Supplementary Information for: Magnetic fields from microscopic sources: a new quantum-based discrete interaction approach

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S1. MICROSCOPIC CURRENT–MAGNETISATION FRAMEWORK

The CMH framework postulates that the magnetostatic field inside the conductor can be written as a superposition of short-range, screened contributions from these sources:

$$\mathbf{B}^{*}_{\mathrm{CMH}}(\mathbf{r}) = \sum_{i=1}^{N_e} \mathbf{C}_i\, b(s_i), \qquad s_i = \|\mathbf{r} - \mathbf{r}_i\|, \tag{1}$$

with $b(s)$ a radial envelope. A convenient baseline choice is a screened-Coulomb form,

$$b(s) = \frac{\kappa}{s+\kappa}, \tag{2}$$

where κ is a screening length of order the Thomas–Fermi or Debye screening length. For $s \ll \kappa$, $b(s) \approx 1$ and the microscopic source acts locally; for $s \gg \kappa$, $b(s) \sim \kappa/s$ and the contribution decays as $1/s$. κ is meant to be fitted as a universal constant.

The specific form in Eq. (2) is chosen as a convenient baseline that is finite at $s = 0$, approaches unity at short range, and reproduces the required $1/s$ asymptotics at large distances once inserted into the divergence-free field expression. Other screened envelopes (e.g. Yukawa-like forms or response-derived kernels) can be used within the same construction and will modify only short-range details, while leaving the long-distance continuum limit unchanged provided $b_{\mathrm{eff}}(s) \to 1$ in Sec. S5. We therefore treat Eq. (2) as a representative minimal choice.

As written, Eq. (1) does not guarantee $\nabla \cdot \mathbf{B}^{*}_{\mathrm{CMH}} = 0$, because each term is a constant vector multiplied by a scalar function of s. To ensure exact compliance with Gauss's law for magnetism, we reconstruct the field from a vector potential.

S2. DIVERGENCE-FREE CONSTRUCTION AND EFFECTIVE CURRENT

We consider a conductor with N_e conduction electrons at positions $\{\mathbf{r}_i\}$ and an ionic background at positions $\{\mathbf{R}_j\}$. At any instant, electron i moves with velocity $\mathbf{v}_i$ in the electric field generated by nearby ions. We associate to this electron a *source vector* $\mathbf{C}_i$ that encodes the correlated motion of the electron relative to its ionic environment. In the original CMH formulation, $\mathbf{C}_i$ is constructed directly from the relative motion of the electron with respect to nearby ions and the local ionic electric field, i.e. the minimal axial structure permitted by symmetry:

$$\mathbf{C}_i = \sum_{j\in\mathrm{ions}} \big(\mathbf{v}_i - \mathbf{v}_j\big) \times \mathbf{E}_j(\mathbf{r}_i) e^{-k|\mathbf{r}_i - \mathbf{r}_j|}. \tag{3}$$

Here $\mathbf{v}_j$ and $\mathbf{E}_j$ are the ionic velocities and electric fields, and the exponential decay factor $e^{-k|\mathbf{r}_i-\mathbf{r}_j|}$ was introduced to represent field screening within the material (with the choice $k = 10^9$). The exponential factor restricts the construction of the microscopic axial source $\mathbf{C}_i$ to local electron–ion correlations. Physically, it represents the finite spatial range over which the electric field of an ion contributes coherently to the correlated motion of a conduction electron. Equation (3) should be understood as a constitutive definition of a local source vector that weights electron–ion correlations. Any additional material dependence enters through (i) the microscopic electric field $\mathbf{E}_j$, (ii) the ion dynamics $\mathbf{v}_j$, and (iii) the screening kernel $b(s)$ introduced below, rather than through explicit pairwise coefficients.

Under proper rotations, $\mathbf{v}_i - \mathbf{v}_j$ and $\mathbf{E}_j$ transform as polar vectors, so their cross product is an axial vector, matching the transformation properties of magnetic induction. Under time reversal, $\mathbf{v} \to -\mathbf{v}$ while $\mathbf{E}$ is unchanged, so $\mathbf{C}_i$ changes sign, consistent with induction by steady currents. Higher-order symmetry-allowed local invariants (e.g. involving $\nabla\mathbf{E}$ or higher velocity moments) can be added if needed but are not required for the divergence-free construction developed below.

To make CMH predictive in practice while retaining the original coefficient-free structure of Eq. (3), we suggest fixing the screening length κ using one reference structure with known geometry and independently measured current (e.g. an NV-reconstructed field map in a wide wire where continuum theory is reliable). With κ fixed, CMH makes geometry-dependent predictions for suppression, asymmetry, and corrugation trends as dimensions approach the $W \sim \kappa$ regime.

We introduce a local vector potential contribution for each electron,

$$\mathbf{A}_i(\mathbf{r}) = \frac{1}{2}\big(\mathbf{r} - \mathbf{r}_i\big) \times \mathbf{C}_i\, b(s_i), \qquad s_i = \|\mathbf{r} - \mathbf{r}_i\|, \tag{4}$$

and define the total vector potential as $\mathbf{A}(\mathbf{r}) = \sum_i \mathbf{A}_i(\mathbf{r})$.

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The CMH magnetic field is then

$$\mathbf{B}_{\mathrm{CMH}}(\mathbf{r}) = \nabla \times \mathbf{A}(\mathbf{r}), \tag{5}$$

which guarantees $\nabla\cdot\mathbf{B}_{\mathrm{CMH}} \equiv 0$.

Evaluating the curl using $\nabla \times (\mathbf{r} \times \mathbf{C}) = 2\mathbf{C}$ for constant $\mathbf{C}$, and $\nabla b(s) = b'(s)\hat{\mathbf{s}}$, one obtains a closed expression for the local CMH field from electron i:

$$\mathbf{B}_{\mathrm{CMH},i}(\mathbf{r}) = \mathbf{C}_i\, b(s) + \frac{b'(s)\, s}{2}\left[\mathbf{C}_i - (\mathbf{C}_i\cdot\hat{\mathbf{s}})\,\hat{\mathbf{s}}\right], \qquad \hat{\mathbf{s}} = \frac{\mathbf{r}-\mathbf{r}_i}{s}, \tag{6}$$

where $b'(s) = db/ds$. The full divergence-free CMH field is

$$\mathbf{B}_{\mathrm{CMH}}(\mathbf{r}) = \sum_{i=1}^{N_e} \mathbf{B}_{\mathrm{CMH},i}(\mathbf{r}). \tag{7}$$

Using Eq. (6), the contribution from electron i satisfies

$$\nabla \times \mathbf{B}_{\mathrm{CMH},i}(\mathbf{r}) = 2\, b'(s)\, \hat{\mathbf{s}} \times \mathbf{C}_i, \tag{8}$$

so that the full field obeys

$$\nabla \times \mathbf{B}_{\mathrm{CMH}}(\mathbf{r}) = \mu_0\, \mathbf{J}_{\mathrm{CMH}}(\mathbf{r}) = 2\sum_{i=1}^{N_e} b'(s_i)\, \hat{\mathbf{s}}_i \times \mathbf{C}_i. \tag{9}$$

We identify $\mathbf{J}_{\mathrm{CMH}}$ as a *microscopic effective current density*.

For the screened envelope in Eq. (2),

$$b'(s) = -\frac{\kappa}{(s+\kappa)^2}, \tag{10}$$

so $b'(s)$ decays as $1/s^2$ for large s: the effective current density is strongly localized, even though the resulting magnetic field has a longer-range $1/s$ component.

S3. QUANTUM MECHANICAL CMH FORMULATION

Negatively charged carriers are described by single-particle orbitals $\psi_\alpha(\mathbf{r},t)$, $\alpha = 1,\ldots,N_{\mathrm{orb}}$, with occupation numbers f_α. The quantity f_α is the state occupation (dimensionless), i.e. the number of electrons populating orbital α. In a spin-degenerate, zero-temperature Kohn–Sham picture one often has $f_\alpha \in \{0,1,2\}$, while at finite temperature or in open systems it can be fractional ($0 \le f_\alpha \le 2$) (e.g. Fermi–Dirac occupations).

The electronic density and probability current are

$$n_e(\mathbf{r},t) = \sum_\alpha f_\alpha\, |\psi_\alpha(\mathbf{r},t)|^2, \tag{11}$$

$$\mathbf{j}_\alpha(\mathbf{r},t) = \frac{\hbar}{m_e}\, \Im\big[\psi_\alpha^*(\mathbf{r},t)\nabla\psi_\alpha(\mathbf{r},t)\big], \tag{12}$$

and the charge current density contributed by orbital α is

$$\mathbf{J}_\alpha(\mathbf{r},t) = (-e)\,\mathbf{j}_\alpha(\mathbf{r},t), \qquad \mathbf{J}(\mathbf{r},t) = \sum_\alpha f_\alpha\, \mathbf{J}_\alpha(\mathbf{r},t). \tag{13}$$

A local (hydrodynamic) velocity field for orbital α is defined by

$$\mathbf{v}_\alpha(\mathbf{r},t) = \frac{\mathbf{j}_\alpha(\mathbf{r},t)}{|\psi_\alpha(\mathbf{r},t)|^2 + \varepsilon}, \tag{14}$$

where ε is a small regulariser used only to avoid division by zero in low-density regions.

Positively charged ions are treated as classical particles with positions $\mathbf{R}_J(t)$, velocities $\mathbf{V}_J(t)$ (often negligible in magnetostatic settings), and charges $Z_J e$.

For each orbital α we define a pointwise CMH source field

$$\mathbf{C}_\alpha(\mathbf{r},t) = \frac{1}{c^2}\, \mathbf{v}_\alpha(\mathbf{r},t) \times \mathbf{E}_{\mathrm{ion}}(\mathbf{r},t) e^{-k|\mathbf{r}|}, \tag{15}$$

and therefore the total source field is given by

$$\mathbf{C}(\mathbf{r},t) = \sum_\alpha f_\alpha\, |\psi_\alpha(\mathbf{r},t)|^2\, \mathbf{C}_\alpha(\mathbf{r},t). \tag{16}$$

The CMH field can be written entirely in terms of a local kernel obtained from the single-particle expression (Eq. (6)) by replacing the discrete source vector $\mathbf{C}_i$ with a continuous source $\mathbf{C}_\alpha(\mathbf{r}',t)$ at position $\mathbf{r}'$.

Define

$$\mathbf{s} = \mathbf{r} - \mathbf{r}', \qquad s = \|\mathbf{s}\|, \qquad \hat{\mathbf{s}} = \mathbf{s}/s, \tag{17}$$

and let $b(s)$ be the dimensionless screening envelope in Eq. 2. Then the *local CMH field contribution* from a source at $\mathbf{r}'$ with source vector $\mathbf{C}$ is

$$\boldsymbol{\mathcal{B}}^*(\mathbf{s};\mathbf{C}) = \mathbf{C}\, b(s) + \frac{b'(s)s}{2}\left[\mathbf{C} - (\mathbf{C}\cdot\hat{\mathbf{s}})\,\hat{\mathbf{s}}\right]. \tag{18}$$

The object $\boldsymbol{\mathcal{B}}(\mathbf{s};\mathbf{C})$ is the vector-valued kernel mapping a source vector at $\mathbf{r}'$ into the magnetic field at $\mathbf{r}$.

The quantum–classical CMH field is obtained by integrating the orbital contributions over space and summing over occupied orbitals:

$$\mathbf{B}_{\mathrm{CMH}}(\mathbf{r},t) = \sum_\alpha f_\alpha \int d^3r'\, |\psi_\alpha(\mathbf{r}',t)|^2\, \boldsymbol{\mathcal{B}}^*(\mathbf{r}-\mathbf{r}';\, \mathbf{C}_\alpha(\mathbf{r}',t)). \tag{19}$$

For comparison, the magnetostatic BS field computed from the same orbital currents is

$$\mathbf{B}_{\mathrm{BS}}(\mathbf{r},t) = \frac{\mu_0}{4\pi}\int d^3r'\, \frac{\mathbf{J}(\mathbf{r}',t)\times(\mathbf{r}-\mathbf{r}')}{\|\mathbf{r}-\mathbf{r}'\|^3}, \tag{20}$$

with $\mathbf{J}$ defined by Eq. (13). Equations (19) and (20) thus provide a like-for-like comparison: both fields are derived from the same underlying quantum state, but CMH incorporates the additional ionic-field correlation encoded in $\mathbf{C}_\alpha(\mathbf{r},t)$.

S4. BENZENE TOY MODEL: HÜCKEL RING CURRENT AND CMH FIELD

We consider benzene as a six-site π-electron ring in a static magnetic field $\mathbf{B}_0 = B_0\hat{\mathbf{z}}$, which induces a circulating aromatic ring current. We compare the resulting field against the CMH construction using discrete carriers on the ring.

We model the π system by a six-site Hückel tight-binding ring with nearest-neighbour hopping t and a Peierls phase corresponding to the flux Φ through the ring,

$$H(\Phi) = -t \sum_{n=1}^{6} \left(e^{i\theta}\, c_{n+1}^{\dagger} c_n + e^{-i\theta}\, c_n^{\dagger} c_{n+1} \right), \qquad \theta = \frac{2\pi}{6}\frac{\Phi}{\Phi_0}, \tag{21}$$

with $c_7 \equiv c_1$ and $\Phi_0 = h/e$. The eigenenergies are

$$\varepsilon_m(\Phi) = -2t \cos\left(\frac{2\pi m}{6} + \theta \right), \quad m = 0, \ldots, 5. \tag{22}$$

At $T = 0$, benzene has six π electrons occupying the three lowest orbitals with spin degeneracy. The ground-state energy is

$$E_{\mathrm{tot}}(\Phi) = 2 \sum_{m \in \mathrm{occ}} \varepsilon_m(\Phi). \tag{23}$$

The equilibrium orbital current is obtained from the flux derivative,

$$I(\Phi) = -\frac{\partial E_{\mathrm{tot}}}{\partial \Phi}. \tag{24}$$

In the weak-field regime $\Phi = B_0 A$ with $A = \pi R^2$ the ring area.

As a reference, we interpret the orbital current as a circular loop current I of radius R in the x–y plane. At the ring centre the BS magnetic field reduces to $B_{\mathrm{BS}}(0) = \mu_0 I/(2R)$.

To calculate the induced CMH field, we represent the orbital current by N_{car} discrete carriers at positions $\mathbf{r}_i$ on the ring, each with tangential velocity $\mathbf{v}_i$ chosen so that the net current equals Eq. (24):

$$I = \frac{N_{\mathrm{car}} e v}{2\pi R}, \qquad \mathbf{v}_i = v\,\hat{\mathbf{t}}_i, \tag{25}$$

where $\hat{\mathbf{t}}_i$ is the unit tangent and $e > 0$ is the elementary charge. The microscopic CMH source vector for carrier i is defined by Eq. 3

S5. CONTINUUM LIMIT AND RECOVERY OF BIOT–SAVART

We replace the discrete sum over electrons by a coarse-grained description. We introduce a smooth number density $n(\mathbf{r}')$ and a coarse-grained source field $\mathbf{C}(\mathbf{r}')$,

$$n(\mathbf{r}')\,\mathbf{C}(\mathbf{r}') = \sum_{i=1}^{N_e} \mathbf{C}_i\, W_\ell(\mathbf{r}' - \mathbf{r}_i), \tag{26}$$

with W_ℓ a normalized kernel of width ℓ. For sufficiently large coarse-graining cells, the sum in Eq. (7) becomes

$$\mathbf{B}_{\mathrm{CMH}}(\mathbf{r}) \simeq \int n(\mathbf{r}')\,\mathbf{b}_{\mathrm{CMH}}(\mathbf{r};\mathbf{r}')\, d^3r', \tag{27}$$

where the kernel from Eq. (6) is

$$\mathbf{b}_{\mathrm{CMH}}(\mathbf{r};\mathbf{r}') = \mathbf{C}(\mathbf{r}')\, b(s) + \frac{b'(s)\, s}{2} \left[\mathbf{C}(\mathbf{r}') - \big(\mathbf{C}(\mathbf{r}')\cdot\hat{\mathbf{s}}\big)\hat{\mathbf{s}} \right], \tag{28}$$

with $s = \|\mathbf{r} - \mathbf{r}'\|$.

At the continuum level, the number density and drift velocity define the usual current density $\mathbf{J}(\mathbf{r}') = \rho(\mathbf{r}')\mathbf{v}(\mathbf{r}')$, with $\rho = -en$. Under standard magnetostatic assumptions (quasistationary transport, ℓ large compared to interparticle spacing yet small compared to device-scale variations, weak vorticity, and slowly varying screening), the CMH kernel can be written as a magnetostatic Green's function acting on $\mathbf{J}$:

$$\mathbf{B}_{\mathrm{CMH}}(\mathbf{r}) = \frac{\mu_0}{4\pi} \int \mathbf{J}(\mathbf{r}') \times \nabla' G(\mathbf{r},\mathbf{r}')\, d^3r', \tag{29}$$

with

$$G(\mathbf{r},\mathbf{r}') = \frac{1}{4\pi} \frac{b_{\mathrm{eff}}(s)}{s}, \qquad s = \|\mathbf{r} - \mathbf{r}'\|. \tag{30}$$

For the screened form Eq. (2), $b_{\mathrm{eff}}(s) \to 1$ as $s \gg \kappa$, so that Eq. (29) reduces to the BS law.

The exponential factor in Eq. (3) ensures that $\mathbf{C}_i$ is already localized on the scale k^{-1} before coarse graining is applied. When the coarse-graining scale ℓ satisfies $\ell \gtrsim k^{-1}$, the exponential weight suppresses nonlocal electron–ion correlations, and the resulting $\mathbf{C}(\mathbf{r}')$ becomes a smooth, slowly varying field. This allows the coarse-grained CMH kernel to be expressed in terms of the macroscopic current density $\mathbf{J}(\mathbf{r}')$ without introducing additional exponential decay in the Green's function.

S6. TRANSFERABILITY AND PREDICTIVE POWER OF THE CMH FRAMEWORK

The CMH evaluation requires only three ingredients: (a) instantaneous electron positions and velocities, or equivalently the orbital wavefunctions ψ_α with associated probability currents $\mathbf{j}_\alpha$ in the quantum formulation of Section S3; (b) ionic positions and their electric fields $\mathbf{E}_j$; and (c) two empirical parameters κ and k. None of these is system-specific, so the framework applies, without modification, to simple and noble metal nanowires (the present work and Ref.[1]), semiconductor and oxide nanowires, molecular wires and single-molecule junctions, aromatic, antiaromatic, and heteroaromatic ring systems, metal clusters and nanoparticles, coordination complexes and organometallic species with metal-centred orbital currents, and two-dimensional materials such as graphene nanoribbons. The framework inherits sensitivity to chemical composition through $\mathbf{E}_j$, to size effects through the ratio W/κ, and to dimensionality through the geometric distribution of the carriers, so that predictive trends with thickness, lateral confinement, and screening length emerge naturally. The principal practical constraint is the availability of microscopic electronic positions and velocities, which is now standard in modern atomistic simulation pipelines.

REFERENCES

[1] S. A. Tawfik, The current magnetization hypothesis as a microscopic theory of the Ørsted magnetic field induction, Eur. Phys. J. Plus **137**, 378.