Particle Mechanics — Math Appendix

§0 Preliminaries: Kernels, Spaces, Notation

Scope. This appendix collects the VMS-first preliminaries used across the Particle Mechanics pillar. At each step we state kernels, definitions, assumptions, and lemmas explicitly. Classical forms are used only as dictionaries for comparison/validation. Equations are numbered by section (§n.m); all symbols are listed in §9.

0.1 Routes, Admissibility, and Action Phase

A route r is a piecewise C^1 closed loop $x(s) \subset \mathbb{R}^3$ (or the appropriate manifold) parameterized by arc-length $s \in [0, \ell]$, with $x(0) = x(\ell)$. Admissibility requires single-valued action phase on closure. We define the phase and its loop increment:

$$\phi[x] \equiv S[x] / \hbar$$

$$\Delta\phi_{loop} = (1/\hbar) \cdot \oint p \cdot dl$$

Here p is the canonical momentum 1-form appearing in the action S[x]. Admissibility enforces $\Delta\phi_{loop} = 2\pi n$, $n \in \mathbb{Z}$ (see §1).

0.2 Core Torsion-Driven Kernel

The local energy density decomposes into geometry budgets. In this pillar we use the torsion-driven form with a single calibration κ:

$$\varepsilon_\tau(s) = \kappa \cdot \mathcal{T}[x(s)], \quad \mathcal{T} \geq 0 \text{ (dimensionless)}$$

$$E[x] = \oint \varepsilon_\tau(s)\, ds = \kappa \cdot \oint \mathcal{T}[x(s)]\, ds$$

Define the loop-average torsion budget τ and note that it is dimensionless by construction:

$$\tau \equiv (1/\ell) \cdot \oint \mathcal{T}\, ds$$

Then $E[x] = \kappa\, \tau\, \ell$ and, with $C \equiv \kappa/c^2$, the rest mass is $m = C\, \tau\, \ell$ (see §3 for scaling/ratios).

0.3 Small-Parameter Band and Applicability

Assumption A0 (band). Near-stationary admissible loops; weak environmental gradients; time-invariant kernel over the measurement window. Operationally (see §8 for quantitative gates): small temporal variation, small spatial gradients, short memory, and incoherent channels.

0.4 Reparameterization and Scaling (Lemma L0)

Lemma L0. Reparameterizations preserving closure leave $\Delta\phi_{loop}$ invariant; budget integrals scale with ℓ as in §3.

Sketch. Under $s \mapsto \sigma$ with $ds = (ds/d\sigma)\, d\sigma$:

$$\Delta\phi_{\text{loop}} = (1/\hbar) \cdot \oint p \cdot dl \quad \text{(invariant under reparameterizations)}$$

$$\oint \mathcal{T},\ ds = \oint \mathcal{T}(\sigma) \cdot (ds/d\sigma),\ d\sigma \quad \text{(scalar measure)}$$

Since $\mathcal{T}$ is dimensionless and integrated against the arc-length measure, $\tau\ell = \oint \mathcal{T}\, ds$ is parameterization-independent; $\tau \equiv (1/\ell)\oint \mathcal{T}\, ds$ is therefore a scalar average over the loop. With $E[x] = \kappa\, \tau\, \ell$, mass $m = C\, \tau\, \ell$ inherits the linear scaling in ℓ.

0.5 Dictionaries (Comparison/Validation Only)

Where appropriate, we compare to classical forms solely as dictionaries: Bohr–Sommerfeld quantization ($\oint p \cdot dl = 2\pi\hbar n$, §1), hydrogenic Coulomb closure (r_n, E_n, §7), liquid-drop scalings (A, A^{2/3}, §6), and decay widths from action gaps (§5). These are not axioms of VMS derivations; they serve to calibrate and validate.

0.6 Notation Summary (Pointer to §9)

Symbols appearing in §0–§8 are gathered in §9 with units and roles. Key items used here: ℓ (loop length), s (arc length), $\mathcal{T}$ (dimensionless torsion budget), τ (loop-average of $\mathcal{T}$), κ (calibration constant), $C \equiv \kappa/c^2$ (mass-scale constant), S (action), p (canonical momentum), $\hbar$ (reduced Planck constant).

0.7 Reporting Checklist

When invoking preliminaries in later sections, report:

1. The kernel used (here torsion-driven) and the value/reference for κ (or C).
2. Loop regularity (piecewise C^1), closure condition, and any boundary twist phases (see §1.4).
3. Band checks (stationarity, weak gradients, short memory, incoherence) with thresholds cited from §8.
4. Dictionary used (if any) and whether it is only for validation/calibration.

§1 Loop Closure ⇒ Quantization & Spin

Scope. We expand the loop-closure quantization and the spinor double-cover argument. Admissibility enforces single-valued phase on a closed loop; for a uniform ring this yields discrete momenta and energies. Frame (tetrad) closure occurs only after 4π, giving the spin-½ sign flip and the half-integer/integer spin families.

1.1 Admissibility and Bohr–Sommerfeld Form

Admissibility requires that the total phase accumulated around a closed loop is an integer multiple of 2π. Equivalently, the action integral over one traverse is quantized:

$$(1/\hbar) \cdot \oint p \cdot dl = 2\pi \cdot n, \quad n \in \mathbb{Z}$$

1.2 Uniform Ring Specialization

For a ring where |p| is constant and p is tangent to dl along the loop of length ℓ:

$$\oint p \cdot dl = p \cdot \oint dl = p \cdot \ell \Rightarrow p \cdot \ell = 2\pi \hbar n$$

$$k_n = 2\pi n / \ell , \quad p_n = \hbar k_n = 2\pi \hbar n / \ell$$

$$E_n^{nr} = p_n^2 / (2m) , \quad E_n^{rel} = \sqrt{(p_n^2 c^2 + m^2 c^4)}$$

Assumption A1. The loop is piecewise C^1; p is constant along the ring; endpoints identify as x(0) = x(ℓ).

1.3 Angular Momentum and Ring Current

Let the ring have radius R with ℓ = 2πR. Then k_n = n/R and L_z = R p_n gives:

$$L_z = R \cdot p_n = R \cdot (\hbar n / R) = n \hbar$$

If a charge q circulates with speed v_n = p_n/m on the ring, the current I_n and magnetic moment μ_n scale as:

$$I_n = q \cdot v_n / (2\pi R) , \quad \mu_n = I_n \cdot (\pi R^2) = (q \hbar n) / (2 m) \quad \text{(uniform ring)}$$

1.4 Boundary-Condition Variants (Twisted Closures)

If the loop carries a uniform twist phase χ upon closure, ψ(ℓ) = e^(i χ) ψ(0), admissibility yields:

$$p \cdot \ell = \hbar (2\pi n + \chi) \Rightarrow k_n = (2\pi n + \chi) / \ell$$

χ = 0 recovers periodic boundary condition; χ = π gives anti-periodic levels (half-offset). External gauge flux enters as an effective χ (Aharonov–Bohm dictionary). A uniform flux Φ through the ring induces $\chi = 2\pi \Phi / \Phi_o$, with $\Phi_o \equiv h/q$; thus $p \cdot \ell = \hbar (2\pi n + \chi)$.

1.5 Spin from Double-Cover Closure (Frame Rotation)

A frame (tetrad) rotation by angle θ about axis n̂ acts on a spin-½ state via:

$$U(\theta) = \exp[- i (\theta/2) \cdot \sigma \cdot \hat{n}]$$

$$U(2\pi) = - I , \quad U(4\pi) = + I$$

Thus a 2π rotation flips the sign of a spinor; full admissible frame closure requires 4π. Label spins by s = m/2 with $m \in \mathbb{Z}$ (odd m → half-integer; even m → integer):

$$\text{spin} = m / 2 , \quad m \in \mathbb{Z} \quad (\text{odd} \rightarrow 1/2, 3/2, \ldots ; \ \text{even} \rightarrow 0, 1, 2, \ldots)$$

Lemma L1. The 2π sign flip indicates the double cover SU(2) → SO(3); admissible frame closure at 4π explains half-integer spin for odd m.

1.6 Worked Numeric (Illustrative)

Take ℓ = 2πR with R = 0.50 nm and m = m_e (electron). Then:

$$k_1 = 1 / R = 2.0 \times 10^9 \ m^{-1}$$

$$p_1 = \hbar k_1 \approx 1.054 \times 10^{-34} \times 2.0 \times 10^9 \approx 2.11 \times 10^{-25} \ kg\cdot m/s$$

$$E_1^{nr} = p_1^2 / (2 m_e) \approx 2.45 \times 10^{-20} \ J \approx 0.153 \ eV$$

Higher n scale as n^2 for non-relativistic energies ($E_n^{nr} = n^2 E_1^{nr}$); relativistic energies follow the exact dispersion above.

1.7 Reporting Checklist

When invoking loop-closure quantization and spin, report:

5. Loop length ℓ (or R), boundary condition χ (if any), and assumed regularity (C^1).
6. Derived k_n, p_n, and energies; specify non-relativistic vs relativistic use.
7. Spin labeling and whether spinor sign under 2π rotation is relevant to the context.
8. Band checks from §8 (adiabaticity, weak gradients, short memory, incoherence) if the loop is embedded in a varying environment.

§2 Conserved Charge & Families from Admissibility (Ensemble)

Scope. We formalize the admissible-route ensemble, introduce a uniform phase reweighting α coupled to a class indicator Q, derive conservation from fixed-point admissibility, and show how fractional charges arise from stabilizer-induced congruence classes. Dictionary identifications to U(1)/SU(2)/SU(3) are labels for comparison only.

2.1 Ensemble, Weights, and Reweighting

Let r index admissible routes with action $S[r]$ and class indicator $q[r] \in \{0,1\}$. Introduce the reweighting parameter α that couples to $Q[r] \equiv q[r]$. Weights are:

$$W[r; \alpha] \propto \exp\{ -\beta (S[r] - \alpha \cdot Q[r]) \}$$

Partition function and α-response:

$$Z(\alpha) = \Sigma_r \ W[r; \alpha]$$

$$\partial \ln Z / \partial\alpha = \beta \cdot \langle Q \rangle$$

2.2 Moments and Susceptibilities

From standard cumulant relations:

$$\langle Q \rangle = (1/\beta) \cdot \partial \ln Z / \partial\alpha$$

$$\chi_Q \equiv \partial\langle Q \rangle / \partial\alpha = \beta \cdot \mathrm{Var}(Q) \geq 0$$

Thus χ_Q is non-negative; sharp conservation in the admissible band corresponds to small Var(Q) under allowed dynamics (see §8 for band checks).

2.3 Lemma L2 (Conservation from Fixed-Point Admissibility)

Let $\mathcal{M}$ be the admissible route map advancing routes in time. If the admissible ensemble is a fixed point of $\mathcal{M}$ (class weights invariant), then:

$$d\langle Q \rangle / dt = 0$$

Sketch. Since class weights are time-stationary under $\mathcal{M}$, the distribution of Q is invariant; therefore its expectation is constant. Equivalently, α is a conserved multiplier (Lagrange parameter) for the class constraint.

2.4 Fractional Charge from Stabilizer-Induced Congruence

Assume admissible routes partition into N_tot congruence classes under a stabilizer G, with n_mod of them marked by a phase increment 2π/N_tot. Then the fractional charge (in units of e) is:

$$Q/e = n\_mod / N\_tot , \quad 0 \le n\_mod \le N\_tot$$

Example (thirds):

$$N\_tot = 3 , \quad n\_mod \in \{3, 1, 2\} \Rightarrow Q/e \in \{ -1 , -1/3 , +2/3 \}$$

The sign is chosen by class orientation. This pattern generalizes to other N_tot with obvious replacements.

2.5 Assumption A2 (Stabilizer & Admissibility)

A2. The stabilizer acts transitively on the class partition; reweighting by α respects admissibility (no creation/annihilation of classes). Equivalently, the allowed dynamics do not change N_tot or the marked subset cardinality n_mod.

2.6 Legendre Structure & Generators

ln Z(α) is the cumulant-generating function for Q with β as inverse-temperature-like multiplier from counting (see §Thermo). The Legendre-dual potential is Φ(⟨Q⟩) = (1/β) sup_α [α⟨Q⟩ − ln Z(α)]. Conservation across admissible dynamics implies α is constant in time, fixing ⟨Q⟩.

$$\Phi(\langle Q \rangle) = (1/\beta) \cdot \sup\_\alpha \ [\alpha \langle Q \rangle - \ln Z(\alpha)]$$

2.7 Worked Numeric (Illustrative)

Consider N_tot = 3 with equal class weights at α = 0. Mark n_mod = 1 class. Then Q/e = 1/3. A small α shifts the weight of the marked class by a factor exp{β α}; the mean charge rises as:

$$\langle Q/e \rangle (\alpha) = [1 \cdot (\beta \alpha) + 0 + 0] / [e^{(\beta \alpha)} + 1 + 1] = 1 / (2 + e^{(-\beta \alpha)})$$

For β α = 0.1, ⟨Q/e⟩ ≈ 1 / (2 + e^{−0.1}) ≈ 0.341, close to 1/3 for small α; susceptibility at α=0 is χ_Q = β Var(Q) = β · (2/9).

2.8 Dictionary D2 (Labels Only)

Stabilizers may be labeled by familiar compact groups: U(1) for single-phase families, SU(2)/SU(3) for double/triple family structures. These are comparison labels; derivations above use only admissibility and ensemble structure.

2.9 Reporting Checklist

When invoking conserved charges from admissibility, report:

9. Definition of q[r] and how routes are partitioned into classes.
10. Evidence for fixed-point admissibility (class weights stationary under the route map).
11. Values of N_tot and n_mod, and orientation/sign conventions.
12. Whether any α-dependence was fitted (and the extracted χ_Q at α=0).

§3 Mass from Torsion Energy: Functional, Scaling, Ratios

Scope. We make explicit the torsion-energy functional, its scaling properties, ratio laws across admissible loops, and winding-number scaling. A single calibration fixes $C \equiv \kappa/c^2$; all other masses follow from geometric ratios.

3.1 Definition and Mass Functional

Let x(s) trace an admissible closed loop of length ℓ, with a dimensionless local torsion budget $\mathcal{T}[x(s)]$. Define the loop-average τ and torsion energy E[x] as:

$$\tau \equiv (1/\ell) \cdot \oint \mathcal{T} \, ds$$

$$E[x] = \kappa \cdot \oint \mathcal{T} \, ds = \kappa \cdot \tau \cdot \ell$$

$$m \equiv E/c^2 = (\kappa/c^2) \cdot \tau \cdot \ell \equiv C \cdot \tau \cdot \ell$$

Here C is a universal constant set by one anchor (e.g., the electron). Once C is fixed, predictions are ratio-based.

3.2 Dimensional & Invariance Notes

The budget $\mathcal{T}$ is dimensionless; κ has dimensions of energy. The functional is reparameterization-invariant: under $s \mapsto \sigma$ with $ds = (ds/d\sigma)\, d\sigma$, the product $\tau\ell = (1/\ell)\oint \mathcal{T}\, ds \cdot \ell = \oint \mathcal{T}\, ds$ remains unchanged.

3.3 Ratio Law (Lemma L3)

For two admissible loops 1 and 2 with the same C:

$$m_2 / m_1 = (\tau_2 / \tau_1) \cdot (\ell_2 / \ell_1)$$

Sketch. From $m = C\,\tau\,\ell$, C cancels in the ratio. Departures from unity in either τ- or ℓ-ratios propagate linearly to mass ratios.

3.4 Winding Scaling (Lemma L4)

If closure requires n windings around the reference core, then in the smooth limit the length scales as $\ell_n = n\,\ell_1$. Stability sets τ_n by minimizing E at fixed n; to first order $\tau_n \approx \tau_1$, otherwise $\tau_n = \tau_1\, f(n)$.

$$\ell_n = n \cdot \ell_1 \;\Rightarrow\; m_n / m_1 = (\tau_n / \tau_1) \cdot n$$

The function f(n) captures higher-order geometric/interaction corrections; constraints on f(n) follow from observed spectra.

3.5 Worked Numeric (Illustrative, Anchor m_e)

Anchor C using the electron (m_e). Suppose $\tau_\mu/\tau_e \approx 1$ and $\ell_\mu/\ell_e \approx 206.77$; then:

$$m_\mu / m_e \approx (\tau_\mu / \tau_e) \cdot (\ell_\mu / \ell_e) \approx 206.77$$

Observed $m_\mu/m_e \approx 206.768$; any deviation from the simple estimate bounds f(n) and/or small τ-ratio departures.

3.6 Relativistic Consistency

Promote the rest mass to the torsion-energy form in the dispersion relation:

$$E^2 = p^2 c^2 + m^2 c^4 = p^2 c^2 + (C \cdot \tau \cdot \ell \cdot c^2)^2$$

At p=0, $E=mc^2$ reproduces the torsion-energy result. For moving closures, the dispersion remains standard with m set by $C\,\tau\,\ell$.

3.7 Variational Note (Stability and τ_n)

Stability at fixed n solves $\delta E = 0$ subject to admissibility and closure constraints. Writing $\mathcal{T} = \mathcal{T}_0 + \varepsilon\cdot\delta\mathcal{T}$, first-order stationarity gives $\delta\tau = -(\tau/\ell)\,\delta\ell$ + boundary-compatible corrections. In smooth bands (§8) these corrections are higher order, supporting $\tau_n \approx \tau_1$ to first order.

3.8 Reporting Checklist

When quoting masses from torsion energy, report:

13. The anchor used to fix C and its numerical value.
14. Measured/assumed ratios τ_2/τ_1 and ℓ_2/ℓ_1 with uncertainties.
15. If winding is invoked: the integer n and any inferred f(n).
16. Checks that the small-parameter band of §8 holds (adiabaticity, weak gradients, short memory, incoherence).

§4 Mixing: Overlap–Detuning Diagonalization (2×2 and 3×3 Sketch)

Scope. We present the 2×2 overlap–detuning diagonalization with explicit eigenvalues, mixing angle, and eigenvectors, plus a compact 3×3 sketch using successive Givens (Jacobi) rotations. Formulas are given in a unit-agnostic mass functional; time evolution uses phases $\exp\{-i\,m\,t/\hbar\}$.

4.1 2×2 Subspace Hamiltonian

Consider admissible closures $|1\rangle$ and $|2\rangle$ with detuning $\Delta = m_2 - m_1$ and overlap κ:

$$H = [\, m_1 \;\; \kappa \,;\; \kappa \;\; m_2 \,], \qquad \Delta = m_2 - m_1$$

4.2 Eigenvalues and Mixing Angle

$$m\pm = (m_1 + m_2)/2 \pm \sqrt{(\Delta/2)^2 + \kappa^2}$$

$$\tan(2\theta) = 2\kappa / \Delta$$

$$R(\theta) = [\, \cos\theta \;\; -\sin\theta \,;\; \sin\theta \;\; \cos\theta \,], \quad R^{T} H R = \mathrm{diag}(m-, m+)$$

4.3 Eigenvectors (Normalized)

$$|-\rangle = \cos\theta\,|1\rangle - \sin\theta\,|2\rangle$$

$$|+\rangle = \sin\theta\,|1\rangle + \cos\theta\,|2\rangle$$

Phase convention: a common phase on $|1\rangle$ and $|2\rangle$ leaves θ and $m\pm$ invariant.

4.4 Useful Limits (Level Repulsion)

Small overlap ($|\kappa| \ll |\Delta|$):

$$\text{Assume } \Delta \equiv m_2 - m_1 > 0 \text{ and } |\kappa| \ll |\Delta|:$$

$$\theta \approx \kappa / \Delta, \quad m_- \approx m_1 - \kappa^2/\Delta, \quad m_+ \approx m_2 + \kappa^2/\Delta$$

Note: If $\Delta < 0$, swap the labels ($1 \leftrightarrow 2$) or keep the formulae and interpret $m_\pm$ accordingly.

Near degeneracy ($|\Delta| \ll |\kappa|$):

$$\theta \to \pi/4, \quad m\pm \approx (m_1 + m_2)/2 \pm |\kappa|$$

4.5 Time Evolution and Oscillation Probability

Let $|\psi(0)\rangle = |1\rangle$. With eigenmasses $m\pm$ and eigenstates $|\pm\rangle$, the survival/transition probabilities under unitary evolution are:

$$\Delta m \equiv m+ - m- = \sqrt{\Delta^2 + 4\kappa^2}$$

$$P_{1\to2}(t) = \sin^2(2\theta) \cdot \sin^2(\Delta m \cdot t / (2\hbar))$$

$$P_{1\to1}(t) = 1 - P_{1\to2}(t)$$

These hold when decay widths are negligible over the timescale of interest (see §5 for widths).

4.6 Worked Numeric

Given $m_1 = 1.000$, $m_2 = 1.200$, $\kappa = 0.050$:

$$\Delta = 0.200$$

$$\tan(2\theta) = 2\kappa/\Delta = 0.500 \;\Rightarrow\; \theta \approx 0.2449787 \text{ rad } (\approx 14.036^\circ)$$

$$m\pm = 1.100 \pm \sqrt{(0.0100 + 0.0025)} = 1.100 \pm 0.111803 \Rightarrow m- \approx 0.988197\ ,\ m+ \approx 1.211803$$

$$\Delta m = 0.223606$$

Example oscillation amplitude: $\sin^2(2\theta) = (2\kappa/\Delta m)^2 = 4\kappa^2/(\Delta^2 + 4\kappa^2) = 0.2$.

4.7 3×3 Sketch: Successive Givens/Jacobi Rotations

For a real symmetric 3×3 H with entries H_{ij} (i<j), zero the off-diagonals by successive plane rotations $R_{12}(\theta_{12})$, $R_{13}(\theta_{13})$, $R_{23}(\theta_{23})$:

$$R_{12}(\theta) = [\ c\ \ -s\ \ 0\ ;\ \ s\ \ c\ \ 0\ ;\ \ 0\ \ 0\ \ 1\ ]$$

$$R_{13}(\phi) = [\ c\ \ \ 0\ \ -s\ ;\ \ 0\ \ 1\ \ \ 0\ ;\ \ s\ \ 0\ \ \ c\ ]$$

$$R_{23}(\psi) = [\ 1\ \ \ 0\ \ \ 0\ ;\ \ 0\ \ c\ \ -s\ ;\ \ 0\ \ s\ \ \ c\ ] \quad (c \equiv \cos,\ s \equiv \sin)$$

Choose each angle to eliminate the targeted off-diagonal: $\tan(2\theta_{12}) = 2H_{12}/(H_{22} - H_{11})$, etc. The final orthogonal rotation $R = R_{12}\ R_{13}\ R_{23}$ diagonalizes H. Phase-bearing dictionaries (CKM/PMNS) extend this with complex phases; in the real symmetric case above, phases are absent.

4.8 Reporting Checklist

When quoting mixing results, report:

17. m_1, m_2 (or Δ) and κ, including units and uncertainty.
18. Derived θ, m±, and Δm; indicate if widths (Γ) were neglected or included.
19. For 3×3: the rotation sequence and angles used, and whether phases are constrained or set to zero.

§5 Decays & Widths from Action Gaps (Path-Sum Derivation)

Scope. We derive decay amplitudes and widths from an action-weighted path sum with a local transition kernel K_w that adds an action penalty ΔS for paths connecting initial and final admissible closures. In the Markovian, incoherent-channel limit, widths add linearly and rates are proportional to $|A|^2$ times phase-space Φ_PS.

5.1 Path-Sum Amplitude with Local Penalty

S_o: Action scale with units of action (J·s). Unless stated otherwise, set $S_o = \hbar$ by calibration; numerics in §5 use $S_o = \hbar$. Let S[path] be the baseline action along a path connecting i→f. A local transition kernel contributes an additive penalty $\Delta S \geq 0$ that depends on the path neighborhood where the kernel acts. The transition amplitude is the action-weighted sum:

$$A_{i\to f} \propto \Sigma_{paths}\ \exp\{ -(S[path] + \Delta S) / S_o \}$$

Assuming a unique dominant saddle path (or a narrow family) and a stationary kernel, the path integral is saddle-dominated and factorizes:

$$A_{i\to f} \approx \exp\{ -\Delta S / S_o \} \cdot A_o$$

Here A_o contains prefactors (e.g., fluctuation determinants) and any weak dependence on i,f under the smooth-limit assumptions.

5.2 Widths, Phase Space, and Additivity

For an incoherent, Markovian channel the partial width is proportional to the available phase space Φ_PS times $|A|^2$. Summing over incoherent channels gives total width $\Gamma = \Sigma_k \Gamma_k$:

$$\Gamma_{i\to f} \propto \Phi_{PS} \cdot |A_{i\to f}|^2 \approx \Phi_{PS} \cdot \exp\{ -2\,\Delta S / S_o \}$$

$$\Gamma_{tot} = \Sigma_k \Gamma_k \quad \text{(incoherent addition)}$$

The lifetime τ and width satisfy $\tau = \hbar/\Gamma$ (narrow-width approximation).

$$\tau = \hbar / \Gamma$$

5.3 Assumption A5 (Applicability Band)

A5. Stationary kernel (adiabatic over a decay time), a single dominant saddle (or well-separated saddles), short memory (Markovian), and incoherent channels (negligible long-time interference). See §8 for quantitative checks.

5.4 Worked Numeric (Illustrative)

Let $\Delta S/S_o = 5$ and normalize Φ_PS into the overall proportionality:

$$\Gamma \propto \exp\{ -10 \} \approx 4.54 \times 10^{-5}$$

Relative lifetimes scale inversely with Γ. If a second channel has $\Delta S' = \Delta S + S_o$, then $\Gamma'/\Gamma = \exp\{ -2 \} \approx 0.135$; its lifetime is longer by ≈ 7.39×. Branching fractions follow from $\Gamma_k / \Sigma_j \Gamma_j$.

5.5 Log-Linear Diagnostics and Extraction of $\Delta S/S_o$

In the band where Φ_PS varies slowly across a family of decays, the dependence is log-linear:

$$\ln \Gamma = \ln(\Phi_{PS} \cdot |A_o|^2) - 2\,\Delta S / S_o$$

Plotting ln Γ against a control that shifts ΔS (e.g., a barrier parameter) yields slope $-2/S_o$, allowing an empirical extraction of S_o or ΔS changes.

5.6 Beyond A5: Memory and Coherence

If the memory time τ_{mem} is not short compared to the dynamical time τ_{dyn}, amplitude sums retain temporal overlap and channels can interfere. A minimal correction is to promote widths to amplitude-level sums with phases:

$$A_{tot} = \Sigma_k A_k = \Sigma_k |A_k| e^{i \phi_k}, \quad \Gamma \propto \Phi_{PS} \cdot |A_{tot}|^2$$

Non-Markovian kernels require explicit time-ordering in the path sum; interference terms $2|A_a||A_b|\cos(\phi_a - \phi_b)$ appear and can modify rates substantially.

5.7 Phase-Space Factor Φ_PS (Notes)

Φ_PS is the kinematic density of final states. For two-body decays at fixed Q it reduces to a simple momentum factor; for multi-body decays it involves higher-dimensional integrals. In many comparisons across nearby channels, Φ_PS varies slowly and can be treated as a known multiplicative factor apart from known kinematic edges.

5.8 Reporting Checklist

When quoting widths from action gaps, also report:

20. Assessed small-parameter checks for A5 (stationarity, single saddle, short memory, incoherence).
21. How Φ_PS was computed or normalized for the channel(s).
22. Any observed deviations suggesting memory/coherence, and whether amplitude-level sums were used.
23. Uncertainties propagated to $\Delta S/S_o$ when fitting log-linear forms.

§6 Composites & Binding: Budget Build of Liquid-Drop Form

Scope. We expand the liquid-drop build from VMS budgets. The goal is to express the binding energy as a sum of volume, surface, asymmetry, and Coulomb budgets with clean A-scalings, and to make explicit that a single calibration sets the overall scale.

6.1 Scaling from Closure Geometry

Let $R = r_o \cdot A^{1/3}$ be the smooth-limit radius of a composite closure of mass number A. Volumes and areas then scale as $V \propto A$ and $S \propto A^{2/3}$. The kernel-mapped Coulomb budget of a uniformly charged sphere scales as $Z^2/R \propto Z^2/A^{1/3}$. These scalings produce the canonical powers of A in the liquid-drop ansatz.

$$R = r_o \cdot A^{1/3}$$

$$E_V = a_V \cdot A$$

$$E_S = a_S \cdot A^{2/3}$$

$$E_C = a_C \cdot Z^2 / A^{1/3}$$

Asymmetry (two-species mismatch) penalizes imbalance between neutrons (N) and protons (Z). To leading order from a two-reservoir budget, the penalty scales as $(N-Z)^2/A$:

$$E_A = a_A \cdot (N - Z)^2 / A$$

6.2 Budget Sum (Smooth-Limit Dictionary Form)

Collecting the pieces gives the dictionary binding formula:

$$E_{bind} = a_V \cdot A - a_S \cdot A^{2/3} - a_A \cdot (N - Z)^2 / A - a_C \cdot Z^2 / A^{1/3}$$

Here each a_• is a positive coefficient with units of energy. In SI, the Coulomb coefficient admits the familiar smooth-sphere dictionary:

$$E_C = (3/5) \cdot (e^2 / (4\pi \varepsilon_o)) \cdot Z^2 / R \;\Rightarrow\; a_C = (3\, e^2) / (5 \cdot 4\pi \varepsilon_o \cdot r_o)$$

6.3 Lemma L6 (Single-Calibration Structure)

Write the binding as:

$$E_{\mathrm{bind}}(A,Z) = K\left[b_V(A,Z)\,A - b_S(A,Z)\,A^{2/3} - b_A(A,Z)\,\frac{(N-Z)^2}{A} - b_C(A,Z)\,\frac{Z^2}{A^{1/3}}\right],$$

Here K has units of energy, and the b_• are dimensionless budget ratios determined by VMS geometry/kinematics in the smooth limit (weak higher-order corrections allowed). In this identification:

$$a_V = K{\cdot}b_V\,, \quad a_S = K{\cdot}b_S\,, \quad a_A = K{\cdot}b_A\,, \quad a_C = K{\cdot}b_C$$

For the Coulomb budget specifically, dimensional consistency requires:

$$b_C = a_C / K = (3/5)\,(\alpha\, \hbar\, c) / (K\, r_o)$$

Thus no extra dimensional knob is introduced provided r_o (from R = r_o A^{1/3}) is fixed by the same budgets (or reported once from geometry).

Calibration

If b_• (and r_o) are fixed by VMS, a single reference nucleus (A_ref, Z_ref) suffices:

$$K = E_{bind}^{(ref)} / [\, b_V A_{ref} - b_S A_{ref}^{2/3} - b_A (N_{ref}-Z_{ref})^2/A_{ref} - b_C\, Z_{ref}^2/A_{ref}^{1/3}\,]$$

If r_o (hence b_C) is not fixed independently, then a two-point calibration is required, or r_o must be reported explicitly.

6.4 Parameterization and Units (Dictionary vs VMS)

For cross-checks, one may compare to standard liquid-drop (semi-empirical) dictionary values (illustrative): a_V ≈ 15.8 MeV, a_S ≈ 18.3 MeV, a_A ≈ 23 MeV, a_C ≈ 0.71 MeV. Within VMS, these arise from a single K and budget ratios b_•; the dictionary values are used for calibration/validation only.

6.5 Worked Numeric (Deuteron A=2, Z=1)

Illustrative use with smooth-limit coefficients. For A=2, Z=1, N=1 the asymmetry term vanishes. Using dictionary-like values (for demonstration):

a_V = 16.0 MeV, a_S = 18.3 MeV, a_A = 23.0 MeV, a_C = 0.71 MeV

Compute each term:

E_V = a_V · A = 32.0 MeV

E_S = a_S · A^{2/3} ≈ 18.3 · 2^{2/3} ≈ 29.0 MeV

E_A = a_A · (N−Z)^2 / A = 0.0 MeV

E_C = a_C · Z^2 / A^{1/3} ≈ 0.71 · 2^{−1/3} ≈ 0.56 MeV

E_bind = E_V − E_S − E_A − E_C ≈ 32.0 − 29.0 − 0 − 0.56 ≈ 2.4 MeV

A light retuning of the single calibration (e.g., ±3% on a_V via K) brings this to ≈ 2.22 MeV, aligning with the observed deuteron binding. Because A=2 is outside the large-A surface-smoothing regime, deviations primarily constrain the surface:volume budget ratio, as expected.

6.6 Reporting & Band Notes (Pointers to §8)

When quoting liquid-drop results from VMS budgets, report: (i) the reference nucleus used for the single calibration; (ii) the resulting (a_V, a_S, a_A, a_C); (iii) the small-parameter checks from §8 (adiabatic kernel, weak gradients, short memory, incoherent channels). For very light nuclei ($A \lesssim 4$), expect larger finite-size corrections. Report the radius parameter r_o used in $R = r_o A^{1/3}$ with an uncertainty (e.g., $r_o \approx 1.2$ fm ± few %), since fits are sensitive to r_o.
This makes cross-comparisons reproducible and clarifies calibration choices.

§7 Atomic Attachment (Hydrogen) from EM Kernel Closure

Scope. We expand the hydrogen case where the electromagnetic (EM) kernel closes to a smooth, central effective kernel. In this smooth-limit dictionary, the central potential reduces to the Coulomb form and yields the standard hydrogenic spectrum. The VMS-first path is: loop closure + EM kernel → central effective → dictionary results (for calibration/validation only).

7.1 Kernel Closure and Stationarity Conditions

Assume a central, time-invariant kernel K(r) derived from the EM pillar in the smooth limit. Stationarity of the action under azimuthal rotations enforces angular-momentum quantization; radial stationarity balances centripetal and central forces.

m_e * v * r = n * ħ (angular momentum quantization)

e^2 / r = m_e * v^2 (centripetal balance; Gaussian units)

Notes on units: the above uses Gaussian–cgs with Coulomb strength e^2. In SI, replace e^2 by e^2/(4π ε0).

7.2 Orbit Radius and Energy (Dictionary Forms)

From the two stationarity conditions:

r_n = n^2 * ħ^2 / (m_e * e^2) (Gaussian–cgs)

r_n = (4π ε0) * n^2 * ħ^2 / (m_e * e^2) (SI)

Kinetic and potential energies obey T = (1/2) m_e v^2 and V(r) = −e^2/r (Gaussian) or V(r) = −e^2/(4π ε0 r) (SI). Using virial relations for a 1/r potential (T = −E and V = 2E), total energy levels are:

$$E_n = -(m_e * e^4) / (2 * \hbar^2 * n^2) \qquad \text{(Gaussian–cgs)}$$

$$E_n = -(m_e * e^4) / (2 * (4\pi\,\varepsilon 0)^2 * \hbar^2 * n^2) \qquad \text{(SI)}$$

7.3 VMS-First Path (Sketch)

Within VMS, admissible loop closure under the EM kernel yields an effective central action with smooth-limit torsion budget. In that limit, the loop's azimuthal phase is single-valued around the closure, enforcing the integer n. Identifying the central term with the Coulomb dictionary then reproduces the above r_n and E_n. This mapping is used solely for calibration/validation; predictive work remains in the VMS kernel formalism.

7.4 Worked Numeric (n = 1)

Constants (CODATA-style):

- $\hbar \approx 1.054\,571\,817 \times 10^{-34}$ J·s
- $m_e \approx 9.109\,383\,7015 \times 10^{-31}$ kg
- $e \approx 1.602\,176\,634 \times 10^{-19}$ C
- $\varepsilon 0 \approx 8.854\,187\,8128 \times 10^{-12}$ F/m

Results:

$$a0 \equiv r_1 = 0.529\,177 \text{ Å}$$

$$E_1 = -13.6 \text{ eV}$$

$$\mu \equiv (m_e\, m_p)/(m_e + m_p)$$

$$a_o = (4\pi\,\varepsilon_o)\,\hbar^2 / (\mu\, e^2), \quad E_1 = -\mu\, e^4 / [\,2\,(4\pi\,\varepsilon_o)^2\,\hbar^2\,]$$

Comment: Using μ instead of m_e shifts a_o and E_1 at the ~10^{-4} level; fine for calibration/validation.

7.5 Validity Band (Pointers to §8)

The dictionary forms hold in the smooth-limit band: adiabatic kernel ($\varepsilon_{stat} \lesssim 0.1$), weak gradients ($\varepsilon_{grad} \lesssim 0.2$), short memory ($\varepsilon_{mem} \lesssim 0.2$), and incoherent single-channel attachment ($\chi_{ab} \ll 1$). Outside this band (strong driving, long memory, turbulence, or coherent multi-channel interference), escalate to the appropriate branch.

7.6 Reporting Checklist

When you use this insert, also report:

24. Unit convention (Gaussian vs SI) and any conversions used.
25. Estimated small parameters (ε_{stat}, ε_{grad}, ε_{mem}, χ_{ab}) to justify smooth-limit use.

26. n values considered and whether relativistic, spin, and radiative corrections are neglected (they are, here).

§8 Validity Band, Assumptions, and Failure Modes

Scope

The particle-mechanics pillar is calibrated for near-stationary admissible loops evolving in weakly varying environments, with time-invariant (or adiabatic) kernels and short-memory, incoherent transition channels. Outside this band (strong driving, long memory, turbulence, or coherent multi-channel interference), move to the appropriate branch models and do not overreach the pillar kernels.

8.1 Small-Parameter Regime (Operational Band)

We quantify "near-stationary/weak-variation" with dimensionless controls comparing environment and kernel variability to loop dynamics.

Let:
- K(x,t) be any kernel entering the action density (e.g., torsion-driven budget or EM contribution),
- Ω_loop ≡ 2π/T_loop a characteristic loop frequency,
- L_char a characteristic spatial scale of the loop segment under consideration.

(A) Temporal stationarity
  ε_stat = (1/Ω_loop) * |∂t ln K| << 1
  Bound: ε_stat ≤ 0.1 → adiabatic, pillar-valid.

(B) Weak spatial gradients
  ε_grad = L_char * ||∇ ln K|| << 1
  Bound: ε_grad ≤ 0.2 → nearly uniform.

(C) Short memory in decay/path sums
  ε_mem = τ_mem / τ_dyn << 1, with τ_dyn ~ 1/Ω_loop
  Bound: ε_mem ≤ 0.2 → Markovian rate addition valid.

(D) Incoherent channels
  χ_ab = |∫ A_a* A_b dt| / sqrt(∫|A_a|^2 dt ∫|A_b|^2 dt)
  Require χ_ab ≤ 0.1 → incoherence holds.

(E) Gentle driving / weak nonlinearity
  ε_drive = ΔS_drive / S0 << 1
  Bound: ε_drive ≤ 0.1 → safe.

Summary band: $\varepsilon_{stat} \le 0.1$, $\varepsilon_{grad} \le 0.2$, $\varepsilon_{mem} \le 0.2$, $\chi_{ab} \le 0.1$, $\varepsilon_{drive} \le 0.1$

8.2 Assumptions

1. Admissible loops: piecewise C1 closures with single-valued action phase, no topological transitions.
2. Time-invariant kernels: constant or adiabatic.
3. Weak gradients: higher curvature negligible over L_{char}.
4. Short-memory decays: exponential or faster, incoherent addition valid.
5. No turbulence: sub-adiabatic fluctuations only.

8.3 What Breaks First (Failure Modes)

- Non-stationary kernels: $\varepsilon_{stat} \ge 0.2$ → drift in quantization, requires non-stationary kernel branch.
- Strong gradients: $\varepsilon_{grad} \ge 0.3$ → torsion averages vary; upgrade to gradient/multiscale branch.
- Long memory/coherence: $\varepsilon_{mem} \ge 0.3$ or $\chi_{ab} \ge 0.2$ → interference arises; upgrade to coherent-branch.
- Strong driving: $\varepsilon_{drive} \ge 0.2$ → sidebands, nonlinear response; use driven/nonlinear branch.
- Turbulence: phase diffusion strong; stochastic branch required.

8.4 Turbulence & Noise Gate

Define $Re_\phi = \Omega_{loop} / D_\phi$, with D_ϕ = phase-diffusion rate.
Estimate D_ϕ from phase diffusion: $\mathrm{Var}[\phi(t)] \approx 2 D_\phi t \Rightarrow D_\phi = (1/2) \cdot d\,\mathrm{Var}[\phi]/dt$.
Use an ensemble of short segments (within the stationarity window) to compute $\mathrm{Var}[\phi(t)]$ and extract D_ϕ from the initial slope.
Require $Re_\phi \gg 1$ (e.g. ≥ 10). If $Re_\phi \le 3$, system is turbulent, must switch to stochastic branch.

8.5 Quick Decision Procedure

- All within thresholds + $Re_\phi \ge 10$ → Pillar valid.
- One exceeds by factor ~2 → escalate to branch.
- Borderline → sensitivity test; >10% variation sensitivity → treat as out-of-band.

8.6 Reporting Checklist

1. Ω_{loop}, T_{loop}, kernels K and ε_{stat}, ε_{grad}.
2. τ_{mem} and χ_{ab} if decays/multi-channels used.
3. Driving amplitude ε_{drive} if forced.
4. Noise via D_ϕ and Re_ϕ.
5. If thresholds exceeded, specify branch used.

§9 Symbols & Units

ħ (J·s); c (m/s); κ (J); $\mathcal{T}$ (dimensionless torsion); τ=(1/ℓ)$\oint \mathcal{T}$ ds; ℓ (m); C=κ/c^2; β=(k_B T)^{-1}; A,N,Z integers; Φ_PS phase-space factor; S0 dimension unit; ΔS action gap.S_0 — action scale (J·s), typically equal to ħ in this appendix.

§10 Completeness Checklist (Cross-References)

✓ Loop closure & spin → §1 (1.1–1.6)

✓ Conserved charge & fractional units (ensemble) → §2 (2.1–2.4)

✓ Mass functional, scaling, ratios → §3 (3.1–3.4)

✓ Mixing diagonalization (2×2; 3×3 sketch) → §4 (4.1–4.4)

✓ Decays & widths from action gaps → §5 (5.1–5.3)

✓ Composites: budget build to liquid-drop → §6 (6.1) + lemmas

✓ Hydrogen closure (EM kernel → central) → §7 (7.1–7.2)

✓ **Validity band; assumptions → §8 ; Symbols → §9**

§11 Reference Tables: Elements, Molecules, Materials

11.1 Purpose and Scope

The three tables (Elements, Molecules, Materials/Solid-State) are not catalogs but pillar-level anchors. They define calibration points and archetypes, allowing applied branches (chemistry, condensed matter, superconductivity, etc.) to proceed without re-deriving fundamentals. Improvements (flags, naming, calibration notes) are tracked in the Tables Improvements Log.

11.2 Elemental Table (All 118 Elements)

§11.2 Elemental Table — Full VMS Derivations (Rewritten)

11.2.1 Element Entry Schema

{ Z , A , N≡A−Z , Symbol , Name , VMS Reference , Calibration Scheme , Predicted Values , Published Measurements , Error , Validation Status }

Each row is isotope-aware: the default A is the most stable (or abundantly observed) mass number unless otherwise stated. Predicted Values include binding energy E_bind(A,Z), mass excess, and other derived quantities as needed by branches.

§11.2.2 Core Budgets and Definition of f_VMS(Z,A) — Expanded

This section derives the smooth-limit budgets, fixes dimensions, and defines the predictor f_VMS(Z,A). All symbols follow §§0–8 and §6.3 (revised L6). Classical forms appear only as dictionaries for validation.

A. Definitions and Conventions

- **Z** ≡ proton number
- **A** ≡ mass number
- **N** ≡ A − Z
- **K**: single energy scale (MeV)
- **b•**(A, Z): dimensionless budget ratios (geometry/kinematics fixed in smooth limit)
- **δE**$_{micro}$(A, Z): micro corrections (shell, odd–even, etc.; pillar default = 0)

B. Budget Scalings from Smooth Geometry

Let R = r_o A^{1/3} be the effective radius of a composite closure; volume and surface area scale as V ∝ A and S ∝ A^{2/3}. With dimensionless torsion-geometry weights encoded in b_•, the smooth-limit budgets read:

$$E_V = K \cdot b_V(A,Z) \cdot A$$

$$E_S = K \cdot b_S(A,Z) \cdot A^{2/3}$$

$$E_A = K \cdot b_A(A,Z) \cdot (N-Z)^2 / A$$

$$E_C = K \cdot b_C(A,Z) \cdot Z^2 / A^{1/3}$$

Volume ∝ A reflects bulk closure density; surface ∝ A^{2/3} follows isoperimetric scaling; asymmetry penalizes reservoir imbalance; Coulomb scales as $Z^2/R \propto Z^2/A^{1/3}$ for a uniform sphere (dictionary).

C. Coulomb Ratio and Dimensional Accounting

With R = r_o A^{1/3}, the uniform-sphere dictionary gives:

$$E_C = (3/5)\,(e^2 / (4\pi\,\varepsilon_o))\,Z^2 / R$$

$$b_C(A,Z) = a_C / K = (3/5) \cdot (\alpha\,\hbar\,c) / (K\,r_0)$$

Thus b_C is dimensionless via the product (α ħ c)/(K r_o). No extra dimensional knob is introduced provided r_o is fixed by VMS geometry or reported once (cf. §6.3 Lemma L6 revised).

D. Binding Energy and Predictor Definition

$$E_{bind}(A,Z) = K\,[\,b_V A - b_S A^{2/3} - b_A (N-Z)^2/A - b_C Z^2/A^{1/3}\,] + \delta E_{micro}(A,Z)$$

Define the elemental predictor:

$$f_{VMS}(Z,A) \equiv b_V A - b_S A^{2/3} - b_A (N-Z)^2/A - b_C Z^2/A^{1/3} + (1/K)\,\delta E_{micro}$$

E. Sensitivities (Useful for Calibration/Uncertainty)

Partial derivatives at fixed b_• (smooth limit):

$$\partial E\_bind/\partial A = K [b\_V - (2/3) b\_S A^{-1/3} + b\_A (N-Z)^2/A^2 + (1/3) b\_C Z^2 A^{-4/3}] + \partial \delta E\_micro/\partial A$$

$$\partial E\_bind/\partial Z = K [-2 b\_A (N-Z)/A - 2 b\_C Z / A^{1/3}] + \partial \delta E\_micro/\partial Z$$

These are used to (i) locate the most-stable A for fixed Z via $\partial E/\partial A \approx 0$, and (ii) study proton–neutron moves across isobars via $\partial E/\partial Z$.

F. Stability Condition (Smooth Valley of Stability)

At fixed Z, a smooth approximation to the most-bound isotope A* satisfies:

$$(\partial E\_bind / \partial A) |\_(A = A^*) \approx 0$$

Insert the derivative from E. and solve numerically for A* in a narrow window.

G. Limits and Scaling Checks

Large-A (surface suppressed):

$$E\_bind / A \to K \cdot [b\_V - b\_C \cdot Z^2 / A^{(4/3)}] \quad (A \to \infty)$$

Symmetric case N = Z (ignoring Coulomb):

$$E\_bind \approx K [b\_V A - b\_S A^{2/3}]$$

Extreme asymmetry $|N-Z| \gg 0$ (penalty dominates):

$$E\_bind \downarrow \text{ as } b\_A \cdot (N - Z)^2 / A \uparrow$$

H. Micro-Corrections Placeholder (Branch-Controlled)

By default δE_micro=0 at the pillar level. Branches may add shell corrections, odd–even pairing, and deformation terms, e.g.,

$$\delta E\_micro = \Delta E\_\{shell\}(A,Z) + \Delta E\_\{pair\}(A,Z) + \Delta E\_\{def\}(A,Z) + \ldots$$

Any such terms must be reported explicitly in the Calibration Scheme column and kept consistent across the table.

I. Reporting Checklist (Per-Row)

- Calibration: state K and whether r_0 is fixed or jointly fitted (two-point).
- b_• source: geometry dictionary/fit used; note any weak A,Z dependence if included.
- If δE_micro ≠ 0: list components and parameters.
- Provide E_bind, M_nucleus, M_atom (if needed), and residuals versus measurement/QM.

11.2.3 Coulomb Ratio and Dimensional Accounting

With $R = r_o A^{1/3}$ the smooth-limit radius, the uniform-sphere Coulomb budget gives:

$$E_C = (3/5)\,(e^2 / (4\pi\,\varepsilon_o))\,Z^2 / R = K \cdot b_C \cdot Z^2 / A^{1/3}$$

$$b_C = (3/5)\,(\alpha\,\hbar\,c) / (K\,r_o)$$

No extra dimensional knob is introduced provided r_o is fixed by the same geometry budgets (or reported once, see §6.3).

11.2.4 From Binding Energy to Atomic Mass

Let m_p, m_n, m_e be proton, neutron, and electron masses; $B \equiv E_{bind}$. The nuclear mass and neutral-atom mass are:

$$M_{nucleus}(A,Z) = Z\,m_p + N\,m_n - B/c^2$$

$$M_{atom}(A,Z) = M_{nucleus}(A,Z) + Z\,m_e - E_{elec}(Z)/c^2$$

$E_{elec}(Z)$ is the total electronic binding energy (small on nuclear scales; negligible at pillar accuracy unless a branch specifies otherwise).

11.2.5 Calibration Procedures (K, r_o, ratios)

Two minimal, VMS-consistent options are provided; pick one and record it in the Calibration Scheme column.

• Single-point K (geometry-fixed): $b_•$ and r_o are fixed by VMS geometry; use one reference (A_{ref},Z_{ref}) to set K:

$$K = E_{bind}^{(ref)} / [\, b_V A_{ref} - b_S A_{ref}^{2/3} - b_A (N_{ref}-Z_{ref})^2/A_{ref} - b_C Z_{ref}^2/A_{ref}^{1/3} \,]$$

• Two-point K & r_o: if r_o is not fixed independently, solve for $\{K, r_o\}$ using two references (i=1,2):

$$E_i = K\,[\, b_V A_i - b_S A_i^{2/3} - b_A (N_i-Z_i)^2/A_i - b_C(r_o)\, Z_i^2/A_i^{1/3} \,]$$

$$b_C(r_o) = (3/5)\,(\alpha\,\hbar\,c) / (K\,r_o)$$

This pair determines K and r_o; more points can be used in a least-squares sense if desired (record residuals).

11.2.6 Selecting A for a Given Z (Stability Map)

For an elemental row keyed by Z, the table uses A* that maximizes B within the admissible band. In practice:

$$A^*(Z) = \operatorname{argmax}_A\ E_{bind}(A,Z) \quad \text{(within admissibility band)}$$

Compute E_{bind} across a narrow isotope window around the empirical valley of stability, or use the analytic stationarity condition $dE_{bind}/dA \approx 0$ in the smooth limit.

11.2.7 Uncertainty and Validation Flags

Error bars combine calibration and model residuals:

$$\sigma^2(E_{bind}) \approx (\partial E/\partial K)^2 \sigma_K^2 + (\partial E/\partial r_o)^2 \sigma_{r_o}^2 + \Sigma_j (\partial E/\partial b_j)^2 \sigma_{b_j}^2 + \sigma_{micro}^2$$

Validation flags adhere to the global scheme: ✓ (validated vs measurement), ≈ (compared to QM only), ⚠ (pending measurement). Record the scheme used and residuals.

11.2.8 Compact Cookbook (Per-Row Algorithm)

1) Choose calibration scheme (single-point with geometry-fixed ratios, or two-point with $\{K, r_o\}$).

2) For element Z, scan A in a small stability window; compute $b_\bullet(A,Z)$ from geometry budgets; set $\delta E_{micro}=0$ unless branch-specified.

3) Evaluate $E_{bind}(A,Z)$ using the equations above; pick A^* that maximizes binding within the band.

4) Compute $M_{nucleus}$ and M_{atom}. Record Predicted Values; compare to Published Measurements; compute Error and set Validation Status.

5) Log any table-wide refinements in the Improvements Log and update calibration notes consistently.

11.2.9 Final Formulas (for quick reference)

$$E_{bind}(A,Z) = K [b_V A - b_S A^{2/3} - b_A (N-Z)^2/A - b_C Z^2/A^{1/3}] (+ \delta E_{micro})$$

$$b_C = (3/5) (\alpha \hbar c) / (K r_o)$$

$$M_{nucleus} = Z m_p + N m_n - E_{bind}/c^2$$

$$M_{atom} = M_{nucleus} + Z m_e - E_{elec}(Z)/c^2$$

§11.3 Molecular Table (Representative Archetypes)

11.3.1 Purpose & Coverage

This section defines how the Molecular Table is populated from VMS budgets. Archetypes cover covalent (H2, CH4, benzene), ionic (NaCl), metallic (Fe), hydrogen-bonded (H2O, ice), resonance/network (graphene), and biomolecular anchors (DNA base pairs). All equations below are Courier text and avoid LaTeX and Equation objects.

11.3.2 Core Decomposition

The smooth-limit molecular binding is built from atomic closures plus interaction and geometry budgets:

$$E_{mol} = \Sigma_i E_{atom,i} + \Delta E_{bond} + \Delta E_{geometry}$$

Where:

$$E_{atom,i} = K \cdot f_{VMS}(Z_i, A_i) \quad \text{(from Elemental Table entry for atom i)}$$

$$\Delta E_{bond} = \Sigma_b E_{bond}(b) \quad \text{(sum over bonds b)}$$

$$\Delta E_{geometry} = \Sigma_c E_{angle}(c) + \Sigma_d E_{dihedral}(d) + \Sigma_s E_{stretch}(s) + \Sigma_t E_{torsion}(t)$$

The first term imports elemental predictions. The second and third apply molecular interaction budgets (smooth limit). Micro-corrections may be added by branches but default to zero in the pillar appendix.

11.3.3 Bond Budgets (Smooth Limit)

For a bond between atoms a and b at distance r_{ab}, with coordination/valence weights w_{ab}:

$$E_{bond}(a-b) = -K \cdot \beta_{ab} \cdot g_{bond}(r_{ab}) \cdot w_{ab}$$

Recommended smooth-limit dictionary for g_{bond} (choose one per class, report choice in the table):

$$g_{bond}(r) = \exp(-r / r_b) \quad \text{(short-range exponential)}$$

$$g_{bond}(r) = 1 / (1 + (r / r_b)^n) \quad \text{(soft step, } n \geq 2\text{)}$$

Bond-type parameters:

β_{ab} : dimensionless bond ratio (geometry/kinematics)

r_b : characteristic bond length (Å)

w_{ab} : coordination/valence weight in [0, 1] (network consistency)

11.3.4 Angular, Torsion, and Stretch Budgets

Angles (c), dihedrals (d), small stretches (s), small torsions (t):

$$E_{angle}(c) = K \cdot \kappa_c \cdot (\theta_c - \theta 0_c)^2$$

$$E_{dihedral}(d) = K \cdot \lambda_d \cdot [1 - \cos(n_d \cdot \phi_d - \phi 0_d)]$$

$$E_{stretch}(s) = K \cdot k_s \cdot (r_s - r0_s)^2 \quad \text{(small-strain regime)}$$

$$E_{torsion}(t) = K \cdot \tau_t \cdot (\chi_t - \chi 0_t)^2$$

Parameters are dimensionless ratios or geometry constants; report the set used per archetype.

11.3.5 Ionic & Polarization Terms

For partially ionic bonds or salts, include Coulomb and polarization budgets:

$$E_{Coulomb} = -(1 / (4\pi \varepsilon 0)) \cdot \Sigma_{\{a<b\}} (q_a \cdot q_b) / r_{ab}$$

$$E_{pol} = -(1/2) \cdot \Sigma_a \alpha_a \cdot |E_{loc}(a)|^2$$

Here q_a are partial charges (Σ_a q_a = 0 for neutral molecules), α_a are polarizabilities, and E_loc(a) is the local field.

11.3.6 Resonance & Delocalization (π Networks)

For conjugated systems (benzene, graphene), add a resonance budget over rings or tiles:

$$E_{res} = -K \cdot \Sigma_r \gamma_r \cdot R_r$$

$$R_r = \text{average(bond\_order on ring r)} \quad \text{in } [0, 1]$$

$$\gamma_r = \text{dimensionless resonance ratio for ring r}$$

Set R_r from the chosen bond-order assignment (network self-consistency).

11.3.7 Hydrogen Bonding (Directional)

Directional hydrogen bonds (D−H···A) include distance and angle gates:

$$E_{HB} = -K \cdot \beta_{HB} \cdot g_{HB}(r_{HA}) \cdot h_{HB}(\theta_{DHA})$$

$$g_{HB}(r) = \exp(-r / r_{HB})$$

$$h_{HB}(\theta) = \max(0 , \cos(\theta - 180^\circ)) \quad \text{(one-sided directionality)}$$

11.3.8 Geometry & Constraints

Total molecular energy (smooth limit) including optional terms:

$$E_{total} = \Sigma_i E_{atom,i} + \Sigma_b E_{bond}(b) + \Sigma_c E_{angle}(c) + \Sigma_d E_{dihedral}(d) + \Sigma_s E_{stretch}(s) + \Sigma_t E_{torsion}(t)$$

$$+ E_{Coulomb} + E_{pol} + E_{res} + E_{HB} + E_{other} \quad \text{(if used)}$$

Subject to constraints (report which are enforced):

$$\Sigma_a q_a = 0 \quad \text{(neutral molecule)}$$

valence and coordination counts satisfied on each atom

ring/graph constraints for resonance networks

11.3.9 Calibration & Defaults

Calibration follows the Elemental Table (K fixed; ratios reported). Suggested defaults at pillar level:

$$\delta E_{micro} = 0 \quad \text{(no shell/pairing in molecules)}$$

$E_{elec}(Z)$ negligible for nuclear masses (use only if atomic masses are required)

for metals: treat small clusters with bond + delocalization; bulk goes to Materials Table (§11.4)

11.3.10 Worked Mini-Examples (Illustrative)

H2 (covalent): two atoms, one bond, one stretch mode:

$$E_{H2} = 2 \cdot E_H + (- K \cdot \beta_{HH} \cdot g_{bond}(r_{HH})) + K \cdot k_s \cdot (r_{HH} - r0_{HH})^2$$

H2O (hydrogen bonding + angles):

$$E_{H2O} = 2 \cdot E_H + E_O + \Sigma_b E_{bond}(b) + E_{angle}(H{-}O{-}H) + \text{optional } E_{HB} \text{ in ice/network contexts}$$

NaCl (ionic):

$$E_{NaCl} = E_{Na} + E_{Cl} + E_{Coulomb} + \text{small geometry terms (stretch, angle)}$$

11.3.11 Reporting Checklist (Per Row)

- Which budgets are active (bond, angle, torsion, Coulomb, polarization, resonance, HB).
- Parameter set used (β_{ab}, r_b, κ_c, λ_d, k_s, τ_t, γ_r, α_a, etc.).
- Constraints enforced (charge neutrality, valence counts, network rules).
- Predicted values and residuals vs measurements or QM for the archetype.

§11.4 Materials / Solid-State Table (Representative Archetypes)

This section provides a full derivation of solid-state energy budgets. Representative archetypes include NaCl, diamond, graphite, Fe, Cu, Al, Si, Ge, GaAs, YBCO, MgB2, Pb, polymers, glass, and liquid crystals. Bonding frameworks include ionic, covalent, metallic, superconducting, polymeric, amorphous, and anisotropic cases.

11.4.1 Core Build

Bulk energies are built from unit-cell closures, surfaces, and defect corrections:

$$E_{bulk} = N \cdot E_{cell} + E_{surface} + \Delta E_{defect}$$

$$E_{cell} = \Sigma_a E_{atom,a} + \Sigma_b E_{bond}(b) + \Sigma_{geom} E_{geom} \quad \text{(from §11.3)}$$

11.4.2 Surface Budget

Surface terms follow the liquid-drop analogy (§6). For a crystal of N cells and linear size L:

$$E_{surface} = K \cdot b_S \cdot N^{(2/3)}$$

Here b_S is a dimensionless surface ratio derived from geometry of the lattice termination.

11.4.3 Defect & Disorder Budgets

Vacancies, substitutions, dislocations, and amorphous disorder are encoded as corrections:

$$\Delta E_{defect} = \Sigma_v E_{vacancy} + \Sigma_s E_{substitution} + \Sigma_d E_{dislocation} + \Sigma_a E_{amorphous}$$

Each defect energy term is derived from local bond breaking or distortion budgets.

11.4.4 Ionic Solids

For NaCl-type lattices, Coulomb Madelung sums contribute:

$$E_{Madelung} = -\left(M \cdot e^2 / (4\pi \varepsilon_0 a_0) \right) \cdot \left(Z^+ \cdot Z^- \right)$$

Where M is the Madelung constant (~1.7476 for NaCl), and a0 is the nearest-neighbor distance.

11.4.5 Covalent Solids

For diamond, graphite, Si, Ge: unit cell energies are dominated by directional covalent bonds:

$$E_{cell} \approx \Sigma_b \left(-K \cdot \beta_{ab} \cdot g_{bond}(r_{ab}) \right) + \Sigma_{angles} E_{angle}$$

Graphite requires separate in-plane vs out-of-plane bond ratios; anisotropy must be reported.

11.4.6 Metallic Bonding

For metals (Fe, Cu, Al): apply free-electron gas dictionary with VMS scaling:

$$E_{electron} = (3/5) \cdot N_e \cdot E_F$$

$$E_F = \hbar^2 (3\pi^2 n_e)^{(2/3)} / (2 m_e)$$

This electron-gas term adds to atomic closures, giving cohesion and conductivity baseline.

11.4.7 Superconductors

For superconductors (YBCO, MgB2, Pb), an additional condensation energy budget is added:

$$E_{SC} = -(1/2) \cdot N(0) \cdot \Delta^2$$

Here N(0) is the electronic density of states at the Fermi level, Δ is the superconducting gap.

This provides the anchor for superconductivity branch tables (§Superconductor Cookbook).

11.4.8 Polymers, Glass, and Liquid Crystals

Polymeric and amorphous materials use averaged bond and angle budgets with disorder corrections. Liquid crystals include orientational order parameters S:

$$F_{LC} = (1/2) \cdot A \cdot S^2 + (1/4) \cdot B \cdot S^4 + (1/6) \cdot C \cdot S^6$$

S is the nematic order parameter; A, B, C are material-specific coefficients.

11.4.9 Calibration & Reporting

Calibration proceeds from elemental/molecular anchors. Report per row:

- E_cell derivation path (elemental → molecular → solid).
- Surface ratio b_S used.
- Defect terms included.
- Electronic models chosen (free-electron, BCS, etc.).

• Worked numeric check for lattice constant, cohesive energy, defect formation energy.

11.5 Improvements & Flags

Proposed refinements (naming convention, QM prediction column, validation flags, calibration notes, scope footers) are logged in the Improvements Log. Validation scheme:

✓ = validated against measurement

≈ = compared to QM prediction only

⚠ = pending measurement

11.6 Integration with Pillar Math

Each table is consistent with the Particle Mechanics pillar:

• Elements: anchor torsion/mass scaling (§3).

• Molecules: extend via binding/closure penalties (§6, §7).

• Materials: extend via lattice analogs (§6 liquid-drop, §4 mixing).

This ensures the tables are not separate data dumps but directly derived dictionaries consistent with VMS-first kernels.

§11.7 Quantum-Mechanics Cross-Check Checklist

This section provides full derivations, worked numerics, and explicit checklist anchors for validating VMS pillar results against standard quantum-mechanics dictionaries.

§11.7.1 Ring Quantization & Boundary Twist

This section derives ring quantization conditions from single-valuedness of the wavefunction, connects to the Aharonov–Bohm dictionary, and provides worked numeric examples

A) Derivation

$$\psi(\ell) = \exp(i \cdot \chi) \cdot \psi(0)$$

$$p \cdot \ell = \hbar \cdot (2\pi \cdot n + \chi)$$

$$k_n = (2\pi \cdot n + \chi) / \ell$$

$$p_n = \hbar \cdot k_n$$

$$\chi = 2\pi \cdot \Phi / \Phi 0 , \quad \Phi 0 = h / q$$

B) Energies

$$E_n = p_n^2 / (2m) = (\hbar^2 / 2m) \cdot ((2\pi \cdot n + \chi) / \ell)^2$$

C) Worked Numerics

Example for ℓ = 1 nm:

$$\chi = 0\,,\ n = 1 \ \Rightarrow\ k_1 = 2\pi / \ell \approx 6.28\times10^{9}\ m^{-1}\,,\ \ E_1 \approx 0.15\ eV$$

$$\chi = \pi\,,\ n = 0 \ \Rightarrow\ k_0 = \pi / \ell \approx 3.14\times10^{9}\ m^{-1}\,,\ \ E_0 \approx 0.038\ eV$$

$$\Phi = \Phi0/2 \ \Rightarrow\ \chi = \pi\,,\ \text{identical to anti-periodic case}$$

D) Checklist

- Confirm χ = 0 → periodic integer spectrum.
- Confirm χ = π → anti-periodic half-integer spectrum.
- Verify Aharonov–Bohm mapping: Φ = Φ0/2 shifts lowest state energy upward by ΔE = ħ^2 π^2 / (2m ℓ^2).
- Declare unit system (SI vs natural) explicitly.

§11.7.2 Hydrogenic Dictionary

This insert expands §11.7.2 with a complete step-by-step derivation in SI, reduced mass μ, and a worked numeric. All formulas are Courier text (no LaTeX, no Equation objects).

A) Setup (SI Units)

$$V(r) = -(1 / (4\pi \cdot \varepsilon0)) \cdot e^2 / r \quad \text{(Coulomb potential)}$$

$$F_C(r) = (1 / (4\pi \cdot \varepsilon0)) \cdot e^2 / r^2 \quad \text{(magnitude of Coulomb force)}$$

$$\mu = (m_e \cdot m_p) / (m_e + m_p) \quad \text{(reduced mass for e–p system)}$$

B) Stationary Orbit (Bohr Conditions)

$$\text{Angular momentum quantization:}\quad \mu \cdot v \cdot r = n \cdot \hbar\,,\ \ n = 1, 2, 3, \ldots$$

$$\text{Centripetal balance:}\quad F_C(r) = \mu \cdot v^2 / r$$

Solve for r_n. From the first line, v = n · ħ / (μ · r). Insert into centripetal balance:

$$(1 / (4\pi \cdot \varepsilon0)) \cdot e^2 / r^2 = \mu \cdot (n^2 \cdot \hbar^2 / (\mu^2 \cdot r^2)) / r = n^2 \cdot \hbar^2 / (\mu \cdot r^3)$$

$$\Rightarrow\ r_n = (4\pi \cdot \varepsilon0) \cdot n^2 \cdot \hbar^2 / (\mu \cdot e^2) \equiv n^2 \cdot a0(\mu)$$

$$\text{Bohr radius (with reduced mass):}\quad a0(\mu) = (4\pi \cdot \varepsilon0) \cdot \hbar^2 / (\mu \cdot e^2)$$

C) Energies

$$\text{Kinetic:}\quad T_n = (1/2) \cdot \mu \cdot v^2 = (1/2) \cdot \mu \cdot (n^2 \cdot \hbar^2 / (\mu^2 \cdot r_n^2)) = n^2 \cdot \hbar^2 / (2 \cdot \mu \cdot r_n^2)$$

$$\text{Potential:}\quad V_n = -(1 / (4\pi \cdot \varepsilon0)) \cdot e^2 / r_n$$

$$\text{Virial (Coulomb):}\quad T_n = -(1/2)\cdot V_n$$

$$\text{Total:}\quad E_n = T_n + V_n = -T_n = -\mu\cdot e^4 / (2\cdot(4\pi\cdot\varepsilon 0)^2\cdot\hbar^2\cdot n^2)$$

D) Auxiliary Relations

$$k_n = n / r_n \quad \text{(wave number magnitude on ring of length } 2\pi\, r_n)$$

$$p_n = \mu\cdot v_n = \hbar\cdot n / r_n$$

$$\text{Orbital period:}\quad T_{orb} = 2\pi\cdot r_n / v_n = 2\pi\cdot\mu\cdot r_n^2 / (n\cdot\hbar)$$

E) Worked Numeric (n = 1, Hydrogen)

Constants (SI): $\varepsilon 0 = 8.8541878128\times10^{-12}$ F/m, $\hbar = 1.054571817\times10^{-34}$ J·s, $e = 1.602176634\times10^{-19}$ C.

$$\mu / m_e = m_p / (m_e + m_p) \approx 1836.152673 / 1837.152673 \approx 0.999455$$

$$a0(\mu) = (4\pi\cdot\varepsilon 0)\cdot\hbar^2 / (\mu\cdot e^2) \approx 0.529\times10^{-10}\ \text{m}$$ (slightly below the m_e value by ~0.055%)

$$E_1 = -\mu\cdot e^4 / (2\cdot(4\pi\cdot\varepsilon 0)^2\cdot\hbar^2) \approx -13.6\ \text{eV}$$ (shifted by $\mu/m_e \approx 0.999455$)

Checklist: state unit system; list excluded corrections (fine structure, spin–orbit, Lamb shift).

F) Dictionary Note (VMS ↔ QM)

These hydrogenic relations are used as a dictionary for calibration/validation in §7. In VMS, the central effective kernel arises from EM closure; no additional QM axioms are invoked beyond the stationary-orbit mapping used for comparison.

11.7.3 Liquid-Drop Budgets vs SEMF (Maps to §6)

Uniform sphere Coulomb derivation:

$$E_C = (3/5)\cdot(e^2 / (4\pi\,\varepsilon 0))\cdot Z^2 / R, \quad R = r0\cdot A^{(1/3)}$$

$$a_C = (3\cdot e^2) / (5\cdot 4\pi\,\varepsilon 0\cdot r0)$$

$$E_{bind} = a_V\cdot A - a_S\cdot A^{(2/3)} - a_A\cdot(N-Z)^2 / A - a_C\cdot Z^2 / A^{(1/3)}$$

Worked numeric: For 56Fe (A = 56, Z = 26), plug values to get binding per nucleon ≈ 8.6 MeV vs measured ≈ 8.8 MeV.

Checklist: specify r0; state calibration scheme; list δE_{micro} terms if included.

§11.7.5 Decays from Action Gaps ↔ WKB

This section provides a detailed derivation and comparison between the VMS path-sum formalism for decays and the quantum-mechanical WKB approximation for barrier penetration. It is expanded beyond the other subsections with extra descriptions, step-by-step math, and two worked numeric examples.

A) Path-Sum Derivation and Interpretation

$$A \propto \exp(- \Delta S / S0)$$

$$\Gamma \propto |A|^2 \propto \exp(- 2 \Delta S / S0)$$

$$\tau = \hbar / \Gamma$$

Here A is the transition amplitude, ΔS is the action penalty associated with moving between admissible closures, and S0 is the natural unit of action (identified with ħ). The exponential form arises from evaluating a path-sum via stationary-phase (saddle-point) approximation: paths with larger ΔS contribute exponentially less. Γ is the decay width and τ is the associated lifetime.

B) WKB Barrier Penetration Derivation

$$\psi(x) \approx \exp(\pm \int \kappa(x) \, dx)$$

$$\kappa(x) = \text{sqrt}(2m (V(x) - E)) / \hbar$$

$$T = \exp(- 2 \int \kappa(x) \, dx)$$

In the WKB approximation, the wavefunction in the classically forbidden region decays exponentially with rate κ(x). The transmission probability T is given by the exponential of twice the integral across the barrier. This structure directly mirrors the VMS path-sum suppression form, with the identification:

$$\Delta S / S0 \leftrightarrow (1/\hbar) \int \text{sqrt}(2m (V - E)) \, dx$$

C) Worked Numeric Examples

Example 1: Abstract scaling with ΔS/S0.

$$\Delta S / S0 = 5$$

$$\Gamma \propto \exp(-10) \approx 4.54 \times 10^{(-5)}$$

$$\tau \propto \hbar / \Gamma \Rightarrow \text{relative scaling across channels}$$

Example 2: Alpha decay through Coulomb barrier (illustrative).

$$\text{Nucleus: } Z_{daughter} \approx 82 , \quad R \approx 7 \text{ fm} , \quad E_{alpha} \approx 5 \text{ MeV}$$

$$\text{Barrier integral } \int \kappa \, dx \approx 50 \text{ (order of magnitude)}$$

$$T \approx \exp(- 2 \times 50) = \exp(-100) \approx 3.7 \times 10^{(-44)}$$

This extreme suppression explains why alpha decay lifetimes span many orders of magnitude. Slight changes in ΔS correspond to exponential changes in observed half-lives.

D) Checklist

- Identify S0 = ħ explicitly in all derivations.
- Verify log-linear scaling: plot ln Γ vs ΔS to confirm straight-line behavior.
- State whether channels are Markovian (incoherent sum) or coherent (interference possible).
- Confirm that saddle approximation assumptions are explicitly declared.
- Include at least one real-world numeric check (e.g. alpha decay, field emission).
- Always declare units (eV, s, fm, J).
- Note that even modest changes in ΔS lead to exponential changes in lifetime, a robust cross-check.

§11.7.5 Decays from Action Gaps ↔ WKB

This section connects the VMS path-sum derivation of decays with the standard WKB barrier penetration formula. All math is presented in Courier font for clarity.

A) Path-Sum Derivation

$$A \propto \exp(- \Delta S / S0)$$

$$\Gamma \propto |A|^2 \propto \exp(- 2 \Delta S / S0)$$

$$\tau = \hbar / \Gamma$$

Here A is the amplitude, ΔS is the action penalty, S0 is the action scale (identified with ħ), Γ is the decay width, and τ is the lifetime.

B) WKB Mapping

$$T \approx \exp(- 2 \int \mathrm{sqrt}(2m (V(x) - E)) dx / \hbar)$$

The integral runs over the classically forbidden region where V(x) > E. This exponential suppression matches the path-sum form with identification: ΔS / S0 ↔ (1/ħ) ∫ sqrt(2m (V−E)) dx.

C) Worked Numeric

$$\Delta S / S0 = 5$$

$$\Gamma \propto \exp(-10) \approx 4.54 \times 10^{(-5)}$$

$$\tau \propto \hbar / \Gamma \Rightarrow \text{relative scaling across channels}$$

A modest increase in ΔS yields exponential suppression of Γ, leading to long lifetimes.

D) Checklist

- Identify S0 = ħ explicitly.

• Plot ln Γ vs ΔS to confirm log-linear dependence.
• State whether channels are Markovian (incoherent sum) or coherent (interference possible).
• Confirm saddle approximation assumptions in path-sum.
• Report τ in physical units when Γ is calibrated.

§11.7.6 Metals (Free Electron) and Superconductors (BCS)

This section provides a full derivation of the free-electron gas model and the BCS condensation energy, including worked numeric examples and a checklist for consistency.

A) Free-Electron Gas Derivation

$$k_F = (3\pi^2 n_e)^{(1/3)}$$

$$E_F = \hbar^2 k_F^2 / (2 m_e)$$

$$DOS = (V / 2\pi^2) \cdot (2m_e / \hbar^2)^{(3/2)} \cdot \sqrt{E}$$

$$E_{avg} = (3/5) E_F$$

$$E_{electron} = N_e \cdot E_{avg} = (3/5) \cdot N_e \cdot E_F$$

Worked Numeric (Aluminum)

$$n_e \approx 18 \times 10^{28}\ m^{(-3)}$$

$$k_F = (3\pi^2 n_e)^{(1/3)} \approx 1.75 \times 10^{10}\ m^{(-1)}$$

$$E_F = \hbar^2 k_F^2 / (2 m_e) \approx 11.7\ eV$$

$$E_{avg} = (3/5) E_F \approx 7.0\ eV$$

B) BCS Condensation Energy

$$E_{SC} = -(1/2) \cdot N(0) \cdot \Delta^2$$

N(0) is the density of states per spin at the Fermi surface. Δ is the superconducting energy gap. Formula holds at T = 0. At finite T, Δ(T) decreases and vanishes at T_c.

Worked Numeric (Lead)

$$\Delta \approx 1.35\ meV = 2.16 \times 10^{(-22)}\ J$$

$$N(0) \approx 10^{47}\ J^{(-1)}\ m^{(-3)}$$

$$E_{SC} = -0.5 \cdot N(0) \cdot \Delta^2$$

$$\approx -0.5 \cdot (10^{47}) \cdot (2.16 \times 10^{(-22)})^2$$

$$\approx -9 \times 10^3\ J/m^3$$

C) Checklist

• Specify n_e explicitly (free-electron density).

• State constants (ħ, m_e) used.
• For BCS, specify N(0) and Δ, and declare whether T-dependence is included.
• Always report condensation energy density in J/m³ for comparability.

§11.7.7 Reporting Template

This subsection provides a standardized reporting template for each QM comparison row. It includes a copy-paste block in Courier font, field notes, a worked example, and a checklist.

A) Template Block (Copy-Paste Ready)

QM-Check: Model = <name> ; Inputs = <list> ; Output = <value> ; Reference = <DOI or source>

Agreement: residual = prediction − measurement ; rel_error = residual / measurement

Scope: corrections excluded = <list> ; band check = <brief statement>

B) Field Notes

• Model: name of QM model used (e.g. Bohr hydrogen, SEMF, BCS).
• Inputs: constants or parameters inserted (n, A, Z, Δ, etc.).
• Output: predicted value (energy, radius, width, etc.).
• Reference: literature source (textbook, DOI, or standard).
• Residual: numerical difference between prediction and measurement.
• rel_error: residual normalized to measurement.
• Scope: corrections or bands excluded (fine structure, shell effects, etc.).

C) Worked Example (Hydrogen n=1)

QM-Check: Model = Bohr hydrogen ; Inputs = { μ, ħ, e, ε0, n=1 } ; Output = E1 = −13.6 eV ; Reference = CODATA

Agreement: residual = −0.007 eV ; rel_error = −0.05%

Scope: corrections excluded = { fine structure, Lamb shift } ; band check = ground-state only

D) Checklist

• Every row that cites QM must include this block.

• Use consistent units (eV, MeV, SI).

• Residuals must include sign (positive or negative).

• Scope must explicitly declare excluded corrections.

• Band check should clarify whether the comparison is ground state, excited state, or continuum.