^{(0)}/\alpha_{yy}^{(0)} &\simeq 0.6882. \end{aligned} \tag{13}$$

In particular $\alpha_{xx}^{(0)} \neq \alpha_{yy}^{(0)}$. Thus the corresponding directional spectral measures differ and their causal response functions cannot be identical. This establishes a reference realization of the polarization-anisotropy target attributed to Article 40. It does not assert these numerical values for arbitrary nonzero on-site shifts in D or T.

Proof. The sum-over-states expression follows from second-order perturbation theory for a gapped, spin-degenerate closed shell; the factor four includes spin degeneracy and the two static response terms. The verification companion computes eigenpair residuals and an independent spectral evaluation. Its exact rational certificate uses rational approximations Q, d to the eigenvectors and eigenvalues, Gershgorin disks of $Q^{-1}H_0Q$ to isolate the real spectrum, and residual/separation bounds to enclose each normalized eigenvector. Propagation through the transition elements and positive denominators gives $4.365 < \alpha_{xx}^{(0)} < 4.367$ and $6.343 < \alpha_{yy}^{(0)} < 6.345$ (block T3); these disjoint rational enclosures prove the inequality. Equality of the two transition measures would give equal integrals with weight $4/\Omega$ on their positive-gap support and hence equal static components, a contradiction. No claim about a particular HOMO–LUMO residue is needed. □

Remark 4.3 (Scope of the response realization)**.** The coordinates and uniform hopping fix this numerical example. Inversion-symmetric substitutions preserve the vanishing permanent dipole under the gap and symmetric-state assumptions below, but they change transition energies and polarizabilities. An off-diagonal α_{xy} in the chosen axes is allowed by C_{2h} and can be removed by rotating to principal polarizability axes; it is not an independent proof of a device-control channel.

Theorem 4.4 (Symmetry-controlled Stark terms across (D, I, T))**. [D]** *Let $\mathcal{P}$ implement the locant inversion and satisfy $\mathcal{P}X_i\mathcal{P}^\dagger = -X_i$. Assume a gapped closed-shell branch near zero field.*

(a) If the on-site shifts are equal on inversion-related sites, then the $D = \{6, 12\}$ and $T = \{3, 6, 9, 12\}$ model Hamiltonians commute with $\mathcal{P}$. Their occupied projectors are inversion invariant, their permanent model dipoles vanish, and

$$\Delta E_S(\mathbf{F}) = -\tfrac{1}{2}\mathbf{F}^T\alpha_S^{(0)}\mathbf{F} + O(|\mathbf{F}|^4). \tag{14}$$

The leading allowed term is quadratic, not an assertion that higher even terms vanish.

(b) A nonzero common on-site shift on $I = \{3, 6, 12\}$ breaks inversion:

$$\mathcal{P}H_I\mathcal{P}^\dagger - H_I = \delta\varepsilon(|v_9\rangle\langle v_9| - |v_3\rangle\langle v_3|) \neq 0. \tag{15}$$

The following geometric locant moments are exact:

$$\begin{aligned} \mathbf{d}_I &= -\tfrac{1}{2}\hat{d}_x, & \|\mathbf{d}_I\|^2 &= 37/4, \\ \mathbf{d}_{Dm} &= \tfrac{1}{2}\hat{d}_y, & \|\mathbf{d}_{Dm}\|^2 &= 13/4, \\ \mathbf{d}_I \cdot \mathbf{d}_{Dm} &= -7/4. \end{aligned} \tag{16}$$

Here $\mathbf{d}_I = \sum_{l\in I}(\hat{r}_{v_l} - c_{\mathrm{mol}})$ and $\mathbf{d}_{Dm} = (\hat{r}_{v_6} - \hat{r}_{v_{12}})/2$. They are coordinate sums, not charge-weighted electronic dipoles. If the occupied-projector calculation or experiment establishes $\boldsymbol{\mu}_I \neq 0$ (hypothesis H_μ), then

$$\begin{aligned} \Delta E_I(\mathbf{F}) = -\boldsymbol{\mu}_I \cdot \mathbf{F} - \tfrac{1}{2}\mathbf{F}^T\alpha_I^{(0)}\mathbf{F} \\ + O(|\mathbf{F}|^3). \end{aligned} \tag{17}$$

The linear term is nonzero only for field directions with $\boldsymbol{\mu}_I \cdot \mathbf{F} \neq 0$. The same conditional statement applies to an asymmetrically substituted Dm model.

Proof. For (a), functional calculus gives $\mathcal{P}P_S\mathcal{P}^\dagger = P_S$, so $\mathrm{Tr}(P_S X_i) = -\mathrm{Tr}(P_S X_i) = 0$. Inversion relates $H_S(\mathbf{F})$ to $H_S(-\mathbf{F})$, making the analytic closed-shell energy even near zero; its Taylor expansion yields (14). For (b), conjugating the diagonal site shifts gives (15). The inversion-paired coordinates at 6 and 12 cancel, leaving the coordinate at 3, which is $-\hat{d}_x/2$; the differential pair is $\hat{d}_y/2$. The stated norms and dot product follow from $\|\hat{d}_x\|^2 = 37$, $\|\hat{d}_y\|^2 = 13$ and $\hat{d}_x \cdot \hat{d}_y = 7$. Finally the Hellmann–Feynman derivative of the gapped oc-

cupied energy is $-\boldsymbol{\mu}_I$, giving (17) under H_μ. Broken inversion permits but does not alone prove a nonzero dipole. □

Remark 4.5 (Molecular and excitonic interpretation)**.** Planar site-potential models may retain a molecular-plane reflection after inversion is broken. A fully decorated molecular point group, including arm conformations and environment, requires its own geometry. For a spectroscopic transition the linear coefficient is the difference between excited- and ground-state dipoles. Exciton dissociation additionally depends on binding energies, charge-transfer states, reorganization, dielectric screening and competing rates. The Stark expansion supplies a candidate field-coupling mechanism, not a proof of photovoltaic charge separation.

5 Registry-gated ballistic transport: registry-dependent transmission in coherent finite chains

Finally, we connect the alignment field $\eta = (\eta_0, \dots, \eta_{l-2}) \in \{0,1\}^{l-1}$ of Articles 84 and 90 [Sch26e, Sch26f] to the reflectionless transmission theorem of Article 15 [Sch26a, Thm. 4].

Definition 5.1 (Registry-modulated vertical tight-binding chain)**. [D]** Consider a column of $l = 2N$ stacked units ($2N-1$ vertical contacts) with alignment field $\eta \in \{0,1\}^{2N-1}$. Let an aligned contact ($\eta_k = 0$) carry vertical π-stacking hopping integral $t_0 > 0$ and an unaligned contact ($\eta_k = 1$) carry hopping integral $t_1 = \tau t_0$ with $\tau \in (0,1)$, so the column Hamiltonian on $\ell^2(\{0,\dots,2N-1\})$ is

$$H_{\mathrm{col}}(\eta) := -\sum_{k=0}^{2N-2} t_{\eta_k}(|k\rangle\langle k+1| + |k+1\rangle\langle k|), \qquad t_{\eta_k} = t_0\tau^{\eta_k}. \tag{18}$$

Attach semi-infinite leads of hopping t_0 to sites 0 and $2N-1$, with both lead-to-chain couplings also t_0. The model is static, phase coherent, single channel and lossless, with zero on-site potentials. The map from a registry bit to a hopping amplitude is the explicit hypothesis H_{hop}, not a consequence of registry combinatorics alone. For this matched-lead model, let $T(E;\eta) \in [0,1]$ denote the Landauer–Büttiker S-matrix transmission probability at energy $E \in (-2t_0, 2t_0)$.

Theorem 5.2 (Ballistic reflectionless transmission of placed stacks vs. endogenous disorder suppression)**. [A], [D]** *In the vertical chain of Definition 5.1 at the band center $E = 0$:*

(a) Exact transfer-product formula: *For any alignment field $\eta \in \{0,1\}^{2N-1}$, let $\Delta m(\eta) := \sum_{j=0}^{N-1}\eta_{2j} - \sum_{j=0}^{N-2}\eta_{2j+1} \in \mathbb{Z}$ be the net difference between even-contact and odd-contact unaligned bits. Then the exact S-matrix transmission probability at $E = 0$ is*

$$T(0;\eta) = \frac{4}{\left(\tau^{\Delta m(\eta)} + \tau^{-\Delta m(\eta)}\right)^2} = \operatorname{sech}^2(\Delta m(\eta)\,\ln\tau). \tag{19}$$

(b) Exogenous Placed Source (H_{place}, [Sch26a, Thm. 4]): *For any placed alignment field satisfying $\Delta m(\eta^0) = 0$ (including the uniform field $\eta^0 = 0^{2N-1}$ and every field with paired equal bits $\eta_{2j} = \eta_{2j+1}$ for $0 \le j \le N-2$ and final bit $\eta_{2N-2} = 0$), the reflection amplitude vanishes identically and the S-matrix achieves* perfect transmission*:*

$$T(0;\eta^0) = 1 \qquad (\forall\,\eta^0 \text{ with } \Delta m(\eta^0) = 0), \tag{20}$$

whereas placing a maximally dimerized SSH field $\eta^{\mathrm{SSH}} = (1,0,1,0,\dots,1)$ ($\Delta m = N$) suppresses transmission exponentially to $T(0;\eta^{\mathrm{SSH}}) = \frac{4}{(\tau^N+\tau^{-N})^2} \le 4\tau^{2N}$ (64/289 at $l = 4$ and 256/4225 ≈ 0.0606 at $l = 6$ for $\tau = 1/2$, realizing the "ON" and "OFF" states of [Sch26a, Thm. 4]).

(c) Endogenous Source (μ_{endo}, Article 79): *Under the uniform endogenous law $\mu_{\mathrm{endo}}(\eta) = 2^{-(2N-1)}$ of [Sch26e, Thm. 7.10(a)], $\Delta m(\eta)$ is the difference of independent* $\mathrm{Bin}(N,1/2)$ *and* $\mathrm{Bin}(N-1,1/2)$ *variables, so the ensemble-averaged transmission $\langle T(0)\rangle_{\mathrm{endo}} = 2^{-(2N-1)}\sum_\eta T(0;\eta)$ is strictly less than* 1 *(0.6559 at $l = 6, \tau = 1/2$) and is $\Theta(N^{-1/2})$ for fixed $0 < \tau < 1$ as $N \to \infty$ (T5, T6).*

Proof. At $E = 0$, the tight-binding Schrödinger equation $(H_{\mathrm{col}}\psi)_k = 0$ relates even and odd site amplitudes by $t_{\eta_{2j}}\psi_{2j} + t_{\eta_{2j+1}}\psi_{2j+2} = 0$ and $t_{\eta_{2j-1}}\psi_{2j-1} + t_{\eta_{2j}}\psi_{2j+1} = 0$ at interior sites; at the ends the lead coupling is t_0. Matching to incoming and outgoing plane waves $\psi_n = e^{i\pi n/2} + re^{-i\pi n/2}$ (left lead, $k_F = \pi/2$) and $\psi_n = t_{\mathrm{tr}}e^{i\pi n/2}$ (right lead) yields $|t_{\mathrm{tr}}|^2 = 4/(\Lambda+\Lambda^{-1})^2$ where $\Lambda = (\prod_{j=0}^{N-1} t_{\eta_{2j}})/(t_0\prod_{j=0}^{N-2} t_{\eta_{2j+1}}) = \tau^{\Delta m(\eta)}$, proving (19). Part (b) follows by substitution. For (c), write $X \sim \mathrm{Bin}(N,1/2)$ and $Y \sim \mathrm{Bin}(N-1,1/2)$ independently, so $\Delta m = X - Y$. Vandermonde's identity gives

$$\mathbb{P}(\Delta m = k) = 2^{-(2N-1)}\binom{2N-1}{N-1+k}. \tag{21}$$

The maximal mass is $O(N^{-1/2})$, while $\sum_{k\in\mathbb{Z}}\operatorname{sech}^2(k\ln\tau) < \infty$ for fixed $0 < \tau < 1$. Multiplying these bounds proves

the upper estimate for the mean. The $k = 0$ term has mass $\Theta(N^{-1/2})$ and transmission one, giving the matching lower estimate. Since nonzero Δm occurs with positive probability and has transmission below one, the finite mean is strictly below one. The independent lead-dressed matrix calculation in block T5 checks the closed form on the declared finite test set. □

Corollary 5.3 (Frame-group invariance of $T(0;\eta)$ and exact binomial spectrum at $l = 6$)**. [A]** *On any $2N$-site column, end-to-end reversal $\mathrm{rev}_\eta(\eta)_i = \eta_{2N-2-i}$ ([Sch26e, Lem. 8.10]) maps even contact indices $2j \mapsto 2(N-1-j)$ to even contact indices and odd contact indices $2j+1 \mapsto 2(N-2-j)+1$ to odd contact indices. Hence $\Delta m(\mathrm{rev}_\eta(\eta)) = \Delta m(\eta)$ and*

$$T(0;\,\mathrm{rev}_\eta(\eta)) = T(0;\,\eta) \qquad (\forall\,\eta \in \{0,1\}^{2N-1}), \tag{22}$$

The global complement of unit orientations leaves every adjacent XOR bit η_k unchanged. Together with reversal invariance, this proves that $T(0;\eta)$ is an exact invariant of the frame classes $\{0,1\}^{2N}/\mathrm{Fr}$ ([Sch26e, Cor. 8.12]). At codon length $l = 6$ ($N = 3$, 32 fields across 20 frame classes), $|\Delta m(\eta)| \in \{0,1,2,3\}$ partitions the 32 fields into:

- $|\Delta m| = 0$*: 10 fields with $T(0) = 1$ (reflectionless resonance);*
- $|\Delta m| = 1$*: 15 fields with $T(0) = \frac{4}{(\tau+\tau^{-1})^2}$ ($16/25 = 0.64$ at $\tau = 1/2$);*
- $|\Delta m| = 2$*: 6 fields with $T(0) = \frac{4}{(\tau^2+\tau^{-2})^2}$ ($64/289 \approx 0.2215$ at $\tau = 1/2$);*
- $|\Delta m| = 3$*: 1 field ($\eta^{\mathrm{SSH}} = (1,0,1,0,1)$) with $T(0) = \frac{4}{(\tau^3+\tau^{-3})^2}$ ($256/4225 \approx 0.0606$ at $\tau = 1/2$; T6).*

Proof. Since $2N-2$ is even, $2N-2-2j = 2(N-1-j)$ is even and $2N-2-(2j+1) = 2(N-2-j)+1$ is odd, so rev_η permutes the two sums in $\Delta m(\eta)$ within themselves, proving (22). For $N = 3$, $\sum_{j=0}^{2} \eta_{2j} \in \{0,1,2,3\}$ has binomial counts $(1,3,3,1)$ and $\sum_{j=0}^{1} \eta_{2j+1} \in \{0,1,2\}$ has binomial counts $(1,2,1)$; convolving the two distributions gives $1\cdot 1 + 3\cdot 2 + 3\cdot 1 = 10$ at $|\Delta m| = 0$, $(3\cdot 1 + 3\cdot 2 + 1\cdot 1) + (1\cdot 2 + 3\cdot 1) = 10 + 5 = 15$ at $|\Delta m| = 1$, $(3\cdot 1 + 1\cdot 2) + (1\cdot 1) = 5 + 1 = 6$ at $|\Delta m| = 2$, and $1\cdot 1 = 1$ at $|\Delta m| = 3$ (T6). □

6 Precedence rulings and targets

Ruling 6.1 (Relation to the earlier operator targets)**.** Theorem 3.3 supplies a uniform-hopping realization of the directional-transfer target attributed to Article 40. Theorem 4.2 supplies a reference closed-shell realization of its polarization target. The exact node and matched-chain formulas refine the channel and transport mechanisms discussed in Article 15. The Stark theorem establishes symmetry selection rules and a conditional linear term, rather than chemical exciton dissociation.

Target 6.2 (Contact-aware molecular transport)**.** Compare 6,12- and 3,9-connected derivatives with matched anchors, charge state and electrode geometry. Measure gate/Fermi-level dependence and substitution-induced level shifts. Test the weak-contact midgap ratio against the full lead-dressed transmission, and separately examine the named interference node rather than assuming universal channel isolation [G+15, FL81].

Target 6.3 (Structure-resolved Stark and exciton measurements)**.** Determine arm conformations and molecular symmetry, then calculate or measure permanent and transition dipoles and polarizabilities. Optical Stark spectra probe excited-minus-ground differences, and isotropic orientational averaging can suppress a net odd-field signal. Oriented or single-molecule measurements and electroabsorption lineshape analysis are appropriate discriminants [B+97]. Test any charge-separation hypothesis separately using excited-state energetics and dissociation/recombination kinetics [Bra84].

7 Conclusion

The reference chrysene graph provides exact directional-transfer and same-sublattice node identities. The C6–C12 and C3–C9 first nonzero path moments occur at orders five and seven, and their band-center isolated amplitudes have magnitudes $1/(2t)$ and $1/(8t)$. Their squared ratio is 16; the corresponding measured conductance interpretation is conditional on contacts and level alignment. The closed-shell reference response is anisotropic, with corrected model ratio $\alpha_{xx}^{(0)}/\alpha_{yy}^{(0)} \simeq 0.6882$. Inversion-symmetric D, T site potentials enforce zero permanent model dipole, whereas asymmetric I, Dm substitutions permit a linear Stark term under a separate nonzero-dipole premise. Finally, the ideal coherent chain has an exact registry-invariant transmission and the hexamer field partition $(10, 15, 6, 1)$. These results connect graph structure, response and registry in defined

Table 1: Results and their realization conditions.

Result	Established statement	Physical premise
Directional transfer	Leading Laurent orders differ; squared isolated ratio 16	Uniform hopping, equal local terminals; conductance ratio needs weak matched contacts at midgap
Sublattice node	$G_{3,12}(0) = G_{6,9}(0) = 0$	Isolated nonsingular chiral Hamiltonian; not arbitrary decorated or lead-dressed models
Polarization	Reference-model diagonal responses differ	Closed-shell occupancy, specified coordinates, positive gap
Stark response	Inversion forces an even energy branch; nonzero dipole gives a linear term	Symmetric Hamiltonian and state for D, T; separate H_μ for I, Dm
Registry transport	Exact $\operatorname{sech}^2(\Delta m \ln \tau)$; finite counts $(10, 15, 6, 1)$	Coherent static chain, zero on-site energies, matched leads, specified hopping map

realizations while identifying the molecular measurements required for implementation.

A Hypothesis register

$H_{\partial\pi}$ and contacts.
The uniform nearest-neighbor Hamiltonian $-tA_{\mathrm{chr}}$, common contact strength and fixed terminal vertices define the transfer realization. If the physical hypothesis fails, graph distances, matching counts and inverse-matrix identities still hold for that formal graph.

H_{gap}.
Nine doubly occupied orbitals are separated from the unoccupied orbitals by a gap; a gapped analytic branch is used for Stark expansions. The graph results do not depend on this response premise.

H_{sym}.
Potentials on inversion-related sites are equal, and the occupied state respects inversion. For atomistic interpretation, substituents and surroundings must also respect it. Locant-set invariance alone does not suffice.

H_{ind} and H_μ.
Substitution is represented by specified diagonal shifts. A nonzero permanent occupied-state dipole is an additional premise for a nonzero linear Stark coefficient. Geometric locant moments remain exact if that premise fails.

H_{hop} and coherent contacts.
The static chain has $2N - 1$ binary contacts, hoppings $t_0\tau^{\eta_k}$, zero on-site energies and matched t_0 leads. This ideal scattering model is lossless for every field, so its S-matrix is always unitary; $T = 1$ means reflectionless transmission. Molecular overlaps and persistence must be independently calibrated. At $\tau = 1$ all fields give $T(0) = 1$.

H_{endo}.
Contact bits are independent and fair for the ensemble calculation. Without this law the pointwise transmission formula remains, but the binomial distribution and its mean need not.

B Verification blocks

The standalone verification companion documents the exact executed source, generated values, tolerances, negative controls and reproducibility commands. It distinguishes exact rational checks from floating-point checks rather than calling numerical diagonalization exact.

`T1` Graph and matching structure.
Reconstructs the 18-vertex, 21-edge bipartite graph, enumerates the eight perfect matchings, checks the determinant -64, and verifies both residual matching counts independently.

`T2` Transfer and inverse identities.
Computes path moments and the exact inverse with its matrix-product residual. Checks the two selected zeros, the isolated ratio and the finite-contact correction; a diagonal-potential perturbation distinguishes the decorated model from the chiral reference.

`T3` Spectrum and response.
Computes floating-point eigenpairs with residual and orthogonality tests, the gap $1.0403\,t$ and response components. An exact rational similarity/Gershgorin and eigenvector-residual certificate encloses the diagonal responses in disjoint intervals. Numerical finite-difference response provides an independent consistency check.

`T4` Geometry and Stark scope.
Checks the exact locant moments and inversion relations. Numerical occupied-projector checks at declared site shifts

are examples, not a proof that every asymmetric parameter choice has nonzero dipole.

T5 Chain and frame action.
Compares the closed transmission formula with an independently formed lead-dressed chain inverse on the stated finite set, and verifies the registry action, matched-lead convention and reflectionless cases.

T6 Field distribution.
Enumerates the hexamer histogram $(10, 15, 6, 1)$, checks normalization and the exact rational mean whose decimal value is 0.6559 at $\tau = 1/2$. The all-length asymptotic statement uses the analytic binomial proof in the manuscript, not finite enumeration alone.

The run contains 18,181 explicit predicates per execution mode, comprising 17,093 exact checks (including 10 negative controls) and 1,088 numerical checks. The separate Lean 4.24 companion freshly compiles 57 finite named theorems with no axioms in their dependency audit; its exact coverage is listed there.

C Molecular commentary and empirical closure

Remark C.1 (Combinatorics and chemical mechanisms)**. [E]** Perfect-matching deletion is an algebraic cofactor construction. It does not describe literal destruction of aromatic sextets by an electron in transit, nor does a conductance amplitude establish an electrophilic substitution mechanism or yield. Clar and Kekulé language is used here as structural interpretation, not as a reaction pathway.

Remark C.2 (Boundary polarity as a hypothesis)**. [E]** An asymmetric cap is a candidate source of a local field after its charge distribution is determined. A dipole field varies spatially and is not automatically a step function. Exciton dissociation requires a separate electron–hole model, dielectric screening, accessible charge-transfer states and favorable competing rates [Bra84]. Flexible arms may lower molecular symmetry further than the planar site model.

Remark C.3 (Empirical closure)**.** The realization program requires conformer-resolved structures, calibrated on-site energies and transfer integrals, dipole and polarizability measurements, contact-aware conductance, and temperature/coherence characterization. Intermolecular hopping can fluctuate strongly with geometry [TO06]. A placed registry is an initial condition; its lifetime and its electronic coupling require separate tests. These measurements distinguish mathematical model consistency from molecular operation.

D Clarifications and verification boundaries

Remark D.1 (Parity and channel matrix elements)**. [A]** Both antisymmetric terminal combinations are odd under inversion. For an inversion-even operator V_{even}, the well-typed parity selection rule is $\langle \psi_{\text{odd}} | V_{\text{even}} | \psi_{\text{even}} \rangle = 0$. It does not imply that two odd channel states cannot couple. The same-sublattice zero in Theorem 3.4 is a distinct band-center identity.

Remark D.2 (Shortest path and registry counts)**. [A]** The C3–C9 distance is seven with one shortest path, while the C6–C12 distance is five with three. A $2N$-site chain has $2N - 1$ bits, so a six-site field has 32 possibilities. Their absolute alternating-sum counts are $(10, 15, 6, 1)$; the mean under the specified uniform law is 0.6559 at $\tau = 1/2$. Reversal preserves contact-index parity, and global unit-orientation complement preserves the contact bits themselves.

Remark D.3 (Computational and formal scope)**.** The new verification companion replaces the original hard-coded response macros by computed values and supplies independent exact and numerical checks with explicit tolerances or enclosures. The Lean companion certifies its stated finite graph and arithmetic statements. It does not formalize the full analytic response theory, arbitrary coherent chains, atomistic chemistry or experimental device behavior. The original files and report are retained as superseded provenance.

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