Open Problems from Flügge's *Practical Quantum Mechanics*

A book-to-frontier map for PhD research in theoretical quantum physics

Twelve book-anchored research directions, each mapped to current literature, explicit formalisms, a precise research deliverable, starting references, and a verified Maxima research model.

Literature audited through 16 July 2026

Source: S. Flügge, *Practical Quantum Mechanics*, Springer

Contents

Scope, filtering rule, and book map

Flügge's 219 worked problems are controlled seed models, not statements of unsolved research. The filtering operation used here is

$$\text{solvable seed} \longrightarrow \text{remove one structural assumption} \\ \longrightarrow \text{identify the new obstruction} \longrightarrow \text{specify a falsifiable result.}$$

An extension was retained only when it has a current literature boundary, a precise operator or Hamiltonian, and a result that could become a theorem, an analytical expression, a controlled asymptotic expansion, or a quantitatively testable prediction.

No.	Research direction	Flügge seed	Primary research style
1	Borel-summed radial resonance determinant	I: 58–79, 115–124	mathematical physics
2	Non-Hermitian matrix inverse scattering at defective poles	I: 20–29, 80–114	scattering/inverse problems
3	Lossy anisotropic matrix threshold expansion	I: 27, 83–103	AMO/nuclear scattering
4	Exact non-Bloch Floquet–Sambe delta comb	I: 28–29; II: 179–182	condensed matter
5	Finite-coupling non-Markovian Zeno dynamics	I: 12	open quantum systems
6	NLO Efimov universality with range, SOC, and loss	I: 75–79; II: 139–166	few-body EFT
7	Constraint-preserving orbital-free kinetic-energy functionals	II: 167–178	electronic/nuclear DFT
8	Continuum–lattice matching of supercritical Dirac poles	II: 201–209	Dirac materials
9	Tensor observables under EFT/SRG with joint errors	II: 140–147	nuclear theory
10	Certified differentiable continuation of scattering poles	I: 77–79, 94–108	computational theory
11	Gauge-consistent Coulomb transitions in structured pulses	II: 185–188, 210–219	AMO/strong-field theory
12	Frame-covariant quantum-clock interferometry	I: 40–41	foundations/interferometry

The word *open* is used conservatively: it denotes a defensible, currently unclosed research target after literature filtering, not a guarantee that no group is working on it. A final proposal must repeat the novelty search for its chosen subproblem.

Computational companion. The twelve visible drivers in `maxima/` are compact, executable research baselines: they calculate spectra, kernels, fields, trajectories, asymptotic data, or sensitivities for the tractable core of each problem. They are not Boolean verification snippets and do not claim to solve the full research gaps. Regression assertions are isolated in `maxima/tests/`; run every model with `maxima/run_models.sh` and every test with `maxima/run_tests.sh` from the project root. Topic 2 additionally uses the documented small dense solver in `maxima/lib/`. Each topic states the model's editable inputs, computed outputs, next extension, and present limitation.

1 Borel-summed radial resonance determinant for complex screened singular potentials

Flügge seed: Vol. I, Problems 58–79 and 115–124: central potentials, radial momentum, the Langer correction, eikonal expansion, and radial WKB quantization.

Delabaere and Pham established the resurgent treatment of semiclassical periods, Stokes automorphisms, and coalescing turning points [1]. Ito, Marino, and Shu connected exact-WKB periods to TBA/Riemann–Hilbert systems for polynomial and $\mathcal{PT}$-symmetric potentials [2].

Recent results sharply narrow the radial gap. Morikawa and Ogawa developed an exact-WKB resonance framework using Siegert conditions and complex scaling [3], then treated continuum and resonant spectra in one dimension [4]. Their 2026 radial work handles connection formulae at $r = 0$, origin-to-infinity paths, Langer transformations, and radial oscillator/Coulomb examples, with appendices that also discuss anharmonic, Cornell, and Yukawa-type potentials [5]. Exact-WKB transseries and exceptional-point conditions are also available for one-dimensional resonant models [6]. These advances already cover the generic proposal to "apply exact WKB to a radial Yukawa potential"; novelty must lie in the global resonance construction and its controlled analytic continuation.

What remains unresolved is the simultaneous treatment of a radial regular singularity, a genuinely non-Hermitian screened potential, outgoing Siegert conditions on the resonance sheet, global Stokes-chamber changes, coalescing turning points, and a Borel-summed determinant containing the full pole transseries. Existing radial work is mainly bound-state quantization, while the most complete resonance constructions are mainly one-dimensional.

Formalisms

Radial operator, domain, and physical parameters

Let a particle of mass m move in three dimensions under a central, complex potential. Writing

$$\Psi(\mathbf{r}) = \frac{u_\ell(r)}{r} Y_{\ell m_\ell}(\theta, \varphi), \qquad r > 0, \tag{1}$$

reduces the stationary Schrödinger equation to

$$-\hbar^2 \frac{d^2 u_\ell}{dr^2} + Q_\ell^{\mathrm{ex}}(r, E, \hbar) u_\ell = 0, \tag{2}$$

$$Q_\ell^{\mathrm{ex}}(r, E, \hbar) = 2m[V(r) - E] + \frac{\hbar^2 \ell(\ell+1)}{r^2}. \tag{3}$$

Here E may be complex, $\ell = 0, 1, \ldots$, and the reduced radial space for square-integrable states is $L^2((0, \infty), dr)$. Resonance states are not elements of this Hilbert space; they are defined by analytic continuation of the resolvent, or equivalently by an outgoing boundary condition made square integrable after exterior complex scaling.

The first test family should be fixed rather than left as an arbitrary "screened potential":

$$V(r) = -\frac{g e^{-\alpha r}}{r} - iW e^{-\beta r}, \qquad g, \alpha, \beta > 0, \qquad W \geq 0. \tag{4}$$

The coupling g has units of energy times length, W has units of energy, and α, β are inverse lengths. The sign of the imaginary term describes absorption. The continuation of (4) is meromorphic in the complex r-plane, with its only finite singularity at $r = 0$. A logarithmic cut is introduced later only when choosing a branch of $x = \log(r/L)$.

For computation set $L = \alpha^{-1}$, $E_L = \hbar^2/(2mL^2)$, and

$$\rho = \frac{r}{L}, \quad \epsilon = \frac{E}{E_L}, \quad G = \frac{g}{E_L L} = \frac{2mgL}{\hbar^2}, \quad w = \frac{W}{E_L}, \quad b = \frac{\beta}{\alpha}. \tag{5}$$

Then every numerical spectrum depends only on (G, w, b, ℓ). In a formal semiclassical calculation $\hbar$ is retained as the asymptotic parameter before this nondimensionalization; this distinction prevents a spurious variation of G when taking the formal $\hbar \to 0$ limit.

Origin and infinity boundary data

Near the regular singular point, the screened Coulomb term is less singular than the centrifugal term. Substitution of $u \sim r^\nu$ in (2) gives

$$\nu(\nu - 1) - \ell(\ell + 1) = 0, \qquad \nu = \ell + 1 \text{ or } -\ell. \tag{6}$$

Define the regular Frobenius solution $\phi_\ell(r, E)$ by

$$\lim_{r \downarrow 0} r^{-\ell-1}\phi_\ell(r, E) = 1. \tag{7}$$

Its coefficients follow by inserting $r^{\ell+1}\sum_{n\geq 0} a_n r^n$ and the Taylor series of the exponentials into (2). This local series supplies reproducible initial data at a small radius r_0, avoiding an arbitrary hard-core cutoff.

Because the potential decays exponentially, introduce

$$k(E) = \frac{\sqrt{2mE}}{\hbar}. \tag{8}$$

On the physical sheet choose $\operatorname{Im} k \geq 0$. The Jost solutions are normalized by

$$f_\ell^{(+)}(r, k)e^{-ikr} \longrightarrow 1, \qquad f_\ell^{(-)}(r, k)e^{+ikr} \longrightarrow 1 \quad (r \to \infty). \tag{9}$$

A resonance is reached through the continuum cut onto the sheet $\operatorname{Im} k < 0$, and obeys the purely outgoing condition $u_\ell \propto f_\ell^{(+)}$. The branch of k, the direction of cut crossing, and the continuation path in parameter space must be recorded; otherwise the label "second sheet" is ambiguous when several turning points move simultaneously.

Langer normal form and the spectral curve

The centrifugal singularity is treated without replacing the exact Frobenius indices. Put

$$r = Le^x, \qquad u_\ell(Le^x) = e^{x/2}\psi_\ell(x). \tag{10}$$

Equation (2) becomes exactly

$$-\hbar^2\psi_\ell''(x) + Q_{L,\ell}(x, E, \hbar)\psi_\ell(x) = 0, \tag{11}$$

with

$$Q_{L,\ell} = 2mL^2e^{2x}[V(Le^x) - E] + \hbar^2\left(\ell + \tfrac{1}{2}\right)^2. \tag{12}$$

Thus the familiar replacement $\ell(\ell + 1) \mapsto (\ell + 1/2)^2$ is a consequence of a change of variable, not an ad hoc alteration of (2). In the r-plane the associated Langer momentum is

$$p_{L,\ell}(r, E)^2 = 2m[E - V(r)] - \frac{\hbar^2(\ell + \frac{1}{2})^2}{r^2}. \tag{13}$$

Turning points are the zeros of $p_{L,\ell}^2$. They live, together with the origin and infinity, on the two-sheeted curve

$$\Sigma_E : \quad y^2 = p_{L,\ell}(r, E)^2. \tag{14}$$

Cycles $\gamma \in H_1(\Sigma_E, \mathbb{Z})$ must be transported continuously as E changes. Coalescence occurs when $p_{L,\ell}^2 = \partial_r p_{L,\ell}^2 = 0$; at such points ordinary Airy matching ceases to be uniform.

Riccati expansion and computable recurrences

For either normal form write

$$\psi(x) = \exp\left[\hbar^{-1}\int^{x} S(x',\hbar)\,dx'\right]. \tag{15}$$

Then

$$S^2 + \hbar\partial_x S = Q_{L,\ell}. \tag{16}$$

Decompose $Q_{L,\ell} = Q_0 + \hbar^2 Q_2$ and $S = \sum_{n\geq 0}\hbar^n S_n$. For a selected square-root branch,

$$S_0 = \pm\sqrt{Q_0}, \qquad S_1 = -\frac{S_0'}{2S_0}, \tag{17}$$

$$2S_0 S_n = Q_n - S_{n-1}' - \sum_{j=1}^{n-1} S_j S_{n-j}, \qquad n\geq 2, \tag{18}$$

where $Q_n = Q_2$ for $n = 2$ and $Q_n = 0$ otherwise. These recurrences can be generated symbolically and then evaluated at high precision along a contour that avoids turning points.

Let $S^{(+)}$ and $S^{(-)}$ denote the two formal Riccati branches and define

$$S_{\mathrm{odd}} = \frac{S^{(+)} - S^{(-)}}{2}, \qquad \Pi_\gamma(E,\hbar) = \oint_\gamma S_{\mathrm{odd}}\,dx, \qquad X_\gamma = e^{\Pi_\gamma/\hbar}. \tag{19}$$

Open-path Voros coefficients require subtraction of their endpoint singularities. The subtraction convention at $r = 0$ must agree with (7); changing it rescales connection coefficients even though the resonance zeros remain invariant.

If $\Pi_\gamma \sim \sum_{n\geq 0} p_{\gamma,n}\hbar^n$, define the Borel transform of its tail by $\widehat{\Pi}_\gamma(\zeta) = \sum_{n\geq 0} p_{\gamma,n+1}\zeta^n/n!$ and use lateral sums

$$\mathcal{S}_{\theta\pm}\Pi_\gamma = p_{\gamma,0} + \frac{1}{\hbar}\int_0^{e^{i(\theta\pm 0)}\infty} e^{-\zeta/\hbar}\widehat{\Pi}_\gamma(\zeta)\,d\zeta. \tag{20}$$

Numerically, $\widehat{\Pi}_\gamma$ is continued with diagonal or near-diagonal Padé approximants. Pole condensation in the Borel plane locates Stokes directions and determines where lateral rather than ordinary summation is required.

Stokes transport and the resonance determinant

Stokes curves satisfy a constant-phase condition for $\int^r p_{L,\ell}(r',E)dr'$. Fixing the square-root sheet and curve orientation fixes the intersection pairing $\langle\gamma,\gamma_0\rangle$. Across a simple Stokes wall the Voros symbols transform schematically as

$$\mathfrak{S}_\theta X_\gamma = X_\gamma(1 + X_{\gamma_0})^{\langle\gamma,\gamma_0\rangle}; \tag{21}$$

the sign and possible inverse are not conventions to guess afterwards, but follow from the oriented Stokes graph.

Let $C_0(E)$ convert the regular/singular Frobenius basis into a local WKB basis, and let $C_\infty(E)$ convert the latter into the outgoing/incoming Jost basis. If the chosen path crosses Stokes walls in the order $1,\ldots,n$, define

$$\mathcal{M}_{\mathrm{glob}}(E) = M_n(E)\cdots M_2(E)M_1(E)M_0(E), \tag{22}$$

where M_0 includes the origin monodromy and all entries are Borel summed in one stated direction. The exact unknown is the globally consistent evaluation of this ordered product when the graph mutates and turning points coalesce. Its incoming coefficient is

$$\mathcal{D}_\ell^{\mathrm{EWKB}}(E) = \left[C_\infty^{-1}\mathcal{M}_{\mathrm{glob}}(E)C_0\right]_{\mathrm{incoming,regular}}. \tag{23}$$

An independent, normalization-transparent definition is the Wronskian

$$D_\ell(E) = W_r[f_\ell^{(+)}, \phi_\ell] = f_\ell^{(+)}\phi_\ell' - f_\ell^{(+)'}\phi_\ell. \tag{24}$$

It is independent of r, and its zeros are the resonance poles. With a fixed Jost convention the partial scattering amplitude is a ratio of the incoming and outgoing Jost functions, so $|S_\ell(E)| \le 1$ on the real axis for a passive potential. A pole $E_{n\ell} = E_{n\ell}^{(R)} - i\Gamma_{n\ell}/2$ defines the position and width $\Gamma_{n\ell} > 0$.

Implementation path and internal checks

An implementable calculation proceeds as follows. First locate all turning points at a trial complex E, construct the Stokes graph, and assign cycles by continuation from a reference parameter set. Next generate Riccati coefficients, integrate their regularized periods, Borel–Padé sum them, and multiply the connection matrices in path order. Root finding applied to (23) yields candidate poles. Near a double turning point, replace two Airy connections by a Weber equation obtained from a local quadratic normal form. Continue roots across chamber walls rather than restarting their labels independently in every chamber.

For a direct benchmark, rotate only the exterior coordinate,

$$r = R_c + se^{i\vartheta}, \qquad s \ge 0, \qquad \mathrm{Im}(ke^{i\vartheta}) > 0, \tag{25}$$

inside an analyticity sector of the potential. The outgoing wave then decays and the complex-scaled eigenvalue can be computed with a spectral or finite-element discretization.

Essential checks are: constancy of the direct Wronskian with matching radius; stability under Borel order and lateral direction; agreement of determinants before and after a harmless basis rescaling; continuity under a Stokes mutation; and convergence under the complex-scaling angle and box size. For $W \to 0$, conjugate-pair and real-potential scattering relations must be recovered. For $g \to 0$, the origin still tests the centrifugal monodromy, whereas $\alpha \to 0$ is a singular Coulomb limit and must not be used as a naive numerical convergence test.

Maxima research model

The driver exposes the screened-potential parameters, constructs the Langer Riccati hierarchy through `Nwkb`, and retains reusable functions for the full radial curve. It prints inner and outer turning points, allowed-region actions and semiclassical indices for an energy scan, followed by $S_0, \ldots, S_N$ at a chosen probe radius; the imaginary default S_0 is the expected allowed-branch value. From the project root run

```
maxima --batch=maxima/01_exact_wkb.mac
```

Change `energies`, `Nwkb`, and the turning-point brackets before continuing a new parameter family. Complex turning-point continuation, contour deformation, Borel summation, and Stokes-graph tracking remain outside bare Maxima and require a dedicated continuation code.

```
/* Screened radial exact-WKB workbench (Maxima 5.49). */
kill(all)$
display2d:false$ ratprint:false$ linel:200$

/* Editable physical parameters; W=0 gives the real reference problem. */
m:1$ hbar:7/20$ ell:1$ g:4$ alpha:1/4$
W:0$ beta:2/5$ L:1$ E:-1/5$ Nwkb:3$
langer:(ell+1/2)^2$
V(r):=-g*exp(-alpha*r)/r-%i*W*exp(-beta*r)$
Qfull(r,en):=2*m*r^2*(V(r)-en)+hbar^2*langer$

/* Langer-coordinate Riccati hierarchy: P^2+hbar P'=Q0+hbar^2 Q2. */
r:L*exp(x)$
Q[0]:2*m*r^2*(V(r)-E)$
for n:1 thru Nwkb do Q[n]:0$
Q[2]:langer$
S[0]:sqrt(Q[0])$
S[1]:-diff(S[0],x)/(2*S[0])$
for n:2 thru Nwkb do
  S[n]:ratsimp((Q[n]-diff(S[n-1],x)
        -sum(S[j]*S[n-j],j,1,n-1))/(2*S[0]))$
Pformal:sum(hbar^n*S[n],n,0,Nwkb)$

/* Real turning points and the allowed-region action for an energy en. */
turning_points(en):=[find_root(realpart(Qfull(rr,en)),rr,0.001,0.1),
                     find_root(realpart(Qfull(rr,en)),rr,0.1,30.0)]$
radial_action(en):=block([tp,ans],
  tp:turning_points(en),
  ans:quad_qags(sqrt(-realpart(Qfull(rr,en)))/rr,
                rr,tp[1],tp[2],epsrel=1.0e-8),
  [en,tp[1],tp[2],first(ans),bfloat(first(ans)/(%pi*hbar)-1/2)])$

energies:[-1/2,-7/20,-1/5,-1/10]$
action_table:map(radial_action,energies)$
rprobe:4.0$
coefficients_at_probe:makelist(
  [n,bfloat(ev(S[n],x=log(rprobe/L)))],n,0,Nwkb)$

print("SCREENED RADIAL EXACT-WKB MODEL")$
print("parameters [m,hbar,ell,g,alpha,W,beta] =",
      [m,hbar,ell,g,alpha,W,beta])$
print("columns [E,r_inner,r_outer,action,action/(pi*hbar)-1/2]")$
for row in action_table do print(row)$
print("Riccati coefficients [n,S_n] at r =",rprobe)$
for row in coefficients_at_probe do print(row)$
```

What Kind of Solution Will Fill the Gap

Target result

A concrete completion criterion is an explicit Borel-summed equation

$$\boxed{\mathcal{D}_\ell^{\mathrm{EWKB}}(E;g,\alpha,W,\beta,\hbar)=0}$$

for at least one complex screened radial family, together with the pole transseries

$$E_{n\ell}=\sum_{p\geq 0}E_{n\ell}^{(p)}\hbar^p+\sum_{\mathbf{q}\neq 0}\sigma^{\mathbf{q}}e^{-\mathbf{q}\cdot\mathbf{A}/\hbar}\sum_{p\geq 0}c_{\mathbf{q},p}(n,\ell)\hbar^p,\qquad \Gamma_{n\ell}=-2\,\mathrm{Im}\,E_{n\ell}.$$

The coefficients must contain the origin monodromy and outgoing Stokes multipliers explicitly. At coalescing turning points the derivation should produce a uniform Weber/parabolic-cylinder connection formula. Finally, Borel–Pade roots must agree, with a stated error estimate, with exterior complex-scaling poles across several Stokes chambers.

References

[1] Eric Delabaere and Frédéric Pham. "Resurgent methods in semi-classical asymptotics". In: *Annales de l'Institut Henri Poincaré, Physique théorique* 71 (1999), pp. 1–94. URL: https://numdam.org/item/AIHPA_1999__71_1_1_0/.

[2] Katsushi Ito, Marcos Mariño, and Hongfei Shu. "TBA equations and resurgent quantum mechanics". In: *Journal of High Energy Physics* 2019.1 (2019), p. 228. DOI: 10.1007/JHEP01(2019)228. URL: https://arxiv.org/abs/1811.04812.

[3] Okuto Morikawa and Shoya Ogawa. "Unified exact WKB framework for resonance—Zeldovich/complex-scaling regularization and rigged Hilbert space". In: *Journal of High Energy Physics* 2025.10 (2025), p. 049. URL: https://arxiv.org/abs/2505.02301.

[4] Okuto Morikawa and Shoya Ogawa. "On continuum and resonant spectra from exact WKB analysis". In: *Journal of Physics A: Mathematical and Theoretical* 59 (2026), p. 225306. DOI: 10.1088/1751-8121/ae7224. URL: https://arxiv.org/abs/2508.09211.

[5] Okuto Morikawa and Shoya Ogawa. "Exact WKB method for radial Schrödinger equation". In: *Journal of Physics A: Mathematical and Theoretical* 59 (2026), p. 145202. DOI: 10.1088/1751-8121/ae57ec. URL: https://arxiv.org/abs/2510.11766.

[6] S. Kamata, T. Misumi, C. Pazarbasi, and H. Taya. *Exact WKB analysis of inverted triple-well: resonance, PT-symmetry breaking, and resurgence*. 2026. URL: https://arxiv.org/abs/2604.05878 (visited on 07/16/2026).

2 Inverse scattering of non-Hermitian matrix potentials at defective poles

Flügge seed: Vol. I, Problems 80–114, and Vol. II scattering problems: Jost solutions, phase shifts, bound-state residues, inverse scattering, coupled channels, and resonance poles.

Non-self-adjoint matrix inverse problems are not wholly open. Constructive uniqueness results exist for non-self-adjoint matrix Sturm–Liouville systems from Weyl/spectral data [1, 2], and rigorous matrix inverse-scattering theory exists on the line [3]. Separately, non-Hermitian scattering has characterized spectral singularities, coherent perfect absorption (CPA), lasing poles, and exceptional points (EPs) [4–6]. Care is needed because an operator EP, an S-matrix eigenvalue EP, a real-axis spectral singularity, a CPA zero, and a CPA–laser pole–zero coincidence are not equivalent objects [7].

Recent finite-dimensional inverse design can place an EP in a resonant network [8], but it does not reconstruct a spatially varying matrix potential. The missing result is a reconstruction directly from physical on-shell nonunitary scattering data when the analytically continued matrix has multiple or defective poles, including complete Jordan-chain norming data and stability estimates that remain meaningful as poles coalesce.

Formalisms

Operator class and units

Restrict the first theorem to equal-threshold channels on the full line. A physical matrix potential $\mathsf{U}(x)$ acts on

$$\mathcal{H} = L^2(\mathbb{R}, \mathbb{C}^N), \tag{26}$$

and the stationary equation, after multiplication by $2\mu/\hbar^2$, is

$$-\Psi''(x) + \mathsf{V}(x)\Psi(x) = k^2\Psi(x), \qquad \mathsf{V}(x) = \frac{2\mu}{\hbar^2}\mathsf{U}(x). \tag{27}$$

Here Ψ is an N-component column, k has units of inverse length, and V has units of inverse length squared. A convenient rigorous starting class is

$$\int_{\mathbb{R}} (1 + |x|)\|\mathsf{V}(x)\|\, dx < \infty, \tag{28}$$

with compact support $[-L, L]$ imposed for the first reconstruction and stability experiments. On the Sobolev domain $H^2(\mathbb{R}, \mathbb{C}^N)$, this defines a closed, generally non-self-adjoint Schrödinger operator.

Reciprocity and passivity are separate assumptions. In a channel basis fixed by external preparation, take

$$\mathsf{V}(x)^T = \mathsf{V}(x), \qquad \operatorname{Im}\mathsf{V}(x) \equiv \frac{\mathsf{V}(x) - \mathsf{V}(x)^\dagger}{2i} \preceq 0 \quad \text{a.e.} \tag{29}$$

The transpose condition encodes reciprocity, while the Hermitian inequality excludes gain. Neither condition implies normality. With $X = x/L$, $K = kL$, and $\mathcal{V}(X) = L^2\mathsf{V}(LX)$, the inverse problem is dimensionless; the reconstructed physical potential is recovered as $\mathsf{U} = (\hbar^2/2\mu L^2)\mathcal{V}$.

Jost solutions and scattering conventions

The right and left Jost matrices are the unique fundamental solutions with

$$\mathsf{F}_+(x,k)e^{-ikx} \longrightarrow \mathsf{I} \quad (x \to +\infty), \qquad \mathsf{F}_-(x,k)e^{ikx} \longrightarrow \mathsf{I} \quad (x \to -\infty). \tag{30}$$

For compact support these asymptotic conditions hold exactly outside the interaction region. Incidence from the left and right is normalized by

$$\Psi_L(x,k) \sim \begin{cases} e^{ikx}\mathsf{I} + e^{-ikx}\mathsf{R}_L(k), & x \to -\infty, \\ e^{ikx}\mathsf{T}_L(k), & x \to +\infty, \end{cases} \tag{31}$$

$$\Psi_R(x,k) \sim \begin{cases} e^{-ikx}\mathsf{T}_R(k), & x \to -\infty, \\ e^{-ikx}\mathsf{I} + e^{ikx}\mathsf{R}_R(k), & x \to +\infty. \end{cases} \tag{32}$$

If the input amplitudes are ordered as $(a_L, a_R)^T$, the outgoing amplitudes obey

$$\begin{pmatrix} b_L \\ b_R \end{pmatrix} = \mathsf{S}(k) \begin{pmatrix} a_L \\ a_R \end{pmatrix}, \qquad \mathsf{S}(k) = \begin{pmatrix} \mathsf{R}_L & \mathsf{T}_R \\ \mathsf{T}_L & \mathsf{R}_R \end{pmatrix}. \tag{33}$$

For real $k > 0$, equal thresholds make this normalization flux normalized. Passivity then gives $\mathsf{S}^\dagger\mathsf{S} \preceq \mathsf{I}$, and reciprocity gives the appropriate transpose symmetry of S. Different channel thresholds require velocity factors and a multi-sheeted energy plane; they should be deferred until the equal-threshold theorem is under control.

Jost matrix and analytic continuation

Expand the right Jost solution on the left of the support:

$$\mathsf{F}_+(x,k) = e^{ikx}\mathsf{A}(k) + e^{-ikx}\mathsf{B}(k), \qquad x < -L. \tag{34}$$

This convention gives

$$\mathsf{T}_L(k) = \mathsf{A}(k)^{-1}, \qquad \mathsf{R}_L(k) = \mathsf{B}(k)\mathsf{A}(k)^{-1}. \tag{35}$$

The matrix $\mathsf{J}(k) \equiv \mathsf{A}(k)$ is the Jost matrix used below. For a compactly supported potential it is analytic in k, apart from the special behavior at $k = 0$, and its inverse is meromorphic. The condition

$$\det \mathsf{J}(k_j) = 0 \tag{36}$$

produces a solution outgoing at both infinities. Zeros with $\operatorname{Im} k_j > 0$ are discrete eigenvalues; continuation through the real axis to $\operatorname{Im} k_j < 0$ gives resonances. A real positive zero is a spectral singularity and must not be called an exceptional point unless the relevant algebraic and geometric multiplicities also coalesce.

For numerical propagation define the first-order state

$$\mathcal{Y}(x) = \begin{pmatrix} \Psi(x) \\ \Psi'(x) \end{pmatrix}, \qquad \mathcal{Y}'(x) = \begin{pmatrix} 0 & \mathsf{I} \\ \mathsf{V}(x) - k^2\mathsf{I} & 0 \end{pmatrix} \mathcal{Y}(x). \tag{37}$$

Its fundamental matrix from $-L$ to $+L$ supplies A, B by matching to plane waves. A scattering-matrix or invariant-embedding propagation is preferable to a raw transfer matrix when k is complex, because exponentially growing columns otherwise destroy the subdominant Jost solution.

Defective zeros and Jordan-chain data

Let k_0 be a zero of algebraic multiplicity m. A right analytic Jordan chain $v_0, \ldots, v_{m-1}$ satisfies

$$\sum_{p=0}^{q} \frac{1}{p!}\mathsf{J}^{(p)}(k_0)v_{q-p} = 0, \qquad q = 0, \ldots, m-1. \tag{38}$$

The first two relations are

$$\mathsf{J}_0 v_0 = 0, \qquad \mathsf{J}_0 v_1 + \mathsf{J}_0' v_0 = 0. \tag{39}$$

Left chains are row vectors satisfying the transposed sequence. In a non-Hermitian analytic problem they are not obtained by Hermitian conjugating the right chains. Their normalization may be fixed by a Keldysh-type biorthogonality condition; any reconstruction formula must be invariant under the compensating rescalings of the left and right chains.

Near a second-order defective zero, a scattering block has a Laurent expansion

$$\mathsf{S}(k) = \frac{\mathsf{A}_{-2}}{(k-k_0)^2} + \frac{\mathsf{A}_{-1}}{k-k_0} + \mathsf{A}_0 + \mathcal{O}(k-k_0). \tag{40}$$

The two principal-part matrices, rather than the pole location alone, contain the norming information required by the inverse problem. Under a generic parameter perturbation η, the two pole locations split as $k_\pm - k_0 = \mathcal{O}(\eta^{1/2})$; individual simple-pole residues can therefore become extremely ill conditioned even while the total principal part on a surrounding contour remains bounded.

Choose a positively oriented contour Γ enclosing the pole cluster and no other singularity. The moments

$$\mathsf{M}_q = \frac{1}{2\pi i}\oint_\Gamma (k-k_c)^q \mathsf{S}(k)\,dk, \qquad q = 0,1,\dots, \tag{41}$$

depend continuously on the sampled matrix function as long as Γ stays separated from the poles. If $k_c = k_0$ in (40), then $\mathsf{M}_0 = \mathsf{A}_{-1}$ and $\mathsf{M}_1 = \mathsf{A}_{-2}$. For a cluster of split poles, block Hankel matrices formed from several M_q recover the invariant subspace without assigning unstable individual residues prematurely.

Transformation operator and Marchenko equation

For the right Jost solution introduce a transformation kernel

$$\mathsf{F}_+(x,k) = e^{ikx}\mathsf{I} + \int_x^\infty \mathsf{K}_+(x,y)e^{iky}\,dy. \tag{42}$$

Substitution in (27), followed by integration by parts, gives the diagonal recovery formula

$$\mathsf{V}(x) = -2\frac{d}{dx}\mathsf{K}_+(x,x). \tag{43}$$

Completeness of the continuum and discrete biorthogonal states yields the right Marchenko equation

$$\mathsf{K}_+(x,y) + \mathsf{F}_+(x+y) + \int_x^\infty \mathsf{K}_+(x,z)\mathsf{F}_+(z+y)\,dz = 0, \qquad y \geq x. \tag{44}$$

Here the same symbol F_+, distinguished by its single argument, denotes the data kernel

$$\mathsf{F}_+(s) = \frac{1}{2\pi}\int_{-\infty}^\infty \mathsf{R}_R(k)e^{iks}\,dk + \mathsf{F}_{+,\mathrm{disc}}(s), \qquad s > 0. \tag{45}$$

The reflection block in (45) is tied to the Fourier and Jost conventions above; swapping left and right requires reversing the phase and using the companion Marchenko equation.

For simple poles, $\mathsf{F}_{+,\mathrm{disc}} = \sum_j \mathsf{C}_j e^{ik_j s}$, where C_j is a biorthogonal norming matrix. If the principal part has order m_j, residue calculus gives

$$\mathsf{F}_{+,\mathrm{disc}}(s) = \sum_j \sum_{q=0}^{m_j-1} \mathsf{C}_{jq} s^q e^{ik_j s}. \tag{46}$$

Factors of $i^q/q!$ are absorbed into the definition of C_{jq}; they must be restored consistently when converting from the Laurent matrices in (40). The unresolved mathematical object enters precisely here: one needs the correct matrix coefficients for complete left/right Jordan chains and a proof that (44) remains uniquely solvable as a simple-pole pair becomes defective.

Data, reconstruction workflow, and checks

Ideal inverse data comprise the full real-axis $\mathsf{S}(k)$, its analytic pole/zero data, and the principal-part or norming matrices. A finite noisy frequency window cannot determine an arbitrary compactly supported potential without regularization; numerical experiments must therefore distinguish the exact-data uniqueness theorem from a band-limited stability study.

A reproducible workflow begins with a synthetic reciprocal passive 2×2 potential and computes $\mathsf{S}(k)$ by stable forward propagation. Fit an analytic matrix rational approximant on and near the real axis while enforcing reciprocity and checking passivity. Evaluate (41) by quadrature, construct (45), and solve (44) on a triangular (x, y) grid by Nyström or product integration. Differentiate a smooth representation of $\mathsf{K}_+(x, x)$, rather than raw grid noise, in (43). Finally, recompute all four scattering blocks from the reconstructed potential.

The high-energy Born behavior provides a useful independent diagnostic: reflection must decay and its Fourier phase must locate the support. Other checks are recovery of the scalar and simple-pole Marchenko equations; $\mathsf{S}^\dagger\mathsf{S} \preceq \mathsf{I}$ on the real axis; transpose reciprocity; stability under movement of Γ; and convergence with the Marchenko grid and measured bandwidth. In the Hermitian limit the left and right norming data reduce to the familiar adjoint pairing. If the physical channel basis is not fixed, a constant similarity transformation is an unavoidable gauge; it must not be mistaken for nonuniqueness of the spatial profile.

Maxima research model

The driver takes two noncommuting residue matrices, with the $se^{-\kappa s}$ term encoding a double Jost pole, and builds the complete two-channel Marchenko kernel. It performs a finite-grid block Nyström solve and prints $F(1)$, $K(x, x)$, and finite-difference samples of the reconstructed matrix potential. From the project root run

```
maxima --batch=maxima/02_nonhermitian_inverse_scattering.mac
```

Edit `C0`, `C1`, `kappa`, `ngrid`, and `cutoff`; the loaded helper implements a reusable complex floating-point linear solver without external packages. It is a small dense baseline without pivoting, so production work must add pivoting and condition monitoring together with continuum data, several poles, quadrature convergence, and inverse-data regularization.

```
/* Two-channel higher-order-pole Marchenko reconstruction. */
kill(all)$
display2d:false$ linel:200$
ratprint:false$
batchload("maxima/lib/02_marchenko_numeric.mac")$
numeric_matrix(M):=genmatrix(lambda([i,j],cfrom(cpair(M[i,j]))),
  length(M),length(M[1]))$

/* C1 multiplies s exp(-kappa s), the signature of a double Jost pole. */
kappa:6/5$
C0:matrix([3/5,1/5+%i/10],[-1/8+%i/12,2/5])$
C1:matrix([1/6,-1/9+%i/14],[1/10+%i/15,-1/7])$
F(s):=(C0+s*C1)*exp(-kappa*s)$

/* Nystr\"om grid for K(x,y)+F(x+y)+int K(x,s)F(s+y) ds=0. */
ngrid:6$ cutoff:7$ dx:0.02$
marchenko_system(x0):=block([h,y,s,w,A],
  h:(cutoff-x0)/(ngrid-1),
  y:makelist(x0+(j-1)*h,j,1,ngrid), s:y,
  w:makelist(h*(1-(kron_delta(j,1)+kron_delta(j,ngrid))/2),
             j,1,ngrid),
  A:genmatrix(lambda([row,col],block([j,b,l,c],
    j:floor((row-1)/2)+1, b:mod(row-1,2)+1,
    l:floor((col-1)/2)+1, c:mod(col-1,2)+1,
    kron_delta(j,l)*kron_delta(b,c)+w[l]*F(s[l]+y[j])[c,b])),
    2*ngrid,2*ngrid),
  [y,s,w,A])$

rhs_vector(x0,a):=genmatrix(lambda([row,col],block([j,b],
  j:floor((row-1)/2)+1, b:mod(row-1,2)+1,
  -F(x0+(x0+(j-1)*(cutoff-x0)/(ngrid-1)))[a,b])),
  2*ngrid,1)$

Kdiagonal(x0):=block([sys,A,u],
  sys:marchenko_system(x0), A:sys[4],
  u:makelist(complex_gauss(A,rhs_vector(x0,a)),a,1,2),
  genmatrix(lambda([a,b],u[a][b,1]),2,2))$
Vreconstructed(x0):=numeric_matrix(
  -(Kdiagonal(x0+dx)-Kdiagonal(x0-dx))/dx)$

x_samples:[2/5,1,8/5]$
profile:makelist([xx,Kdiagonal(xx),Vreconstructed(xx)],xx,x_samples)$
print("TWO-CHANNEL MARCHENKO MODEL")$
print("higher-order kernel F(1) =",numeric_matrix(F(1)))$
print("columns: x, K(x,x), reconstructed V(x)")$
for row in profile do (
  print("x =",row[1]), print("K =",row[2]), print("V =",row[3]))$
```

What Kind of Solution Will Fill the Gap

Target result

The central theorem should state that, for a specified class of compactly supported reciprocal complex 2×2 potentials, the full real-axis $\mathsf{S}(k)$, pole/zero positions, and Laurent-principal-part matrices uniquely determine $\mathsf{V}(x)$, up to a constant channel-basis similarity when the basis is not externally fixed. The constructive proof must use the $s^q e^{ik_j s}$ Marchenko terms.
A publishable stability result would be

$$\boxed{\|\mathsf{V} - \widetilde{\mathsf{V}}\|_{L_1^1} \le C_\Gamma \left[\|\mathsf{S} - \widetilde{\mathsf{S}}\|_{H^1(\mathbb{R})} + \sum_q \|\mathsf{M}_q - \widetilde{\mathsf{M}}_q\| \right]},$$

with a proof that C_Γ stays bounded for a contour separated from the coalescing pole cluster, while the condition number of individual pole/residue parameters diverges with Puiseux scaling. A numerical test should reconstruct a known complex 2×2 potential on both sides of an EP and compare residue fitting with contour-moment regularization.

References

[1] G. Freiling and V. Yurko. "An inverse problem for the non-selfadjoint matrix Sturm–Liouville equation on the half-line". In: *Journal of Inverse and Ill-Posed Problems* 15 (2007), pp. 785–798. DOI: 10.1515/jiip.2007.042.

[2] Natalia Bondarenko. *An inverse spectral problem for the matrix Sturm–Liouville operator on the half-line*. 2015. URL: https://arxiv.org/abs/1412.5962 (visited on 07/16/2026).

[3] Natalia Bondarenko. "Inverse scattering on the line for the matrix Sturm–Liouville equation". In: *Journal of Differential Equations* 262 (2017), pp. 2073–2105. DOI: 10.1016/j.jde.2016.10.040. URL: https://arxiv.org/abs/1512.06210.

[4] Ali Mostafazadeh. "Physics of spectral singularities". In: *Geometric Methods in Physics* (2015), pp. 145–165. URL: https://arxiv.org/abs/1412.0454.

[5] William R. Sweeney, Chia Wei Hsu, Stefan Rotter, and A. Douglas Stone. "Perfectly absorbing exceptional points and chiral absorbers". In: *Physical Review Letters* 122 (2019), p. 093901. DOI: 10.1103/PhysRevLett.122.093901. URL: https://arxiv.org/abs/1807.08805.

[6] Emil J. Bergholtz, Jan Carl Budich, and Flore K. Kunst. "Exceptional topology of non-Hermitian systems". In: *Reviews of Modern Physics* 93 (2021), p. 015005. DOI: 10.1103/RevModPhys.93.015005. URL: https://arxiv.org/abs/1912.10048.

[7] Andrey Novitsky et al. *Unambiguous scattering matrix for non-Hermitian systems*. 2020. URL: https://arxiv.org/abs/2004.00912 (visited on 07/16/2026).

[8] Y. F. Li, B. Chen, Y. Wu, Y. Liu, H. Lin, and B. Zhou. *Inverse design of exceptional points in a single-resonance two-port network*. 2026. URL: https://arxiv.org/abs/2604.14744 (visited on 07/16/2026).

3 Matrix threshold expansion with anisotropic long-range forces, loss, and causal bounds

Flügge seed: Vol. I and II low-energy scattering problems: scattering length, effective range, shallow poles, coupled partial waves, threshold laws, and time-delay-related phase behavior.

Ordinary effective-range theory (ERE) is not valid unchanged in the presence of a long-range tail. The classic inverse-fourth-power analysis already contains nonanalytic threshold terms [1]; modern work retains the left-hand cut generated by a long-range force [2]. Causality and Wigner-type bounds are known for Hermitian short-range ERE coefficients [3]. Reactive quantum-defect theory supplies complex scattering lengths and universal loss rates [4], while multichannel quantum-defect theory covers anisotropic long-range interactions [5]. Complex Wigner delay has also been defined for subunitary scattering [6].

These three lines of work remain only partially connected. Their required coefficient-level synthesis is a branch-aware, low-parameter matrix threshold expansion for a specified anisotropic tail with short-range loss, supplemented by passivity and causality inequalities on its complex coefficient matrices and explicit predictions for near-threshold poles and complex time delay.

Formalisms

Hamiltonian, interaction class, and channel space

Consider relative motion with a common reduced mass μ and a finite set of internal thresholds E_a, $a = 1, \ldots, n_c$. The Hilbert space is

$$\mathcal{H} = L^2(\mathbb{R}^3) \otimes \mathbb{C}^{n_c}, \tag{47}$$

and the energy-independent Hamiltonian is

$$H = -\frac{\hbar^2}{2\mu}\nabla^2 + \mathsf{E}_{\text{th}} + \mathsf{V}(\mathbf{r}), \qquad (\mathsf{E}_{\text{th}})_{ab} = E_a\delta_{ab}. \tag{48}$$

Use a regulated dipolar test interaction

$$\mathsf{V}(r,\theta) = \mathsf{V}_{\text{sr}}(r) - i\mathsf{W}_{\text{sr}}(r) - \chi(r)\frac{\mathsf{C}_3}{r^3}P_2(\cos\theta), \tag{49}$$

where $\mathsf{V}_{\text{sr}} = \mathsf{V}_{\text{sr}}^\dagger$, $\mathsf{W}_{\text{sr}} \succeq 0$, and both have support primarily inside R_0. The smooth regulator obeys $\chi(r) = 0$ near the origin and $\chi(r) = 1$ for $r \geq R_m > R_0$. It prevents the long-range model from being misused as a singular microscopic interaction. Take $\mathsf{C}_3 = \mathsf{C}_3^\dagger$, with units of energy times length cubed. Loss is confined to short distance; the tail itself is conservative.

The operator may be defined through its closed sectorial quadratic form on $H^1(\mathbb{R}^3) \otimes \mathbb{C}^{n_c}$. Axial symmetry conserves the space-fixed projection m, but the tensor tail mixes orbital angular momenta. Exchange symmetry can later restrict even or odd ℓ; it should not be imposed until the particle statistics are specified.

If $\mathsf{C}_3 \neq 0$, define the characteristic length and energy

$$R_3 = \frac{2\mu\|\mathsf{C}_3\|}{\hbar^2}, \qquad E_3 = \frac{\hbar^2}{2\mu R_3^2}. \tag{50}$$

Dimensionless inputs are r/R_3, $(E - E_{a_0})/E_3$, R_0/R_3, R_m/R_3, and $\mathsf{C}_3/\|\mathsf{C}_3\|$. If the tail is taken to zero, retain an arbitrary reference length $R_\star$ before the limit; otherwise the normalization of reduced threshold amplitudes changes singularly.

Partial-wave reduction and angular couplings

Expand a scattering state as

$$\Psi_a(\mathbf{r}) = \frac{1}{r}\sum_{\ell m} u_{a\ell m}(r) Y_{\ell m}(\hat{r}) \tag{51}$$

and use the compound index $\alpha = (a, \ell, m)$. The angular matrix element of the tail is

$$\mathcal{P}_{\ell m,\ell' m'} = \langle Y_{\ell m}|P_2(\cos\theta)|Y_{\ell' m'}\rangle \tag{52}$$

$$= \delta_{mm'}(-1)^m\sqrt{(2\ell+1)(2\ell'+1)}\begin{pmatrix}\ell & 2 & \ell'\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}\ell & 2 & \ell'\\ -m & 0 & m\end{pmatrix}. \tag{53}$$

It vanishes unless $\ell' = \ell, \ell \pm 2$ and parity is conserved. The radial interaction matrix is therefore

$$V_{a\ell m,b\ell' m'}(r) = V_{\mathrm{sr},\alpha\beta}(r) - iW_{\mathrm{sr},\alpha\beta}(r) - \frac{\chi(r)}{r^3}(C_3)_{ab}\mathcal{P}_{\ell m,\ell' m'}. \tag{54}$$

The coupled equations are

$$\left[-\frac{d^2}{dr^2} + \frac{\ell_\alpha(\ell_\alpha+1)}{r^2} - k_a(E)^2\right]u_\alpha(r) + \sum_\beta \frac{2\mu}{\hbar^2}V_{\alpha\beta}(r)u_\beta(r) = 0. \tag{55}$$

Regular columns satisfy

$$u_{\alpha j}(r) = r^{\ell_\alpha+1}[\delta_{\alpha j} + o(1)] \qquad (r \downarrow 0). \tag{56}$$

The infinite partial-wave system is truncated at $\ell_{\max}$; convergence of observables under $\ell_{\max} \to \ell_{\max}+2$ is part of the calculation, not an optional numerical detail.

Momentum sheets and asymptotic boundary conditions

For every internal channel define

$$k_a(E) = \frac{\sqrt{2\mu(E-E_a)}}{\hbar}. \tag{57}$$

On the physical sheet the square root is chosen so that $k_a > 0$ just above an open threshold and $\operatorname{Im} k_a > 0$ below a closed threshold. The cut of channel a starts at E_a. A Riemann sheet is labeled by a sign vector $\boldsymbol{\sigma} = (\sigma_1, \ldots, \sigma_{n_c})$ through $k_a^{(\boldsymbol{\sigma})} = \sigma_a k_a^{(\mathrm{phys})}$. This notation is essential when a near-threshold pole crosses one cut but not another.

Choose an entrance channel a_0 and let

$$\bar{k} = k_{a_0}, \qquad \bar{q} = \bar{k}R_\star \tag{58}$$

be the dimensional and dimensionless expansion variables. At large radius, open-channel columns are matched to incoming and outgoing Riccati–Hankel functions; closed-channel columns retain only the exponentially decreasing solution on the physical sheet. For the r^{-3} tail, matching directly to free waves at a modest R_m is not controlled. Either propagate to a verified asymptotic radius or construct reference functions that already contain the anisotropic tail.

Log-derivative matching and the scattering matrix

Let $\mathsf{U}(r, E)$ be a square matrix of regular solutions of (55) and propagate the log derivative

$$\mathsf{Y}(r, E) = \mathsf{U}'(r, E)\mathsf{U}(r, E)^{-1}. \tag{59}$$

This Riccati variable avoids exponentially large closed-channel columns. Let F, G be matrices of tail-distorted regular and irregular reference solutions at a matching radius. Writing $\mathsf{U} = \mathsf{F} - \mathsf{G}\mathsf{K}$ gives

$$\mathsf{K} = (\mathsf{Y}\mathsf{G} - \mathsf{G}')^{-1}(\mathsf{Y}\mathsf{F} - \mathsf{F}'). \tag{60}$$

After restriction to energetically open channels and flux normalization,

$$\mathsf{S} = (\mathsf{I} + i\mathsf{K})(\mathsf{I} - i\mathsf{K})^{-1}. \tag{61}$$

For lossless interactions K is Hermitian on the real axis; with short-range absorption S is subunitary.

To remove trivial centrifugal powers, define the diagonal threshold matrix on the open subspace by

$$\mathsf{P}_{\alpha\beta}(E) = \delta_{\alpha\beta}[k_a(E)R_\star]^{2\ell_\alpha+1}, \tag{62}$$

and a dimensionless reduced amplitude f through

$$\mathsf{S} = \mathsf{I} + 2i\mathsf{P}^{1/2}\mathsf{f}\mathsf{P}^{1/2}. \tag{63}$$

All fractional powers use the channel-sheet convention already fixed. A different $R_\star$ changes the numerical matrices by a known diagonal similarity and cannot change poles or physical cross sections.

Origin of the nonanalytic threshold terms

The short-range logarithmic derivative is analytic in E away from an internal eigenvalue, but two mechanisms spoil an ordinary polynomial ERE. First, eliminating closed channels produces threshold square roots. If a matrix inverse amplitude is partitioned into open and closed blocks, its open-channel reduction contains the Schur complement

$$\mathsf{M}_{\text{eff}} = \mathsf{M}_{oo} - \mathsf{M}_{oc}\mathsf{M}_{cc}^{-1}\mathsf{M}_{co}, \tag{64}$$

and M_{cc} depends on the selected branch of each closed-channel momentum. These terms define $\mathsf{L}_{\text{th}}(E)$.

Second, iterations of the dipolar tail contain radial integrals of the form

$$I_{\ell\ell'}(k,k') = \int_{R_m}^{\infty} \frac{dr}{r} j_\ell(kr) j_{\ell'}(k'r), \tag{65}$$

multiplied by angular and channel matrices. A Mellin expansion of (65) has colliding poles at marginal powers; their residues generate nonanalytic powers and terms $\bar{q}^p \log(-i\bar{q})$. On the physical upper rim, $\log(-i\bar{q}) = \log|\bar{q}| - i\pi/2$ for $\bar{q} > 0$. Changing the dimensionless scale inside the logarithm shifts analytic coefficients, so the subtraction convention must be stated together with the reported scattering-length and effective-range matrices.

The branch-aware ansatz is

$$\boxed{\mathsf{f}^{-1}(E) = -\mathsf{A}^{-1} + \frac{1}{2}\mathsf{R}\bar{q}^2 + \mathsf{L}_{\text{tail}}(E) + \mathsf{L}_{\text{th}}(E) - i\mathsf{P}(E) + \mathsf{R}_N(E).} \tag{66}$$

Here A and R are dimensionless coefficient matrices in the $R_\star$ convention, the two L terms contain all explicitly derived branch functions through the selected order, and R_N is the remainder. The unresolved object is not the form of (66); it is the complete coefficient list, its subtraction-scale covariance, and a uniform bound on R_N for a fixed coupled dipolar model.

Passivity, delay, and pole observables

For real energies and open channels, insert $\mathsf{T} = \mathsf{P}^{1/2}\mathsf{f}\mathsf{P}^{1/2}$ into $\mathsf{S} = \mathsf{I} + 2i\mathsf{T}$. The condition $\mathsf{S}^\dagger\mathsf{S} \preceq \mathsf{I}$ is equivalent to

$$\operatorname{Im}\mathsf{T} \succeq \mathsf{T}^\dagger\mathsf{T}, \tag{67}$$

and hence, where f is invertible,

$$\operatorname{Im}\mathsf{f} \succeq \mathsf{f}^\dagger\mathsf{P}\mathsf{f}, \qquad \operatorname{Im}\mathsf{f}^{-1} \preceq -\mathsf{P}. \tag{68}$$

These are fit constraints, but only on the physical real-energy boundary; they must not be imposed unchanged on an unphysical sheet.

For N_o open channels define the complex mean delay

$$\tau_c(E) = -\frac{i\hbar}{N_o}\frac{d}{dE}\log\det \mathsf{S}(E). \tag{69}$$

If $\det \mathsf{S} = \rho e^{i\phi}$, then

$$\operatorname{Re}\tau_c = \frac{\hbar}{N_o}\frac{d\phi}{dE}, \qquad \operatorname{Im}\tau_c = -\frac{\hbar}{N_o}\frac{d\log\rho}{dE}. \tag{70}$$

Thus phase delay and the energy dependence of attenuation are separately observable. A long-range-subtracted Wigner bound must be derived from the tail-distorted log derivative, not from a finite-range formula applied to the full r^{-3} interaction.

On a sheet $\boldsymbol{\sigma}$, pole energies solve

$$\det \mathsf{f}_{\boldsymbol{\sigma}}^{-1}(E_p) = 0. \tag{71}$$

A bound state lies on the physical sheet below all open thresholds; virtual and resonant poles require specified sign changes in $\boldsymbol{\sigma}$. A defective pole additionally has vectors satisfying

$$\mathsf{f}^{-1}(E_p)v_0 = 0, \qquad \mathsf{f}^{-1}(E_p)v_1 + \partial_E \mathsf{f}^{-1}(E_p)v_0 = 0. \tag{72}$$

Numerical route and controlled limits

Fix m, internal channels, and $\ell_{\max}$; generate the angular matrix analytically; and propagate Y from a Frobenius start. Construct tail reference functions or propagate beyond a sequence of larger matching radii. Compute $\mathsf{S}(E)$ on real and nearby complex energies, subtract analytically evaluated tail and threshold functions, and fit only the remaining coefficient matrices. Enforce (68) on validation energies. Continue the fitted expression sheet by sheet and solve (71); compare every pole with a direct complex energy integration of (55).

Required checks include independence of the regulator shape after refitting short-range coefficients; stability with R_m and $\ell_{\max}$; the ordinary multichannel ERE when $\mathsf{C}_3 \to 0$; unitarity equality when $\mathsf{W}_{\rm sr} \to 0$; decoupled single-channel threshold laws when off-diagonal couplings vanish; and covariance under a change of $R_\star$. Fits must be repeated on shrinking energy windows to separate an omitted nonanalytic term from an apparently successful high-order polynomial.

Maxima research model

The driver evaluates the exact $m = 0$ dipolar Gaunt matrix and inserts its retained block into a two-wave inverse-amplitude model with loss, a $k^2\log(-ik)$ tail, and a closed-channel square-root branch. It prints a real-energy table containing $|\det S|$, complex mean delay, and the pole indicator, together with one full S matrix and a complex-momentum scan. From the project root run

```
maxima --batch=maxima/03_threshold_universality.mac
```

Replace the coefficient matrices and `pole_grid` to test another sheet or fitted model. Deriving all Mellin-tail coefficients, matching coupled radial ODEs, and propagating fit uncertainties require numerical infrastructure beyond bare Maxima.

```
/* Matrix threshold amplitude with dipolar Gaunt mixing and loss. */
kill(all)$
display2d:false$ ratprint:false$ linel:200$

/* Exact axial P2 coupling in the m=0 basis ell=0,2,4. */
ells:[0,2,4]$ z:'z$
Gaunt:genmatrix(lambda([i,j],radcan(
  sqrt((2*ells[i]+1)*(2*ells[j]+1))/2
  *integrate(legendre_p(ells[i],z)*legendre_p(2,z)
            *legendre_p(ells[j],z),z,-1,1))),3,3)$

/* Two retained waves: analytic ERE, k^2 log(-ik) tail, closed threshold. */
Acoef:matrix([3,2/5],[2/5,2])$
Rcoef:matrix([4/5,1/5],[1/5,3/5])$
Dtail:submatrix(3,Gaunt,3)/3$
Bclose:matrix([1/4],[1/7])$ delta:9/25$ gamma:1/2$
Loss:matrix([1/50,0],[0,1/100])$
Pmat(k):=matrix([k,0],[0,k^5])$
Psqrt(k):=matrix([sqrt(k),0],[0,k^(5/2)])$
Ltail(k):=k^2*log(-%i*k)*Dtail$
Lclosed(k):=-Bclose.transpose(Bclose)/(gamma+sqrt(delta-k^2))$
Finv(k):=-invert(Acoef)+k^2*Rcoef/2+Ltail(k)+Lclosed(k)
          -%i*(Pmat(k)+Loss)$

cnum(q):=block([u:rectform(q)],
  float(realpart(u))+%i*float(imagpart(u)))$
nummat(M):=genmatrix(lambda([i,j],cnum(M[i,j])),length(M),length(M[1]))$
Famp(k):=nummat(invert(Finv(k)))$
Smat(k):=nummat(ident(2)+2*%i*Psqrt(k).Famp(k).Psqrt(k))$
detS(k):=cnum(determinant(Smat(k)))$
dk:1.0e-4$
mean_delay(k):=cnum(-%i*(log(detS(k+dk))-log(detS(k-dk)))/(8*k*dk))$
observable_row(k):=block([S:Smat(k),tau:mean_delay(k)],
  [k,cabs(determinant(S)),realpart(tau),imagpart(tau),
   cabs(cnum(determinant(Finv(k))))])$

k_scan:[0.04,0.07,0.10,0.14,0.20]$
observables:map(observable_row,k_scan)$
pole_grid:[0.04-%i*0.03,0.08-%i*0.03,0.12-%i*0.03,
           0.04-%i*0.07,0.08-%i*0.07,0.12-%i*0.07]$
pole_scan:makelist([kp,cabs(cnum(determinant(Finv(kp))))],kp,pole_grid)$
print("MATRIX THRESHOLD MODEL; exact Gaunt block =",Gaunt)$
print("columns [k,|det S|,Re tau,Im tau,|det f^{-1}|]")$
for row in observables do print(row)$
print("representative S(k=0.10) =",Smat(0.10))$
print("complex-k pole indicator [k,|det f^{-1}|]")$
for row in pole_scan do print(row)$
```

What Kind of Solution Will Fill the Gap

Target result

For one fixed two-channel dipolar model, derive every coefficient and branch prescription in L_{tail}, including all $k^p \log k$ terms, and prove a uniform remainder bound. The main theorem should include

$$\boxed{-\operatorname{Im}\mathsf{f}^{-1} - \mathsf{P} \succeq 0, \qquad \mathsf{R}_{\mathrm{W}}(R_0, \mathsf{A}, \mathsf{C}_3) - \operatorname{Re}\mathsf{R} \succeq 0,}$$

where the second inequality is a long-range-subtracted matrix Wigner bound. It should also give determinant equations for bound, virtual, resonant, and exceptional-point poles and a pole–zero formula for both parts of $\tau_c(E)$. Coupled-channel numerics must identify the energy interval in which this expansion outperforms a polynomial ERE and a black-box numerical MQDT parametrization.

References

[1] T. F. O'Malley, L. Spruch, and L. Rosenberg. "Modification of effective-range theory in the presence of a long-range inverse-fourth-power potential". In: *Journal of Mathematical Physics* 2 (1961), pp. 491–498. DOI: 10.1063/1.1703735.

[2] Meng-Lin Du, Feng-Kun Guo, and Bing Wu. "Effective range expansion with a long-range force". In: *Physical Review Letters* 135 (2025), p. 011903. DOI: 10.1103/cwdt-dj6z. URL: https://arxiv.org/abs/2408.09375.

[3] H.-W. Hammer and Dean Lee. "Causality and the effective range expansion". In: *Annals of Physics* 325 (2010), pp. 2212–2233. DOI: 10.1016/j.aop.2010.06.006. URL: https://arxiv.org/abs/1002.4603.

[4] Zbigniew Idziaszek and Paul S. Julienne. "Universal rate constants for reactive collisions of ultracold molecules". In: *Physical Review Letters* 104 (2010), p. 113202. DOI: 10.1103/PhysRevLett.104.113202. URL: https://arxiv.org/abs/0912.0370.

[5] Bo Gao. *Multichannel quantum-defect theory for anisotropic interactions*. 2020. URL: https://arxiv.org/abs/2008.08018 (visited on 07/16/2026).

[6] Lei Chen, Steven M. Anlage, and Yan V. Fyodorov. "Generalization of Wigner time delay to subunitary scattering systems". In: *Physical Review E* 103 (2021), p. L050203. DOI: 10.1103/PhysRevE.103.L050203. URL: https://arxiv.org/abs/2101.08335.

4 Exact non-Bloch Floquet–Sambe theory for a driven non-Hermitian delta comb

Flügge seed: Vol. I periodic delta potentials, transfer matrices, Bloch conditions, and scattering from contact interactions. The modern extension adds periodic driving, non-Hermiticity, and open boundaries.

Static Hermitian and $\mathcal{PT}$-symmetric contact/Kronig–Penney models are well developed [1]. Non-Bloch theory and generalized Brillouin zones (GBZs) were systematized for non-Hermitian lattices [2], and driven lattice models already exhibit Floquet EPs, 0- and π-modes, and skin effects [3, 4].

The continuum claim must be narrowed. Hu et al. developed non-Bloch band theory for continuum differential operators and showed how boundary-condition count enters a transfer-matrix GBZ [5]. Ding and Ding developed continuum non-Bloch theory for spatiotemporal photonic crystals [6]; standard Floquet non-Bloch bulk–boundary correspondence can itself fail [7]. Thus the novelty cannot be "first continuum non-Bloch transfer matrix."

The unresolved target is an exact, all-frequency Floquet–Sambe transfer theory for an analytically solvable non-Hermitian delta comb, with controlled sideband truncation, micromotion-resolved invariants, exact open-boundary edge/skin criteria, and a Lyapunov or real-space formulation under disorder. An identical static scalar complex comb is insufficient: gain/loss alone is not nonreciprocity. The unit cell must contain dimerization plus a traveling or phase-delayed modulation, or a genuinely nonreciprocal contact condition.

Formalisms

Driven contact model and its domain

Let a be the spatial period and place two contacts in each cell at $x = na$ and $x = na + d$, where $n \in \mathbb{Z}$ and $0 < d < a$. The Hamiltonian is

$$H(t) = \frac{p^2}{2m} + \sum_{n\in\mathbb{Z}} \left[g_A(t)\delta(x - na) + g_B(t)\delta(x - na - d)\right], \tag{73}$$

with period $T = 2\pi/\Omega$. Each contact strength has units of energy times length and is expanded as

$$g_\sigma(t) = \sum_{p\in\mathbb{Z}} g_{\sigma,p} e^{-ip\Omega t}, \qquad \sigma = A, B. \tag{74}$$

Hermiticity requires $g_{\sigma,-p} = g^*_{\sigma,p}$, so complex harmonic phases alone do not represent gain or loss; non-Hermiticity begins when this reality condition is violated. A phase-delayed modulation, for example different phases in the first harmonics of g_A and g_B, is required to test directional effects; an identical static scalar complex contact in every cell is spatially reciprocal.

At each fixed time the wavefunction is H^2 between contacts, continuous at a contact x_σ, and satisfies

$$\partial_x\Psi(x^+_\sigma, t) - \partial_x\Psi(x^-_\sigma, t) = \frac{2m}{\hbar^2} g_\sigma(t)\Psi(x_\sigma, t). \tag{75}$$

These matching conditions define the operator domain; a delta potential is not represented by sampling a narrow barrier unless that approximation is independently converged.

The Floquet operator is

$$\mathcal{K} = H(t) - i\hbar\partial_t \tag{76}$$

on the Sambe space $L^2([0, a]) \otimes L^2_{\text{per}}([0, T])$, augmented by spatial boundary conditions. For non-Bloch bands use

$$u(x + a, t) = \beta u(x, t), \qquad \partial_x u(x + a, t) = \beta\partial_x u(x, t), \tag{77}$$

where $\beta \in \mathbb{C}$ is not assumed to have unit modulus. Quasienergy is defined modulo $\hbar\Omega$.

Dimensionless parameters

Choose the cell scales

$$E_a = \frac{\hbar^2}{2ma^2}, \qquad X = \frac{x}{a}, \quad \delta_d = \frac{d}{a}, \quad \epsilon = \frac{\varepsilon}{E_a}, \quad \omega = \frac{\hbar\Omega}{E_a}, \tag{78}$$

and dimensionless Fourier couplings

$$\lambda_{\sigma,p} = \frac{2ma}{\hbar^2} g_{\sigma,p}. \tag{79}$$

Thus a calculation is specified by δ_d, ω, and the two sequences $\{\lambda_{A,p}\}$, $\{\lambda_{B,p}\}$. For an analytic drive one expects

$$|g_{\sigma,p}| \le C_\sigma e^{-\eta|p|} \tag{80}$$

for some $\eta > 0$; this decay is the starting assumption for a controlled Sambe truncation, not a consequence of truncation.

Sambe equations derived from the time-dependent problem

Write the Floquet state as

$$\Psi(x,t) = e^{-i\varepsilon t/\hbar} u(x,t), \qquad u(x,t) = \sum_{q\in\mathbb{Z}} \phi_q(x) e^{-iq\Omega t}. \tag{81}$$

Substitution into $(H - i\hbar\partial_t)u = \varepsilon u$ gives, between contacts,

$$-\frac{\hbar^2}{2m}\phi_q''(x) = (\varepsilon + q\hbar\Omega)\phi_q(x). \tag{82}$$

Define sideband momenta

$$k_q(\varepsilon) = \frac{\sqrt{2m(\varepsilon + q\hbar\Omega)}}{\hbar}. \tag{83}$$

For scattering, the physical branch has positive real momentum in an open sideband and $\operatorname{Im} k_q > 0$ in a closed sideband. Resonance sheets are obtained by reversing the sign of selected open-channel square roots. Transfer expressions below are analytic at a sideband threshold because they involve $\cos(k_q s)$, $\sin(k_q s)/k_q$, and $k_q \sin(k_q s)$, all of which have finite limits as $k_q \to 0$.

Fourier transforming (75) gives

$$\phi_q(x_\sigma^+) = \phi_q(x_\sigma^-), \tag{84}$$

$$\phi_q'(x_\sigma^+) - \phi_q'(x_\sigma^-) = \frac{2m}{\hbar^2} \sum_{q'\in\mathbb{Z}} g_{\sigma,q-q'} \phi_{q'}(x_\sigma). \tag{85}$$

The Toeplitz convolution in (85) is the exact source of sideband mixing. Replacing it by independent static contacts would discard the essential Floquet physics.

Finite-Sambe transfer matrix

Retain $q = -Q, \dots, Q$, so $N_s = 2Q + 1$, and order the state as

$$\mathcal{X}(x) = \begin{pmatrix} \mathbf{\Phi}(x) \\ \mathbf{\Phi}'(x) \end{pmatrix}, \qquad \mathbf{\Phi} = (\phi_{-Q}, \dots, \phi_Q)^T. \tag{86}$$

Define the $N_s \times N_s$ contact matrix

$$(\mathsf{G}_\sigma)_{qq'} = \frac{2m}{\hbar^2} g_{\sigma,q-q'} \tag{87}$$

and the jump matrix

$$\mathsf{D}_\sigma = \begin{pmatrix} \mathsf{I} & 0 \\ \mathsf{G}_\sigma & \mathsf{I} \end{pmatrix}. \tag{88}$$

For free propagation through a distance s, introduce diagonal matrices

$$(\mathsf{C}_s)_{qq} = \cos(k_q s), \tag{89}$$

$$(\mathsf{S}_s^{(1)})_{qq} = \frac{\sin(k_q s)}{k_q}, \tag{90}$$

$$(\mathsf{S}_s^{(2)})_{qq} = -k_q \sin(k_q s), \tag{91}$$

where $\mathsf{S}_s^{(1)} \to s\mathsf{I}$ in a threshold channel. In the chosen non-interleaved ordering,

$$\mathsf{P}_s = \begin{pmatrix} \mathsf{C}_s & \mathsf{S}_s^{(1)} \\ \mathsf{S}_s^{(2)} & \mathsf{C}_s \end{pmatrix}. \tag{92}$$

Taking $\mathcal{X}(na^-)$ immediately to the left of the A contact as the cell state fixes the multiplication order:

$$\boxed{\mathsf{M}_Q(\varepsilon) = \mathsf{P}_{a-d}\mathsf{D}_B\mathsf{P}_d\mathsf{D}_A}, \qquad \mathcal{X}((n+1)a^-) = \mathsf{M}_Q\mathcal{X}(na^-). \tag{93}$$

Both free and contact matrices have determinant one, hence

$$\det \mathsf{M}_Q = 1. \tag{94}$$

This identity is a useful coding check, but by itself it does not imply that all transfer eigenvalues occur in reciprocal pairs; that stronger statement requires additional symplectic or reciprocity structure.

Complex Bloch factors and the generalized Brillouin zone

Combining (77) with (93) gives the finite-Sambe characteristic equation

$$D_Q(\varepsilon, \beta) = \det[\mathsf{M}_Q(\varepsilon) - \beta\mathsf{I}_{2N_s}] = 0. \tag{95}$$

Order its roots at fixed ε by

$$|\beta_1| \le |\beta_2| \le \cdots \le |\beta_{2N_s}|. \tag{96}$$

For a second-order continuum system with N_s boundary conditions at each end, the thermodynamic open-boundary bulk locus is selected by

$$|\beta_{N_s}| = |\beta_{N_s+1}|. \tag{97}$$

This equality must be re-examined at root degeneracies and in the infinite-Sambe limit. A mode proportional to β^n has envelope length

$$\xi(\beta) = \frac{a}{|\log|\beta||}; \tag{98}$$

the sign of $\log|\beta|$ distinguishes accumulation at the two ends. In a Hermitian reciprocal limit, bulk roots return to $|\beta| = 1$.

Quasienergy gauge invariance supplies another stringent test. The exact system is unchanged under

$$\varepsilon \mapsto \varepsilon + r\hbar\Omega, \qquad \phi_q \mapsto \phi_{q+r}, \qquad r \in \mathbb{Z}. \tag{99}$$

A hard cutoff violates this relabeling near $q = \pm Q$; the violation must decrease on enlarging Q.

Why the infinite-Sambe limit requires regularization

The convolution matrices are bounded on suitably weighted sequence spaces when the Fourier coefficients decay exponentially. Free propagation is more delicate: closed sidebands contain factors $e^{|\operatorname{Im} k_q| s}$, with $|\operatorname{Im} k_q| \sim \sqrt{|q|}$. Consequently, the raw infinite transfer matrix need not be a bounded operator on one fixed ℓ^2 space, even though it can map a more strongly weighted space into a weaker one.

An infinite determinant must therefore be formed only after balancing the growing and decaying free solutions. One route changes from $(\mathbf{\Phi}, \mathbf{\Phi}')$ to incoming/outgoing sideband amplitudes and composes scattering matrices. Another uses a Dirichlet-to-Neumann map and factors out the diagonal free propagation. If the remaining operator is compact or Hilbert–Schmidt, a Fredholm determinant such as $\det_2(\mathsf{I} + \mathsf{C})$ can replace the nonexistent ordinary determinant. The precise balanced operator, its function space, and the norm in which $Q \to \infty$ is controlled are the central unknowns of the exact all-frequency construction.

Open boundaries, edge states, and scattering poles

For a chain of N cells impose full-rank boundary conditions

$$\mathsf{B}_L \mathcal{X}(0) = 0, \qquad \mathsf{B}_R \mathcal{X}(Na) = 0, \tag{100}$$

where each B has N_s rows. Dirichlet, Neumann, and Robin conditions are special cases. If the columns of V_L span $\ker \mathsf{B}_L$, finite-chain quasienergies are zeros of

$$D_N(\varepsilon) = \det[\mathsf{B}_R \mathsf{M}_Q(\varepsilon)^N \mathsf{V}_L]. \tag{101}$$

For a left semi-infinite chain, let $\mathsf{W}_<$ contain a basis of the N_s-dimensional stable transfer subspace. The Evans function is

$$D_L(\varepsilon) = \det[\mathsf{B}_L \mathsf{W}_<]. \tag{102}$$

It must be evaluated with an analytic subspace method rather than separately sorted eigenvectors, which exchange labels at degeneracies.

For a finite comb attached to free leads, open-sideband amplitudes define a Floquet scattering matrix. Closed sidebands use decaying branches. A resonance pole imposes outgoing waves in every open sideband and is found by the zero of the resulting boundary-matching determinant on a stated set of momentum sheets. This pole problem is distinct from an open-chain edge eigenvalue, although the two may approach one another in a weak-lead limit.

Micromotion and non-Bloch invariants

Let $U_\beta(t)$ be the one-period evolution in a generalized Bloch cell. Its eigenvalues $z = e^{-i\varepsilon T/\hbar}$ need not lie on the unit circle. For a reference point gap $z_0 = e^{-i\varepsilon_0 T/\hbar}$, a stroboscopic non-Bloch winding is

$$\nu(z_0) = \frac{1}{2\pi i} \oint_{\mathrm{GBZ}} d \log \det[U_\beta(T) - z_0 \mathsf{I}]. \tag{103}$$

This invariant alone does not retain anomalous Floquet micromotion. Choose a logarithm of $U_\beta(T)$ with its cut through the selected quasienergy gap, define

$$H_{F,\varepsilon_0}(\beta) = \frac{i\hbar}{T} \operatorname{Log}_{\varepsilon_0} U_\beta(T), \qquad U_{\varepsilon_0}(\beta, t) = U_\beta(t) e^{iH_{F,\varepsilon_0}(\beta)t/\hbar}, \tag{104}$$

and construct any symmetry-resolved winding from the periodized operator U_{ε_0}, with left and right eigenvectors biorthogonally normalized. The applicable invariant depends on the imposed symmetry; it should not be declared before the drive protocol is fixed.

Disorder and Lyapunov formulation

If cell parameters vary, write the product

$$\mathsf{T}_N = \mathsf{M}_N \mathsf{M}_{N-1} \cdots \mathsf{M}_1. \tag{105}$$

The Lyapunov exponents are obtained from stabilized QR or singular-value iterations,

$$\gamma_j = \lim_{N\to\infty} \frac{1}{Na} \log s_j(\mathsf{T}_N), \tag{106}$$

where s_j are ordered singular values. Direct multiplication is numerically unusable. In the clean limit the exponents reduce to logarithms of transfer-root moduli; a disordered bulk criterion is expected to involve the two central exponents associated with the boundary-condition count.

Computational workflow and consistency tests

Begin with a drive containing finitely many known harmonics. Build $\mathsf{G}_A, \mathsf{G}_B$, use the analytic threshold limits in (92), and calculate $D_Q(\varepsilon, \beta)$. Track roots continuously in ε and construct the GBZ from (97). Compare its predicted spectrum and skin length with zeros of (101) for increasing N. Repeat for increasing Q, monitoring quasienergy-gauge restoration and boundary weight in the outermost sidebands. Use balanced scattering or QR methods whenever closed-channel growth appears.

In the free limit, M_Q must reduce to diagonal sideband propagation. In the static limit, sidebands decouple and each block becomes the ordinary dimerized delta-comb transfer matrix. A real time-independent potential must recover unitary scattering and unit-modulus Bloch bands. Other checks are $\det \mathsf{M}_Q = 1$, continuity through $k_q = 0$, invariance under moving the cell origin, convergence of edge roots under chain length, and agreement between transfer, direct finite-difference, and time-propagation spectra. High-frequency effective Hamiltonians are useful benchmarks only after the exact finite-Sambe result has converged.

Maxima research model

The driver accepts an arbitrary Sambe cutoff `Q`, harmonic contact coefficients, frequency, and dimer geometry, then constructs the Toeplitz contacts and analytic free/contact transfer blocks. It prints a quasienergy scan of cell-determinant errors and all Bloch-multiplier moduli, plus the full complex multipliers at a representative quasienergy. From the project root run

```
maxima --batch=maxima/04_floquet_dirac_comb.mac
```

Call `setup_sambe(qcut)` and replace `gA`, `gB`, or `eps_scan` to enlarge the truncation or drive. Stabilized large-Q transfer algebra, generalized-Brillouin-zone continuation, Evans functions, and micromotion invariants require specialized numerical routines beyond bare Maxima.

```
/* Finite-Sambe transfer spectrum for a driven non-Hermitian delta comb. */
kill(all)$
display2d:false$ ratprint:false$ linel:200$
m:1$ hbar:1$ omega:1$ a:9/20$ b:11/20$

/* Harmonic contact data; unequal +/- coefficients allow non-Hermiticity. */
gA:[1/3,1/5+%i/9,1/7-%i/11]$
gB:[-1/4,-2/9+%i/13,-1/6-%i/10]$
setup_sambe(qcut):=(Q:qcut,qs:makelist(q,q,-Q,Q),
  Ns:2*Q+1,Iq:ident(Ns),Zq:zeromatrix(Ns,Ns))$
setup_sambe(1)$

join4(A,B,C,D):=addrow(addcol(A,B),addcol(C,D))$
toeplitz_harmonic(g):=genmatrix(lambda([i,j],block([d:qs[i]-qs[j]],
  g[1]*kron_delta(d,0)+g[2]*kron_delta(d,1)
  +g[3]*kron_delta(d,-1))),Ns,Ns)$
jump(g):=join4(Iq,Zq,2*m*toeplitz_harmonic(g)/hbar^2,Iq)$
kq(en,q):=sqrt(2*m*(en+q*omega))/hbar$
sine_kernel(k,s):=block([x],limit(sin(x*s)/x,x,k))$

free_transfer(en,s):=block([C,U,V],
  C:genmatrix(lambda([i,j],kron_delta(i,j)*cos(kq(en,qs[i])*s)),Ns,Ns),
  U:genmatrix(lambda([i,j],kron_delta(i,j)
      *sine_kernel(kq(en,qs[i]),s)),Ns,Ns),
  V:genmatrix(lambda([i,j],-kron_delta(i,j)*kq(en,qs[i])
      *sin(kq(en,qs[i])*s)),Ns,Ns), join4(C,U,V,C))$
cell_transfer(en):=bfloat(free_transfer(en,b).jump(gB)
                          .free_transfer(en,a).jump(gA))$

floquet_multipliers(en):=block([lam:'lam,p,roots],
  p:expand(charpoly(cell_transfer(en),lam)),
  roots:map(rhs,allroots(p)),roots)$
multiplier_row(en):=block([M:cell_transfer(en),r],
  r:floquet_multipliers(en),
  [en,cabs(rectform(determinant(M)-1)),sort(map(cabs,r))])$

eps_scan:[0.35,0.55,0.75]$
spectrum_table:map(multiplier_row,eps_scan)$
roots_mid:floquet_multipliers(0.55)$
print("FLOQUET-SAMBE DELTA-COMB MODEL: Q =",Q,"sidebands =",qs)$
print("contact Toeplitz block A =",toeplitz_harmonic(gA))$
print("columns [quasienergy, |det(M)-1|, sorted |Bloch multipliers|]")$
for row in spectrum_table do print(row)$
print("multipliers [beta,|beta|] at quasienergy 0.55")$
for root in roots_mid do print([root,cabs(root)])$
```

What Kind of Solution Will Fill the Gap

Target result

The key mathematical result is a weighted infinite-Sambe Fredholm/Evans determinant plus a truncation theorem. Let $\mathcal{H}_\eta = \{\mathbf{v} : \sum_q e^{2\eta|q|}\|\mathbf{v}_q\|^2 < \infty\}$, let P_Q project onto $|q| \le Q$, and let ι_Q be the corresponding inclusion. Because closed-sideband transfer blocks grow exponentially, formulate a stabilized cell-matching or scattering operator $\mathsf{K}_\infty(\varepsilon)$, with truncation K_Q, rather than taking an undefined norm difference between raw finite- and infinite-dimensional transfer matrices. For an analytic drive, away from sideband thresholds, prove for $0 < \eta' < \eta$

$$\boxed{\|\mathsf{K}_\infty(\varepsilon) - \iota_Q \mathsf{K}_Q(\varepsilon) P_Q\|_{\mathcal{B}(\mathcal{H}_\eta, \mathcal{H}_{\eta'})} \le C(\varepsilon, \eta, \eta') e^{-\sigma Q},}$$

with a separate algebraic estimate at thresholds. From it derive: an exact quasienergy–β determinant; an open-boundary condition and skin length; Evans functions at $\varepsilon = 0$ and $\varepsilon = \hbar\Omega/2$; a periodized, micromotion-resolved winding evaluated on the GBZ; and a disordered criterion in terms of the two central Lyapunov exponents. A phase diagram must quantify where high-frequency or effective-medium approximations fail.

References

[1] F. Thompson, K. Jones-Smith, H. Mathur, and K. McKee. "Contact interactions and Kronig–Penney models in Hermitian and PT-symmetric quantum mechanics". In: *Journal of Physics A: Mathematical and Theoretical* 51 (2018), p. 495204. DOI: 10.1088/1751-8121/aaeaa6. URL: https://arxiv.org/abs/1804.06681.

[2] Kazuki Yokomizo and Shuichi Murakami. "Non-Bloch band theory of non-Hermitian systems". In: *Physical Review Letters* 123 (2019), p. 066404. DOI: 10.1103/PhysRevLett.123.066404. URL: https://arxiv.org/abs/1902.10958.

[3] Xizheng Zhang and Jiangbin Gong. "Non-Hermitian Floquet topological phases: exceptional points, coalescent edge modes, and the skin effect". In: *Physical Review B* 101 (2020), p. 045415. DOI: 10.1103/PhysRevB.101.045415. URL: https://arxiv.org/abs/1909.10234.

[4] Longwen Zhou and Da-Jian Zhang. *Non-Hermitian Floquet topological matter: a review.* 2023. URL: https://arxiv.org/abs/2305.16153 (visited on 07/16/2026).

[5] Y.-M. Hu, Y.-Q. Huang, W.-T. Xue, and Z. Wang. "Non-Bloch band theory for non-Hermitian continuum systems". In: *Physical Review B* 110 (2024), p. 205429. DOI: 10.1103/PhysRevB.110.205429. URL: https://arxiv.org/abs/2310.08572.

[6] H. Ding and K. Ding. "Non-Bloch theory for spatiotemporal photonic crystals assisted by continuum effective medium". In: *Physical Review Research* 6 (2024), p. 033167. DOI: 10.1103/PhysRevResearch.6.033167. URL: https://arxiv.org/abs/2401.12536.

[7] H. Wu, X.-M. Yang, and H. Liu. "Breakdown of non-Bloch bulk–boundary correspondence and emergent topology in Floquet non-Hermitian systems". In: *Physical Review B* 113 (2026), p. 235123. DOI: 10.1103/f37j-l6wp. URL: https://arxiv.org/abs/2510.09193.

5 Finite-coupling non-Markovian Zeno dynamics from structured reservoirs

Flügge seed: Vol. I, Problem 12, which computes the return probability after a projective measurement followed by unitary evolution. The modern question replaces ideal projections by microscopic reservoirs.

The ideal quantum-Zeno effect and quantum-Zeno dynamics are mature: frequent projections, kicks, or continuous strong coupling confine motion to spectral subspaces of a measurement operator [1]. The anti-Zeno effect also shows that the reservoir spectral density can enhance, rather than inhibit, decay [2]. General diagnostics of memory and information backflow are reviewed in [3].

Finite-coupling corrections are already known for Markovian strong dissipation. Effective Lindblad motion inside a dark/Zeno subspace and the large-dissipation Liouvillian spectrum were derived in [4, 5]. A further expansion of a strongly dissipative Lindblad generator would therefore duplicate established results.

The required extension is a measurement generated by an explicit bath without assuming a semigroup. Marcantoni and Merkli proved that ultrastrong bosonic coupling produces an instantaneous nonselective measurement followed by a Zeno Hamiltonian; additional reservoirs can leave non-Markovian reduced dynamics [6]. Gaikwad et al. engineered a non-Markovian-to-Markovian crossover and a Zeno-stabilized decoherence-free subspace [7]. Crucially, the 2026 fine-time analysis now resolves the initial one-reservoir transient on $t = O(\lambda^{-1})$ [8]. What remains is a uniform finite-λ theory on physical times $t = O(1)$ for several structured reservoirs, especially competing noncommuting strong couplings, with an explicit memory kernel, complete-positivity control, and leakage error bars.

Formalisms

Microscopic model, spaces, and scales

Set $\hbar = 1$. Let the measured system have finite-dimensional Hilbert space $\mathcal{H}_S$, while reservoir ν is a bosonic Fock space $\mathcal{F}_\nu$. A concrete starting Hamiltonian is

$$H_\lambda = H_S + \sum_{\nu=0}^{M} H_{R,\nu} + \lambda A \otimes B_0 + \sum_{\nu=1}^{M} g_\nu S_\nu \otimes B_\nu, \tag{107}$$

$$H_{R,\nu} = \int_0^\infty \omega b_\nu^\dagger(\omega) b_\nu(\omega)\, d\omega, \tag{108}$$

$$B_\nu = \int_0^\infty \left[h_\nu(\omega) b_\nu^\dagger(\omega) + \overline{h_\nu(\omega)} b_\nu(\omega) \right] d\omega. \tag{109}$$

Here λ is the dimensionless strong-measurement parameter, g_ν are fixed weak or moderate couplings, and h_ν has units that make B_ν an energy. More general bounded system operators and fermionic reservoirs may be used, but the domain of H_λ must be independent of λ; a sufficient bosonic assumption is relative boundedness of each field operator with respect to $(H_{R,\nu} + 1)^{1/2}$.

Write the measured observable and its spectral projections as

$$A = \sum_a a P_a, \qquad P_a P_b = \delta_{ab} P_a, \qquad \sum_a P_a = I_S. \tag{110}$$

The initial state is first taken to be factorized,

$$\rho(0) = \rho_S(0) \otimes \rho_R, \qquad \rho_R = \bigotimes_{\nu=0}^{M} \rho_{R,\nu}, \qquad [\rho_{R,\nu}, H_{R,\nu}] = 0, \tag{111}$$

with $\rho_S \geq 0$ and $\operatorname{Tr}\rho_S = 1$. Shift each bath operator so that $\operatorname{Tr}_R(B_\nu \rho_R) = 0$. The stationary correlation matrix is

$$C_{\mu\nu}(t) = \operatorname{Tr}_R[B_\mu(t) B_\nu(0)\rho_R], \qquad B_\nu(t) = e^{iH_R t} B_\nu e^{-iH_R t}. \tag{112}$$

For an independent thermal bath of inverse temperature β_ν,

$$C_{\nu\nu}(t) = \int_0^\infty d\omega\, J_\nu(\omega) \left[(n_\nu(\omega)+1)e^{-i\omega t} + n_\nu(\omega)e^{i\omega t}\right], \quad J_\nu = |h_\nu|^2, \tag{113}$$

where $n_\nu = (e^{\beta_\nu \omega} - 1)^{-1}$. A rigorous expansion must state whether $C \in L^1(\mathbb{R}_+)$, whether its first moments are integrable, and how any infrared behavior $J(\omega) \sim \omega^s$ is handled. Those choices determine the power of $1/\lambda$.

Measurement channel and boundary layer

The ideal nonselective measurement is the conditional expectation

$$\mathcal{M}(X) = \sum_a P_a X P_a, \qquad \mathfrak{A}_Z = \{X \in \mathcal{B}(\mathcal{H}_S) : [X, A] = 0\}. \tag{114}$$

Thus $\mathcal{M}$ projects onto the block-diagonal Zeno algebra, not onto a single outcome. The Hamiltonian surviving inside that algebra is

$$H_Z = \mathcal{M}(H_S) = \sum_a P_a H_S P_a. \tag{115}$$

For the exactly soluble pure-dephasing part $H_R + \lambda A \otimes B_0$, an off-diagonal block has the form

$$P_a \rho_S(t) P_b = \chi_{ab}^{(\lambda)}(t) P_a \rho_S(0) P_b, \qquad \chi_{ab}^{(\lambda)}(t) = \operatorname{Tr}_R[U_a(t)\rho_R U_b(t)^\dagger], \tag{116}$$

where $U_a(t) = \exp[-it(H_R + \lambda a B_0)]$. For a Gaussian bath,

$$|\chi_{ab}^{(\lambda)}(t)| = \exp[-\lambda^2 (a-b)^2 G(t)], \tag{117}$$

$$G(t) = \int_0^\infty d\omega\, \frac{J_0(\omega)}{\omega^2}(1 - \cos\omega t) \coth\left(\frac{\beta_0 \omega}{2}\right). \tag{118}$$

If $G(t) = g_2 t^2 + O(t^4)$, coherence is removed on the inner scale $\tau = \lambda t = O(1)$. Algebraic infrared correlations can produce a different inner scale, which must be derived rather than assumed. The outer initial condition is consequently $\mathcal{M}\rho_S(0)$, augmented by an initial-slip correction obtained by matching to the inner solution.

Exact projection equation

Define the Liouvillian $\mathcal{L}_\lambda X = -i[H_\lambda, X]$. A Zeno-adapted projection on trace-class operators is

$$\mathsf{P}X = \sum_a P_a \operatorname{Tr}_R(P_a X P_a) P_a \otimes \rho_R, \qquad \mathsf{Q} = I - \mathsf{P}. \tag{119}$$

Apply P and Q to $\dot\rho = \mathcal{L}_\lambda \rho$, solve the Q equation by Duhamel's formula, and substitute it into the P equation. This gives the exact Nakajima–Zwanzig identity

$$\frac{d}{dt}\mathsf{P}\rho(t) = \mathsf{P}\mathcal{L}_\lambda \mathsf{P}\rho(t) + \int_0^t \mathcal{K}_\lambda(t-s)\mathsf{P}\rho(s)\, ds + \mathcal{I}_\lambda(t), \tag{120}$$

$$\mathcal{K}_\lambda(t) = \mathsf{P}\mathcal{L}_\lambda \mathsf{Q} e^{t\mathsf{Q}\mathcal{L}_\lambda \mathsf{Q}} \mathsf{Q}\mathcal{L}_\lambda \mathsf{P}, \tag{121}$$

$$\mathcal{I}_\lambda(t) = \mathsf{P}\mathcal{L}_\lambda \mathsf{Q} e^{t\mathsf{Q}\mathcal{L}_\lambda \mathsf{Q}} \mathsf{Q}\rho(0). \tag{122}$$

Even a factorized initial state has $\mathsf{Q}\rho(0) \neq 0$ when it contains coherences between distinct P_a blocks, so the inhomogeneous term is precisely where the rapid measurement transient enters. If one uses the simpler reservoir projector $\mathrm{Tr}_R(X) \otimes \rho_R$, that term vanishes initially, but the subsequent projection onto $\mathfrak{A}_Z$ must then be performed separately.

In Laplace space, for $\mathrm{Re}\, z > 0$, the memory self-energy is

$$\widetilde{\mathcal{K}}_\lambda(z) = \mathsf{P}\mathcal{L}_\lambda\mathsf{Q}(z - \mathsf{Q}\mathcal{L}_\lambda\mathsf{Q})^{-1}\mathsf{Q}\mathcal{L}_\lambda\mathsf{P}. \tag{123}$$

This resolvent representation is preferable to a pointwise expansion of $\mathcal{K}_\lambda(t)$, because the latter generally contains a narrowing boundary-layer contribution. A matched form is

$$\mathcal{K}_\lambda(t) = \lambda^p \mathcal{K}_{\mathrm{bl}}^{(0)}(\lambda^p t) + \mathcal{K}_{\mathrm{out}}^{(0)}(t) + \lambda^{-p}\mathcal{K}_{\mathrm{out}}^{(1)}(t) + \cdots, \tag{124}$$

with p fixed by the short-time bath correlation. Its time integral, not its pointwise height, determines the finite outer correction.

Dressed kernels and competing measurements

Split $H_\lambda = H_{\mathrm{str},\lambda} + V$, treating the strong bath exactly and $V = H_S + \sum_{\nu \geq 1} g_\nu S_\nu \otimes B_\nu$ perturbatively only when the stated g_ν counting permits it. In the strong interaction picture,

$$V_\lambda(t) = U_{\mathrm{str},\lambda}(t)^\dagger V U_{\mathrm{str},\lambda}(t), \tag{125}$$

and the second-order convolution kernel acting on a system block X is

$$\mathcal{K}_\lambda^{(2)}(t)X = -\mathcal{M}\,\mathrm{Tr}_R[V_\lambda(t), [V_\lambda(0), X \otimes \rho_R]]. \tag{126}$$

Decomposing $S_\nu = \sum_{ab} P_a S_\nu P_b$ makes every transition carry a strong-bath overlap $\chi_{ab}^{(\lambda)}$. This is the calculable link between the spectral densities and leakage out of a Zeno block.

For two measurement reservoirs consider

$$H_{\mathrm{str},\lambda} = \lambda A \otimes B + \lambda^\alpha C \otimes D, \qquad [A, C] \neq 0. \tag{127}$$

For $0 < \alpha < 1$, the A boundary layer occurs first, at $t_A \sim \lambda^{-1}$; the slower layer $t_C \sim \lambda^{-\alpha}$ then acts on the already projected A-algebra. Its generator contains the A-block-diagonal part of C and strong-bath dressing, so a naive second projection by C need not be correct. For $\alpha > 1$ the order is reversed. At $\alpha = 1$ there is no sequential limit; under faithful, independent dephasing the surviving algebra is

$$\mathfrak{A}_{AC} = \{X : [X, A] = [X, C] = 0\}. \tag{128}$$

Correlated baths or a singular correlation matrix can leave a larger decoherence-free algebra, so the general construction is the kernel of the joint quadratic decoherence form. For $\alpha \leq 0$, the C coupling is not itself a divergent measurement on physical times and belongs in the outer dynamics.

Observables, complete positivity, and workflow

The exact reduced map

$$\Phi_\lambda(t)[\rho_S] = \mathrm{Tr}_R\Big(e^{-itH_\lambda}(\rho_S \otimes \rho_R)e^{itH_\lambda}\Big) \tag{129}$$

is completely positive and trace preserving. A truncated memory equation need not share that property. For a finite system, compute its Choi matrix

$$C_\Phi(t) = \sum_{mn} |m\rangle\langle n| \otimes \Phi(t)(|m\rangle\langle n|) \tag{130}$$

and check $C_\Phi(t) \geq 0$ and $\mathrm{Tr}_2\, C_\Phi = I$. Negative time-local rates diagnose failure of CP divisibility, but do not alone imply that $\Phi(t)$ is nonpositive.

For a chosen Zeno projector P, directly measurable diagnostics are

$$L_P(t) = 1 - \mathrm{Tr}[P\rho_S(t)], \qquad C_{ab}(t) = \|P_a\rho_S(t)P_b\|_1, \qquad \Delta_O(t) = \mathrm{Tr}[O(\rho_S(t) - \rho_Z(t))]. \quad (131)$$

An implementable calculation proceeds as follows: specify $J_\nu(\omega)$ and temperatures; evaluate $C_{\mu\nu}(t)$; obtain the inner dephasing solution; construct the Laplace-space projected resolvent; invert it by a stable contour method; and compare with a nonperturbative reduced-dynamics solver. A Lorentzian J admits a pseudomode embedding, while sums of exponentials permit hierarchical equations or tensor-network influence functionals.

Mandatory checks are trace and Hermiticity preservation, convergence as the pseudomode or memory cutoff grows, recovery of unitary dynamics at zero bath coupling, the Markovian limit for a delta-correlated weak reservoir, and the projective Zeno limit as $\lambda \to \infty$. The unresolved mathematical object is the composite inner–outer expansion of $\widetilde{\mathcal{K}}_\lambda(z)$ and its inverse Laplace transform, uniform for physical times and expressed in terms of the structured correlation matrix, including the noncommuting-coupling algebra.

Maxima research model

The driver evaluates finite-coupling coherence and the time-local dephasing rate for a zero-temperature Ohmic bath augmented by exponentially correlated structured noise. Its editable inputs are the two bath strengths, cutoff, memory time, coupling grid, and time grid; it prints an outer-time table, an inner Zeno-layer comparison, and the rational structured-memory kernel. Run it from the project root with

```
maxima --batch=maxima/05_nonmarkovian_zeno.mac
```

Replace `Goh`, `Gstr`, and `Cstr_tilde` together to insert another measured spectral density and carry the same finite-coupling scan into a parameter fit. This is an exactly soluble commuting pure-dephasing baseline; noncommuting Zeno projectors require replacing the scalar exponent by the projected operator-valued memory kernel.

```
/* Finite-coupling dephasing with Ohmic and exponential memory. */
kill(all)$
display2d:false$
ratprint:false$
linel:200$

/* Editable reservoir parameters (dimensionless units). */
eta:1/10$                         /* Ohmic strength */
wc:4$                             /* Ohmic cutoff */
sigma2:1/20$                      /* C_str(0) */
tc:3/2$                           /* structured-memory time */

Goh(t):=eta*log(1+wc^2*t^2)/2$
Gstr(t):=sigma2*tc^2*(exp(-t/tc)+t/tc-1)$
Gtot(t):=Goh(t)+Gstr(t)$
coherence(lam,t):=exp(-lam^2*Gtot(t))$
rate(lam,t):=lam^2*(eta*wc^2*t/(1+wc^2*t^2)
                  +sigma2*tc*(1-exp(-t/tc)))$

/* Rational Laplace transform of C_str(t)=sigma2 exp(-t/tc). */
Cstr_tilde(z):=sigma2/(z+1/tc)$
memory_kernel(z,lam):=lam^2*Cstr_tilde(z)$

lambda_grid:[1/2,1,2,4]$
inner_lambda_grid:[2,4,8,16,32]$
time_grid:[1/50,1/10,1/2,1]$
print("outer table: [lambda,t,coherence,instantaneous_rate]")$
for lam in lambda_grid do
  for tv in time_grid do
    print([lam,tv,float(coherence(lam,tv)),float(rate(lam,tv))])$

/* The inner coordinate tau=lambda*t resolves the Zeno layer. */
tau0:1$
short_variance:eta*wc^2+sigma2$
inner_gaussian(tau):=exp(-short_variance*tau^2/2)$
inner_exact(lam,tau):=coherence(lam,tau/lam)$
print("inner table: [lambda,tau,C_exact,C_Gaussian]")$
for lam in inner_lambda_grid do
  print([lam,tau0,float(inner_exact(lam,tau0)),
         float(inner_gaussian(tau0))])$

print("structured Laplace kernel at lambda=2:",
      memory_kernel(z,2))$
```

What Kind of Solution Will Fill the Gap

Target result

A decisive result is a theorem constructing explicit effective maps through first correction order and proving, under stated correlation-decay and regularity assumptions,

$$\boxed{\sup_{0\le t\le T}\left\|\Phi_\lambda(t)-\Phi_{\rm eff}^{(0)}(t)-\lambda^{-1}\Phi_{\rm eff}^{(1)}(t)\right\|_\diamond \le \frac{C_T}{\lambda^2}.}$$

It should give $\mathcal{K}^{(0)}$ and $\mathcal{K}^{(1)}$ in terms of measurable spectral densities $J_\nu(\omega)$, state when the truncated description is completely positive, and prove a leakage estimate

$$L_P(t)=\mathrm{Tr}[(1-P)\rho_S(t)]\le C_T\lambda^{-p}.$$

For two noncommuting strong couplings, the work must classify the surviving algebra generated by (A) and (C), including the possibility that no nontrivial Zeno subsystem survives at $\alpha=1$. An exactly solvable Lorentzian-bath qubit or pseudomode model should benchmark the expansion and turn the bound into predictions for coherence and entanglement lifetimes.

References

[1] Paolo Facchi and Saverio Pascazio. "Quantum Zeno dynamics: mathematical and physical aspects". In: *Journal of Physics A: Mathematical and Theoretical* 41 (2008), p. 493001. DOI: 10.1088/1751-8113/41/49/493001. URL: https://arxiv.org/abs/0903.3297.

[2] A. G. Kofman and G. Kurizki. "Acceleration of quantum decay processes by frequent observations". In: *Nature* 405 (2000), pp. 546–550. DOI: 10.1038/35014537.

[3] Heinz-Peter Breuer, Elsi-Mari Laine, Jyrki Piilo, and Bassano Vacchini. "Non-Markovian dynamics in open quantum systems". In: *Reviews of Modern Physics* 88 (2016), p. 021002. DOI: 10.1103/RevModPhys.88.021002. URL: https://arxiv.org/abs/1505.01385.

[4] Vladislav Popkov, Sander Essink, Carlo Presilla, and Gunter M. Schütz. "Effective quantum Zeno dynamics in dissipative quantum systems". In: *Physical Review A* 98 (2018), p. 052110. DOI: 10.1103/PhysRevA.98.052110. URL: https://arxiv.org/abs/1806.10422.

[5] Vladislav Popkov and Carlo Presilla. "Full spectrum of the Liouvillian of open dissipative quantum systems in the Zeno limit". In: *Physical Review Letters* 126 (2021), p. 190402. DOI: 10.1103/PhysRevLett.126.190402. URL: https://arxiv.org/abs/2101.05708.

[6] Stefano Marcantoni and Marco Merkli. *Ultrastrong coupling, nonselective measurement and quantum Zeno dynamics*. 2024. URL: https://arxiv.org/abs/2411.06817 (visited on 07/16/2026).

[7] Chandrashekhar Gaikwad, Daria Kowsari, Carson Brame, Xingrui Song, Haimeng Zhang, Martina Esposito, Arpit Ranadive, Giulio Cappelli, Nicolas Roch, Eli M. Levenson-Falk, and Kater W. Murch. *Entanglement assisted probe of the non-Markovian to Markovian transition in open quantum system dynamics*. 2024. URL: https://arxiv.org/abs/2401.13735 (visited on 07/16/2026).

[8] Stefano Marcantoni and Marco Merkli. *Ultrastrongly coupled open systems and fine grained time*. Accepted in Open Systems & Information Dynamics. 2026. URL: https://arxiv.org/abs/2606.16634 (visited on 07/16/2026).

6 NLO Efimov universality with finite range, one-dimensional spin–orbit coupling, and loss

Flügge seed: Vol. I, Problems 75–79, and Vol. II, Problems 139–166: central-force models, momentum-space integral equations, spin/tensor interactions, three-particle spin functions, and few-particle scattering.

Zero-range Efimov universality, its renormalization-group limit cycle, and the usual inelasticity parameter are established [1, 2]. Finite-effective-range corrections are established as well: NLO renormalization of the three-boson system requires additional three-body information when the scattering length is varied [3, 4].

Spin–orbit coupling (SOC) alone is likewise a developed deformation. For one-dimensional SOC, Guan and Blume showed that a generalized discrete scaling law survives when the scattering length, SOC momentum, Raman coupling, detuning, and center-of-mass momentum are rescaled together [5]. Loss has progressed beyond a purely phenomenological η_*: complex two-body scattering lengths generate non-Hermitian Efimov poles [6], and dissipative SOC three-body models have now been considered [7]. Dipolar anisotropy is a separate long-range problem; recent calculations show that portions of van der Waals universality survive after appropriate two-body parameters are renormalized [8].

A proposal combining "finite range plus anisotropy, SOC, and loss" would be too broad. A tractable target is the NLO renormalization of finite effective range, experimentally relevant one-dimensional SOC, and a complex two-body scattering length, followed by a derivation of the complex correction to the generalized Efimov radial law. Weak dipolar anisotropy belongs in a later extension with its own power counting.

Formalisms

Three-body model and conventions

Take three identical bosons of mass m, each carrying two internal states. After fixing the total wave vector $\mathbf{K}$ (total momentum $\hbar\mathbf{K}$), the relative wave function belongs to

$$\mathcal{H}_{\rm rel} = L^2(\mathbb{R}^3_{\mathbf{x}} \times \mathbb{R}^3_{\mathbf{y}}) \otimes \mathcal{S}_{\rm B}, \tag{132}$$

where $\mathbf{x}, \mathbf{y}$ are Jacobi coordinates and $\mathcal{S}_{\rm B} \subset (\mathbb{C}^2)^{\otimes 3}$ has the required bosonic permutation symmetry. The one-particle Hamiltonian is

$$h_{\rm sp}(\mathbf{p}) = \frac{\mathbf{p}^2}{2m} + \frac{\hbar k_{\rm so}}{m} p_z \sigma_z + \frac{\Omega}{2}\sigma_x + \frac{\delta}{2}\sigma_z, \tag{133}$$

where $k_{\rm so}$ is an inverse length and Ω, δ are energies. The many-body Hamiltonian before zero-range reduction is

$$H = \sum_{i=1}^{3} h_{\rm sp}(\mathbf{p}_i) + \sum_{i<j} V_{ij} + V_3, \qquad \sum_i \mathbf{p}_i = \hbar\mathbf{K}. \tag{134}$$

Assume that a specified symmetric two-body spin channel is resonant and all other channels are natural. The potential range r_0 is the ultraviolet length. Universal calculations require

$$r_0 \ll |a_c|, \quad r_0 k_{\rm so} \ll 1, \quad m|\Omega| r_0^2/\hbar^2 \ll 1, \quad m|\delta| r_0^2/\hbar^2 \ll 1. \tag{135}$$

Time dependence is $e^{-iEt/\hbar}$, and a decaying pole is written $E_* = E_R - i\Gamma/2$, with $\Gamma > 0$.

Two-body input and the two distinct loss mechanisms

Without SOC, the on-shell amplitude in the resonant channel is normalized as

$$f(k) = \frac{1}{k\cot\delta_0(k) - ik}, \qquad k\cot\delta_0(k) = -a_c^{-1} + \frac{1}{2} r_e k^2 + O(k^4 r_0^3). \tag{136}$$

Here a_c may be complex, while r_e is taken real in the minimal model. With the stated time convention, passive two-body absorption has $a_c = a_R - ia_I$, $a_I \geq 0$. If range-dependent absorption matters, r_e must also be complex and introduces another independently fitted parameter.

Two-body absorption is not the same as loss into unresolved deeply bound three-body channels. The latter is imposed at small hyperradius by the pair (R_0, η_*), or equivalently (Λ_*, η_*), where R_0 and $\Lambda_* \propto R_0^{-1}$ are real and $\eta_* \geq 0$. These parameters must remain separately visible:

$$F(R) \underset{R\to R_0^+}{\propto} \sqrt{R}\left[\left(\frac{R}{R_0}\right)^{is_0} - e^{-2\eta_*}\left(\frac{R}{R_0}\right)^{-is_0}\right]. \tag{137}$$

The factor $e^{-2\eta_*}$ is the short-distance reflection amplitude; $\eta_* = 0$ conserves hyperradial flux. Replacing the real phase by a complex three-body parameter is merely another representation of Eq. (137); adding a second deep-loss counterterm would double count the same physics. If both $\operatorname{Im} a_c$ and η_* are retained, two-body and three-body loss data are needed to identify them.

Auxiliary-dimer EFT and renormalized propagator

A practical zero-range formulation introduces a spinor atom field ψ and an auxiliary dimer d_α for each retained pair-spin channel α. Schematically,

$$\begin{aligned}\mathcal{L} = \psi^\dagger(i\hbar\partial_t - h_{\rm sp})\psi + d_\alpha^\dagger\left[\Delta_{\alpha,0} + \eta_\alpha\left(i\hbar\partial_t + \frac{\hbar^2\nabla^2}{4m}\right)\right]d_\alpha \\ - g_\alpha(d_\alpha^\dagger\psi^T P_\alpha\psi + \text{h.c.}) - \frac{mg_\alpha g_\beta}{\hbar^2\Lambda^2}H_{\alpha\beta}(\Lambda)d_\alpha^\dagger d_\beta\psi^\dagger\psi.\end{aligned} \tag{138}$$

Repeated channel labels are summed, and P_α projects onto the resonant pair spin. Let $Q_{\rm IR}$ be the largest external wave number among $|a_c|^{-1}$, $k_{\rm so}$, $|\mathbf{K}|$, and the pole momenta. Choose a cutoff in the EFT window $Q_{\rm IR} \ll \Lambda \lesssim r_0^{-1}$. Bare quantities Δ_0, η, g are matched to a_c, r_e; predictions must become independent of Λ to the calculated order as the window is widened.

In a helicity basis of Eq. (133), the dressed dimer propagator is a channel matrix,

$$\mathcal{D}^{-1}_{\alpha\beta}(E,\mathbf{q};\mathbf{K}) = \mathcal{D}^{-1}_{0,\alpha\beta}(E,\mathbf{q}) - g_\alpha g_\beta \Pi_{\alpha\beta}(E,\mathbf{q};\mathbf{K}), \tag{139}$$

with pair bubble

$$\Pi_{\alpha\beta} = \sum_{\lambda_1\lambda_2}\int_{|\mathbf{l}|<\Lambda}\frac{d^3l}{(2\pi)^3}\frac{\mathcal{C}_\alpha^{\lambda_1\lambda_2}(\mathbf{l},\mathbf{q})\overline{\mathcal{C}_\beta^{\lambda_1\lambda_2}(\mathbf{l},\mathbf{q})}}{E - \epsilon_{\lambda_1}(\mathbf{q}/2+\mathbf{l}) - \epsilon_{\lambda_2}(\mathbf{q}/2-\mathbf{l}) + i0}. \tag{140}$$

The spin overlaps $\mathcal{C}_\alpha$ follow from P_α, and ϵ_λ are the two helicity dispersions. Subtract the linear ultraviolet divergence before taking $\Lambda \to \infty$. In the limits $k_{\rm so}, \Omega, \delta \to 0$, matching must reduce $\mathcal{D}$ to Eq. (136).

STM equation with broken Galilean invariance

Let $\mathcal{F}_\alpha(\mathbf{p})$ be the amplitude for a spectator with wave vector $\mathbf{p}$ and a dimer in channel α. The homogeneous Skorniakov–Ter-Martirosian equation for a trimer pole is

$$\begin{aligned}\mathcal{F}_\alpha(\mathbf{p}) = \sum_{\beta\gamma}\int_{|\mathbf{q}|<\Lambda}\frac{d^3q}{(2\pi)^3}\left[\mathcal{Z}_{\alpha\beta}(\mathbf{p},\mathbf{q};E,\mathbf{K}) + \frac{H_{\alpha\beta}(\Lambda)}{\Lambda^2}\right] \\ \times\mathcal{D}_{\beta\gamma}(E - \epsilon_{\rm sp}(\mathbf{p}), \mathbf{K}-\mathbf{p};\mathbf{K})\mathcal{F}_\gamma(\mathbf{q}).\end{aligned} \tag{141}$$

The exchange kernel $\mathcal{Z}$ is obtained from the propagator of the exchanged atom and the helicity-spin overlaps. Because one-dimensional SOC breaks Galilean invariance, E and $\mathbf{K}$ are independent inputs, and the kernel cannot in general be reduced to a function of $|\mathbf{p}|, |\mathbf{q}|$ alone. Axial symmetry about z still permits blocks of fixed total azimuthal quantum number.

After quadrature, define

$$\mathsf{A}_\Lambda(E) = I - \mathsf{K}_\Lambda(E), \qquad D_\Lambda(E) = \det \mathsf{A}_\Lambda(E). \tag{142}$$

Bound states are zeros on the physical sheet below all thresholds. For a resonance, continue each helicity-channel momentum through its cut. The physical convention is $\sqrt{-m(E+i0)/\hbar^2} > 0$ below a simple zero-SOC threshold; changing its sign selects the adjacent outgoing sheet. With SOC, a sheet is specified by the sign choice for every open helicity momentum. Complex a_c then moves the pole further into the lower half-plane without changing that convention.

Hyperradial limit cycle and generalized scaling

In the window

$$r_0 \ll R \ll \min(|a_c|, k_{\mathrm{so}}^{-1}, \hbar/\sqrt{m|\Omega|}, \hbar/\sqrt{m|\delta|}), \tag{143}$$

the SOC and threshold scales drop out of the hyperangular equation. For three identical bosons its attractive eigenvalue is $-s_0^2$, $s_0 \simeq 1.00624$, and

$$\left[-\frac{d^2}{dR^2} - \frac{s_0^2 + \frac{1}{4}}{R^2}\right] F(R) = \frac{2\mu_3 E}{\hbar^2} F(R), \qquad \lambda_0 = e^{\pi/s_0} \simeq 22.694. \tag{144}$$

Here μ_3 depends only on the Jacobi-coordinate normalization. Cutoff independence at leading order gives the limit-cycle coupling

$$H_0(\Lambda) = \frac{\cos[s_0 \ln(\Lambda/\Lambda_*) + \arctan s_0]}{\cos[s_0 \ln(\Lambda/\Lambda_*) - \arctan s_0]}, \tag{145}$$

where the real Λ_* fixes the phase modulo multiplication by λ_0, while η_* independently fixes short-range loss.

For a pole scale $\kappa_n = \sqrt{-mE_n}/\hbar$, useful dimensionless variables are

$$\mathbf{y}_n = \left(\frac{1}{\kappa_n a_c}, \kappa_n r_e, \frac{k_{\mathrm{so}}}{\kappa_n}, \frac{m\Omega}{\hbar^2\kappa_n^2}, \frac{m\delta}{\hbar^2\kappa_n^2}, \frac{K_{\mathrm{cm}}}{\kappa_n}, \eta_*\right). \tag{146}$$

At zero range the simultaneous rescaling of all dimensional arguments gives

$$E_{n+1}(a_c, k_{\mathrm{so}}, \Omega, \delta, K_{\mathrm{cm}}) = \lambda_0^{-2} E_n\left(\frac{a_c}{\lambda_0}, \lambda_0 k_{\mathrm{so}}, \lambda_0^2\Omega, \lambda_0^2\delta, \lambda_0 K_{\mathrm{cm}}\right). \tag{147}$$

NLO insertion and location of the unknown counterterm

Use the explicit counting

$$Q_{\mathrm{EFT}} = \max\left(\kappa_n|r_e|, \frac{|\operatorname{Im} a_c^{-1}|}{\kappa_n}, \eta_*\right) \ll 1, \tag{148}$$

while holding the finite SOC ratios in $\mathbf{y}_n$ fixed. Expand the dimer and STM kernels as

$$\mathcal{D} = \mathcal{D}_0 + \mathcal{D}_0 \delta\mathcal{D}_r^{-1} \mathcal{D}_0 + \cdots, \qquad \mathsf{K} = \mathsf{K}_0 + r_e \mathsf{K}_r + \mathsf{K}_3^{(1)} + \cdots. \tag{149}$$

The NLO amplitude satisfies

$$(I - \mathsf{K}_0)\mathcal{F}_1 = (r_e \mathsf{K}_r + \mathsf{K}_3^{(1)})\mathcal{F}_0. \tag{150}$$

Dimensionally, the running three-body coupling can contain

$$H(\Lambda) = H_0(\Lambda;\Lambda_*) + (\Lambda r_e)h_{10}(\Lambda) + \frac{r_e}{a_c}h_{11}(\Lambda) + (r_e k_{\rm so})h_{\rm so}(\Lambda) + \cdots . \tag{151}$$

The first two structures occur already without SOC when the scattering length is varied. The unresolved renormalization question is whether axial SOC and broken Galilean symmetry make $h_{\rm so}$, or another spin-dependent three-body operator, independently necessary rather than fixed by the usual NLO datum.

For a simple pole with right and left null vectors v_n, w_n, its NLO shift is computed without repeatedly searching the complex plane:

$$\delta E_n = -\frac{w_n^\dagger \delta\mathsf{A}(E_n)v_n}{w_n^\dagger(\partial_E\mathsf{A})(E_n)v_n}, \qquad \delta\mathsf{A} = -\delta\mathsf{K}. \tag{152}$$

The real and imaginary parts give the feature shift and width correction.

Numerical workflow and controlled limits

Diagonalize the single-particle helicity Hamiltonian; construct and renormalize Eq. (140); discretize momentum logarithmically and polar angles with axial-symmetry blocks; fit Λ_* and η_* to one real three-body feature and one deep-loss observable; fit any NLO finite part to an additional feature; then locate zeros of $D_\Lambda(E)$ on specified sheets. Repeat for several Λ values well above every infrared scale. Residual cutoff variation must decrease by one EFT order.

Report $E_n^{(R)}$, Γ_n, the threshold locations $a_{-,n}$ and $a_{*,n}$, and atom–dimer or three-atom loss obtained from the flux deficit of the corresponding S matrix. Checks include recovery of the standard STM equation as SOC vanishes, Eq. (145) under $\Lambda \mapsto \lambda_0\Lambda$, zero width when both loss mechanisms vanish, correct two-body unitarity when $\operatorname{Im} a_c = 0$, and Eq. (147) at $r_e = 0$. The research object is the cutoff-independent NLO kernel and its minimal counterterm set, from which the complex violation of generalized discrete scaling follows.

Maxima research model

The driver samples the complex three-body running coupling over one cutoff cycle and generates a lossy, NLO-deformed Efimov ladder. The inputs `s0`, `LambdaStar`, `etaStar`, `re`, and `kso` control the cycle, while the printed tables give complex running, level momenta, energies, widths, and an EFT validity parameter. Run it from the project root with

```
maxima --batch=maxima/06_efimov_corrections.mac
```

Replace `range_shift` and `soc_shift` by corrections extracted from a discretized NLO STM kernel, then use `validity` to retain only controlled levels. The displayed corrections are parameterized EFT ansatzes, not a discretized STM solve with cutoff renormalization and complex-sheet pole searches.

```
/* Complex Efimov limit cycle and an NLO-deformed level ladder. */
kill(all)$
display2d:false$
ratprint:false$
linel:200$

/* Editable EFT inputs; hbar^2/m=1. */
s0:1.00624$
LambdaStar:1$
etaStar:0.08$                    /* deep-channel loss phase */
kappaStar:1$
re:0.05$                         /* effective range */
kso:1.0e-5$                      /* infrared SOC momentum */
cr:0.4$
cso:0.2$

u(L):=s0*log(L/LambdaStar)+%i*etaStar$
Hrun(L):=cos(u(L)+atan(s0))/cos(u(L)-atan(s0))$
lambda0:exp(%pi/s0)$

print("cutoff table: [Lambda,Re(H),Im(H)]")$
for q:0 thru 4 do block([Lv,Hv],
  Lv:LambdaStar*exp(q*%pi/(4*s0)),
  Hv:float(rectform(Hrun(Lv))),
  print([float(Lv),realpart(Hv),imagpart(Hv)]))$

kappaLO(n):=kappaStar*exp(-%pi*n/s0)$
range_shift(n):=cr*re*kappaLO(n)$
soc_shift(n):=cso*(kso/kappaLO(n))^2$
kappaNLO(n):=kappaLO(n)*(1+range_shift(n)+soc_shift(n))$
validity(n):=abs(re*kappaLO(n))+(kso/kappaLO(n))^2$
Elevel(n):=-kappaNLO(n)^2*exp(2*%i*etaStar/s0)$
width(n):=-2*imagpart(rectform(Elevel(n)))$

print("level table: [n,kappa_NLO,Re(E),width,EFT_parameter]")$
for n:0 thru 3 do block([En],
  En:float(rectform(Elevel(n))),
  print([n,float(kappaNLO(n)),realpart(En),
         float(width(n)),float(validity(n))]))$

print("LO discrete factors: momentum =",float(1/lambda0),
      ", energy =",float(1/lambda0^2))$
```

What Kind of Solution Will Fill the Gap

Target result

The first formal deliverable is the renormalized NLO interaction

$$\boxed{H_{\rm NLO}(\Lambda) = H_0(\Lambda;\Lambda_*) + r_e H_r(\Lambda) + \cdots\,,}$$

with complex a_c entering the two-body propagator, and a demonstration that the complex STM pole energies are cutoff independent. In the alternative deep-loss scheme, promote the real short-distance phase to a complex one parameterized by (Λ_*, η_*); do not append a redundant $H_{\rm loss}$. The central question is whether broken Galilean and spin symmetry requires an additional independent NLO three-body operator.
The analytical output should be a corrected radial law,

$$E_{n+1}(\mathbf{x}) - \lambda_0^{-2} E_n(S^{-1}\mathbf{x}) = \frac{\hbar^2\kappa_n^2}{2\mu}\,\mathcal{C}_n(\mathbf{y}),$$

$$\mathcal{C}_n(\mathbf{y}) = C_r r_e \kappa_n + C_{r\rm so} r_e k_{\rm so} + C_{2L}\frac{\operatorname{Im} a_c^{-1}}{\kappa_n} + C_{3L}\eta_* + \cdots\,.$$

where $E_n = E_n^{(R)} - i\Gamma_n/2$, S^{-1} is the generalized scaling map, all $C_i = C_i(\mathbf{y})$, and $\mathbf{y}$ contains dimensionless SOC and loss variables. It must predict both feature shifts and widths

$a_{-,n}, a_{*,n}, E_n^{(R)}, \Gamma_n$, with EFT truncation errors. A later dipolar extension is controlled only when $a_{\rm dd}\kappa_n \ll 1$.

References

[1] Eric Braaten and H.-W. Hammer. "Universality in few-body systems with large scattering length". In: *Physics Reports* 428 (2006), pp. 259–390. DOI: 10.1016/j.physrep.2006.03.001. URL: https://arxiv.org/abs/cond-mat/0410417.

[2] Pascal Naidon and Shimpei Endo. "Efimov physics: a review". In: *Reports on Progress in Physics* 80 (2017), p. 056001. DOI: 10.1088/1361-6633/aa50e8. URL: https://arxiv.org/abs/1610.09805.

[3] Chen Ji, Daniel R. Phillips, and Lucas Platter. "The three-boson system at next-to-leading order in an effective field theory for systems with a large scattering length". In: *Annals of Physics* 327 (2012), pp. 1803–1824. DOI: 10.1016/j.aop.2012.02.001. URL: https://arxiv.org/abs/1106.3837.

[4] Chen Ji, Eric Braaten, Daniel R. Phillips, and Lucas Platter. "Universal relations for range corrections to Efimov features". In: *Physical Review A* 92 (2015), p. 030702. DOI: 10.1103/PhysRevA.92.030702. URL: https://arxiv.org/abs/1506.02334.

[5] Q. Guan and D. Blume. "Three-boson spectrum in the presence of one-dimensional spin-orbit coupling: Efimov's generalized radial scaling law". In: *Physical Review X* 8 (2018), p. 021057. DOI: 10.1103/PhysRevX.8.021057. URL: https://arxiv.org/abs/1807.07653.

[6] Mingyuan Sun, Chang Liu, and Zhiyuan Shi. "Non-Hermitian Efimov physics in dissipative three-body systems". In: *Physical Review Research* 5 (2023), p. 043010. DOI: 10.1103/PhysRevResearch.5.043010.

[7] X. Zhao. "Three-body physics under dissipative spin-orbit coupling". In: *Chinese Physics B* 34 (2025), p. 033101. DOI: 10.1088/1674-1056/ada43e.

[8] K. Oi, P. Naidon, and S. Endo. "Universality of Efimov states in highly mass-imbalanced cold-atom mixtures with van der Waals and dipole interactions". In: *Physical Review A* 110 (2024), p. 033305. DOI: 10.1103/PhysRevA.110.033305. URL: https://arxiv.org/abs/2404.02441.

7 Constraint-preserving and variationally stable orbital-free kinetic-energy functionals

Flügge seed: Vol. II, Problems 167–178: the electron gas, Thomas–Fermi approximation, Amaldi correction, virial theorem, and variational approximations to atomic screening.

The central unknown in orbital-free DFT (OFDFT) is the noninteracting kinetic functional $T_s[n]$. Thomas–Fermi, von Weizsaecker, gradient expansions, and density-response kernels establish important limits but no traditional functional is uniformly accurate for metals, molecules, density tails, shell structure, and strongly inhomogeneous regions. Exact Pauli-potential properties, including positivity for physical ground-state densities, were derived in [1]; the modern status and limits of nonlocal kernels are reviewed in [2].

Machine learning has advanced the frontier. KineticNet learned a transferable molecular functional and demonstrated self-consistent optimization in a restricted setting [3]. Remme et al. subsequently obtained stable optimized densities and near-Kohn–Sham energies over a substantial QM9 domain [4]. Periodic constrained-search and Pauli-potential machinery has also progressed [5], while a 2026 jellium-with-gap nonlocal functional improves finite-cluster energies and Pauli potentials [6]. A recent perspective emphasizes interpretable and symbolic functional discovery [7].

Taken together, these results make unconstrained neural approximation of $T_s[n]$ an insufficient research objective. The sharper target is a density-only, size-consistent nonlocal functional with exact scaling and limiting constraints by construction, stable first and second functional derivatives during unconstrained minimization, broad transferability, and a controlled warning when a trial density leaves its domain of validity.

Formalisms

Units, density domain, and constrained search

Use Hartree atomic units, $\hbar = m_e = e = 4\pi\epsilon_0 = 1$, and first consider a spin-unpolarized system. A mathematically natural density domain is

$$\mathcal{D}_N = \left\{ n : \mathbb{R}^3 \to [0,\infty); \left| \int n(\mathbf{r}) d^3r = N, \sqrt{n} \in H^1(\mathbb{R}^3) \right. \right\}. \tag{153}$$

For periodic matter, replace $\mathbb{R}^3$ by a unit cell, impose periodic boundary conditions, and normalize to the electrons per cell. The exact noninteracting kinetic functional is the constrained search

$$T_s[n] = \inf_{\{\varphi_i, f_i\} \to n} \frac{1}{2} \sum_i f_i \int |\nabla \varphi_i(\mathbf{r})|^2 d^3r, \tag{154}$$

$$n(\mathbf{r}) = \sum_i f_i |\varphi_i(\mathbf{r})|^2, \qquad \langle \varphi_i | \varphi_j \rangle = \delta_{ij}, \qquad \sum_i f_i = N. \tag{155}$$

The occupation convention may use spin orbitals $0 \le f_i \le 1$, or spatial orbitals $0 \le f_i \le 2$; it must be kept fixed in all reference data. Equation (154) defines the research target independently of any Kohn–Sham potential or machine-learning representation.

Introduce

$$T_W[n] = \frac{1}{8} \int \frac{|\nabla n|^2}{n} d^3r = \frac{1}{2} \int |\nabla \sqrt{n}|^2 d^3r, \tag{156}$$

$$T_P[n] = T_s[n] - T_W[n], \tag{157}$$

$$T_{\mathrm{TF}}[n] = C_F \int n^{5/3} d^3r, \qquad C_F = \frac{3}{10}(3\pi^2)^{2/3}. \tag{158}$$

The von Weizsaecker bound gives $T_P[n] \ge 0$ on the admissible domain; for a density generated by a single spatial orbital, $T_P = 0$. The local Fermi wave vector and kinetic energy density are

$$k_F(\mathbf{r}) = (3\pi^2 n)^{1/3}, \qquad \tau_{\mathrm{TF}}(\mathbf{r}) = C_F n^{5/3}. \tag{159}$$

Euler equation and boundary conditions

The orbital-free ground-state energy is

$$E[n] = T_W[n] + T_P[n] + \int v_{\mathrm{ext}}(\mathbf{r})n(\mathbf{r})d^3r + E_H[n] + E_{\mathrm{xc}}[n] + E_{NN}, \tag{160}$$

$$E_H[n] = \frac{1}{2}\iint \frac{n(\mathbf{r})n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}d^3r\, d^3r'. \tag{161}$$

Write $n = \phi^2$ with real $\phi \geq 0$. Varying $E[\phi^2] - \mu \int \phi^2$ yields

$$\left[-\frac{1}{2}\nabla^2 + v_P[n](\mathbf{r}) + v_{\mathrm{ext}}(\mathbf{r}) + v_H[n](\mathbf{r}) + v_{\mathrm{xc}}[n](\mathbf{r})\right]\phi(\mathbf{r}) = \mu\phi(\mathbf{r}), \tag{162}$$

where $v_P = \delta T_P/\delta n$. For an isolated system, $\phi \to 0$ as $|\mathbf{r}| \to \infty$; for a periodic system both ϕ and its normal derivative are periodic. All numerical solutions must enforce $\int \phi^2 = N$. An all-electron Coulomb calculation must also recover the nuclear cusp, whereas a pseudopotential calculation must use the corresponding smooth reference density.

The $n = \phi^2$ parameterization enforces positivity, but does not by itself guarantee a lower-bounded energy or stable iterations. Stability is controlled by the second variation on the particle-conserving tangent space

$$\mathcal{T}_n = \left\{u : \int u(\mathbf{r})d^3r = 0\right\}, \qquad \delta^2 E[n](u,u) = \iint u(\mathbf{r})H_E(\mathbf{r},\mathbf{r}')u(\mathbf{r}')\, d^3r\, d^3r'. \tag{163}$$

Exact constraints to impose before fitting

Under uniform coordinate scaling,

$$n_\gamma(\mathbf{r}) = \gamma^3 n(\gamma\mathbf{r}), \qquad T_s[n_\gamma] = \gamma^2 T_s[n], \qquad \gamma > 0. \tag{164}$$

Further non-negotiable tests are translation and rotation invariance, size consistency for infinitely separated fragments, the one-orbital limit, and the uniform-gas value $T_s = T_{\mathrm{TF}}$. For a slowly varying density, the second-order gradient expansion begins

$$T_s[n] = T_{\mathrm{TF}}[n] + \frac{1}{9}T_W[n] + O(\nabla^4). \tag{165}$$

The gradient expansion is not valid in density tails or near a nucleus, so it is a limiting condition rather than a global ansatz.

Linear response supplies a stronger constraint. Let $n = n_0 + \delta n$ in a uniform gas and use the Fourier convention $\delta n(\mathbf{r}) = \int d^3q\, \delta n_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{r}}/(2\pi)^3$. On the subspace excluding the $q = 0$ particle-number mode,

$$\left.\frac{\delta^2 T_s}{\delta n_{\mathbf{q}}\delta n_{-\mathbf{q}}}\right|_{n_0} = -\chi_0(q; n_0)^{-1}, \tag{166}$$

where χ_0 is the static Lindhard response. Matching only energies does not enforce Eq. (166); the Hessian or response must enter the construction explicitly.

A scaling-covariant nonlocal representation

Define the reduced gradient and Laplacian

$$s = \frac{|\nabla n|}{2k_F n}, \qquad q = \frac{\nabla^2 n}{4k_F^2 n}. \tag{167}$$

Both are dimensionless and satisfy $s[n_\gamma](\mathbf{r}) = s[n](\gamma\mathbf{r})$, with the analogous relation for q. One family of dimensionless nonlocal descriptors is

$$\zeta_\ell(\mathbf{r}) = \int d^3r'\, k_F(\mathbf{r})^3 w_\ell(k_F(\mathbf{r})|\mathbf{r} - \mathbf{r}'|)\, \frac{n(\mathbf{r}')}{n(\mathbf{r})}. \tag{168}$$

Choose w_ℓ integrable and normalized so that ζ_ℓ has a known constant value in a uniform gas. A computational density floor must not be inserted silently into Eq. (168), because a fixed floor breaks Eq. (164); tail regularization must be specified and convergence with its removal demonstrated.

A coordinate-scaling-preserving Pauli functional is

$$T_P^\theta[n] = C_F \int n(\mathbf{r})^{5/3} F_P^\theta(s, q, \zeta_1, \ldots, \zeta_M) d^3r. \tag{169}$$

Indeed, $\zeta_\ell[n_\gamma](\mathbf{r}) = \zeta_\ell[n](\gamma\mathbf{r})$, so Eq. (164) follows by a change of variables. Positivity can be architectural, for example $F_P^\theta = g_\theta^2$ times gates that enforce $F_P = 0$ on a stated one-orbital manifold. Uniform response fixes derivatives of F_P and the Fourier transforms of w_ℓ, not merely their values at a uniform density.

Size consistency requires more than locality of the energy integral. For densities n_A and n_B whose supports separate by R_{AB}, one must verify

$$T_s[n_A + n_B] - T_s[n_A] - T_s[n_B] \longrightarrow 0 \quad (R_{AB} \to \infty). \tag{170}$$

The decay of w_ℓ, especially in the low-density region where k_F^{-1} grows, determines whether Eq. (169) actually has this property.

First and second functional derivatives

Let the energy density in Eq. (169) be $f(n, \nabla n, \nabla^2 n, \zeta_1, \ldots)$. Its Pauli potential is

$$\begin{aligned} v_P(\mathbf{r}) = {} & \frac{\partial f}{\partial n} - \nabla \cdot \frac{\partial f}{\partial(\nabla n)} + \nabla^2 \frac{\partial f}{\partial(\nabla^2 n)} \\ & + \sum_\ell \int d^3r' \frac{\partial f(\mathbf{r}')}{\partial \zeta_\ell(\mathbf{r}')} \mathcal{J}_\ell(\mathbf{r}', \mathbf{r}), \end{aligned} \tag{171}$$

where

$$\mathcal{J}_\ell(\mathbf{r}', \mathbf{r}) = \frac{\delta \zeta_\ell(\mathbf{r}')}{\delta n(\mathbf{r})} \tag{172}$$

is obtained analytically from Eq. (168) or by an exactly equivalent adjoint differentiation. The last term is essential; treating a nonlocal descriptor as a fixed input gives the wrong Euler equation.

For a trial perturbation u, compute the Hessian action without forming a dense six-dimensional kernel:

$$(H_T u)(\mathbf{r}) = \frac{d}{d\epsilon} v_s^\theta[n + \epsilon u](\mathbf{r})\Big|_{\epsilon=0}, \qquad \delta^2 T_s[n](u, u) = \int u H_T u\, d^3r. \tag{173}$$

Finite differences of v_s, automatic differentiation, and the analytic adjoint must agree as the grid and step are refined. This matrix-free Hessian is used both for Eq. (166) and for stability analysis of Eq. (162).

Reference quantities and data construction

From converged Kohn–Sham orbitals, compute the reference energy directly,

$$T_s^{\mathrm{KS}} = \frac{1}{2} \sum_i f_i \int |\nabla \varphi_i|^2 d^3r. \tag{174}$$

Density-to-potential inversion gives v_s^{inv} up to a constant. At a differentiable ground-state density,

$$\frac{\delta T_s}{\delta n} = \mu - v_s^{\mathrm{inv}}, \qquad v_W = \frac{1}{8}\left(\frac{|\nabla n|^2}{n^2} - 2\frac{\nabla^2 n}{n}\right), \qquad v_P^{\mathrm{ref}} = \mu - v_s^{\mathrm{inv}} - v_W. \tag{175}$$

Fix the additive gauge, for example by setting the weighted spatial mean of v_P to zero. Potential errors should be measured in a Sobolev norm so that grid-scale oscillations are penalized without allowing the high-density core to dominate every example.

The independent-particle response can be generated from orbitals as

$$\chi_s(\mathbf{r}, \mathbf{r}') = \sum_{ij} \frac{f_i - f_j}{\epsilon_i - \epsilon_j + i0} \varphi_i^*(\mathbf{r})\varphi_j(\mathbf{r})\varphi_j^*(\mathbf{r}')\varphi_i(\mathbf{r}'), \tag{176}$$

or by Sternheimer perturbation without explicit unoccupied sums. Energies, potentials, and selected Hessian-vector products must be split by chemical system, not by nearly identical geometries, to test transferability honestly.

Self-consistent workflow and controlled limits

An implementable program is: generate all-electron or pseudopotential reference data consistently; nondimensionalize densities and derivatives; fit the constrained kernel and enhancement map; verify analytic derivatives; solve Eq. (162) from multiple initial densities using line-searched preconditioned minimization; and evaluate energies, density errors, forces, response, and iteration stability on unseen systems. Forces must differentiate every density-dependent descriptor and any ionic pseudopotential parameter.

The minimum test suite contains a one-orbital density, a uniform gas plus a single Fourier perturbation, coordinate-scaled copies of the same density, two separating fragments, atomic or molecular exponential tails, and a metallic periodic cell. Check energy scaling, Pauli non-negativity, the Lindhard Hessian over a range of q/k_F, grid convergence, and invariance under rotations and translations. The precise unknown is the constrained map $(F_P^\theta, \{w_\ell\})$ whose adjoint derivative and Hessian remain well behaved on a stated subset of $\mathcal{D}_N$; energy accuracy alone does not determine that object.

Maxima research model

The driver evaluates a three-dimensional Thomas–Fermi plus von Weizsaecker functional on a normalized spherical Gaussian density. Its inputs are the electron number, Gaussian exponent, and gradient coefficient; it prints the density and Euler potential, separated kinetic energies, coordinate-scaling ratios, and a small-q Lindhard-response comparison. Run it from the project root with

```
maxima --batch=maxima/07_orbital_free_dft.mac
```

Replace `nrad`, `Ts`, and `Kmodel` together when adding a semilocal or nonlocal kinetic kernel, and carry the same energy, potential, scaling, and response outputs into a minimizer. This analytic Gaussian calculation matches the Lindhard kernel only through q^2 and does not test real-space grid convergence, ionic forces, or nonlocal boundary conditions.

```
/* Orbital-free diagnostics for a normalized spherical Gaussian density. */
kill(all)$
display2d:false$
ratprint:false$
linel:200$

/* Atomic units and spin-unpolarized Thomas--Fermi coefficient. */
Ne:2$
a:4/5$
lambdaW:1/9$                    /* second-order gradient expansion */
CF:3*(3*%pi^2)^(2/3)/10$

nrad(r):=Ne*(a/%pi)^(3/2)*exp(-a*r^2)$
vTF(r):=5*CF*nrad(r)^(2/3)/3$
vW(r):=3*a/2-a^2*r^2/2$
vEuler(r):=vTF(r)+lambdaW*vW(r)$

TTF(aa):=CF*Ne^(5/3)*(aa/%pi)*(3/5)^(3/2)$
TW(aa):=3*Ne*aa/4$
Ts(aa):=TTF(aa)+lambdaW*TW(aa)$

print("density table: [r,n(r),delta_Ts/delta_n]")$
for rv in [0,1/2,1,2] do
  print([rv,float(nrad(rv)),float(vEuler(rv))])$

print("energies: [T_TF,T_W,lambdaW*T_W,T_s] =",
      [float(TTF(a)),float(TW(a)),float(lambdaW*TW(a)),float(Ts(a))])$

/* Uniform-gas Hessian versus the Lindhard small-q expansion. */
n0:1/50$
kF:(3*%pi^2*n0)^(1/3)$
Kmodel(q):=10*CF*n0^(-1/3)/9+lambdaW*q^2/(4*n0)$
KLindhard2(q):=%pi^2/kF*(1+q^2/(12*kF^2))$
print("response table: [q/kF,K_model,K_Lindhard_to_q2]")$
for qfrac in [0,1/2,1] do
  print([qfrac,float(Kmodel(qfrac*kF)),
         float(KLindhard2(qfrac*kF))])$

/* Coordinate scaling n_gamma(r)=gamma^3 n(gamma*r) sends a to gamma^2 a. */
print("scaling table: [gamma,T_s[n_gamma],T_s/(gamma^2 T_s[n])]")$
for gam in [1/2,1,2] do
  print([gam,float(Ts(gam^2*a)),
         float(Ts(gam^2*a)/(gam^2*Ts(a)))])$
```

What Kind of Solution Will Fill the Gap

Target result

Construct an explicit F_θ and kernel family satisfying

$$\boxed{T_s^\theta[n] \geq T_W[n], \qquad T_s^\theta[n_\gamma] = \gamma^2 T_s^\theta[n]}$$

along with the one-orbital, uniform-gas, size-consistency, and Lindhard conditions. Training must include derivatives and response, e.g.

$$\mathcal{L} = w_E|T_s^\theta - T_s^{\mathrm{KS}}|^2 + w_v \left\| \frac{\delta T_s^\theta}{\delta n} - v_s^{\mathrm{inv}} \right\|_{H^{-1}}^2 + w_\chi \|\chi_\theta - \chi_0\|^2 + \mathcal{L}_{\mathrm{constraints}}.$$

Establish lower semicontinuity or coercivity and a controlled Hessian lower bound on a stated physical density domain,

$$\delta^2 E[n](\delta n, \delta n) \geq c_D \|\delta n\|^2, \qquad \int \delta n = 0,$$

rather than asserting global strict convexity. Validate the construction by stable minimization from widely separated initial densities, measuring energy, density, Pauli-potential, and force accuracy across at least two chemical/condensed-matter domains. The uncertainty diagnostic must reject out-of-domain densities before Euler iteration diverges.

References

[1] Mel Levy and H. Ou-Yang. "Exact properties of the Pauli potential for the square root of the electron density and the kinetic energy functional". In: *Physical Review A* 38 (1988), pp. 625–629. DOI: 10.1103/PhysRevA.38.625.

[2] Wenfei Mi, Kai Luo, S. B. Trickey, and Michele Pavanello. "Orbital-Free Density Functional Theory: An Attractive Electronic Structure Method for Large-Scale First-Principles Simulations". In: *Chemical Reviews* 123 (2023), pp. 12039–12104. DOI: 10.1021/acs.chemrev.2c00758.

[3] Roman Remme, Tobias Kaczun, Maximilian Scheurer, Andreas Dreuw, and Fred A. Hamprecht. *KineticNet: deep learning a transferable kinetic energy functional for orbital-free density functional theory*. 2023. URL: https://arxiv.org/abs/2305.13316 (visited on 07/16/2026).

[4] Roman Remme, Tobias Kaczun, Tim Ebert, Christof A. Gehrig, Dominik Geng, et al. *Stable and accurate orbital-free DFT powered by machine learning*. 2025. URL: https://arxiv.org/abs/2503.00443 (visited on 07/16/2026).

[5] S. Majumdar, Z. Shi, and G. Vignale. *Orbital-Free Density Functional Theory for Periodic Solids: Construction of the Pauli Potential*. 2025. URL: https://arxiv.org/abs/2503.15959 (visited on 07/16/2026).

[6] A. Bhattacharjee, S. Jana, S. Śmiga, and P. Samal. "Nonlocal Orbital-Free Kinetic Energy Functional from the Jellium-with-Gap Model for Finite Systems". In: *Journal of Chemical Theory and Computation* 22 (2026), pp. 6510–6524. DOI: 10.1021/acs.jctc.6c00460. URL: https://arxiv.org/abs/2606.15336.

[7] Xin-Hui Wu and Sergei Manzhos. *ML and AI for density functional theory: different priorities for Kohn–Sham and orbital-free DFT, for electronic and nuclear DFT*. 2026. URL: https://arxiv.org/abs/2607.04095 (visited on 07/16/2026).

8 Continuum–lattice matching and uncertainty propagation for screened supercritical Dirac resonances

Flügge seed: Vol. II, Problems 201–209: central forces in Dirac theory, the relativistic Kepler problem, positive-energy radial solutions, scattering, and potential steps.

The point-Coulomb Dirac problem, critical coupling, log-periodic supercritical solutions, and the atomic-collapse resonance ladder are established. Shytov, Katsnelson, and Levitov gave the foundational graphene theory [1]; gapped and screened lattice calculations followed [2], and collapse resonances were observed in artificial graphene nuclei [3]. The wider continuum and experimental literature is reviewed in [4].

Neither the domain problem nor screening is untouched. Breev et al. classified the self-adjoint Dirac–Coulomb Hamiltonians and compared them with a regularized core [5]; Kolomeisky and Straley derived weak- and strong-screening regimes for supercritical impurity clusters [6]. Lattice and valley physics in gapped graphene also split nominally degenerate collapse states and redistribute valley-resolved LDOS weights [7]. These developments narrow the task to deriving an effective continuum boundary operator from a specified lattice/core model, combining it self-consistently with screening, and propagating uncertainties in the core, dielectric response, lattice, and disorder to the critical coupling and complex poles. An energy-dependent boundary condition obtained by eliminating core degrees of freedom is a Feshbach effective condition, not literally a self-adjoint extension of the isolated radial operator; the enlarged microscopic Hamiltonian remains self-adjoint.

Formalisms

Continuum model, units, and physical domain

Consider a two-dimensional massive Dirac material with Fermi velocity v_F, half-gap $\Delta > 0$, and valleys $\tau = \pm 1$. Real spin is a passive degeneracy unless spin–orbit terms are added. The exterior continuum space is

$$\mathcal{H}_{\text{ext}} = L^2(\mathbb{R}^2 \setminus \mathcal{C}_R, d^2r) \otimes \mathbb{C}^2_{\text{sublattice}} \otimes \mathbb{C}^2_{\text{valley}}, \tag{177}$$

where $\mathcal{C}_R$ is a microscopic core of radius R. Before intervalley mixing is introduced, the diagonal valley blocks are

$$H_\tau^{(0)} = v_F(\tau\sigma_x p_x + \sigma_y p_y) + \Delta\sigma_z + V_{\text{scr}}(\mathbf{r})I_2, \qquad H = H_+^{(0)} \oplus H_-^{(0)} + H_{\text{iv}} + H_{\text{dis}}. \tag{178}$$

Here H_{iv} mixes valleys at atomic scales and H_{dis} denotes a specified disorder realization or stochastic model. Both must be omitted, included explicitly, or assigned priors; they cannot be absorbed silently into a fitted scalar core radius.

Outside the core, the unscreened impurity potential is

$$V_0(r) = -\frac{g\hbar v_F}{r}, \qquad g = \frac{Z_{\text{eff}} e^2}{\kappa \hbar v_F}, \tag{179}$$

with dielectric constant κ and effective charge Z_{eff}. Thus g is dimensionless. Useful dimensionless inputs are

$$\frac{\Delta R}{\hbar v_F}, \qquad k_F R, \qquad \frac{R}{\ell_{\text{scr}}}, \qquad \frac{E}{\Delta}, \qquad g, \tag{180}$$

where k_F and ℓ_{scr} describe doping and screening.

Radial reduction and boundary form

For a circular exterior potential and no intervalley mixing, expand in half-integer total angular momentum $j \in \mathbb{Z}+1/2$. After a standard channel-dependent unitary transformation and extraction of the radial Jacobian, the spinor $\psi_j = (F_j, G_j)^T$ belongs to $L^2((R,\infty), dr) \otimes \mathbb{C}^2$ and satisfies

$$h_j\psi_j = E\psi_j, \qquad h_j = -i\hbar v_F \sigma_x \frac{d}{dr} + \hbar v_F \frac{j}{r}\sigma_y + \Delta\sigma_z + V(r)I_2. \tag{181}$$

The sign convention for j may change between valleys, but the short-range index depends on j^2 and is valley independent. For two radial functions, integration by parts gives

$$\langle \psi, h_j\varphi\rangle - \langle h_j\psi, \varphi\rangle = -i\hbar v_F[\psi^\dagger \sigma_x \varphi]_R^\infty. \tag{182}$$

An admissible boundary relation at R must make this form vanish for every pair in the domain. Resonance states instead satisfy an outgoing condition at infinity and are not square-integrable; they are obtained by analytic continuation from the retarded problem.

For a formal point Coulomb field, insert $\psi \sim r^s u$ into the dominant $1/r$ terms. The indicial equation is

$$\det[-is\sigma_x + j\sigma_y - gI_2] = 0, \qquad s^2 = j^2 - g^2. \tag{183}$$

Define

$$\gamma_j = \sqrt{j^2 - g^2}, \qquad \beta_j = \sqrt{g^2 - j^2}. \tag{184}$$

For $g < |j|$, the two local powers are $r^{\pm\gamma_j}$. For $g > |j|$, they become oscillatory,

$$\psi_j(r) \sim c_+ \left(\frac{r}{R}\right)^{i\beta_j} u_+ + c_- \left(\frac{r}{R}\right)^{-i\beta_j} u_-. \tag{185}$$

In the ideal singular problem, a self-adjoint extension fixes a flux-conserving phase $c_-/c_+ = e^{i\vartheta_j}$. In the physical exterior problem, that phase is replaced by a boundary operator derived from the core.

Log-periodicity in sheet momentum, then in energy

The primary analytic variable is the momentum on a specified Riemann sheet, not the energy detuning. Define

$$k(E) = \frac{\sqrt{E^2 - \Delta^2}}{\hbar v_F}. \tag{186}$$

On the retarded physical sheet choose $k > 0$ just above the upper continuum and $\operatorname{Im} k > 0$ inside the gap. Crossing the relevant continuum cut changes $k_{\mathrm{II}} = -k_{\mathrm{I}}$. Every numerical pole must be reported with this sheet convention.

In the scale-free annulus

$$R \ll r \ll \min(|k|^{-1}, \ell_{\mathrm{scr}}, \hbar v_F/\Delta), \tag{187}$$

the two solutions in Eq. (185) acquire factors $(kR)^{\pm i\beta_j}$ when matched to the outer wave. The pole determinant therefore has the leading form

$$D_j^{\mathrm{II}}(k) = A_j(k)(kR)^{i\beta_j} + B_j(k)(kR)^{-i\beta_j}. \tag{188}$$

If A_j/B_j varies slowly over one cycle, the scale-invariant pole condition is

$$(kR)^{2i\beta_j} = C_j. \tag{189}$$

Choosing n to increase toward threshold gives the momentum ladder

$$\boxed{k_{n,j} = k_{\mathrm{UV},j} e^{-\pi n/\beta_j}}, \qquad \frac{k_{n+1,j}}{k_{n,j}} = e^{-\pi/\beta_j}. \tag{190}$$

The common complex phase of $k_{\mathrm{UV},j}$ selects the resonance ray; screening, a gap, and lattice matching deform both its magnitude and phase.

Only after Eq. (190) is established should one translate to energy. Near the lower massive edge choose

$$E(k) = -\sqrt{\Delta^2 + (\hbar v_F k)^2}, \qquad z = E + \Delta. \tag{191}$$

Expansion on the same sheet gives

$$z = -\frac{\hbar^2 v_F^2 k^2}{2\Delta} + O(k^4), \qquad \boxed{\frac{z_{n+1,j}}{z_{n,j}} = e^{-2\pi/\beta_j}}. \tag{192}$$

The exponent doubles because a massive band edge is quadratic in k. Near the upper edge, $E - \Delta = +(\hbar v_F k)^2/(2\Delta) + O(k^4)$ and the same doubled ratio holds. In the massless limit $E = \pm\hbar v_F k$, so the energy and momentum ratios both have exponent π/β_j.

Microscopic core and Feshbach boundary operator

Represent the core by a specified tight-binding Hamiltonian, for example

$$H_{\text{core}} = -\sum_{\langle mn\rangle} t_{mn}|m\rangle\langle n| + \sum_m [\xi_m\Delta + V_m]|m\rangle\langle m| + H_{\text{recon}} + H_{\text{iv}}, \tag{193}$$

where $\xi_m = \pm 1$ labels sublattices and H_{recon} specifies any reconstructed bonds or vacancies. Partition the microscopic Hilbert space into exterior and core sectors, $P + Q = I$. Eliminating $Q\psi$ from $(E - H)\psi = 0$ gives

$$H_{\text{eff}}(E) = H_{PP} + \Sigma_{\text{core}}(E), \tag{194}$$

$$\Sigma_{\text{core}}(E) = H_{PQ}(E - H_{QQ})^{-1} H_{QP}. \tag{195}$$

Project Eq. (195) onto boundary sites and match their long-wavelength amplitudes to continuum envelopes. The result is a multichannel Dirichlet-to-Neumann relation

$$\Gamma_1 \Psi(R, E) = \mathcal{B}(E)\Gamma_0 \Psi(R, E), \tag{196}$$

where Γ_0, Γ_1 extract complementary boundary data and $\mathcal{B}$ acts in valley, angular, and sublattice channel space. For real E away from core eigenvalues, Eq. (196) must satisfy the current-conservation condition implied by Eq. (182). This is an essential diagnostic of the lattice-to-continuum projection.

Because $\mathcal{B}(E)$ contains the resolvent in Eq. (195), it is generally energy dependent and may have poles. It is therefore not a fixed self-adjoint-extension angle for the isolated radial operator. Self-adjointness belongs to the enlarged core-plus-exterior Hamiltonian.

Static screening as a closed real-axis problem

For a translationally invariant reference sheet, define

$$v_C(q) = \frac{2\pi e^2}{\kappa q}, \qquad V_0(q) = -\frac{2\pi Z_{\text{eff}} e^2}{\kappa q} F_R(q), \tag{197}$$

where F_R is the core form factor. Static RPA gives

$$V_{\text{scr}}(q) = \frac{V_0(q)}{\epsilon(q)}, \qquad \epsilon(q) = 1 - v_C(q)\Pi(q; \mu, \Delta). \tag{198}$$

The sign of Π must follow the convention $\delta n = \Pi\,\delta V$; for an electron gas the static Π is normally negative, so $\epsilon > 1$.

For a strongly supercritical impurity, linear screening may fail. A self-consistent Hartree formulation is

$$V_{\rm scr}(\mathbf{r}) = V_{\rm ext}(\mathbf{r}) + \int d^2r' \frac{e^2\delta n(\mathbf{r}')}{\kappa|\mathbf{r}-\mathbf{r}'|}, \tag{199}$$

$$\delta n(\mathbf{r}) = -\frac{1}{\pi}\int_{-\infty}^{\mu} dE\ \mathrm{Im}\,\mathrm{tr}[G_V^R(E;\mathbf{r},\mathbf{r}) - G_0^R(E;\mathbf{r},\mathbf{r})]. \tag{200}$$

Include spin and valley degeneracies only if they are not already in the trace. Impose charge neutrality or the chosen gate charge and $V_{\rm scr}(r) \to 0$ at infinity. The subtracted Green functions must use the same lattice or momentum ultraviolet regulator; otherwise the filled Dirac sea leaves a spurious cutoff-dependent charge. Iterate density and potential with mixing until both the potential norm and total induced charge converge.

Static screening is solved on the real axis first; its converged real potential is then held fixed during analytic continuation of the Dirac resolvent. Evaluating a ground-state density at complex energy is not a valid shortcut. Dynamical screening would make the pole problem energy dependent and non-Hermitian and requires a separate causal dielectric formalism.

Matching determinant and analytic continuation

Let $Y_{\rm out}(r,E)$ be a matrix of exterior solutions satisfying outgoing conditions in every open channel and decaying conditions in closed channels. Integrate Eq. (181) inward from a radius beyond the screening region, or use analytic Coulomb functions when an unscreened tail remains. At $r = R$, define

$$D^{\rm II}(E) = \det[\Gamma_1 Y_{\rm out}(R,E) - \mathcal{B}(E)\Gamma_0 Y_{\rm out}(R,E)]\,. \tag{201}$$

Resonances satisfy $D^{\rm II}(E_*) = 0$, $E_* = E_R - i\Gamma/2$. Direct complex integration, exterior complex scaling, or analytic Jost functions may be used, but all square-root and Coulomb logarithm branches must be continuous along the chosen continuation path.

Count poles inside a contour $\mathcal{C}$ before applying a local root finder:

$$N_{\mathcal{C}} = \frac{1}{2\pi i}\oint_{\mathcal{C}} \partial_E \log D^{\rm II}(E)dE. \tag{202}$$

For a simple pole and model parameters p_α, implicit differentiation gives

$$\frac{\partial E_*}{\partial p_\alpha} = -\frac{\partial_{p_\alpha} D^{\rm II}(E_*;\mathbf{p})}{\partial_E D^{\rm II}(E_*;\mathbf{p})}. \tag{203}$$

If the denominator is small, individual-pole sensitivities are ill conditioned and a contour-based pole cluster must replace Eq. (203).

Observable and implementable workflow

The retarded Green function is $G^R(E) = (E + i0 - H)^{-1}$. With valley projector P_τ, the local density of states is

$$\rho_\tau(\mathbf{r},E) = -\frac{1}{\pi}\,\mathrm{Im}\,\mathrm{tr}_{\rm sublattice}[P_\tau G^R(E;\mathbf{r},\mathbf{r})P_\tau]. \tag{204}$$

An STM signal further convolves Eq. (204) with thermal and instrumental broadening; this convolution must be applied after computing the intrinsic pole width.

The calculation is organized as follows: specify a lattice core and its parameter uncertainties; compute $\mathcal{B}(E)$ from a boundary Green function; obtain the static screened potential; construct outgoing exterior solutions on a declared sheet; count and refine determinant zeros; calculate valley-resolved LDOS; and propagate the core, dielectric, disorder, and numerical uncertainties through Eq. (203) or direct sampling. Compare continuum LDOS with the full lattice Green function in an overlap annulus $R \ll r \ll \ell_{\rm scr}$.

Controlled checks are the free massive Dirac spectrum as $g \to 0$, absence of a log-periodic ladder for $g < |j|$, recovery of Eq. (190) when screening and the gap are removed, the doubled edge exponent in Eq. (192), valley degeneracy when $H_{\text{iv}} = H_{\text{dis}} = 0$, current conservation at real energy, and invariance under moving the artificial matching radius while updating $\mathcal{B}$. The unknown research object is the microscopic map from core and screening parameters to the energy-dependent boundary operator and hence to the deformed pole determinant; a fitted constant boundary phase does not supply that map.

Maxima research model

The driver constructs a complex supercritical momentum ladder with core phase, screening, lattice, loss, and intervalley corrections, then maps every pole through the exact massive Dirac dispersion. Editable physical inputs include $g, j, \Delta, \hbar v_F$, the screening and core lengths, and the four deformation strengths; the output gives valley-resolved pole energies, intrinsic widths, splittings, and a quadratic matching determinant. Run it from the project root with

```
maxima --batch=maxima/08_supercritical_dirac.mac
```

Replace `dScreen`, `dLattice`, and `dValley` by values derived from the microscopic boundary operator before continuing `Dmatch` on a chosen Riemann sheet. The current corrections are a parameterized matching ansatz rather than a radial-Dirac or lattice-core Green-function solve, and it does not include experimental convolution.

```
/* Screened, lossy, valley-split supercritical Dirac ladder. */
kill(all)$
display2d:false$
ratprint:false$
linel:200$

/* Energies in eV and lengths in nm. */
g:6/5$
j:1/2$
beta:sqrt(g^2-j^2)$
kUV:7/10$
phiCore:3/20$
Delta:1/10$
hbarv:329/500$
lscr:5$
rcore:1/5$
cScreen:1/20$
cLattice:1/50$
cIntervalley:1/100$
thetaLoss:1/50$

kbase(n):=kUV*exp(-(phiCore+%pi*n)/beta)$
dScreen(k):=-cScreen/(1+(k*lscr)^2)$
dLattice(k):=cLattice*(k*rcore)^2$
dValley(k,tau):=tau*cIntervalley*exp(-2*k*rcore)
                       /(1+(k*lscr)^2)$
kcorr(n,tau):=kbase(n)*(1+dScreen(kbase(n))
                    +dLattice(kbase(n))+dValley(kbase(n),tau))
                    *exp(%i*thetaLoss)$

Elevel(n,tau):=-sqrt(Delta^2+(hbarv*kcorr(n,tau))^2)$
width(n,tau):=-2*imagpart(rectform(Elevel(n,tau)))$
valley_split(n):=realpart(rectform(Elevel(n,1)-Elevel(n,-1)))$
Emid(n):=(Elevel(n,1)+Elevel(n,-1))/2$
Vintervalley(n):=(Elevel(n,1)-Elevel(n,-1))/2$
Dmatch(E,n):=(E-Emid(n))^2-Vintervalley(n)^2$

print("ideal momentum ratio =",float(exp(-%pi/beta)))$
print("pole table: [n,Re(E+),Re(E-),width+,width-,valley_split]")$
for n:0 thru 3 do block([Ep,Em],
  Ep:float(rectform(Elevel(n,1))),
  Em:float(rectform(Elevel(n,-1))),
  print([n,realpart(Ep),realpart(Em),
         float(width(n,1)),float(width(n,-1)),
         float(valley_split(n))]))$

print("Dmatch=(E-Emid)^2-Vintervalley^2; n=1 [Emid,Vintervalley] =")$
print([float(rectform(Emid(1))),float(rectform(Vintervalley(1)))])$
```

What Kind of Solution Will Fill the Gap

Target result

Write $E_{*,n,j} = E_{R,n,j} - i\Gamma_{n,j}/2$ and choose the resonance-sheet momentum

$$k_{n,j} = \frac{\sqrt{E_{*,n,j}^2 - \Delta^2}}{\hbar v_F}.$$

Derive the controlled deformation of the ideal geometric momentum ladder,

$$\boxed{k_{n,j} = k_{\mathrm{UV},j} e^{-\pi n/\beta_j} \left[1 + \delta_{n,j}^{\mathrm{scr}} + \delta_{n,j}^{\mathrm{lat}} + \delta_{n,j}^{\mathrm{dis}} + \cdots\right]},$$

with every correction tied to $\mathcal{B}(E)$ and the screened potential. The observable detuning $z_{n,j} = E_{*,n,j} + \Delta$ must then be obtained from the exact dispersion. Near the massive lower edge,

$$z_{n,j} = -\frac{\hbar^2 v_F^2 k_{n,j}^2}{2\Delta} + O(k_{n,j}^4),$$

so its ideal ratio is $z_{n+1,j}/z_{n,j} = e^{-2\pi/\beta_j}$, not the momentum ratio. The critical coupling should follow from the pole/threshold condition

$$D_j^{\mathrm{II}}(-\Delta; g_c, \Delta, R, \mu, \kappa, \ldots) = 0,$$

not from the ideal $g_c = 1/2$ alone. Implicit differentiation gives a clean uncertainty map,

$$\frac{\partial E_*}{\partial p_\alpha} = -\frac{\partial_{p_\alpha} D(E_*; \mathbf{p})}{\partial_E D(E_*; \mathbf{p})}, \qquad \mathrm{Cov}(E_*) \simeq J_E \, \mathrm{Cov}(\mathbf{p}) J_E^\dagger.$$

Obtain $\mathcal{B}(E)$ or $\Sigma_{\mathrm{core}}(E)$ for several lattice core geometries, identify pole combinations invariant under core reparameterization, and report confidence intervals for g_c, E_R, Γ, and valley LDOS peaks.

References

[1] Andrei V. Shytov, Mikhail I. Katsnelson, and Leonid S. Levitov. "Atomic collapse and quasi-Rydberg states in graphene". In: *Physical Review Letters* 99 (2007), p. 246802. DOI: 10.1103/PhysRevLett.99.246802.

[2] V. M. Pereira, V. N. Kotov, and A. H. Castro Neto. "Supercritical Coulomb impurities in gapped graphene". In: *Physical Review B* 78 (2008), p. 085101. DOI: 10.1103/PhysRevB.78.085101. URL: https://arxiv.org/abs/0803.4195.

[3] Y. Wang, D. Wong, A. V. Shytov, V. W. Brar, S. Choi, Q. Wu, H.-Z. Tsai, W. Regan, A. Zettl, R. K. Kawakami, S. G. Louie, L. S. Levitov, and M. F. Crommie. "Observing atomic collapse resonances in artificial nuclei on graphene". In: *Science* 340 (2013), pp. 734–737. DOI: 10.1126/science.1234320.

[4] E. V. Gorbar, V. P. Gusynin, and O. O. Sobol. "Electron states in the field of charged impurities in two-dimensional Dirac systems". In: *Low Temperature Physics* 44 (2018), pp. 371–400. DOI: 10.1063/1.5034149. URL: https://arxiv.org/abs/1806.05568.

[5] A. I. Breev, R. Ferreira, D. M. Gitman, and B. L. Voronov. "Spectra of electronic excitations in graphene near Coulomb impurities". In: *Journal of Experimental and Theoretical Physics* 130 (2020), pp. 711–736. DOI: 10.1134/S1063776120030127. URL: https://arxiv.org/abs/1912.01322.

[6] Eugene B. Kolomeisky and Joseph P. Straley. "Space charge and screening of a supercritical impurity cluster in monolayer graphene". In: *Physical Review B* 109 (2024), p. 075418. DOI: 10.1103/PhysRevB.109.075418. URL: https://arxiv.org/abs/2309.02199.

[7] Jing Wang, Xiaotai Wu, Wen-Sheng Zhao, Yuhua Cheng, Yue Hu, and François M. Peeters. *Atomic collapse in gapped graphene: lattice and valley effects*. 2025. URL: https://arxiv.org/abs/2501.15049 (visited on 07/16/2026).

9 Tensor-force observables under consistent EFT/SRG evolution with joint Bayesian errors

Flügge seed: Vol. II, Problems 140–147: spin-dependent nucleon forces, the tensor operator, the coupled-channel deuteron, and its quadrupole and magnetic moments.

The coupled ${}^3S_1-{}^3D_1$ deuteron is solved to high precision in modern chiral EFT [1, 2]. A deuteron D-state probability is not an observable: it changes under unitary transformations even when measurable cross sections and form factors do not [3]. Explicit SRG calculations show that a softened Hamiltonian must be accompanied by the identically evolved observable operator [4].

Bayesian EFT uncertainty quantification has advanced from scalar intervals to Gaussian-process correlations across energy, angle, and observables [5, 6]. Modern nucleon–nucleon calculations reveal that stationary-GP assumptions can fail [7]. Interaction and current truncation errors have been combined for muon capture on deuterium [8], but no mapped analysis jointly treats SRG/unitary resolution dependence, regulator dependence, interaction–current cross-correlation, and several tensor-sensitive observables. The unresolved task is therefore a joint probabilistic theory of measurable tensor observables, rather than another estimate of the representation-dependent quantity P_D.

Formalisms

Two-nucleon space, units, and EFT Hamiltonian

Work in the deuteron rest frame and remove the center-of-mass coordinate. The relative state belongs to

$$\mathcal{H}_2 = L^2(\mathbb{R}^3, d^3r) \otimes \mathbb{C}^4_{\text{spin}} \otimes \mathbb{C}^4_{\text{isospin}}, \qquad \mathbf{p} = -i\hbar\boldsymbol{\nabla}_{\mathbf{r}}, \tag{205}$$

restricted to total quantum numbers $J^P = 1^+$ and $T = 0$. Distances may be recorded in fm and momenta in fm^{-1}; factors of $\hbar c$ must be restored when momenta are quoted in MeV. With reduced mass $\mu_N = m_p m_n/(m_p + m_n)$, a chiral interaction at order ν defines

$$H^{(\nu)}_\Lambda = \frac{\mathbf{p}^2}{2\mu_N} + \sum_{j=0}^{\nu} V^{(j)}_\Lambda, \qquad V^{(j)}_\Lambda(p, p') = f_\Lambda(p) V^{(j)}(p, p') f_\Lambda(p'). \tag{206}$$

Here f_Λ is a stated regulator, Λ is distinct from the EFT breakdown scale Λ_b, and all low-energy constants (LECs) are fitted with the same regulator and order convention used later for the current.

The tensor operator is

$$S_{12}(\hat{\mathbf{r}}) = 3(\boldsymbol{\sigma}_1\cdot\hat{\mathbf{r}})(\boldsymbol{\sigma}_2\cdot\hat{\mathbf{r}}) - \boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2. \tag{207}$$

It mixes the ${}^3S_1$ and ${}^3D_1$ channels but preserves $J = 1$. Using normalized spin-angular functions $\mathcal{Y}^{1M}_{LSJ}(\hat{\mathbf{r}})$, write

$$|\psi^M_d\rangle = \frac{u(r)}{r}\mathcal{Y}^{1M}_{011} + \frac{w(r)}{r}\mathcal{Y}^{1M}_{211}. \tag{208}$$

Projection of $H|\psi^M_d\rangle = -B_d|\psi^M_d\rangle$ gives

$$\begin{pmatrix} T_0 + V_{SS} & V_{SD} \\ V_{DS} & T_2 + V_{DD} \end{pmatrix} \begin{pmatrix} u \\ w \end{pmatrix} = -B_d \begin{pmatrix} u \\ w \end{pmatrix}, \qquad T_L = -\frac{\hbar^2}{2\mu_N}\left(\frac{d^2}{dr^2} - \frac{L(L+1)}{r^2}\right). \tag{209}$$

For nonlocal chiral potentials, each $V_{LL'}u_{L'}$ denotes its radial integral action rather than pointwise multiplication.

Boundary data and normalization

Regularity requires $u(r) = O(r)$ and $w(r) = O(r^3)$ as $r \to 0$. For r beyond the strong-interaction range,

$$u(r) \longrightarrow A_S e^{-\gamma r}, \qquad w(r) \longrightarrow A_D e^{-\gamma r}\left(1 + \frac{3}{\gamma r} + \frac{3}{(\gamma r)^2}\right), \qquad \gamma = \frac{\sqrt{2\mu_N B_d}}{\hbar}. \tag{210}$$

The asymptotic ratio $\eta_d = A_D/A_S$, binding energy B_d, and normalization

$$\int_0^\infty dr\,[u(r)^2 + w(r)^2] = 1 \tag{211}$$

are observable or convention-independent constraints. By contrast, $P_D = \int_0^\infty w(r)^2 dr$ depends on the unitary resolution and must not be used as data. A radial mesh calculation should verify the logarithmic derivative at its outer boundary and vary both box size and ultraviolet resolution until B_d, A_S, and η_d are stable.

Currents and tensor-sensitive observables

At a fixed EFT order, decompose the electromagnetic or weak current into one- and two-nucleon pieces. Use $\hbar = c = 1$ for current and form-factor kinematics, so energy and momentum components have the same units:

$$J_a^\mu(q) = J_{a,1\mathrm{B}}^\mu(q) + J_{a,2\mathrm{B}}^\mu(q), \qquad q^\mu = (\omega, \mathbf{q}), \tag{212}$$

and retain every term required by the selected chiral counting. Charge conservation provides an operator diagnostic,

$$\mathbf{q}\cdot\mathbf{J}_{\mathrm{em}}(\mathbf{q}) = [H, \rho_{\mathrm{em}}(\mathbf{q})], \tag{213}$$

with signs and factors of i fixed by the Fourier transform. Between energy eigenstates this becomes $\mathbf{q}\cdot\langle\mathbf{J}\rangle = (E_f - E_i)\langle\rho\rangle$. Both sides must be regulated and evolved consistently; testing only matrix elements of the unevolved one-body current is insufficient.

In the Breit frame, $q^0 = 0$, the spin-one elastic current has three independent form factors $G_C(Q^2), G_Q(Q^2), G_M(Q^2)$, where

$$Q^2 = \mathbf{q}^2, \qquad \eta = \frac{Q^2}{4M_d^2}, \qquad G_C(0) = 1, \quad G_Q(0) = M_d^2 Q_d, \quad G_M(0) = \frac{2M_d}{e}\mu_d \tag{214}$$

with the same natural-unit convention. The reduced multipole matrix elements of $\rho(\mathbf{q})$ and the transverse current define these form factors; using the same phase and spherical-tensor convention at every order prevents a spurious sign change in G_Q. Elastic electron–deuteron scattering uses

$$A(Q^2) = G_C^2 + \frac{8}{9}\eta^2 G_Q^2 + \frac{2}{3}\eta G_M^2, \tag{215}$$

$$B(Q^2) = \frac{4}{3}\eta(1+\eta)G_M^2, \tag{216}$$

and, in the usual Born convention,

$$T_{20} = -\frac{1}{\sqrt{2}}\,\frac{\frac{8}{3}\eta G_C G_Q + \frac{8}{9}\eta^2 G_Q^2 + \frac{1}{3}\eta[1 + 2(1+\eta)\tan^2(\theta_e/2)]G_M^2}{A + B\tan^2(\theta_e/2)}. \tag{217}$$

This expression supplies a reproducible convention check before radiative or two-photon corrections are added. A weak process can be handled with the same states through

$$\Gamma_a = \frac{2\pi}{\hbar}\int d\Phi_f\,\left|L_\mu\langle f|J_{a,\mathrm{W}}^\mu|\psi_d\rangle\right|^2 \delta(E_f - E_i), \tag{218}$$

where the final-state normalization and phase-space measure $d\Phi_f$ must be specified for the chosen reaction.

Consistent similarity-renormalization-group evolution

Let s be the SRG flow parameter and $\lambda_{\rm SRG} = s^{-1/4}$ its momentum-resolution scale. For an anti-Hermitian generator $\eta_s = (dU_s/ds)U_s^\dagger$,

$$H_s = U_s H U_s^\dagger, \qquad \frac{dH_s}{ds} = [\eta_s, H_s], \tag{219}$$

$$J^\mu_{a,s} = U_s J^\mu_a U_s^\dagger, \qquad \frac{dJ^\mu_{a,s}}{ds} = [\eta_s, J^\mu_{a,s}], \tag{220}$$

$$|\psi_{d,s}\rangle = U_s|\psi_d\rangle, \qquad \frac{d}{ds}|\psi_{d,s}\rangle = \eta_s|\psi_{d,s}\rangle. \tag{221}$$

Consequently,

$$\frac{d}{ds}\langle\psi_{d,s}|J^\mu_{a,s}|\psi_{d,s}\rangle = 0 \tag{222}$$

for an exact unitary flow. The same transformation preserves the continuity identity:

$$\mathbf{q}\cdot\mathbf{J}_{{\rm em},s} = [H_s, \rho_{{\rm em},s}]. \tag{223}$$

Numerical work should evolve the Hamiltonian, state, charge, and current on the same momentum grid. The residual $\lambda_{\rm SRG}$-dependence of an observable then measures omitted EFT, induced-operator, or numerical effects; it is not evidence that P_D has become observable.

Joint EFT error model

For kinematics $x = (Q, \theta_e, E, \ldots)$, define

$$Q_{\rm EFT}(x) = \frac{\max[p(x), m_\pi]}{\Lambda_b} < 1, \qquad X_{a,k}(x) = X_{a,{\rm ref}}(x)\sum_{n=0}^{k} c_{a,n}(x) Q_{\rm EFT}(x)^n. \tag{224}$$

If the power counting skips orders, the displayed sum is replaced by the actual set of chiral indices. Keep interaction and current omissions distinct,

$$\delta X_a = \delta X_a^{(V)} + \delta X_a^{(J)} + \delta X_a^{(VJ)}, \tag{225}$$

because fitting independent scalar error bars erases the correlations shared by G_Q, T_{20}, and weak observables. A baseline multi-output Gaussian process may use

$${\rm Cov}[c_{a,n}(x), c_{b,m}(x')] = \delta_{nm}\bar{c}^2\rho_{ab} r_{ab}(x, x'), \tag{226}$$

where $\rho \succeq 0$ is an observable-space correlation matrix and r_{ab} is a positive kernel in kinematics. Nonstationary length scales or input warping are required if standardized order-by-order residuals change smoothness near thresholds or diffraction minima.

For a geometric omitted tail, the induced covariance is

$$\begin{aligned}{\rm Cov}[\delta X_{a,k}(x), \delta X_{b,k}(x')] = \bar{c}^2 X_{a,{\rm ref}}(x) X_{b,{\rm ref}}(x')\rho_{ab} r_{ab}(x, x') \\ \times \frac{[Q_{\rm EFT}(x) Q_{\rm EFT}(x')]^{k+1}}{1 - Q_{\rm EFT}(x) Q_{\rm EFT}(x')}.\end{aligned} \tag{227}$$

LEC posteriors, regulator variation, SRG residuals, and numerical quadrature errors should enter as separately labelled covariance blocks, with cross blocks retained whenever the same calibration data determine both interaction and current LECs.

Reproducible calculation and validation

An implementable sequence is: fit or sample the LECs; solve the coupled bound state at every EFT order and regulator; construct currents at matching order; evolve all operators and states over several λ_{SRG} values; evaluate reduced multipoles and weak matrix elements; and infer the joint error kernel from standardized order increments. Cache wave functions and operator matrix elements separately so that LEC and hyperparameter sampling does not hide a basis-convergence error.

Essential checks are charge normalization, the deuteron pole residue, continuity-equation residuals, independence of exact matrix elements under SRG flow, recovery of the unevolved result as $s \to 0$, regulator stability within the predicted EFT band, and empirical coverage of held-out orders or kinematics. The unresolved formal object is the cross-observable probability law for omitted interaction, current, and SRG-induced contributions after all these identities are imposed; independent error bars cannot represent it.

Maxima research model

The driver takes a two-channel S–D Hamiltonian, a mixed state and current, a flow scale, the EFT parameter Q, and shared omitted-order loadings. It prints the suppression of H_{SD} with flow, both consistent and inconsistent current expectations, and the joint covariance and correlation matrices for three tensor observables. Replace the small matrices by momentum-grid reductions and infer the loading matrix from order-by-order calculations to extend the model. The exact two-channel rotation is a diagnostic surrogate, not a full SRG differential-equation solver. From the project root run the following full command.

```
maxima --batch=maxima/09_tensor_force_eft.mac
```

```
/* Two-channel S--D similarity flow and correlated EFT predictions. */
kill(all)$
display2d:false$
ratprint:false$
linel:200$

H0 : matrix([-2.2246,0.62],[0.62,1.15])$  /* MeV */
psi0 : matrix([sqrt(0.94)],[sqrt(0.06)])$
J0 : matrix([1.00,0.18],[0.18,-0.35])$
theta_inf : 0.5*atan(2*H0[1,2]/(H0[2,2]-H0[1,1]))$
theta(s) := theta_inf*(1-exp(-s/0.8))$
U(s) := matrix([cos(theta(s)),-sin(theta(s))],
               [sin(theta(s)), cos(theta(s))])$
H(s) := U(s).H0.transpose(U(s))$
psi(s) := U(s).psi0$
Jflow(s) := U(s).J0.transpose(U(s))$
expect(p,O) := transpose(p).O.p$

print("SRG-like two-channel flow (energies in MeV)")$
print(" s       H_SD       <J> coevolved    <J0> inconsistent")$
for sv in [0,0.25,0.5,1,2,4] do block([hs:H(sv),ps:psi(sv)],
  printf(true,"~5,2f  ~10,6f    ~12,8f      ~12,8f~%",
    float(sv),float(hs[1,2]),float(expect(ps,Jflow(sv))),
    float(expect(ps,J0))))$

/* Shared omitted-order modes correlate three tensor observables. */
Q : 0.28$
kdone : 3$
L : matrix([1.00,0.25],[0.72,-0.18],[0.42,0.55])$
yref : matrix([1.00],[0.31],[0.86])$
tail : Q^(2*(kdone+1))/(1-Q^2)$
Y : matrix([yref[1,1],0,0],[0,yref[2,1],0],[0,0,yref[3,1]])$
Ceft : tail*Y.L.transpose(L).Y$
Cnum : matrix([2e-8,0,0],[0,4e-9,0],[0,0,1e-8])$
Ctot : Ceft+Cnum$
Corr : genmatrix(lambda([i,j],Ctot[i,j]/sqrt(Ctot[i,i]*Ctot[j,j])),3,3)$
print("Correlated truncation covariance for [G_C,T_20,G_M]")$
print(matrixmap('float,Ctot))$
print("Corresponding correlation matrix")$
print(matrixmap('float,Corr))$
```

What Kind of Solution Will Fill the Gap

Target result

Construct a multivariate posterior for

$$\boxed{\{G_C(q), G_Q(q), G_M(q), T_{20}(q), Q_d, \mu_d, \Gamma_{\mu d}, \ldots\}}$$

that separately exposes LEC, interaction-truncation, current-truncation, regulator, SRG, and numerical covariances. Prove and validate $X_{a,k}(s) - X_{a,k}(s_0) = O(Q^{k+1})$ when currents are consistently evolved and truncated. Extend the analytical covariance above to explicit interaction–current cross-correlations and infer tensor-sector LECs only from observables, never from P_D. An initial application should jointly use $G_Q(q)$, $T_{20}(q)$, and one weak process because they probe different combinations of tensor mixing and two-body currents.

References

[1] R. Machleidt and D. R. Entem. "Chiral effective field theory and nuclear forces". In: *Physics Reports* 503 (2011), pp. 1–75. DOI: 10.1016/j.physrep.2011.02.001. URL: https://arxiv.org/abs/1105.2919.

[2] H.-W. Hammer, Sebastian König, and U. van Kolck. "Nuclear effective field theory: status and perspectives". In: *Reviews of Modern Physics* 92 (2020), p. 025004. DOI: 10.1103/RevModPhys.92.025004. URL: https://arxiv.org/abs/1906.12122.

[3] R. J. Furnstahl and A. Schwenk. *How should one formulate, extract, and interpret non-observables for nuclei?* 2010. URL: https://arxiv.org/abs/1001.0328 (visited on 07/16/2026).

[4] E. R. Anderson, S. K. Bogner, R. J. Furnstahl, and R. J. Perry. "Operator evolution via the similarity renormalization group I: The deuteron". In: *Physical Review C* 82 (2010), p. 054001. DOI: 10.1103/PhysRevC.82.054001. URL: https://arxiv.org/abs/1008.1569.

[5] R. J. Furnstahl, D. R. Phillips, and S. Wesolowski. "A recipe for EFT uncertainty quantification in nuclear physics". In: *Journal of Physics G: Nuclear and Particle Physics* 42 (2015), p. 034028. DOI: 10.1088/0954-3899/42/3/034028. URL: https://arxiv.org/abs/1407.0657.

[6] J. A. Melendez, R. J. Furnstahl, D. R. Phillips, M. T. Pratola, and S. Wesolowski. "Quantifying correlated truncation errors in effective field theory". In: *Physical Review C* 100 (2019), p. 044001. DOI: 10.1103/PhysRevC.100.044001. URL: https://arxiv.org/abs/1904.10581.

[7] P. J. Millican, R. J. Furnstahl, J. A. Melendez, D. R. Phillips, and M. T. Pratola. "Assessing correlated truncation errors in modern nucleon-nucleon potentials". In: *Physical Review C* 110 (2024), p. 044002. DOI: 10.1103/PhysRevC.110.044002. URL: https://arxiv.org/abs/2402.13165.

[8] Alex Gnech, Laura Elisa Marcucci, and Michele Viviani. "Bayesian analysis of muon capture on the deuteron in chiral effective field theory". In: *Physical Review C* 109 (2024), p. 035502. DOI: 10.1103/PhysRevC.109.035502. URL: https://arxiv.org/abs/2305.07568.

10 Certified differentiable analytic continuation of momentum-space scattering poles

Flügge seed: Vol. I, Problems 77–79 and 94–108, plus Vol. II, Problem 184: momentum-space integral equations, Schwinger/Kohn variational ideas, and Born approximations.

Projection and eigenvector-continuation emulators now reproduce real-energy scattering for local, nonlocal, charged, complex optical, and multichannel potentials [1–3]. Separate mathematical work provides contour algorithms for nonlinear eigenvalue problems [4] and guaranteed-convergent algorithms for scattering resonances [5]. Differentiable resonance and inverse-scattering calculations are also emerging [6, 7]. These advances shift the target from differentiability alone to a certified framework for nonlocal or energy-dependent momentum-space potentials. It must supply the correct unphysical-sheet continuation, derivatives of simple poles, cluster treatment at coalescence, a posteriori discretization/continuation bounds, and a verified pole count or pole-containing disk.

Formalisms

Partial-wave operator and admissible kernels

Consider two particles of reduced mass μ after separating their center-of-mass motion. In a fixed partial wave ℓ, or in a finite set of coupled channels $c = 1, \ldots, N_c$, use

$$\mathcal{H} = \bigoplus_{c=1}^{N_c} L^2([0,\infty), p^2 dp), \qquad \|\psi\|^2 = \sum_c \int_0^\infty p^2 |\psi_c(p)|^2 dp. \tag{228}$$

Channel thresholds are E_c, momenta are

$$k_c(E) = \frac{\sqrt{2\mu_c(E - E_c)}}{\hbar}, \tag{229}$$

and a Riemann sheet is fixed by specifying the sign of every square root. Energies are measured relative to a declared entrance threshold; momenta and nonlocal cutoffs must use one consistent unit system.

Let $\boldsymbol{\theta} \in \Theta \subset \mathbb{R}^{n_\theta}$ parameterize a possibly complex, nonlocal, and energy-dependent interaction $V^{\ell}_{cc'}(p, p'; E, \boldsymbol{\theta})$. A useful mathematical starting class is: the kernel is analytic in E on a sheet domain Ω away from thresholds and left-hand singularities, continuously differentiable in $\boldsymbol{\theta}$, and Hilbert–Schmidt after multiplication by stated momentum weights. Trace-class assumptions are stronger and are invoked only when an ordinary Fredholm determinant is used. Unscreened Coulomb interactions must first be treated with a Coulomb-distorted resolvent or screening and renormalization; the free-resolvent formulas below do not apply to them unchanged.

Lippmann–Schwinger equation and sheet continuation

With the convention

$$G_{0,c}(E; q) = \left(E - E_c - \frac{\hbar^2 q^2}{2\mu_c} \right)^{-1}, \tag{230}$$

the coupled Lippmann–Schwinger equation is

$$\begin{aligned} T^{\ell}_{cc'}(p, p'; E) &= V^{\ell}_{cc'}(p, p'; E) \\ &\quad + \frac{2}{\pi} \sum_d \int_{\mathcal{C}_d} dq\, q^2 V^{\ell}_{cd}(p, q; E) G_{0,d}(E; q) T^{\ell}_{dc'}(q, p'; E). \end{aligned} \tag{231}$$

The factor $2/\pi$ fixes the radial momentum normalization and must be changed together with the definitions of V and T if another convention is chosen. On the physical upper rim of an open-channel cut, $G_0(E+i0)$ enforces outgoing boundary conditions. Bound states lie on the physical sheet below all open thresholds; virtual states and resonances require the corresponding unphysical signs of k_c.

Continuation can be implemented by deforming each momentum contour $\mathcal{C}_c$ into the complex plane without crossing kernel singularities. For a rotation $q = e^{-i\varphi_c}x$, the angle must expose the requested pole while leaving exchange and regulator singularities on the correct side. A piecewise contour is safer when a moving propagator pole approaches a branch point. Record the contour, orientation, square-root convention, and every crossed residue: these data are part of the definition of the sheet, not numerical tuning parameters.

Define the compact integral operator

$$K(E,\boldsymbol{\theta}) = V(E,\boldsymbol{\theta})G_0(E), \qquad A(E,\boldsymbol{\theta}) = I - K(E,\boldsymbol{\theta}). \tag{232}$$

Then $A(E)T(E) = V(E)$. Analytic Fredholm theory implies that $A(E)^{-1}$ is meromorphic in Ω. If K is trace class,

$$D(E,\boldsymbol{\theta}) = \det[I - K(E,\boldsymbol{\theta})] \tag{233}$$

is defined and its zeros locate poles with algebraic multiplicity. If only Hilbert–Schmidt regularity is available, use a regularized determinant or work directly with the analytic operator pencil.

Simple poles, residues, and exact derivatives

At a simple pole E_*, choose right and left null vectors

$$A(E_*,\boldsymbol{\theta})v = 0, \qquad w^\dagger A(E_*,\boldsymbol{\theta}) = 0, \qquad w^\dagger A_E(E_*,\boldsymbol{\theta})v \neq 0. \tag{234}$$

The scale freedom may be fixed by $w^\dagger A_E(E_*)v = 1$. The singular part of the inverse is then

$$A(E)^{-1} = \frac{vw^\dagger}{E - E_*} + A_{\mathrm{reg}}(E), \tag{235}$$

with the denominator restored if a different normalization is used. For a real parameter θ_j, implicit differentiation gives

$$\boxed{\frac{\partial E_*}{\partial \theta_j} = -\frac{w^\dagger A_{\theta_j}(E_*,\boldsymbol{\theta})v}{w^\dagger A_E(E_*,\boldsymbol{\theta})v}}. \tag{236}$$

Both derivatives contain all explicit energy or parameter dependence:

$$A_E = -V_E G_0 - V G_{0,E}, \tag{237}$$
$$A_{\theta_j} = -V_{\theta_j} G_0. \tag{238}$$

Automatic differentiation may evaluate the discretized numerator and denominator, but the pole derivative must still be obtained from this implicit formula; differentiating iterations of a root finder is neither necessary nor stable. A useful condition indicator is

$$\kappa_*(E_*) = \frac{\|w\|\,\|v\|}{|w^\dagger A_E(E_*)v|}. \tag{239}$$

Its growth signals loss of an individually differentiable pole label.

Multiple poles and contour invariants

For a defective zero, vectors satisfy nonlinear Jordan-chain relations such as

$$A_* v_0 = 0, \qquad A_* v_1 + A_{E,*} v_0 = 0. \tag{240}$$

Generic perturbations then produce Puiseux, rather than Taylor, expansions. Stable quantities are associated with the entire cluster enclosed by a positively oriented contour $\Gamma \subset \Omega$. The operator-valued argument principle gives

$$N_\Gamma = \frac{1}{2\pi i} \operatorname{tr} \oint_\Gamma A(E)^{-1} A_E(E)\, dE, \tag{241}$$

provided the trace and contour assumptions hold. For a probing matrix or finite-rank map B, form moments

$$M_j = \frac{1}{2\pi i} \oint_\Gamma E^j A(E)^{-1} B\, dE, \qquad j = 0, 1, \dots . \tag{242}$$

An SVD of M_0, followed by the projected small pencil built from M_0, M_1, returns the pole cluster without assigning unstable individual residues. Under parameter variation, derivatives of the contour projector and of symmetric quantities such as $\sum_r E_r$ remain finite as long as no pole crosses Γ.

Nyström discretization on a deformed contour

Parameterize $q = z_c(t)$, $0 \le t < 1$, with a map that resolves the origin, on-shell neighborhood, and ultraviolet tail. A quadrature $\{t_i, \omega_i\}_{i=1}^{N_h}$ gives a block matrix

$$[K_h(E)]_{ci,dj} = \frac{2}{\pi} V^\ell_{cd}(p_i, z_d(t_j); E) G_{0,d}(E; z_d(t_j)) z_d(t_j)^2 z_d'(t_j) \omega_j, \qquad A_h = I - K_h. \tag{243}$$

Square-root quadrature weights may be distributed symmetrically between rows and columns to improve conditioning, but this similarity scaling must be undone when reconstructing continuum vectors. The mesh cannot contain a propagator singularity, and a moving contour requires differentiating its parameterization or proving that contour invariance removes that term.

Refine radial mapping, node number, contour angle, and ultraviolet cutoff independently. Residuals $\|A_h(\widehat{E})\widehat{v}\|$ test the discrete nonlinear eigenpair; they do not by themselves bound the continuum pole. Introduce sampling and reconstruction maps $P_h : \mathcal{H} \to \mathbb{C}^{N_h N_c}$ and $I_h : \mathbb{C}^{N_h N_c} \to \mathcal{H}$, and compare operators on one space, with $P_h I_h = I$ on the discrete space. Define $\widetilde{K}_h = I_h K_h P_h$ and $\widetilde{A}_h = I - \widetilde{K}_h$. Compact-operator approximation then requires

$$\|K(E) - \widetilde{K}_h(E)\|_{\mathcal{B}(\mathcal{H})} = \|A(E) - \widetilde{A}_h(E)\|_{\mathcal{B}(\mathcal{H})} \le \varepsilon_h(E), \qquad E \in \Gamma. \tag{244}$$

Certification, uncertainty, and workflow

If $A_h(E)$ is invertible on Γ and the lifted inverse is controlled, a sufficient homotopy condition has the form

$$\boxed{\sup_{E\in\Gamma} \|\widetilde{A}_h(E)^{-1}\|\, \varepsilon_h(E) < 1.} \tag{245}$$

For $P_h I_h = I$, the lifted inverse can be evaluated from the finite matrix,

$$\widetilde{A}_h^{-1} = I + I_h(A_h^{-1} - I)P_h. \tag{246}$$

It prevents a zero from crossing the contour during interpolation between the continuum and discrete pencils, so the enclosed multiplicity is preserved. The bound ε_h must include quadrature, tail truncation, contour interpolation, and floating-point effects; comparing two meshes estimates but does not certify it.

An implementable calculation therefore proceeds as follows: specify the sheet and analytic domain; validate the deformed kernel; build a sequence of Nyström operators; count poles on a coarse contour; extract clusters from moments; refine simple poles with left/right vectors; evaluate implicit derivatives; and only then propagate a parameter posterior. Numerical enclosures and parameter uncertainty should be reported separately, especially when a posterior sample changes the number of poles within Γ.

Checks include an exactly soluble separable kernel, real-axis unitarity for a Hermitian interaction, subunitarity for a passive optical potential, invariance under allowed contour deformations, conjugation or sheet symmetries, and stable threshold limits from domains that exclude the branch point itself. The unresolved mathematical object is a computable continuum-level error majorant $\varepsilon_h(E, \boldsymbol{\theta})$ that remains uniform over the inference domain and interfaces correctly with cluster, rather than scalar-pole, differentiation.

Maxima research model

The driver takes two bare channel energies, an energy-dependence coefficient, a coupling, a finite-difference step, and a diagnostic disk radius. It returns both poles, implicit sensitivities, finite-difference benchmarks, residuals, condition factors, and a floating Rouché margin that includes the residual $|D(E_p)|$. Replace `A(E,g)` by a separable or Nyström operator on the chosen sheet; this quadratic real-axis example has no threshold branch cut. A rigorous disk certificate requires interval or directed-rounding bounds for every term, not the displayed floating margin. If `aa(g)` vanishes use the linear equation, while a zero discriminant requires cluster rather than simple-pole differentiation. From the project root run the following full command.

```
maxima --batch=maxima/10_differentiable_scattering.mac
```

```
/* Energy-dependent rank-two inverse amplitude: poles and sensitivities. */
kill(all)$
display2d:false$
ratprint:false$
linel:200$

e1 : -1.20$ e2 : 0.45$ beta : 0.25$ g0 : 0.35$
A(E,g) := matrix([E-e1,-g*(1+beta*E)],
                 [-g*(1+beta*E),E-e2])$
D(E,g) := expand(determinant(A(E,g)))$
aa(g) := coeff(D(E,g),E,2)$
bb(g) := coeff(D(E,g),E,1)$
cc(g) := coeff(D(E,g),E,0)$
pole(branch,g) := (-bb(g)+branch*sqrt(bb(g)^2-4*aa(g)*cc(g)))/(2*aa(g))$
DEexpr : diff(D(E,g),E)$
Dgexpr : diff(D(E,g),g)$
dEdg(Ep,gv) := -subst([E=Ep,g=gv],Dgexpr)/subst([E=Ep,g=gv],DEexpr)$

hfd : 1e-5$
radius : 0.08$
print("Energy-dependent two-channel pole map")$
print("branch       E_pole       dE/dg analytic    dE/dg finite-diff")$
for branch in [-1,1] do block([Ep,sa,sf],
  Ep:pole(branch,g0),
  sa:dEdg(Ep,g0),
  sf:(pole(branch,g0+hfd)-pole(branch,g0-hfd))/(2*hfd),
  printf(true," ~2d      ~12,8f      ~12,8f        ~12,8f~%",
    branch,Ep,sa,sf))$

/* Floating Rouche diagnostic; rigorous certification needs interval bounds. */
print("Floating pole-isolation diagnostic for radius",radius)$
print("branch     residual        condition 1/|D_E|    diagnostic margin")$
for branch in [-1,1] do block([Ep,res,cond,diag_margin],
  Ep:pole(branch,g0),
  res:abs(D(Ep,g0)),
  cond:1/abs(subst(Ep,E,diff(D(E,g0),E))),
  diag_margin:abs(subst(Ep,E,diff(D(E,g0),E)))*radius
              -abs(aa(g0))*radius^2-res,
  printf(true," ~2d      ~12,4e       ~12,6f        ~12,6e~%",
    branch,res,cond,diag_margin))$
print("Pole separation =",float(abs(pole(1,g0)-pole(-1,g0))))$
```

What Kind of Solution Will Fill the Gap

Target result

For a stated class of analytic, nonlocal, possibly energy-dependent partial-wave kernels, prove that the contour-deformed Nystrom operator $A_h(E,\theta)$ produces a disk $B(\widehat{E}, r_h)$ containing exactly one continuum pole, with

$$\boxed{|E_* - \widehat{E}| \le r_h, \qquad \left|\partial_{\theta_j} E_* - \widehat{d}_j\right| \le C_j(\varepsilon_h, \|A_h(\widehat{E})\widehat{v}\|, \kappa, \mathrm{sep}).}$$

The code must refuse a misleading scalar derivative near multiplicity and instead return a certified cluster, Puiseux data, or derivatives of symmetric cluster invariants. Demonstrate the method by Bayesian inference of a nonlocal optical/EFT interaction from phase shifts, propagating the certified pole disk into the posterior for a bound, virtual, or resonant state.

References

[1] R. J. Furnstahl, A. J. Garcia, P. J. Millican, and Xilin Zhang. "Efficient emulators for scattering using eigenvector continuation". In: *Physics Letters B* 809 (2020), p. 135719. DOI: 10.1016/j.physletb.2020.135719. URL: https://arxiv.org/abs/2007.03635.

[2] C. Drischler, M. Quinonez, P. G. Giuliani, A. E. Lovell, and F. M. Nunes. "Toward emulating nuclear reactions using eigenvector continuation". In: *Physics Letters B* 823 (2021), p. 136777. DOI: 10.1016/j.physletb.2021.136777. URL: https://arxiv.org/abs/2108.08269.

[3] K. Hagino, S. Yoshida, M. Kimura, and K. Uzawa. *Emulating multi-channel scattering based on the eigenvector continuation in the discrete basis formalism*. 2025. URL: https://arxiv.org/abs/2504.14922 (visited on 07/16/2026).

[4] Wolf-Jürgen Beyn. "An integral method for solving nonlinear eigenvalue problems". In: *Linear Algebra and its Applications* 436 (2012), pp. 3839–3863. DOI: 10.1016/j.laa.2011.03.030.

[5] Jonathan Ben-Artzi, Marco Marletta, and Frank Rösler. "Computing scattering resonances". In: *Journal of the European Mathematical Society* (2023). DOI: 10.4171/JEMS/1258. URL: https://arxiv.org/abs/2006.03368.

[6] Julius D. Fischbach et al. "A framework to compute resonances arising from multiple scattering". In: *Advanced Theory and Simulations* (2025). DOI: 10.1002/adts.202400989. URL: https://arxiv.org/abs/2409.05563.

[7] A. Awasthi, I. Kant, A. Sharma, M. R. Ganesh Kumar, and O. S. K. S. Sastri. *Constructing inverse potentials from scattering phase shifts using physics-informed neural networks: application to neutron-alpha scattering*. 2026. URL: https://arxiv.org/abs/2605.02264 (visited on 07/16/2026).

11 Gauge-consistent Coulomb-continuum transitions driven by finite structured pulses

Flügge seed: Vol. II, Problems 185–188 and 210–219: photoionization, oscillator strengths, spin flips, emission, dipole selection rules, Compton scattering, and bremsstrahlung.

Twisted-photon selection rules and impact-parameter dependence are established for hydrogenic excitation and ionization [1, 2], and optical OAM transfer to a bound electron has been observed [3]. The Power–Zienau–Woolley literature clarifies that minimal and multipolar descriptions remain equivalent when basis and multipole truncations are transformed consistently; inconsistent truncations can break that equivalence [4].

The strong-field frontier already includes nondipole descriptions for spatially structured fields [5], measured electric nondipole momentum shifts [6], few-cycle nondipole SFA [7], nonparaxial vector-beam multipoles [8], and ionization by few-cycle twisted pulses [9]. Together they leave a narrower task: a gauge-audited finite-energy pulse theory with Maxwell-consistent longitudinal fields, a Coulomb- or screened-Coulomb-distorted continuum, and a controlled E1–E2–M1/$1/c$ truncation.

Formalisms

Target space, Hamiltonian, and continuum convention

Begin with a specified one-active-electron target rather than a generic plane wave. For a fixed nucleus and, when needed, electron spin,

$$\mathcal{H}_{\rm e} = L^2(\mathbb{R}^3, d^3r)\otimes\mathbb{C}^2, \qquad H_0 = \frac{\mathbf{p}^2}{2m_e} + V_{\rm eff}(r) + H_{\rm so}, \qquad \mathbf{p} = -i\hbar\boldsymbol{\nabla}. \tag{247}$$

The effective potential must be declared: examples are $-Ze^2/(4\pi\epsilon_0 r)$, a screened Coulomb potential, or a local one-electron model potential fitted to binding energies and phase shifts. A nonlocal pseudopotential needs its own gauge link and cannot be coupled by the naive substitution $\mathbf{p}\mapsto\mathbf{p}+e\mathbf{A}$.

Let $|i\rangle = |n_iL_iJ_iM_i\rangle$ be normalized to one and satisfy $H_0|i\rangle = E_i|i\rangle$. The exact final scattering solution used in a photoionization bra is $|\psi^{(-)}_{E\widehat{\mathbf{p}}\sigma}\rangle$, where the $(-)$ boundary condition is the time-reversed convention that produces an outgoing detected electron. Adopt energy–angle normalization,

$$\langle\psi^{(-)}_{E\widehat{\mathbf{p}}\sigma}|\psi^{(-)}_{E'\widehat{\mathbf{p}}'\sigma'}\rangle = \delta(E-E')\delta^{(2)}(\widehat{\mathbf{p}}-\widehat{\mathbf{p}}')\delta_{\sigma\sigma'}. \tag{248}$$

For a Coulomb tail, its large-r phase contains the logarithmic Coulomb term and partial-wave phase $\sigma_L = \arg\Gamma(L+1+i\eta_C)$, with $\eta_C = -Z_{\rm eff}\alpha c/v$ for an electron in an attractive effective charge $Z_{\rm eff}$. Imposing a plane-wave boundary at a finite box edge gives the wrong phase and Wigner delay. If momentum-normalized states are used instead, the corresponding density of states must be retained explicitly in every probability.

A finite-energy Maxwell pulse

Place the atomic center a transverse displacement $\mathbf{b}$ from the beam axis. In radiation gauge, represent the positive-frequency vector potential by

$$\mathbf{A}^{(+)}(\mathbf{r},t;\mathbf{b}) = \sum_\lambda\int_0^\infty d\omega\int_{|\mathbf{k}_\perp|<\omega/c} d^2k_\perp\, a_\lambda(\mathbf{k}_\perp,\omega)\boldsymbol{\epsilon}_\lambda(\mathbf{k}) \times e^{i[\mathbf{k}_\perp\cdot(\mathbf{r}_\perp-\mathbf{b})+k_zz-\omega t]}, \qquad k_z = \sqrt{(\omega/c)^2-k_\perp^2}, \tag{249}$$

and set $\mathbf{A} = \mathbf{A}^{(+)}+\mathbf{A}^{(-)}$. The polarization vectors obey

$$\mathbf{k}\cdot\boldsymbol{\epsilon}_\lambda(\mathbf{k}) = 0, \qquad \boldsymbol{\epsilon}^*_\lambda\cdot\boldsymbol{\epsilon}_{\lambda'} = \delta_{\lambda\lambda'}. \tag{250}$$

Thus $\mathbf{E} = -\partial_t \mathbf{A}$ and $\mathbf{B} = \boldsymbol{\nabla} \times \mathbf{A}$ satisfy the source-free Maxwell equations, including the nonparaxial longitudinal field. Evanescent components may be admitted for a near-field source, but then their source geometry and normalization must replace the propagating support above.

A finite Bessel–Gauss example is specified by

$$a_\lambda(\mathbf{k}_\perp, \omega) = \mathcal{N} F(\omega) e^{i m_\gamma \varphi_k} \exp\left[-\frac{w_0^2}{4}(k_\perp - \kappa_0)^2\right] c_\lambda(\mathbf{k}), \tag{251}$$

where m_γ is the beam's azimuthal index, F fixes its duration and carrier-envelope phase, and $\mathcal{N}$ fixes pulse energy. Confirm numerically that

$$U_{\text{pulse}} = \frac{\epsilon_0}{2} \int d^3 r \left(|\mathbf{E}|^2 + c^2 |\mathbf{B}|^2\right) \tag{252}$$

is finite and time independent when integrated over all space in vacuum. On a finite numerical domain, include the outgoing Poynting flux so that the energy balance closes. The useful control parameters are

$$\epsilon_{ka} = k_0 a, \qquad \epsilon_w = \frac{a}{w_0}, \qquad \epsilon_v = \frac{v}{c}, \qquad \epsilon_\omega = \frac{\Delta\omega}{\omega_0}, \tag{253}$$

where a is a target length scale and v a characteristic continuum velocity. These parameters, rather than "nondipole" as a label, determine the truncation.

Minimal and multipolar interactions

For electron charge $q_e = -e$, the Pauli Hamiltonian in minimal coupling is

$$H_{\min}(t) = \frac{[\mathbf{p} - q_e \mathbf{A}(\mathbf{r}, t)]^2}{2m_e} + q_e \phi(\mathbf{r}, t) + V_{\text{eff}}(r) - \boldsymbol{\mu}_s \cdot \mathbf{B}(\mathbf{r}, t). \tag{254}$$

Its interaction separates into

$$H_I^{(1)} = -\frac{q_e}{2m_e}(\mathbf{p} \cdot \mathbf{A} + \mathbf{A} \cdot \mathbf{p}) + q_e \phi - \boldsymbol{\mu}_s \cdot \mathbf{B}, \tag{255}$$

$$H_I^{(2)} = \frac{q_e^2}{2m_e} \mathbf{A}^2. \tag{256}$$

The $\mathbf{A}^2$ term does not enter a strictly first-order, one-photon amplitude, but it is required for a consistent second-order or strong-classical field comparison. Recoil requires adding the nucleus and transforming to center-of-mass and internal coordinates before expanding.

The Power–Zienau–Woolley transformation is a unitary transformation of the full matter–field Hilbert space. When its operators, states, and basis are transformed consistently, it gives the same amplitudes as minimal coupling. Expanding the transformed interaction about the center $\mathbf{R}$ gives

$$H_I^{\text{PZW}} = -\mathbf{d} \cdot \mathbf{E}(\mathbf{R}, t) - \frac{1}{2}\Theta_{ij} \partial_i E_j(\mathbf{R}, t) - \boldsymbol{\mu} \cdot \mathbf{B}(\mathbf{R}, t) + H_{\text{Röntgen}} + \cdots, \tag{257}$$

where $\epsilon_s = \max(\epsilon_{ka}, \epsilon_w, \epsilon_v)$ and

$$\Theta_{ij} = \int d^3 r \, \rho(\mathbf{r}) r_i r_j. \tag{258}$$

For the traceless convention $Q_{ij} = \int \rho(3 r_i r_j - r^2 \delta_{ij}) d^3 r$, the quadrupole term is $-Q_{ij} \partial_i E_j / 6$ in a source-free region. The Röntgen term is tied to center-of-mass motion and must accompany recoil at the same order. Projecting one gauge before applying the unitary transformation, or retaining E2 in one gauge but omitting terms of the same order in the other, destroys equivalence.

Finite-pulse transition amplitude

In first-order perturbation theory the ionization amplitude is

$$\mathcal{A}_{E\widehat{\mathbf{p}}\sigma,i}(\mathbf{b}) = -\frac{i}{\hbar}\int_{-\infty}^{\infty} dt\, e^{i(E-E_i)t/\hbar}\langle\psi^{(-)}_{E\widehat{\mathbf{p}}\sigma}|H_I^{(+)}(t;\mathbf{b})|i\rangle. \tag{259}$$

Equivalently, for an exactly conserved transition current,

$$\mathcal{A}_{fi} = -\frac{i}{\hbar}\int dt\, d^3r\, [\rho_{fi}(\mathbf{r},t)\phi(\mathbf{r},t) - \mathbf{j}_{fi}(\mathbf{r},t)\cdot\mathbf{A}(\mathbf{r},t)]\,, \qquad \partial_t\rho_{fi} + \boldsymbol{\nabla}\cdot\mathbf{j}_{fi} = 0. \tag{260}$$

The bandwidth integral enforces energy conservation only in the long-pulse limit; replacing it prematurely by a delta function removes pulse broadening.

Expand each plane-wave component in vector spherical waves about the displaced target. Angular reduction then has the form

$$\begin{aligned}\mathcal{A}_{fi}(\mathbf{b}) = \sum_{p=E,M}\sum_{L,M}\int_0^{\infty} d\omega\, \widetilde{f}^{(p)}_{LM}(\omega;\mathbf{b})(-1)^{J_f-M_f}\begin{pmatrix} J_f & L & J_i \\ -M_f & M & M_i\end{pmatrix} \\ \times \langle\alpha_f J_f\|T_L^{(p)}(\omega)\|\alpha_i J_i\rangle.\end{aligned} \tag{261}$$

All beam dependence, including $m_\gamma, w_0, F(\omega)$, helicity, and impact parameter, belongs to $\widetilde{f}$. Target structure and Coulomb phases belong to the reduced matrix element. In a central one-electron model, an electric radial factor is, schematically,

$$R_L^E(E, L_f; n_i, L_i) = \int_0^{\infty} dr\, P_{EL_f}(r) r^L P_{n_iL_i}(r), \tag{262}$$

with the exact finite-frequency operator replacing r^L beyond the long-wavelength limit.

Gauge audit and continuum diagnostics

Under $\mathbf{A}\to\mathbf{A}+\boldsymbol{\nabla}\chi$, $\phi\to\phi-\partial_t\chi$, the exact state also transforms by its charge phase. Current conservation makes the change of $\mathcal{A}_{fi}$ a vanishing boundary term for a finite pulse and properly normalized scattering states. For the spin-independent local Hamiltonian $H_0 = \mathbf{p}^2/(2m_e) + V(r)$, the length–velocity identity

$$\langle f|\mathbf{p}|i\rangle = \frac{im_e}{\hbar}(E_f - E_i)\langle f|\mathbf{r}|i\rangle \tag{263}$$

follows from $[H_0,\mathbf{r}] = -i\hbar\mathbf{p}/m_e$. If spin–orbit or nonlocal terms are retained, replace $\mathbf{p}/m_e$ by the exact velocity $\mathbf{v} = (i/\hbar)[H_0,\mathbf{r}]$ and gauge those terms consistently. The finite-basis residual,

$$\mathcal{R}_{fi} = \left\langle f\left|[H_0,\mathbf{r}] + \frac{i\hbar}{m_e}\mathbf{p}\right|i\right\rangle, \tag{264}$$

separates target-basis error from a multipole-order mismatch. Exterior complex scaling, an R-matrix surface, or analytic Coulomb functions must supply the continuum surface term; simply enlarging an L^2 box can create false gauge agreement.

Observables, computation, and controlled limits

With the energy–angle normalization above,

$$\frac{dP}{dE\, d\Omega_{\mathbf{p}}} = \sum_\sigma |\mathcal{A}_{E\widehat{\mathbf{p}}\sigma,i}|^2. \tag{265}$$

Branching ratios follow by angular and energy integration over stated windows. An OAM-odd momentum signal is obtained from the normalized distribution,

$$\Delta p_z^{(m_\gamma)} = \langle p_z\rangle_{m_\gamma} - \langle p_z\rangle_{-m_\gamma}. \tag{266}$$

It cancels many beam-even systematics but not helicity or displacement asymmetries, which must be reversed independently.

An implementable workflow is to solve and normalize bound and distorted continuum radial functions; tabulate reduced E1, E2, and M1 matrix elements; construct the angular spectrum and verify Maxwell residuals and pulse energy; perform the $(\omega, \mathbf{k}_\perp)$ quadrature; assemble the angular distribution; and repeat in minimal and multipolar representations with matched orders. Vary radial box or matching radius, partial-wave cutoff, multipole cutoff, frequency and transverse-momentum meshes, and pulse calibration.

Checks must recover the ideal-Bessel limit $w_0 \to \infty$ at fixed κ_0, the plane-wave limit when the angular spectrum also collapses to $\mathbf{k}_\perp = 0$, the monochromatic limit $\Delta\omega \to 0$, the paraxial limit $k_\perp/k_0 \to 0$, the dipole limit $k_0 a \to 0$, and known Coulomb photoionization results. Gauge discrepancy is a diagnostic conditional on basis convergence, not an independent physical uncertainty. The missing formal object is a uniform, order-by-order remainder that includes longitudinal-field, recoil, continuum-surface, and transformed-basis effects for a finite structured pulse.

Maxima research model

The driver uses λ_0 as its length unit, sets $c = 1$, and takes the cone angle, helicity, quasi-OAM index, target size a, multipole tensors, and sample points as inputs. It scales the quadrupole as dipole times a, reports ka, synthesizes complex electric and magnetic fields, and prints E2/E1 and M1/E1 amplitude ratios. Four azimuthal rays possess only C_4 quasi-OAM; a continuous angular-spectrum quadrature is required for a true OAM mode. Replace the equal weights by that quadrature and a measured frequency spectrum to extend the calculation. The relative field normalization and illustrative target tensors do not yet predict a pulse-normalized continuum yield. From the project root run the following full command.

```
maxima --batch=maxima/11_structured_light.mac
```

```
/* Four-ray nonparaxial angular spectrum and E1/E2/M1 diagnostics. */
kill(all)$
display2d:false$
ratprint:false$
linel:200$

c : 1.0$ lambda0 : 1.0$ k0 : 2*%pi/lambda0$ /* relative units */
cone : 0.55$ kt : cone*k0$ kz : sqrt(k0^2-kt^2)$
ell_oam : 1$ helicity : 1$
phis : [0,%pi/2,%pi,3*%pi/2]$
dot3(a,b) := sum(a[i,1]*b[i,1],i,1,3)$
cross3(a,b) := matrix([a[2,1]*b[3,1]-a[3,1]*b[2,1]],
 [a[3,1]*b[1,1]-a[1,1]*b[3,1]],
 [a[1,1]*b[2,1]-a[2,1]*b[1,1]])$
kvec(ph) := matrix([kt*cos(ph)],[kt*sin(ph)],[kz])$
svec(ph) := matrix([-sin(ph)],[cos(ph)],[0])$
pvec(ph) := matrix([kz*cos(ph)/k0],[kz*sin(ph)/k0],[-kt/k0])$
eps(ph) := (svec(ph)+%i*helicity*pvec(ph))/sqrt(2)$
weight(ph) := exp(%i*ell_oam*ph)/4$
phase(ph,x,y,z) := exp(%i*dot3(kvec(ph),matrix([x],[y],[z])))$
Efield(x,y,z) := sum(weight(phis[q])*eps(phis[q])
                         *phase(phis[q],x,y,z),q,1,4)$
Bfield(x,y,z) := sum(weight(phis[q])*cross3(kvec(phis[q]),eps(phis[q]))
                         *phase(phis[q],x,y,z)/(c*k0),q,1,4)$
gradE(i,j,x,y,z) := sum(%i*kvec(phis[q])[i,1]*weight(phis[q])
                         *eps(phis[q])[j,1]*phase(phis[q],x,y,z),q,1,4)$

d_scale : 1.0$ a_target : 0.02*lambda0$ ka : k0*a_target$
d : d_scale*matrix([1.0],[0.30],[0.15])$
mu : matrix([0.02],[0.01],[0.03])$
Qt : d_scale*a_target
     *matrix([0.35,0.08,0.00],[0.08,-0.20,0.05],[0.00,0.05,-0.15])$
AE1(x,y,z) := -dot3(d,Efield(x,y,z))$
AE2(x,y,z) := -sum(sum(Qt[i,j]*gradE(i,j,x,y,z),j,1,3),i,1,3)/6$
AM1(x,y,z) := -dot3(mu,Bfield(x,y,z))$
samples : [[0.08,0.03,0],[0.20,-0.05,0.10],[0.35,0.12,0.20]]$
print("Lengths use lambda0; c=1; E,B,d,mu are relative and Q has d*length units")$
printf(true,"target size a = ~8,5f; ka = ~8,5f; four rays give C4 quasi-OAM~%",
       a_target,float(ka))$
print("Nonparaxial four-ray field and multipole diagnostics")$
print(" (x,y,z)             Re(E_x)     Im(E_x)     |E2/E1|    |M1/E1|")$
for r in samples do block([ef:Efield(r[1],r[2],r[3]),a1,a2,am],
  a1:AE1(r[1],r[2],r[3]), a2:AE2(r[1],r[2],r[3]),
  am:AM1(r[1],r[2],r[3]),
  printf(true,"~a  ~10,6f  ~10,6f  ~10,6f  ~10,6f~%",r,
    realpart(float(ef[1,1])),imagpart(float(ef[1,1])),
    float(abs(a2/a1)),float(abs(am/a1))))$
Elast : Efield(0.35,0.12,0.20)$
Blast : Bfield(0.35,0.12,0.20)$
print("Last sample components: j, Re(E_j), Im(E_j), Re(B_j), Im(B_j)")$
for j thru 3 do printf(true,"~2d  ~11,6f ~11,6f  ~11,6f ~11,6f~%",j,
  realpart(float(Elast[j,1])),imagpart(float(Elast[j,1])),
  realpart(float(Blast[j,1])),imagpart(float(Blast[j,1])))$
```

What Kind of Solution Will Fill the Gap

Target result

For one specified system, such as a screened one-active-electron atom in a finite Bessel–Gauss pulse, derive the factorized amplitude through E2 and M1 while retaining every term of the same order in ka, a/w_0, and v/c. Prove the gauge audit

$$\boxed{\mathcal{A}^{(N)}_{\text{minimal}} - \mathcal{A}^{(N)}_{\text{PZW}} = O(\epsilon_s^{N+1}), \qquad \epsilon_s = \max(ka, a/w_0, v/c),}$$

uniformly across the chosen bandwidth, including diamagnetic, seagull, Röntgen, and transformed-state terms. Report pulse-broadened E1/E2/M1 branching ratios and a measurable OAM-odd nondipole observable, for example $\Delta p_z^{(\ell)} = \langle p_z \rangle_\ell - \langle p_z \rangle_{-\ell}$, with its Coulomb correction and a parameter window where it exceeds the gauge/truncation uncertainty.

References

[1] Andrei Afanasev, Carl E. Carlson, and Asmita Mukherjee. *Off-axis excitation of hydrogenlike atoms by twisted photons*. 2013. URL: https://arxiv.org/abs/1305.3650 (visited on 07/16/2026).

[2] Andrei Afanasev, Carl E. Carlson, and Asmita Mukherjee. "High-multipole excitations of hydrogen-like atoms by twisted photons near phase singularity". In: *Journal of Optics* 18 (2016), p. 074013. DOI: 10.1088/2040-8978/18/7/074013. URL: https://arxiv.org/abs/1604.05623.

[3] Christian T. Schmiegelow, Jonas Schulz, Hendrik Kaufmann, Thomas Ruster, Ulrich G. Poschinger, and Ferdinand Schmidt-Kaler. "Transfer of optical orbital angular momentum to a bound electron". In: *Nature Communications* 7 (2016), p. 12998. DOI: 10.1038/ncomms12998.

[4] R. G. Woolley. "Power–Zienau–Woolley representations of nonrelativistic QED for atoms and molecules". In: *Physical Review Research* 2 (2020), p. 013206. DOI: 10.1103/PhysRevResearch.2.013206.

[5] B. Böning, W. Paufler, and S. Fritzsche. "Nondipole strong-field approximation for spatially structured laser fields". In: *Physical Review A* 99 (2019), p. 053404. DOI: 10.1103/PhysRevA.99.053404.

[6] A. Hartung et al. "Electric nondipole effect in strong-field ionization". In: *Physical Review Letters* 126 (2021), p. 053202. DOI: 10.1103/PhysRevLett.126.053202. URL: https://arxiv.org/abs/2008.07638.

[7] D. F. Dar, B. Minneker, and S. Fritzsche. "Nondipole strong-field approximation for above-threshold ionization in a few-cycle pulse". In: *Physical Review A* 107 (2023), p. 053102. DOI: 10.1103/PhysRevA.107.053102. URL: https://arxiv.org/abs/2304.08234.

[8] M. Verde, C. T. Schmiegelow, U. Poschinger, and F. Schmidt-Kaler. "Trapped atoms in spatially-structured vector light fields". In: *Scientific Reports* 13 (2023). DOI: 10.1038/s41598-023-48589-1.

[9] D. F. Dar, A. Weber, S. Ramakrishna, and S. Fritzsche. "Photoionization dynamics in intense few-cycle twisted laser pulses". In: *Physical Review A* 111 (2025), p. 053113. DOI: 10.1103/PhysRevA.111.053113.

12 Frame-covariant quantum-clock interferometry with gradients, rotations, finite packets, and noise

Flügge seed: Vol. I, Problems 40–41: a quantum particle in uniform free fall and in an accelerating electric field.

Modern formulations promote rest, inertial, and gravitational internal energies to operators [1]. Independent atom-interferometer theory already supplies exact phase-space treatments of quadratic potentials, gradients, rotations, open geometries, and Gaussian packets [2]. A composite atom's post-Newtonian Hamiltonian has been derived systematically rather than by a heuristic mass substitution [3]; Roura provided a relativistic clock-interferometer and a doubly differential redshift observable [4].

Recent work includes finite-duration clock pulses, delocalized center-of-mass motion, position-dependent intensities, and mass defect [5], as well as distinct Doppler, Shapiro, and Einstein terms in linearized gravity [6]. Dynamical curvature can generate internal–COM couplings not reducible to a simple mass operator [7]. These ingredients have not been assembled into one closed device signal containing a composite post-Newtonian Hamiltonian, gravity gradients, rotations, finite packets, finite pulse duration, and a noise transfer function. The scope is relativistic quantum metrology in a classical weak field; claims about quantized gravity lie outside it.

Formalisms

Composite Hilbert space and weak-field domain

Use a center-of-mass (COM) coordinate $\mathbf{X}$, conjugate momentum $\mathbf{P}$, and a finite internal clock space spanned by $H_{\text{int}}|n\rangle = \epsilon_n|n\rangle$. The state belongs to

$$\mathcal{H} = L^2(\mathbb{R}^3, d^3X) \otimes \mathcal{H}_{\text{int}}, \qquad [X_i, P_j] = i\hbar\delta_{ij}, \qquad [H_{\text{int}}, \mathbf{X}] = [H_{\text{int}}, \mathbf{P}] = 0. \tag{267}$$

Choose the zero of H_{int} explicitly and let m be the rest mass associated with that reference state. A clock level n then has mass $m_n = m + \epsilon_n/c^2$ to the retained order.

The gravitational field is classical and weak. Over the apparatus, expand the Newtonian potential about a stated origin,

$$\Phi(\mathbf{X}, t) = \Phi_0(t) + \mathbf{g}(t) \cdot \mathbf{X} + \frac{1}{2}\mathbf{X}^T\mathbf{\Gamma}(t)\mathbf{X} + O(X^3/L_\Gamma^3), \qquad \Gamma_{ij} = \partial_i\partial_j\Phi. \tag{268}$$

With this sign convention the acceleration is $-\boldsymbol{\nabla}\Phi$. Require $|\Phi|/c^2 \ll 1$, $|\dot{\mathbf{X}}|/c \ll 1$, and wave-packet support small enough that the neglected spatial derivatives are bounded. Laboratory rotation is described by $\mathbf{\Omega}(t)$, kept to the same perturbative order as gradients and recoil.

Post-Newtonian composite Hamiltonian

Introduce the mass operator

$$\widehat{M} = m + \frac{H_{\text{int}}}{c^2}. \tag{269}$$

Expanding $\widehat{M}c^2 + \mathbf{P}^2/(2\widehat{M}) + \widehat{M}\Phi$ to first order in c^{-2} gives

$$\begin{aligned} H_{\text{PN}} = mc^2 + H_{\text{int}} + \frac{\mathbf{P}^2}{2m} + m\Phi(\mathbf{X}, t) - \mathbf{\Omega} \cdot (\mathbf{X} \times \mathbf{P}) \\ + \frac{H_{\text{int}}}{c^2}\left[\Phi(\mathbf{X}, t) - \frac{\mathbf{P}^2}{2m^2}\right] + H^{\text{int}}_{\text{tidal}} + H_{\text{PN,ext}} + O(c^{-4}). \end{aligned} \tag{270}$$

The term $H_{\text{PN,ext}}$ collects state-independent post-Newtonian corrections, such as $-\mathbf{P}^4/(8m^3c^2)$, if required by the target accuracy. The internal tidal term must be derived from the chosen composite model; it is not automatically represented by replacing m with $\widehat{M}$. Rotation of intrinsic angular momentum may likewise be added when it is not common to the clock states.

For a semiclassical trajectory $\mathbf{X}_\alpha(t)$ on arm α,

$$\tau_\alpha = \int dt \left[1 + \frac{\Phi(\mathbf{X}_\alpha, t)}{c^2} - \frac{\dot{\mathbf{X}}_\alpha^2}{2c^2} + O(c^{-4})\right]. \tag{271}$$

The internal coherence generated by a proper-time difference $\Delta\tau = \tau_\alpha - \tau_\beta$ is

$$\mathcal{C}_{\text{clock}}(\Delta\tau) = \text{Tr}_{\text{int}}\left[\rho_{\text{int}} e^{-iH_{\text{int}}\Delta\tau/\hbar}\right]. \tag{272}$$

This expression assumes the same internal Hamiltonian on both arms; finite clock pulses and state-dependent light shifts must instead be included in the ordered arm propagators.

Laser pulses and path labels

For two clock states $|g\rangle, |e\rangle$, a finite traveling-wave pulse can be modeled in the rotating-wave approximation by

$$H_L(t) = \frac{\hbar\Omega_L(t)}{2}\left[e^{i(\mathbf{k}_L\cdot\mathbf{X} - \omega_L t + \phi_L(t))}|e\rangle\langle g| + \text{h.c.}\right] + \hbar\Delta_L(t)|e\rangle\langle e|. \tag{273}$$

Here Ω_L is a Rabi frequency, Δ_L includes detuning and differential light shifts, and all pulse times, phases, wave vectors, and durations define the device. The short-pulse limit is a conditional momentum kick $\mathbf{\Delta P} = \pm\hbar\mathbf{k}_L$ plus the laser phase at the pulse event. Finite pulses require integration of $H_{\text{PN}} + H_L$; assigning the kick at the pulse midpoint is only an approximation whose order must be stated.

An interferometer path label α records the internal state and the sign of every recoil kick between pulses. Beam-splitter amplitudes are multiplied along the path, while propagation phases and final external states are kept until recombination. This prevents premature use of a classical "area" formula in an open or state-dependent geometry.

Quadratic phase-space propagation

For a fixed internal eigenstate and path segment, truncate the external Hamiltonian at quadratic order,

$$H_{n,\alpha}(t) = \frac{1}{2}\boldsymbol{\xi}^T h_{n,\alpha}(t)\boldsymbol{\xi} + \mathbf{f}_{n,\alpha}(t)^T\boldsymbol{\xi} + c_{n,\alpha}(t), \qquad \boldsymbol{\xi} = \begin{pmatrix}\mathbf{X}\\ \mathbf{P}\end{pmatrix}, \tag{274}$$

where $h = h^T$ and

$$J = \begin{pmatrix} 0 & I_3 \\ -I_3 & 0\end{pmatrix}. \tag{275}$$

The Heisenberg evolution is affine symplectic,

$$\boldsymbol{\xi}(t) = S_{n,\alpha}(t,t_0)\boldsymbol{\xi}(t_0) + \mathbf{d}_{n,\alpha}(t,t_0), \tag{276}$$

$$\dot{S}_{n,\alpha} = Jh_{n,\alpha}S_{n,\alpha}, \qquad S_{n,\alpha}(t_0,t_0) = I_6, \tag{277}$$

$$\dot{\mathbf{d}}_{n,\alpha} = J(h_{n,\alpha}\mathbf{d}_{n,\alpha} + \mathbf{f}_{n,\alpha}), \qquad \mathbf{d}_{n,\alpha}(t_0) = 0. \tag{278}$$

Monitor $S^T JS = J$; its violation measures integration error. Classical actions are evaluated from

$$\mathcal{S}_{n,\alpha} = \int_{t_0}^{t_f} [\mathbf{P}_\alpha \cdot \dot{\mathbf{X}}_\alpha - H_{n,\alpha}(t)]dt, \tag{279}$$

including the phase convention of each kick. A metaplectic phase must be tracked when the symplectic map crosses a caustic.

Take an initial Gaussian external state with mean $\bar{\boldsymbol{\xi}}$ and covariance

$$\Sigma_{ij} = \frac{1}{2}\langle \Delta\xi_i \Delta\xi_j + \Delta\xi_j \Delta\xi_i \rangle, \qquad \Sigma + \frac{i\hbar}{2} J \succeq 0. \tag{280}$$

Its normalization, temperature, position–momentum correlations, and any internal–external correlation must be declared. A thermal mixture is not, in general, reproduced by inserting a single "effective width."

Recombination phase and finite-packet contrast

For two paths ending with affine maps $(S_\alpha, \mathbf{d}_\alpha)$ and $(S_\beta, \mathbf{d}_\beta)$, first bring them to a common output coordinate system. If their linear symplectic parts agree to the retained order, define the final phase-space centers and residual displacement by

$$\boldsymbol{\chi}_{n,\alpha} = S_{n,\alpha}\bar{\boldsymbol{\xi}} + \mathbf{d}_{n,\alpha}, \qquad \delta\boldsymbol{\chi}_n = \boldsymbol{\chi}_{n,\alpha}(t_f) - \boldsymbol{\chi}_{n,\beta}(t_f). \tag{281}$$

In their common output frame the propagated covariance is $\Sigma_n = S_{n,\alpha}\Sigma S_{n,\alpha}^T = S_{n,\beta}\Sigma S_{n,\beta}^T$ to this order. With the Weyl convention $D(\chi) = \exp[-i\chi^T J\boldsymbol{\xi}/\hbar]$, a Gaussian characteristic function is

$$\langle D(\delta\chi_n)\rangle = \exp\left[-\frac{\delta\chi_n^T J\Sigma_n J^T \delta\chi_n}{2\hbar^2} - \frac{i}{\hbar}\delta\chi_n^T J\bar{\boldsymbol{\xi}}_n\right]. \tag{282}$$

The full complex fringe amplitude is a coherent sum over internal states and paths. To display the clock contribution without double counting it, decompose the action obtained from the full conditional Hamiltonian as

$$\mathcal{S}_{n,\alpha} - \mathcal{S}_{n,\beta} = \Delta\mathcal{S}_n^{\text{ext}} - \epsilon_n \Delta\tau_n + O(c^{-4}). \tag{283}$$

This equation defines the external part; if the full action is used directly, the proper-time term must not be added again. For a diagonal internal preparation with populations p_n, a representative split form is

$$\begin{aligned}\mathcal{C} = \sum_n p_n \exp&\left[i\left(\frac{\Delta\mathcal{S}_n^{\text{ext}}}{\hbar} + \Phi_{L,n} + \Phi_{\text{sep},n}\right) - \frac{i\epsilon_n\Delta\tau_n}{\hbar}\right] \\ \times \exp&\left[-\frac{\delta\chi_n^T J\Sigma_n J^T\delta\chi_n}{2\hbar^2} - \frac{i}{\hbar}\delta\chi_n^T J\bar{\boldsymbol{\xi}}_n\right].\end{aligned} \tag{284}$$

For coherent internal superpositions, replace the population sum by the trace of the two ordered arm propagators with ρ_{int}. The detected port probability is

$$P = \frac{1}{2}[1 + \operatorname{Re}\mathcal{C}] = \frac{1}{2}[1 + \mathcal{V}\cos\Phi_{\text{tot}}], \qquad \mathcal{V} = |\mathcal{C}|. \tag{285}$$

Perfect phase-space closure means $\delta\chi_n = 0$ for every populated clock state, not merely for the reference mass. If $S_\alpha \neq S_\beta$, the relative metaplectic map also changes the covariance; evaluate the full Gaussian overlap rather than applying the displacement-only expression above.

Frame transformations

A time-dependent translation, boost, or rotation is represented by a unitary $\mathcal{U}_F(t)$ implementing an affine canonical map. If $|\psi'\rangle = \mathcal{U}_F|\psi\rangle$, then

$$H' = \mathcal{U}_F H \mathcal{U}_F^\dagger + i\hbar\dot{\mathcal{U}}_F\mathcal{U}_F^\dagger. \tag{286}$$

The second term generates the inertial potentials and endpoint phases. The laser phase must be transformed at the same spacetime event, and the initial and detected projectors must be transformed with the state. Propagation, laser, and separation phases are individually frame dependent; their sum and $\mathcal{C}$ are invariant to the retained order. A direct laboratory/free-fall comparison should therefore transform trajectories, kicks, clock couplings, and boundary states, not only replace $m\mathbf{g}\cdot\mathbf{X}$ in the Hamiltonian.

Sensitivity functions and stochastic motion

For a small acceleration perturbation $\delta\mathbf{a}(t)$, define the device response by

$$\delta\Phi_a = \int_{-\infty}^{\infty} dt\, \mathbf{h}_a(t)^T \delta\mathbf{a}(t), \qquad \mathbf{H}_a(\omega) = \int dt\, \mathbf{h}_a(t) e^{i\omega t}. \tag{287}$$

The response $\mathbf{h}_a$ follows from differentiating the finite-pulse propagator, not from inserting delta-function pulses after the fact. For a zero-mean stationary Gaussian process with one-sided spectral-density matrix $S^{(1)}_{a,ij}(\omega)$, use the convention

$$\mathrm{Var}(\delta\Phi_a) = \int_0^{\infty} \frac{d\omega}{2\pi} H^*_{a,i}(\omega) S^{(1)}_{a,ij}(\omega) H_{a,j}(\omega), \qquad \mathcal{V}_{\mathrm{noise}} = e^{-\mathrm{Var}(\delta\Phi_a)/2}. \tag{288}$$

Laser-frequency, phase, timing, rotation, and gradient noise can be added as a multichannel sensitivity matrix. Cross spectra must be retained when sensors or control loops share a reference oscillator.

Calculation sequence and internal checks

Specify a pulse sequence and internal manifold; derive the state-conditioned quadratic coefficients; propagate $S, \mathbf{d}$, actions, and proper times on every path; apply finite-pulse scattering matrices; assemble $\mathcal{C}$; and then evaluate transfer functions and parameter derivatives. Compare the affine method with a split-operator wave-packet calculation for selected points where cubic gravity terms or pulse inhomogeneity may matter.

Mandatory checks are symplecticity, probability conservation, closure in the ideal limit, recovery of the standard $\mathbf{k}_{\mathrm{eff}} \cdot \mathbf{g}T^2$ phase for instantaneous pulses, agreement of laboratory and freely falling frames, vanishing clock phase as $H_{\mathrm{int}}/c^2 \to 0$, and smooth limits $\mathbf{\Gamma}, \mathbf{\Omega} \to 0$. Calibration covariance should be propagated with the Jacobian of the complete signal, while wave-packet and finite-pulse truncation errors remain separately identifiable. The unresolved formal object is the frame-covariant ordered arm propagator, or equivalent influence functional, that combines state-dependent mass, gradients, rotations, finite pulses, packet mismatch, and correlated noise without assigning a frame-dependent phase component physical meaning.

Maxima research model

The driver takes an atomic mass, recoil wave number, pulse separation, initial packet covariance, free-fall acceleration, and a signed constant gravity gradient. Entire hypergeometric sinc/cosc functions make the affine segment exactly finite at zero gradient and analytically continue it to either sign. The model propagates both arms and the covariance, then prints trajectories, phase response, closure, Σ_f, and the resulting symplectic Gaussian overlap. Extend the ordered segment list with state-conditioned masses, rotations, finite-pulse propagators, and noise realizations. The model remains one-dimensional, quadratic, and instantaneous-kick, so it is not a finite-pulse relativistic clock prediction. From the project root run the following full command.

```
maxima --batch=maxima/12_accelerated_quantum_dynamics.mac
```

```
/* Affine symplectic Mach--Zehnder model with signed gravity gradient. */
kill(all)$
display2d:false$
ratprint:false$
linel:200$

m : 1.44316060e-25$ hbar : 1.054571817e-34$
keff : 8.055e6$ recoil : hbar*keff$
T : 0.20$ Gamma : 3.0e-6$ g0 : 9.81$
z0 : 0.0$ v0 : 0.05$ sigma_z : 1.0e-4$
J : matrix([0,1],[-1,0])$

/* Entire sinc/cosc continuations: exact at G=0 and valid for signed G. */
Cfun(t,G) := hypergeometric([],[1/2],-G*t^2/4)$
Sfun(t,G) := t*hypergeometric([],[3/2],-G*t^2/4)$
Kfun(t,G) := t^2*hypergeometric([1],[3/2,2],-G*t^2/4)/2$
Sseg(t,G) := matrix([Cfun(t,G),Sfun(t,G)/m],
                    [-m*G*Sfun(t,G),Cfun(t,G)])$
dseg(t,grav,G) := matrix([-grav*Kfun(t,G)],[-m*grav*Sfun(t,G)])$
prop(x,t,grav,G) := Sseg(t,G).x+dseg(t,grav,G)$
kick(x,dp) := x+matrix([0],[dp])$
xinit : matrix([z0],[m*v0])$

xA0 : kick(xinit,recoil)$ xB0 : xinit$
xAT : prop(xA0,T,grav,Gamma)$ xBT : prop(xB0,T,grav,Gamma)$
xA2 : prop(kick(xAT,-recoil),T,grav,Gamma)$
xB2 : prop(kick(xBT, recoil),T,grav,Gamma)$
zbar2 : (xA2[1,1]+xB2[1,1])/2$
phase : keff*(z0-xAT[1,1]-xBT[1,1]+zbar2)$
phase_value : subst(g0,grav,phase)$ scale_g : diff(phase,grav)$
gradient_shift : phase_value+keff*g0*T^2$
delta : matrix([xA2[1,1]-xB2[1,1]],
               [xA2[2,1]-xB2[2,1]+recoil])$
S2 : Sseg(T,Gamma).Sseg(T,Gamma)$
d2 : Sseg(T,Gamma).dseg(T,g0,Gamma)+dseg(T,g0,Gamma)$
Sigma0 : matrix([sigma_z^2,0],[0,hbar^2/(4*sigma_z^2)])$
Sigmaf : S2.Sigma0.transpose(S2)$
overlap_exponent : transpose(delta).J.Sigmaf.transpose(J).delta/(2*hbar^2)$
contrast : exp(-overlap_exponent)$

print("Light-pulse arms: z in m and v in m/s")$
print("time       z_A          v_A          z_B          v_B")$
for row in [[0,xA0,xB0],[T,xAT,xBT],[2*T,xA2,xB2]] do
  printf(true,"~5,2f  ~12,6e ~12,6e ~12,6e ~12,6e~%",float(row[1]),
    subst(g0,grav,row[2][1,1]),subst(g0,grav,row[2][2,1]/m),
    subst(g0,grav,row[3][1,1]),subst(g0,grav,row[3][2,1]/m))$
print("Composed S(2T), d(2T), and propagated covariance Sigma_f")$
print(matrixmap('float,S2))$ print(matrixmap('float,d2))$
print(matrixmap('float,Sigmaf))$
printf(true,"phase = ~14,7e rad; gradient shift = ~12,5e rad~%",phase_value,gradient_shift)$
printf(true,"dPhi/dg = ~14,7e; closure = (~10,3e m, ~10,3e kg m/s)~%",
       scale_g,subst(g0,grav,delta[1,1]),subst(g0,grav,delta[2,1]))$
printf(true,"covariance-propagated contrast = ~12,9f~%",float(subst(g0,grav,contrast)))$
```

What Kind of Solution Will Fill the Gap

Target result

For a specified device, preferably a strontium single-photon Mach–Zehnder or clock-initialization geometry, derive

$$\boxed{P = \tfrac{1}{2}[1 + \mathcal{V}\cos\Phi_{\rm tot}],}$$

where $\Phi_{\rm tot}$ explicitly contains laser, propagation, separation, clock, gradient, rotation, finite-pulse, and tidal terms. Provide a doubly differential phase isolating $\omega_0\Delta\tau$, the Gaussian contrast above with state-dependent closure errors, and a proof that propagation+laser+separation is invariant to the retained order under time-dependent translations/rotations between the laboratory and freely falling frames. Finally, derive $H_a(\omega)$ and numerical thresholds at which tidal, rotational, finite-pulse, or mass-defect terms imitate the redshift signal.

References

[1] Magdalena Zych and Časlav Brukner. *Quantum formulation of the Einstein equivalence principle.* 2015. URL: https://arxiv.org/abs/1502.00971 (visited on 07/16/2026).

[2] Stephan Kleinert, Enno Kajari, Albert Roura, and Wolfgang P. Schleich. "Representation-free description of light-pulse atom interferometry including non-inertial effects". In: *Physics Reports* 605 (2015), pp. 1–50. DOI: 10.1016/j.physrep.2015.09.004. URL: https://arxiv.org/abs/1512.00260.

[3] Philipp K. Schwartz and Domenico Giulini. "Post-Newtonian Hamiltonian description of an atom in a weak gravitational field". In: *Physical Review A* 100 (2019), p. 052116. DOI: 10.1103/PhysRevA.100.052116. URL: https://arxiv.org/abs/1908.06929.

[4] Albert Roura. "Gravitational redshift in quantum-clock interferometry". In: *Physical Review X* 10 (2020), p. 021014. DOI: 10.1103/PhysRevX.10.021014. URL: https://arxiv.org/abs/1810.06744.

[5] G. Janson, A. Friedrich, and R. Lopp. "Finite pulse-time effects in long-baseline quantum clock interferometry". In: *Journal of Vacuum Science & Technology B* (2024). DOI: 10.1116/5.0178230. URL: https://arxiv.org/abs/2309.14426.

[6] L. Badurina, Y. Du, V. S. H. Lee, Y. Wang, and K. M. Zurek. "Signatures of linearized gravity in atom interferometers: a simplified computational framework". In: *Physical Review D* 111 (2025), p. 042002. DOI: 10.1103/PhysRevD.111.042002. URL: https://arxiv.org/abs/2409.03828.

[7] L. M. van Manen and A. Grossardt. *The Hamiltonian for an atom interacting with gravitational waves.* 2026. URL: https://arxiv.org/abs/2601.17891 (visited on 07/16/2026).