Geometric Spin Filtering in Chiral Molecules: A VERSF Interpretation of the CISS Effect

VERSF Theoretical Physics Program

For the General Reader

Molecules can come in two mirror-image forms — like a left hand and a right hand. These "chiral" molecules are identical in almost every way, but they are not superimposable on each other. One of the most surprising discoveries in modern physics is that this geometric difference — handedness — can act as a spin filter for electrons.

Electrons carry a quantum property called spin, which can point in one of two directions: up or down. Normally, when electrons flow through a material, both spin directions pass through equally. But when electrons are passed through a helical (corkscrew-shaped) chiral molecule — such as a strand of DNA — one spin direction passes through far more readily than the other. This is the Chiral-Induced Spin Selectivity, or CISS, effect. Polarizations of 10–80% have been measured experimentally, meaning that most of the transmitted electrons share the same spin. Change the handedness of the molecule, and the preferred spin flips.

Why does this happen? The conventional explanation — that the molecule's atoms create a tiny magnetic environment that nudges the electron's spin — predicts effects thousands of times too small. Something more fundamental must be at work.

This paper argues that the answer lies in geometry itself. When an electron is forced to travel along a helical path, the corkscrew shape of that path generates a kind of rotational influence on the electron's spin. The helix's twist — its torsion — is the operative quantity: it enters the effective spin connection and generates a gauge-like coupling between the electron's spin and its direction of motion. We show that this geometric effect has the correct symmetry structure and can naturally reach the experimentally relevant range of spin filtering, that it reverses exactly when the handedness of the molecule is reversed, and that it vanishes when the electron is not moving — consistent with the experimental observation that CISS requires an applied voltage.

We then place this result within the Void Energy-Regulated Space Framework (VERSF), which proposes that physical structures do not merely provide a backdrop for processes — they actively define which outcomes are possible. In this view, a chiral molecule is not a passive tunnel through which electrons happen to flow. It is a geometric filter that constitutes the landscape of available pathways, giving one spin orientation preferential access. Geometry, in this picture, is not background. It is participant.

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Abstract

The Chiral-Induced Spin Selectivity (CISS) effect — the experimentally robust observation that chiral molecules preferentially transmit electrons of one spin orientation — remains incompletely explained by conventional spin–orbit coupling arguments. We present two complementary analyses. First, we derive a minimal effective Hamiltonian for an electron constrained to a helical path directly from the three-dimensional Pauli equation in the Frenet–Serret frame, showing that a spin-dependent gauge potential — the spin connection of the rotating frame — emerges from the geometric structure of the constrained helical path upon projection to the lowest transverse mode. We derive the dispersion relation, establish that the spin-splitting reverses exactly under chirality reversal, and compute spin-resolved transmission

coefficients in the Landauer picture, showing that sizable spin polarization is achievable when the dimensionless control parameter η is of order unity, with DNA-like parameters placing the system near the experimentally relevant regime. Second, we interpret these results within the Void Energy-Regulated Space Framework (VERSF), where structural geometry plays a constitutive role in determining which physical transitions are admissible. We argue that CISS is not merely a spin-transport curiosity but an instance of a broader principle: physical structures do not passively host processes — they regulate which processes can occur.

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1. Introduction

When electrons pass through a chiral molecule — one possessing a left- or right-handed helical structure — the transmitted electrons are not spin-random. One spin orientation is strongly favoured. This is the Chiral-Induced Spin Selectivity (CISS) effect, and it has been reproduced across a wide range of molecular systems including DNA, peptides, and helicene derivatives.

The central puzzle is one of magnitude. Standard estimates of spin–orbit coupling (SOC) in light organic molecules yield spin-mixing energies many orders of magnitude below what would be required to produce the observed polarizations, which routinely reach 10–80% in transport experiments. Something beyond weak atomic SOC must be at work — and whatever it is must be chemically nonspecific, since CISS appears across systems with radically different elemental compositions and electronic structures.

Several mechanisms have been proposed: collective SOC amplification along extended helical chains, helically symmetric electrostatic potentials, dephasing-assisted transport, and — most recently — purely geometric mechanisms in which the helical constraint on electron motion generates an effective spin–orbit-like coupling without invoking atomic-scale interactions. This last class of explanation is particularly compelling because it roots the effect in molecular topology rather than chemistry, providing a natural account of the observed universality.

In this paper we pursue two goals. We first derive the geometric mechanism from the constrained Pauli Hamiltonian, working through the Frenet–Serret frame, projection to the lowest transverse mode, and spin-resolved Landauer transmission, in enough detail to establish internal consistency and show that the resulting control parameter lies in the experimentally relevant regime for molecular systems such as DNA. We then interpret the results within the VERSF framework, arguing that the geometric picture is sharpened by VERSF's core claim that structural geometry is constitutive — not merely constraining — of the admissible transitions in a physical process.

The mathematical mechanism developed here is aligned in spirit with prior curved-geometry analyses of CISS, including the helical-confinement work of Brandt et al. [8] and the geometric-SOC interplay studied by Volosniev et al. [11]. The novelty of the present paper is not the claim that geometry matters per se, but rather: (i) the organisation of the helical Pauli reduction into a minimal VERSF-compatible effective Hamiltonian with a single dimensionless control parameter $\eta = C\tau/(2k_F)$; (ii) the explicit derivation of the perturbative Fermi wavevector

splitting $\delta k = m\lambda/\hbar$ and its implications for spin-resolved Landauer transport; and (iii) the interpretation of the resulting spin selectivity as an admissibility effect in the VERSF sense, with the geometry-first scaling prediction $P \propto \tau/k_F$ as the key experimentally testable consequence.

Throughout, we are careful to distinguish what the derivation establishes from what remains open. Helical geometry is **sufficient** to generate a spin-selective transport term of the correct symmetry and potentially of experimentally relevant magnitude; whether geometry alone accounts for all of CISS in every real molecular system is a separate, and still open, empirical question.

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2. Constrained Pauli Dynamics on a Helical Curve

2.1 The Helical Curve and Frenet–Serret Frame

Consider a uniform helix in $\mathbb{R}^3$, parameterised by arc length s:

$$\mathbf{r}(s) = \left(R\cos(s/\Lambda),\ R\sin(s/\Lambda),\ d\cdot s/\Lambda \right)$$

where R is the helix radius, d is the pitch parameter (axial rise per radian), and $\Lambda = \sqrt{(R^2 + d^2)}$ is the normalisation factor ensuring $|d\mathbf{r}/ds| = 1$. The axial rise per full turn is $2\pi d$, and the arc length per turn is $L = 2\pi\Lambda = 2\pi\sqrt{(R^2 + d^2)}$.

For B-DNA: axial rise per turn ≈ 3.4 nm (so $d \approx 0.54$ nm), $R \approx 1$ nm, giving $L \approx 7.1$ nm. Note carefully: 3.4 nm is the axial pitch, not the arc length.

At every point along the helix, the Frenet–Serret frame $\{\hat{T}, \hat{N}, \hat{B}\}$ is defined by:

$$\hat{T} = d\mathbf{r}/ds \qquad \text{(unit tangent)}$$
$$\hat{N} = (d\hat{T}/ds)/|d\hat{T}/ds| \qquad \text{(unit normal, pointing inward toward the helix axis)}$$
$$\hat{B} = \hat{T} \times \hat{N} \qquad \text{(unit binormal)}$$

The frame evolves along s according to the Frenet–Serret equations:

$$d\hat{T}/ds = \kappa_c \hat{N}$$
$$d\hat{N}/ds = -\kappa_c \hat{T} + \tau \hat{B}$$
$$d\hat{B}/ds = -\tau \hat{N}$$

The two fundamental geometric invariants of the helix are:

$$\kappa_c = R / (R^2 + d^2) \qquad \text{(curvature)}$$
$$\tau = d / (R^2 + d^2) \qquad \text{(torsion)}$$

For a right-handed helix $\tau > 0$; for a left-handed helix $\tau < 0$. The handedness label $h = \mathrm{sgn}(\tau)$ encodes the chirality. For a uniform helix, the Frenet–Serret frame rotates at a constant rate along the curve. The binormal $\hat{B}(s)$ is not itself constant — it evolves according to $d\hat{B}/ds = -\tau\hat{N}$ — but

its motion is periodic and governed entirely by the fixed curvature and torsion. After transforming to the co-rotating frame, the effective spin quantisation axis becomes fixed, which allows the spin-dependent term in the projected Hamiltonian to be written in a constant-axis form. It is this co-rotating-frame axis, aligned with the helix axis, that plays the role of $\hat{B}$ in the effective 1D description below.

2.2 Constrained Pauli Hamiltonian

Start with the three-dimensional Pauli Hamiltonian for an electron in the Frenet–Serret coordinate system (s, ρ, φ), where ρ and φ are polar coordinates in the transverse plane spanned by $\{\hat{N}, \hat{B}\}$:

$$H = p^2 / (2m) + V_{conf}(\rho) + H_{spin}$$

The confinement potential $V_{conf}(\rho)$ restricts the electron to a thin tube of radius ρ_0 around the helical curve. In the thin-tube limit $\rho_0 \to 0$, one projects onto the lowest transverse mode $\chi_0(\rho, \varphi)$. The spin Hamiltonian H_{spin} contains the Zeeman coupling and any intrinsic SOC; for the geometric mechanism we set all atomic SOC to zero, retaining only the kinematic spin coupling induced by the moving frame.

2.3 Projection to the Lowest Transverse Mode

When the electron is tightly confined to the curve, the three-dimensional kinetic operator in curvilinear coordinates generates two contributions upon projecting onto χ_0:

i. The da Costa geometric scalar potential. Curvature of the confinement surface yields an attractive scalar shift:

$$V_g = -\hbar^2 \kappa_c^2 / (8m)$$

This term is spin-independent and shifts both spin branches equally. It does not contribute to spin polarization.

ii. The spin connection. The rotating Frenet–Serret frame generates a non-Abelian gauge structure for the spin degrees of freedom. Parallel transport of the spinor along the helix accumulates a spin-dependent phase determined by the Darboux vector — the angular velocity of the frame — which for a helix has components along both $\hat{B}$ and $\hat{T}$ involving both κ_c and τ. In the co-rotating frame, the spin connection reduces to an effective gauge potential along the transport direction. For a uniform helix, working in the frame where the spin quantisation axis is fixed, this takes the effective reduced form:

$$A_s = (\hbar/2)\, \tau\, (\vec{\sigma} \cdot \hat{B})$$

where $\hat{B}$ here denotes the fixed co-rotating-frame axis. The curvature κ_c enters through the scalar potential V_g and through basis-dependent corrections that are absorbed into the coefficient C of the coupling λ defined below. The spin connection A_s acts as a vector potential for the spin

degree of freedom. Upon projection, the longitudinal kinetic operator $-i\hbar\,\partial_s$ shifts to $-i\hbar\,\partial_s - A_s$, producing a momentum-dependent spin coupling. The coefficient C introduced in the effective Hamiltonian below should be understood as encoding the difference between this simplest reduced connection term and the fully projected lowest-mode result, including confinement-profile and basis-dependent corrections.

2.4 Effective 1D Hamiltonian and Handedness Dependence

Combining the projected kinetic term, da Costa potential, and spin connection, the effective 1D Hamiltonian takes the gauge-covariant form:

$$H_{eff} = (1/2m)(-i\hbar\,\partial_s - A_s)^2 + V_g$$

Expanding and retaining only the linear cross-term (the quadratic A_s^2 term contributes a small scalar shift) and working in the minimal single-coupling model:

$$H_{eff} = p_s^2/(2m) + V_g + \lambda\,(\vec{\sigma}\cdot\hat{B})\,p_s$$

where the spin-momentum coupling constant is:

$$\lambda \equiv C\,\hbar\tau\,/\,(2m)$$

Here C is a dimensionless projection coefficient that collects corrections beyond the simplest reduced spin-connection term. Two distinct effects contribute to it. First, there are *confinement-induced corrections* from the finite transverse width of the wavefunction in the curved tube geometry, scaling as $O(\rho_0^2/R^2)$ and parametrically small when $\rho_0 \ll R$. Second, there are *frame-mixing corrections* from the curvature–torsion interplay in the co-rotating-frame reduction: for B-DNA the ratio $\kappa c/\tau \sim 1.75$ is not small, so this second source can produce an order-unity correction to C even when confinement corrections are modest. Accordingly, the statement $C \sim 1$ should be read as a controlled scaling statement — the sign structure and torsion-dominant functional dependence are robust, while the exact magnitude remains uncertain at order unity until C is computed from a realistic molecular electronic structure. A fully explicit curved-frame reduction also generates a subleading spin term proportional to curvature × torsion and independent of k — schematically $\delta H_{sub} \sim (\hbar^2\kappa c\tau/m)(\vec{\sigma}\cdot\hat{T})$ — which does not affect the leading chirality-dependent spin-momentum coupling and is omitted from the minimal model; it is absorbed into C. A schematic calculation of the confinement-induced part of C under a harmonic transverse potential is given in Appendix C.

Dimensional check. λ has units of (m/s), since $\hbar/m$ has units of m^2/s and τ has units of m^{-1}. The coupling term $\lambda\,(\vec{\sigma}\cdot\hat{B})\,p_s$ then has units of $(m/s)(kg\cdot m/s) = kg\cdot m^2/s^2 = J$, as required for an energy.

Handedness reversal. Under chirality reversal — replacing a right-handed helix with its left-handed mirror image — the torsion changes sign: $\tau \to -\tau$. Since $\lambda \propto \tau$, we have $\lambda \to -\lambda$. The spin-momentum coupling term then changes sign:

$$\lambda\ (\vec{\sigma}\cdot\hat{B})\ p_s \ \rightarrow\ -\lambda\ (\vec{\sigma}\cdot\hat{B})\ p_s$$

This reverses the energetic preference between spin-up and spin-down propagation, predicting exactly opposite spin polarizations for enantiomeric molecules. In the idealized uniform-helix model, the sign reversal under chirality inversion is symmetry-exact and independent of the numerical value of the coupling coefficient C.

Relationship to Rashba convention. The Hamiltonian can be rewritten in the Rashba form by defining $\alpha_R \equiv \hbar\lambda$ (units: eV·m):

$$H_{eff} = p_s^2/(2m) + V_g + (\alpha_R/\hbar)(\vec{\sigma}\cdot\hat{B})\ p_s$$

This connects the geometric derivation to the phenomenological Rashba literature, where α_R is typically treated as a fit parameter. The derivation here shows that, geometrically, $\alpha_R = \hbar\lambda = C\hbar^2\tau/m$ — a quantity whose leading geometric dependence is set by torsion, with curvature-dependent corrections entering through V_g and through the effective coefficient C.

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3. Dispersion Relation and Spin Splitting

3.1 Spin-Split Bands

Choosing spin eigenstates along the fixed co-rotating-frame axis — so that $(\vec{\sigma}\cdot\hat{B})|\pm\rangle = \pm|\pm\rangle$, where $\hat{B}$ denotes this effective quantisation axis — and substituting $p_s = \hbar k$, the eigenvalues of H_{eff} are:

$$E_\pm(k) = \hbar^2k^2/(2m) + V_g \pm \lambda\hbar k$$

This dispersion has three immediate structural consequences:

1. **Spin splitting for $k \neq 0$.** The ± branches are energetically non-degenerate whenever there is directed motion. The splitting $2\lambda\hbar k$ is linear in k and in the torsion.
2. **Exact reversal with chirality.** Under $\tau \rightarrow -\tau$ (hence $\lambda \rightarrow -\lambda$), the + and − branches exchange. The left-handed helix favours the opposite spin from the right-handed helix. In the idealized uniform-helix model this is a symmetry-exact result, not a perturbative approximation.
3. **Vanishing at k = 0.** At zero net momentum both spins are degenerate. Spin polarization requires directed, nonequilibrium transport — a bias voltage, contact asymmetry, or nonequilibrium injection condition. This is consistent with experimental observations that CISS signals depend on bias voltage and contact geometry.

3.2 Group Velocities

Taking the k-derivative of $E_\pm(k)$:

$$v_{\pm}(k) = (1/\hbar)\, dE_{\pm}/dk = \hbar k/m \pm \lambda$$

The ± spin branch propagates faster or slower by the fixed velocity offset $\lambda = C\hbar\tau/(2m)$. For a right-handed helix ($\tau > 0$), the + spin propagates faster; for a left-handed helix ($\tau < 0$), the preference reverses. This velocity splitting is linear and immediately feeds into the transport asymmetry.

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4. Spin-Resolved Transport in the Landauer Picture

4.1 Landauer Formalism for Spin-Polarized Transport

The semiclassical velocity ratio provides useful intuition but is not rigorous for a quantum transport calculation. We replace it with the Landauer framework, which is the appropriate formalism for phase-coherent single-molecule transport.

For a two-spin-channel 1D conductor, define spin-resolved transmission coefficients $T_{\pm}(E)$ — the probability that an electron with energy E and spin ± is transmitted through the molecule. The spin-resolved Landauer currents are:

$$I_{\pm} = (e/h) \int dE \; T_{\pm}(E) \, [f_L(E) - f_R(E)]$$

where $f_L(E)$ and $f_R(E)$ are Fermi–Dirac distributions for the left and right electrodes at chemical potentials $\mu_L = E_F + eV/2$ and $\mu_R = E_F - eV/2$ respectively. The measurable spin polarization is:

$$P = (I_+ - I_-) / (I_+ + I_-)$$

In the narrow-bias, low-temperature limit ($eV \ll k_BT$, $k_BT \to 0$), the Fermi window collapses to a delta function at E_F and the currents simplify:

$$I_{\pm} \approx (e^2/h)\, V \cdot T_{\pm}(E_F)$$

giving:

$$P \approx [T_+(E_F) - T_-(E_F)] / [T_+(E_F) + T_-(E_F)]$$

The task now is to determine how the helical Hamiltonian shifts $T_{\pm}$ away from equality.

4.2 Transmission Coefficients from the Spin-Split Dispersion

For a finite helical segment of length $\ell = NL$ (N turns, L arc length per turn) connected to spin-unpolarized contacts, the spin-split dispersion generates different Fermi wavevectors for the two spin channels. From $E_{\pm}(k_{\pm}) = E_F$:

$$\hbar^2 k_\pm^2/(2m) \pm \lambda\hbar k_\pm + V_g = E_F$$

Solving perturbatively for small λ, define k_F by $E_F = \hbar^2 k_F^2/(2m) + V_g$ and write $k_\pm = k_F + \delta k_\pm$. Expanding to first order and equating to zero:

$$(\hbar^2 k_F/m)\,\delta k_\pm \pm \lambda\hbar k_F = 0$$

giving the first-order Fermi wavevector shifts:

$$\delta k_\pm = \mp m\lambda/\hbar$$

and therefore:

$$k_\pm \approx k_F \mp m\lambda/\hbar = k_F (1 \mp \eta)$$

where the dimensionless control parameter is defined as the fractional wavevector splitting:

$$\eta \equiv m\lambda / (\hbar\, k_F) = C\tau / (2k_F)$$

The second equality follows from substituting $\lambda = C\hbar\tau/(2m)$ and confirms that η is dimensionless: it is the ratio of torsion τ (units m^{-1}) to Fermi wavevector k_F (units m^{-1}), scaled by the order-unity factor C.

The transmission amplitude for each spin channel through a segment of length ℓ acquires a spin-dependent phase $\varphi_\pm = k_\pm \ell$. For any smooth transmission function $T(\varphi)$ depending on the accumulated phase, the spin-dependent wavevector shifts $\delta k_\pm = \mp m\lambda/\hbar$ produce phase shifts $\delta\varphi_\pm = \mp\delta k\, \ell$ where $\delta k = m\lambda/\hbar = \eta k_F$. Taylor expanding $T_\pm$ to first order around the spin-averaged phase $\varphi_0 = k_F \ell$:

$$T_\pm = T(\varphi_0 \pm \delta\varphi) \approx T_0 \pm \delta\varphi\, (\partial T/\partial\varphi) = T_0 \pm (k_F \ell)(\partial T/\partial\varphi) \cdot \eta$$

Defining the contact-dependent asymmetry factor:

$$\delta T \equiv k_F \ell \cdot (\partial T/\partial\varphi) \quad [\text{evaluated at } \varphi = k_F \ell]$$

gives the first-order result:

$$T_\pm(E_F) \approx T_0 \pm \delta T \cdot \eta$$

This parametrization is not an arbitrary ansatz: it follows directly from the smoothness of $T(\varphi)$, the first-order wavevector splitting, and the definition of phase accumulation. The quantity δT is a defined function of the contact geometry and the operating phase $\varphi_0 = k_F \ell$; it oscillates with $k_F \ell$ and is governed by the contact reflectivity. In the presence of dephasing over a length $\ell_\varphi < \ell$, the oscillatory interference is suppressed and the expansion remains valid with ℓ replaced by ℓ_φ. The reduction $T_\pm \approx T_0 \pm \delta T \cdot \eta$ is the leading-order consequence of a first-order expansion in the small parameter η, once the transmission is treated as a smooth function of accumulated phase. The spin polarization then becomes:

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P ≈ δT · η / T₀  =  (δT / T₀) · (Cτ / (2k_F))
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This is the central transport result. Polarization is proportional to $\eta = C\tau/(2k_F)$, the ratio of geometric torsion to Fermi wavevector. Strong CISS — $P \sim 1$ — requires $\eta \sim T_0/\delta T \sim 1$. For DNA-like parameters with $\eta \sim 0.2$, achieving sizable polarization requires $\delta T/T_0$ to be a non-negligible fraction of unity. Physically, $\delta T/T_0 \sim 1$ corresponds to a strongly reflective contact (reflection amplitude r not small), in which the Fabry–Pérot phase sensitivity $\partial T/\partial\varphi$ is large. For nearly transparent contacts ($r \to 0$), $\delta T \to 0$ and polarization is suppressed regardless of η.

4.3 The Dimensionless Control Parameter and Experimental Range

The control parameter $\eta = C\tau/(2k_F)$ has a transparent physical meaning: it measures the fractional splitting of the two spin-channel Fermi wavevectors induced by the helical geometry. When $\eta \sim 1$, the geometric coupling is strong enough to shift the wavevectors of the two spin channels by a fraction of themselves, producing order-unity phase difference and transmission asymmetry.

Substituting DNA parameters ($\tau = d/(R^2 + d^2) \approx 0.44$ nm^{-1}, $k_F \sim 1$ nm^{-1} for a typical injection energy of a few eV, $C \sim 1$):

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η ~ 0.44 / (2 × 1)  ~  0.22
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This places DNA firmly within the regime $\eta \sim 0.1$–1, in which the geometric mechanism can support experimentally relevant polarization provided the contact-dependent asymmetry factor $\delta T/T_0$ is not too small. Longer molecules (larger N) accumulate a larger spin-dependent phase difference $\Delta\varphi = (k_+ - k_-)\,\ell = 2\eta\, k_F\, \ell$, which can enhance transmission asymmetry even when the local control parameter η itself is fixed by molecular geometry. This provides a natural account of the observed length dependence of CISS polarization without additional parameters.

Claim. Helical geometry is sufficient to generate a spin-selective transport term of the correct symmetry and of potentially experimentally relevant magnitude. Whether the bare geometric coupling η, without renormalization from contacts, dephasing, or atomic SOC, quantitatively accounts for all observed CISS in every molecular system is a separate empirical question that the present toy model does not settle.

4.4 Summary of the Mathematical Chain

The logical structure of the derivation is:

1. The helix defines a nontrivial rotating frame with curvature κc and torsion τ.
2. Constraining an electron to this curve induces, upon projection to the lowest transverse mode, a geometric scalar potential $V_g = -\hbar^2\kappa c^2/(8m)$ and a spin connection $A_s = (\hbar/2)\tau(\vec{\sigma} \cdot \hat{B})$.
3. The spin connection produces an effective spin-dependent gauge potential along the transport direction, yielding the coupling $\lambda = C\hbar\tau/(2m)$.
4. For uniform helices this gives spin-split bands: $E_\pm(k) = \hbar^2k^2/(2m) + V_g \pm \lambda\hbar k$.

5. The sign of λ reverses with chirality ($\tau \to -\tau$), so enantiomers produce opposite polarizations.
6. Under bias, spin-resolved transmissions differ: $T_{+}(E_F) \neq T_{-}(E_F)$, hence $P \neq 0$.
7. Strong CISS corresponds to $\eta = m\lambda/(\hbar k_F) = C\tau/(2k_F) \sim 1$, while DNA-like parameters place the system in the experimentally relevant regime $\eta \sim 0.1–0.5$.

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5. VERSF Interpretation

5.1 Admissible Transitions and Structural Constraints

Within the Void Energy-Regulated Space Framework, physical processes are not merely particles traversing a neutral background space. All processes consist of irreversible commitments — transitions from one distinguishable state to another — occurring within a structured field that constrains which transitions are possible. The framework introduces the concept of an **admissibility condition**: a physical transition can occur only if it is compatible with the structural constraints of the system in which it takes place.

This differs from conventional selection rules in a specific sense. VERSF holds that structural constraints are **constitutive**: they do not filter transitions from a pre-given neutral catalogue, but rather enter the definition of the operative transition landscape itself — including the energetic weighting, phase structure, and transport accessibility of possible outcomes. In the present context, "constitutive" does not imply that incompatible transitions are strictly forbidden by a sharp rule. It means instead that the geometry determines the effective state space: the relative measure of different outcomes, the accessibility of different propagation modes, and the phase relationships between interfering pathways. The geometry does not simply filter an otherwise-fixed catalogue; it helps constitute what the operative catalogue is.

The derivation in Sections 2–4 gives this claim a precise mathematical form: the spin connection A_s of the rotating Frenet–Serret frame is the operator through which molecular geometry enters the quantum dynamics of the transiting electron. It is not a force; it is a structural feature of the configuration space that the electron must navigate.

5.2 The Chiral Molecule as an Admissibility Filter

A chiral molecule constrains any transiting electron to follow a helical trajectory. This trajectory carries intrinsic angular momentum — the Darboux vector of the Frenet–Serret frame — whose sign is fixed by the torsion τ of the helix. Electron spin is itself a form of angular momentum. The helical constraint therefore couples three quantities — propagation direction, structural handedness ($\mathrm{sgn}\,\tau$), and spin — into a relationship that the electronic state must respect throughout its transit.

In VERSF language: the molecular geometry restricts the set of admissible transition pathways. The two spin channels acquire different effective wavevectors and therefore different phase accumulation and transmission conditions. Because transmission depends on the accumulated

phase $k \pm \ell$, the spin-dependent wavevector shifts place the two channels at different points on the contact-dependent transmission curve, thereby favouring one channel over the other. Which spin is favoured depends on the sign of the torsion — and reverses exactly when the handedness is reversed.

The spin connection A_s derived in §2.3 is the precise operator encoding this admissibility structure. The molecule does not exert a spin-dependent force in any conventional sense. Instead, it defines a gauge potential that modifies the phase accumulated by each spin channel — a modification that is geometric, not dynamical, and that persists as long as the helical structure is maintained.

5.3 Geometry as Information Structure

A deeper VERSF reading focuses on information rather than force. A chiral molecule encodes directional information — handedness — into its physical structure through the sign of its torsion. This is not merely a label; it is a structural asymmetry that any transiting electron must navigate through the accumulated spin-dependent phase. The process of transmission is therefore not spin-neutral: it is a process in which the molecule's structural information is imprinted onto the transmitted electron population.

VERSF describes this as structural information shaping the available state space. The molecule does not push the electron's spin; it defines a spin-dependent configuration space in which the two spin channels acquire different effective wavevectors, different phase accumulation, and consequently different transmission amplitudes. The electron traverses a spin-dependent geometry, not a spin-dependent force field.

This is the sense in which CISS is geometric rather than dynamical. The selectivity is not produced by an interaction that could be switched off; it is encoded in the topology of the available state space and persists as long as the molecular geometry does.

5.4 Irreversibility and Directed Transport

VERSF places significant weight on the irreversibility of physical commitments. The mathematical result in §3.1 — that spin splitting vanishes at $k = 0$ and requires directed transport — fits naturally into this picture.

In a system at equilibrium, electron flow proceeds in both directions with equal probability, and the geometric imprint on the population averages to zero. Spin polarization requires directed irreversibility: a preferred direction of electron flow enforced by a bias, contact asymmetry, or nonequilibrium injection. The geometry provides the differential between spin channels; directed transport provides the irreversibility that converts this differential into a macroscopic population difference.

Neither element alone is sufficient. A chiral molecule in equilibrium — no applied bias — produces no net polarization ($k = 0$ degeneracy). A bias applied to an achiral conductor — $\tau = 0$,

hence $\lambda = 0$ — produces no spin asymmetry. The conjunction of structural handedness and directed irreversibility is what the framework requires, and what the derivation confirms.

5.5 What VERSF Adds Beyond Conventional Accounts

Unifying language across systems. The geometric mechanism is a model of CISS specifically. VERSF generalizes the underlying principle: any physical structure that encodes asymmetric information will generate admissibility conditions that selectively favour certain state transitions. CISS is one instance. The broader VERSF suggestion — that structurally asymmetric processes such as transmission through topological defects or chiral selection in prebiotic chemistry may belong to the same class — is a direction for future investigation that lies beyond the scope of the present paper.

Predictive sharpening. If the admissibility-constraint picture is correct, CISS polarization should correlate with the geometric control parameter $\eta = C\tau/(2k\_F)$, independently of molecular chemistry. A specific prediction follows: two molecules with identical chemical composition but different helical parameters should show different CISS polarizations in proportion to their geometric asymmetry. This is testable using synthetic helical polymers of controlled pitch and radius. More directly: the polarization should scale with $|\tau| = d/(R^2+d^2)$, and should vanish for any molecular conformation in which the torsion is zero, regardless of chemical composition.

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6. Open Questions and Limitations

Magnitude of C. The coefficient C receives two distinct contributions: confinement-induced corrections scaling as $O(\rho_0^2/R^2)$, and potentially order-unity frame-mixing corrections associated with the curvature–torsion structure of the full Darboux vector. Appendix C shows that the former are modest for tight confinement; Appendix A explains why the latter remain the dominant quantitative uncertainty for B-DNA-like geometry. Thus $C \sim O(1)$ is a controlled scaling statement, not a precision estimate.

Multi-mode transport. The analysis is explicitly single-mode. In real molecules multiple electronic orbitals contribute, and mode averaging generically reduces polarization from the single-mode maximum. A complete theory requires summing over all relevant transverse modes and accounting for their different geometric couplings.

The role of atomic SOC. Setting atomic SOC to zero isolates the geometric mechanism. Whether atomic SOC is necessary to seed or amplify the geometric effect in real molecules remains open. In the VERSF interpretation, both contributions shape the admissibility landscape and need not be mutually exclusive; they may be multiplicatively coupled in the effective control parameter η.

Equilibrium vs. nonequilibrium. The vanishing of spin splitting at $k = 0$ predicts no macroscopic spin polarization in purely equilibrium measurements. Systematic comparison with

equilibrium spectroscopic data (circular dichroism, magneto-optical measurements) would provide a sharper test of the geometric picture.

Dephasing. The Landauer analysis assumes phase coherence over the entire molecular length — an idealized limit that is far from satisfied in real organic molecules at room temperature, where dephasing lengths are typically much shorter than molecular lengths. The coherent single-mode Landauer picture developed here is a minimal theoretical model, not a quantitative description of room-temperature CISS. That said, the geometric effect does not require full coherence over the entire molecule. If the phase coherence length $\ell_\varphi < \ell$, the effective interference length is ℓ_φ rather than ℓ, and the accumulated spin-dependent phase difference is:

$$\Delta\varphi = (k_+ - k_-)\,\ell_\varphi = 2\eta\, k_F\, \ell_\varphi$$

Spin polarization scales as $P \sim \sin(\Delta\varphi)$ for a single coherent segment, so appreciable polarization requires:

$$\eta\, k_F\, \ell_\varphi \gtrsim 1$$

For B-DNA parameters ($k_F \sim 1$ nm^{-1}, $\eta \sim 0.2$), this requires only:

$$\ell_\varphi \gtrsim 1/(\eta\, k_F) \sim 2\text{–}3 \text{ nm}$$

This indicates that the geometric mechanism need not be extremely fragile to partial room-temperature dephasing. Dephasing suppresses the Fabry–Pérot interference that enhances polarization through $\partial T/\partial\varphi$, but the k-vector splitting between spin channels — and hence some residual polarization — persists even in the incoherent limit. A quantitative account of the full dephasing-length dependence requires going beyond the present model.

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7. Conclusion

The Chiral-Induced Spin Selectivity effect demonstrates that molecular geometry can govern quantum transport outcomes. Starting from the three-dimensional Pauli Hamiltonian in the Frenet–Serret frame of the helix, we have derived that constraining an electron to a helical path generates, upon projection to the lowest transverse mode, a da Costa geometric scalar potential and a spin connection that acts as a spin-dependent gauge potential along the transport direction. The effective spin-momentum coupling is $\lambda = C\hbar\tau/(2m)$, controlled by torsion and reversing exactly under chirality reversal $\tau \to -\tau$. In the Landauer picture, this coupling shifts the Fermi wavevectors of the two spin channels by $\pm m\lambda/\hbar$, generating a dimensionless splitting $\eta = m\lambda/(\hbar k_F) = C\tau/(2k_F)$ and spin-resolved transmission asymmetry. For DNA-like parameters, $\eta \sim 0.2$, placing the geometric mechanism in the experimentally relevant regime.

Helical geometry is sufficient to generate a spin-selective transport term of the correct symmetry and of potentially experimentally relevant magnitude. Whether the bare geometric coupling,

without renormalization, quantitatively accounts for all CISS in every molecular system is a separate empirical question; the present derivation does not claim to settle it.

Within the VERSF framework, CISS is an instance of a general principle: physical structures constitute the admissibility landscape of possible transitions. The spin connection of the helical Frenet–Serret frame is the mathematical object through which molecular geometry enters the quantum dynamics of the transiting electron — not as a force, but as a modification of the configuration space itself. Directed, nonequilibrium transport then converts this geometric asymmetry into a macroscopic physical fact. The chiral molecule does not push spin; it defines a state space in which the two spin channels acquire different effective wavevectors, different phase accumulation, and consequently different transmission amplitudes — with the favoured spin channel reversing with the sign of the molecular torsion in the minimal model.

The broader implication is this: geometry is not a passive background for quantum processes. It is an active participant — one that defines, weights, and selects the transitions that physical processes can make. The CISS effect makes this principle visible and mathematically precise at the molecular scale. The VERSF framework suggests it operates at every scale at which physical structure can be said to exist.

Appendix A: Spin Connection for a Constrained Pauli Spinor on a Helix

This appendix sketches the reduction from the three-dimensional Pauli Hamiltonian to the effective 1D spin-coupled form, making explicit the role of the Darboux vector and the co-rotating frame transformation.

A.1 Frenet–Serret frame and Darboux vector. For a space curve parameterised by arc length s, the Frenet–Serret frame $\{\hat{T}, \hat{N}, \hat{B}\}$ satisfies:

$$\frac{d\hat{T}}{ds} = \kappa c\, \hat{N}$$
$$\frac{d\hat{N}}{ds} = -\kappa c\, \hat{T} + \tau\, \hat{B}$$
$$\frac{d\hat{B}}{ds} = -\tau\, \hat{N}$$

These equations can be written compactly in terms of the Darboux vector Ω, defined by $d\hat{e}_i/ds = \Omega \times \hat{e}_i$ for each frame vector $\hat{e}_i \in \{\hat{T}, \hat{N}, \hat{B}\}$. Matching to the Frenet–Serret equations gives:

$$\Omega = \tau\, \hat{T} + \kappa c\, \hat{B}$$

For a uniform helix, both κc and τ are constant, so $|\Omega| = \sqrt{(\kappa c^2 + \tau^2)} = 1/\Lambda$ is constant as well.

A.2 Spinor covariant derivative. A Pauli spinor transported along the curve must be differentiated covariantly with respect to the rotating frame. The covariant derivative along s is:

$$\nabla_s = \partial_s - (i/2)(\Omega \cdot \vec{\sigma})$$

so the longitudinal kinetic term becomes:

$$-(\hbar^2/2m)\ \nabla_s^2 = -(\hbar^2/2m)(\partial_s - (i/2)(\Omega \cdot \vec{\sigma}))^2$$

Substituting $\Omega = \tau\,\hat{T} + \kappa c\,\hat{B}$ and writing $\sigma\_T = \vec{\sigma} \cdot \hat{T}$, $\sigma\_B = \vec{\sigma} \cdot \hat{B}$:

$$\nabla_s = \partial_s - (i/2)(\tau\ \sigma\_T + \kappa c\ \sigma\_B)$$

Note the component assignment: torsion τ multiplies σ_T (along $\hat{T}$) because torsion measures rotation around $\hat{T}$; curvature κc multiplies σ_B (along $\hat{B}$) because curvature measures rotation around $\hat{B}$. Before any frame transformation or projection, both torsion and curvature enter the spin connection.

A.3 Co-rotating-frame transformation. Introduce a unitary transformation U(s) that rotates the spinor into a frame whose fixed axis is aligned with the helix axis. For a uniform helix, U(s) is the spin-space rotation by accumulated torsional angle $\varphi(s) = \tau s$ about the fixed helix axis $\hat{B}\_axis$:

$$U(s) = \exp[-(i/2)\ \varphi(s)\ (\vec{\sigma} \cdot \hat{B}\_axis)], \quad \varphi(s) = \tau s$$

Setting $\psi(s) = U(s)\,\tilde{\psi}(s)$, then $\partial_s\psi = U(\partial_s + U^\dagger\partial_s U)\tilde{\psi}$, and the covariant derivative becomes:

$$\nabla_s\ \psi = U\ [\partial_s - (i/2)(\Omega eff \cdot \vec{\sigma})]\ \tilde{\psi}$$

with the effective Darboux vector in the transformed frame:

$$\Omega eff = U^\dagger\ \Omega\ U - 2i\ U^\dagger\ \partial_s\ U$$

For a uniform helix, the co-rotating choice of U removes the explicit s-dependence of the frame, so the effective connection is constant in the transformed basis. Concretely, the unitary U tracks the helical rotation of angle $\varphi(s) = \tau s$ about the fixed helix axis, acting on the spin part as a rotation. The frame-vector projections transform as:

$$U^\dagger\ \sigma\_T\ U = \sigma\_\{B\_eff\}$$
$$U^\dagger\ \sigma\_B\ U = \cos\varphi(s)\ \sigma\_\perp + \sin\varphi(s)\ \sigma\_\perp'$$

where $\sigma\_\{B\_eff\} = \vec{\sigma} \cdot \hat{B}\_eff$ is the fixed-axis spin projection and $\sigma\_\perp$, $\sigma\_\perp'$ are spin projections onto the two transverse directions perpendicular to the helix axis. The torsional term $\tau\sigma\_T$ therefore maps to the fixed-axis term $\tau\sigma\_\{B\_eff\}$, while the curvature term $\kappa c\sigma\_B$ maps to oscillatory transverse spin components rotating at frequency τ in s. Upon projection onto the rotationally symmetric lowest transverse mode χ_0, which has no preferred azimuthal orientation, the oscillatory transverse terms average to zero at leading order: $\langle\chi_0|e^{\pm i\varphi(s)}|\chi_0\rangle = 0$. Accordingly, the leading projected connection takes the reduced form:

$$\Omega eff = \tau\ \hat{B}\_eff + \delta\Omega\kappa$$

where $\delta\Omega\kappa$ denotes curvature-dependent residual terms.

A.4 Effective gauge potential and one-dimensional Hamiltonian. Projecting onto the rotationally symmetric lowest transverse mode χ_0, the leading spin connection term becomes:

$$A_s = (\hbar/2)\,\tau\,(\vec{\sigma}\cdot \hat{B}_{eff})$$

so the longitudinal momentum shifts as $-i\hbar\partial_s \rightarrow -i\hbar\partial_s - A_s$. Expanding the square in the kinetic term:

$$H_{eff} = p_s^2/(2m) + (1/2m)(-p_s A_s - A_s p_s) + A_s^2/(2m) + V_g + \delta H_\kappa$$

For constant A_s, the cross-term simplifies to:

$$(1/2m)(-p_s A_s - A_s p_s) = -(A_s/m)\,p_s = -(\hbar\tau/2m)(\vec{\sigma}\cdot \hat{B}_{eff})\,p_s$$

This is the origin of the spin-momentum coupling in the main text, written as $\lambda(\vec{\sigma}\cdot\hat{B})\,p_s$ with $\lambda \equiv C\hbar\tau/(2m)$. The leading-order reduced-connection calculation gives a prefactor of exactly $\hbar\tau/(2m)$, which matches the main-text definition with $C = 1$ at leading order. The coefficient C absorbs the difference between this leading-order result and the fully projected lowest-mode Hamiltonian, including confinement-profile dependence, basis-choice corrections, and the curvature-dependent frame-mixing terms discussed in A.3. With the consistent definition $\lambda \equiv C\hbar\tau/(2m)$, there is no numerical-prefactor ambiguity between Appendix A and the main text; C is genuinely a correction coefficient starting from unity rather than a device for hiding a conventional factor.

A.5 What is controlled and what is not. The derivation above establishes three things cleanly: (i) both curvature and torsion enter the full spin connection before projection; (ii) after transformation to the co-rotating frame, the leading constant-axis term is torsion-controlled; (iii) the resulting one-dimensional Hamiltonian necessarily contains a chirality-sensitive spin-momentum coupling linear in τ. What this appendix does not provide is a first-principles value of C for a real molecule — that depends on how the full curved-frame spin connection is projected onto the actual molecular transverse state and is therefore model-dependent. The two distinct sources of uncertainty in C are characterised in Appendix C.

Appendix B: Key Symbols and Parameters

(See also Appendix A for the spin connection derivation and Appendix C for the toy calculation of C.)

Symbol	Meaning	Typical Value (B-DNA)
R	Helix radius	~1 nm
d	Pitch parameter (axial rise per radian)	~0.54 nm
$2\pi d$	Axial rise per turn	~3.4 nm

Symbol	Meaning	Typical Value (B-DNA)
$\Lambda = \sqrt{(R^2+d^2)}$	Normalisation factor	~1.14 nm
$L = 2\pi\Lambda$	Arc length per turn	~7.1 nm
$\kappa c = R/(R^2+d^2)$	Curvature	~0.77 nm^{-1}
$\tau = d/(R^2+d^2)$	Torsion	~0.44 nm^{-1}
$h = sgn(\tau)$	Handedness	±1
$\hat{T}, \hat{N}, \hat{B}$	Frenet–Serret tangent, normal, binormal	—
$A_s = (\hbar/2)\tau(\vec{\sigma}\cdot\hat{B})$	Spin connection (gauge potential)	—
$Vg = -\hbar^2\kappa c^2/(8m)$	da Costa geometric scalar potential	spin-independent
$\lambda = C\hbar\tau/(2m)$	Spin-momentum coupling velocity	~ C × 0.04 nm/ps
$\alpha\_R = \hbar\lambda$	Rashba-like geometric coupling (eV·m)	parameter
C	Dimensionless confinement/projection factor	O(1)
$E_0 = \hbar^2/(2mL^2)$	Geometric energy scale	~0.75 meV
$\eta = m\lambda/(\hbar k\_F) = C\tau/(2k\_F)$	Dimensionless control parameter	~0.2 (DNA)
$T\pm(E\_F)$	Spin-resolved Landauer transmission coefficients	—
P	Spin polarization	10–80% (experiment)

Appendix C: Toy Calculation of the Confinement Coefficient C

The coefficient C in $\lambda = C\hbar\tau/(2m)$ collects corrections beyond the simplest reduced spin-connection result. It is important to distinguish two conceptually different contributions:

(i) **Confinement-induced corrections**, controlled by the finite transverse width of the wavefunction and scaling as $O(\rho_0^2/R^2)$. These are parametrically small when $\rho_0 \ll R$.

(ii) **Frame-mixing corrections**, arising from the interplay between the curvature and torsion components of the full Darboux vector in the co-rotating-frame reduction. For B-DNA, the ratio $\kappa c/\tau \sim 0.77/0.44 \sim 1.75$ is not small, so this mixing can produce an order-unity correction to C even when the confinement corrections are modest.

The toy harmonic calculation in this appendix constrains only the first of these. It shows that transverse-confinement corrections are naturally small in the tight-confinement limit, supporting the statement that C is generically of order unity. It does not eliminate the separate order-unity uncertainty associated with curvature–torsion mixing in the full projected Hamiltonian.

C.1 Setup. Take the transverse confining potential to be harmonic:

$$V_{conf}(\rho) = (1/2)\, m\, \omega_0^2\, \rho^2$$

with confinement frequency ω_0. The transverse ground state is a Gaussian:

$$\chi_0(\rho) = (1 / (\sqrt{\pi}\, \rho_0))\, \exp(-\rho^2 / 2\rho_0^2), \quad \rho_0 = \sqrt{(\hbar / m\, \omega_0)}$$

normalized so that $\int |\chi_0(\rho)|^2\, d^2\rho = 1$ (integration over the full 2D transverse plane).

with characteristic confinement radius ρ_0.

C.2 Projection with coordinate corrections. In the curvilinear Frenet–Serret coordinates, the metric along the helical curve acquires a correction due to the finite tube radius. At radial offset ρ from the curve, the arc-length element scales as $(1 + \kappa c\, \rho \cos\varphi)$, where φ is the azimuthal angle in the transverse plane. This modifies the effective spin-connection coupling so that the projected coupling becomes:

$$\lambda = (\hbar\tau/m) \cdot \langle \chi_0 \mid f(\rho) \mid \chi_0 \rangle$$

where $f(\rho)$ encodes the curvature-dependent modification of the integration measure. Expanding to leading order in ρ/R:

$$f(\rho) \approx 1 + O(\rho^2/R^2)$$

The azimuthally averaged correction $\langle \cos\varphi \rangle = 0$ eliminates the linear term, giving:

$$\langle \chi_0 \mid f(\rho) \mid \chi_0 \rangle = 1 + O(\rho_0^2/R^2)$$

C.3 Result from harmonic confinement. For the harmonic transverse ground state, the projection gives:

$$C_{conf} \approx 1 + O(\rho_0^2/R^2)$$

For representative molecular parameters:

$$\rho_0 \sim 0.2\ \text{nm},\ R \sim 1\ \text{nm} \rightarrow \rho_0^2/R^2 \sim 0.04 \quad \text{(tight confinement)}$$
$$\rho_0 \sim 0.5\ \text{nm},\ R \sim 1\ \text{nm} \rightarrow \rho_0^2/R^2 \sim 0.25 \quad \text{(looser estimate)}$$

These values confirm that the confinement-induced renormalization of the coupling remains modest across the physically relevant range.

C.4 Interpretation and scope. The full coefficient C may be written schematically as:

$$C = C_{conf} \cdot C_{mix}$$

where C_conf is the confinement part calculated above and C_mix represents the additional renormalization from curvature–torsion mixing in the co-rotating-frame reduction. The harmonic model gives C_conf ≈ 1 with corrections of order ρ_0^2/R^2. It does not fix C_mix.

For B-DNA, $\kappa c/\tau \approx 0.77/0.44 \approx 1.75$, so the curvature–torsion mixing is not parametrically small. As a result, the full coefficient C is expected to remain of order unity but may carry an order-unity uncertainty in magnitude. The correct interpretation is therefore:

- the functional dependence $\lambda \propto \tau$ is robust and symmetry-exact;
- the confinement correction C_conf is modest in the tight-confinement regime;
- the overall numerical prefactor C = C_conf · C_mix remains uncertain at order unity until a realistic molecular projection is carried out.

This is sufficient for the purposes of the present paper, which aims to establish symmetry structure and scaling rather than precision prediction.

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