Gauge-invariant perturbation expansion in powers of electric charge for the density-of-states of a network model for charged-particle motion in a uniform background magnetic flux density

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An explicitly-gauge-invariant expansion in powers of $e/\hbar$ times the magnetic flux density is formally obtained for the density of states (as characterized by the trace of the resolvent $\hat{G} = (\omega - \hat{h})^{-1}$) of a charged particle moving on a Hermitian quantum network that is embedded in a Euclidean background that supports a uniform magnetic flux density. The explicit expressions, given here up to third order in the flux density, are also valid for the “local trace” (the trace of $P_i \hat{G}$, where $P_i$ is the projector on a network node), and do not appear to have been previously given.
This paper addresses the formal problem of the gauge-invariant expansion, in powers of \( e/\hbar \) times the magnetic flux density, of the density of states or spectrum of a quantum network on which a particle tunnels or “hops” between orbitals located at the network nodes, when the particle is given an electric change \( e \), and the network is embedded in a Euclidean background that supports a uniform magnetic flux density that “dresses” the amplitude of a closed hopping path on the network with a geometric Bohm-Ahanorov phase that depends on the embedding of the network in the background. (The phase is for Euclidean straight-line geodesic tunneling paths between embedding positions of network nodes.) Surprisingly, the explicitly-gauge-invariant result given here does not appear to have appeared previously, at least to the knowledge of the author, and is required for a modern discussion (in terms of Berry geometry) of Landau diamagnetism of Bloch states, which will be reported elsewhere. However, the results and derivation reported here apply more generally, without requiring Bloch periodicity or a thermodynamic limit, and may have other applications, for example to disordered systems, so it is useful to present them as a separate work.

While a continuum Schrödinger equation with a spatially-varying potential was the original microscopic description of electronic motion in solid materials, both spatially periodic and non-periodic, the more common modern approach takes account of atomic structure, and views the problem of electron motion inside rigid solid matter as finite-range tunneling (or “hopping”) between atomic-like localized orbitals of various point-symmetries centered at positions defined by the atomic nuclei (these are the “Wannier orbitals” if the system is periodic and its electronic structure has been approximated by a single isolated Bloch band).

The restriction of the electronic single-particle Hilbert space to a finite density of localized orbitals is a “renormalization” procedure that thins out the electronic spatial degrees of freedom and replaces continuous electronic motion in Euclidean space by hopping motion on a quantum network of orthogonal localized spin-1/2 orbitals \( |i\sigma\rangle \) defined at network nodes, with links between nodes (and onsite terms at nodes) provided by the matrix elements

\[
\langle i\sigma | \hat{h} | j\sigma' \rangle = \sum_{k=0}^{3} h_{ij}^{(k)} \sigma_{\sigma\sigma'},
\]

where \( \{\sigma^k, k = 1, 2, 3\} \) are the \( 2 \times 2 \) unitary Hermitian Pauli matrices, and \( \sigma^0 \) is the \( 2 \times 2 \) identity matrix. In general the matrices \( h^{(k)} \) are complex Hermitian, \( (h^{(k)}_{ij})^* = h^{(k)}_{ji} \), but if there is antiunitary time-reversal symmetry, \( h^{(0)} \) can generically be chosen real symmetric,
and, for \( k \in \{1, 2, 3\} \), \( h^{(k)} \) can be chosen imaginary antisymmetric; the eigenvalue spectrum then has Kramers degeneracy. The network description makes the inclusion of spin-orbit coupling easier, and is the primary tool for describing topologically-non-trivial band structures.

The free-fermion thermodynamics of the quantum network can be entirely expressed in terms of the quantity

\[
\text{Tr} \left( \hat{G}(\omega) \right) = \sum_i \text{Tr}_i \left( \hat{G}(\omega) \right) \equiv \sum_{i\sigma} \langle i\sigma| (\omega - \hat{h})^{-1} |i\sigma \rangle,
\]

the (extensive) trace of the single-particle Green’s function, which is expressible as a sum of local contributions from each network node, using the orthogonal projectors

\[
\hat{P}_i \equiv \sum_{i\sigma} |i\sigma\rangle\langle i\sigma|, \quad \sum_i \hat{P}_i = 1, \quad \hat{P}_i \hat{P}_j = \delta_{ij} \hat{P}_i,
\]

which define the “local trace” \( \text{Tr}_i(\hat{O}) \equiv \text{Tr}(\hat{P}_i \hat{O}) \) of an operator \( \hat{O} \). (All results given here for the trace apply equally to the “local trace”, which greatly simplifies taking the thermodynamic limit.) Note that the trace (and the local trace) has a “locator” expansion as a weighted sum over closed paths on the network. The free-fermion free energy (grand canonical thermodynamic potential) \( \Omega(T, \mu) \) at fixed temperature \( T \) and chemical potential \( \mu \), with \( \beta = 1/k_B T \), is given in terms of \( \text{Tr}(\hat{G}(\omega)) \) by

\[
-\beta \Omega(T, \mu) = \int_C \frac{d\omega}{2\pi i} \text{Tr} \left( \hat{G}(\omega) \right) \ln(1 + e^{(\beta(\mu-\omega))}).
\]

Generally, the spectrum of real eigenvalues \( \varepsilon_\nu \) of a Hermitian network Hamiltonian has both a lower and an upper bound, \( E_{\min} < \varepsilon_\nu < E_{\max} \), that remain finite in the large-network limit if the number of network neighbors that a node is connected is finite. Then (at finite \( \beta \)) the contour \( C \) in the complex \( \omega \)-plane can be taken as a closed contour that encloses all the poles of \( \text{Tr}(\hat{G}(\omega)) \) at \( \omega = \varepsilon_\nu \), which lie on the real axis in the range \( [E_{\min}, E_{\max}] \), but none of the poles of the integrand at \( \omega = \mu \pm i(2n + 1)\pi\beta^{-1}/2, \ n = 0, 1, \ldots, \infty \).

So far the network is an abstract network, and its thermodynamics is entirely a property of the spectrum of the Hermitian single-particle operator \( \hat{h} \), contained in \( \text{Tr}(\hat{G}(\omega)) \). What has been lost in restricting the electron dynamics to a network is any notion of how that network is embedded in a background Euclidean space. Specification of the details of the embedding only becomes necessary when the fermions are given an electric charge \( e \) that
allows them to interact with background electromagnetic fields as they tunnel between nodes on the network. Unlike the electron states which are now localized on the network nodes, the electromagnetic fields are supported throughout the background continuous Euclidean space.

The embedding is a key ingredient of Bloch’s theorem that (provided there is no uniform component of the electric or magnetic field if the particle carries electric charge) the eigenstates of the one-body Hamiltonian of a periodic system, which are quasiperiodic, can be factorized into a quasiperiodic unitary factor (that depends on the embedding) and a periodic factor. In the continuum Schrödinger description, Bloch’s theorem seems so “obvious” that it is not immediately apparent that it involves an embedding. This becomes clearer in the case of network or “tight-binding” models. However, it is often overlooked there too, as calculations of Bloch energy bands (and their topological invariants) do not require specification of the embedding, and for those calculations, a common practice is to implicitly embed all the orbitals in the unit cell at its nominal origin, which conveniently makes the wavefunctions periodic (as opposed to quasiperiodic) functions of the Bloch vector in the Brillouin zone. In contrast, the Berry curvatures of Bloch bands, which are part of the semiclassical description of the dynamics of wavepackets in the presence of quasi-uniform electromagnetic fields, are fundamentally embedding-dependent quantities.

The embedding will formally be in $d$-dimensional Euclidean space, parametrized as

$$\mathbf{x} = x^a \mathbf{e}_a, \quad \mathbf{e}_a \cdot \mathbf{e}_b = \delta_{ab}. \quad (5)$$

The results will in fact be independent of the spatial dimension $d$, so long as it is at least 2, the minimum Euclidean dimension that supports a magnetic flux density. Here $\{x^a, a = 1, 2, \ldots, d\}$ is a Cartesian coordinate system, $\{\mathbf{e}_a, a = 1, 2, \ldots, d\}$ is a position-independent basis of unit vectors, and $\delta_{ab}$ is a unimodular (determinant 1) position-independent Euclidean metric tensor. The unimodular metric defines rotational properties, and plays no role in the discussion here, which will involve Euclidean straight-line paths, which are a metric-independent construction, so long as the metric tensor is not spatially varying (straight-line paths are minimum-length geodesics for all choices of the Euclidean metric tensor). Since the metric will not be used to raise and lower spatial indices, contravariant (upper) and covariant (lower) indices will be distinguished, as in $x^a$ and $\partial_a \equiv \partial/\partial x^a$, with implied summation over repeated upper/lower index pairs.
The embedding of the network in Euclidean space associates each network node with a location $\mathbf{x}_i$, and is defined by the single-particle operators

$$\hat{X}^a = \sum_i x_i^a \hat{p}_i, \quad [\hat{X}^a, \hat{X}^b] = [\hat{X}^a, \hat{p}_i] = 0.$$  \hspace{1cm} (6)

Now introduce a uniform background magnetic flux density in $(d \geq 2)$-dimensional Euclidean space as the gauge-invariant antisymmetric covariant tensor

$$F_{ab} = \partial_a A_b(\mathbf{x}) - \partial_b A_a(\mathbf{x}), \quad \text{constant},$$  \hspace{1cm} (7)

where $A_a(\mathbf{x}) = e_a \cdot \mathbf{A}(\mathbf{x})$ are the covariant components of a gauge-dependent vector potential, the components of a Bohm-Aharonov differential 1-form $A_a(\mathbf{x}) d\mathbf{x}^a$. Then define the modified one-particle Hamiltonian $\hat{h}^A$ by

$$\langle i\sigma | \hat{h}^A | j\sigma' \rangle = \hbar^{i\sigma,j\sigma'} U(\mathbf{x}_i, \mathbf{x}_j),$$

$$U(\mathbf{x}_i, \mathbf{x}_j) = \exp \left( i \frac{e}{\hbar} \int \mathbf{A} \cdot d\mathbf{x} \right),$$

$$\int \mathbf{A} \cdot d\mathbf{x} = \int_0^1 d\lambda (x_i^a - x_j^a) A_a(\lambda \mathbf{x}_i + (1 - \lambda) \mathbf{x}_j),$$  \hspace{1cm} (9)

where $U(\mathbf{x}_i, \mathbf{x}_j)$ is the Bohm-Aharonov factor for a charge-$e$ particle to tunnel along the Euclidean straight-line path from the embedding position $\mathbf{x}_j$ of network node $j$ to position $\mathbf{x}_i$ of network node $i$. Note that because it is a covariant antisymmetric tensor, the magnetic flux density defines a metric-independent Faraday 2-form $\frac{1}{2} F_{ab} d\mathbf{x}^a \wedge d\mathbf{x}^b$.

The mathematical goal here is to obtain an explicitly-gauge-invariant form of the expansion

$$\text{Tr}_i \left( \hat{G}^A \right) = \text{Tr}_i \left( \hat{G} \right) + \sum_{n=1}^\infty \Gamma_i^{(n)}(\omega; F_{ab}),$$  \hspace{1cm} (10)

where $\Gamma_i^{(n)}(\omega, \lambda F_{ab}) = \lambda^n \Gamma_i^{(n)}(\omega, F_{ab})$; $\hat{G}^A = (\omega - \hat{h}^A)^{-1}$ is the network Green’s function when the Hamiltonian is modified by the Bohm-Aharonov phase factor, and $\hat{G} = (\omega - \hat{h})^{-1}$ is the Green’s function of the network Hamiltonian $\hat{h}$ without this factor. This quantity is gauge-invariant because it can be expressed as a sum of closed paths on the network, starting and finishing at node $i$, so the Bohm-Aharonov factor can be expressed in a gauge-invariant way in terms of the magnetic flux linked with the path. It is also invariant under a translation $\hat{X}^a \mapsto \hat{X}^a + \delta x^a I$ of the embedding, because the flux density is taken to be uniform.

In a physical system, the tunneling paths will not be simple Euclidean straight-line geodesic paths. However, the effect of a difference between the true tunneling path between two orbitals and the Euclidean straight-line path is a local effect, which does not
involve the embedding. It merely affects the network parameters in a gauge-invariant way. The applied magnetic field will also in principle locally change the shape and energy of the network orbitals. These gauge-invariant local effects (which only depend on the magnetic flux-density in the immediate neighborhood of points along the path taken by the particle) will be here assumed to have already been included as implicit $F_{ab}$-dependence of the network model parameters, on top of which the geometrical Bohm-Aharonov phase factors (which are non-local, as they depend on the total flux linked with the closed path of Euclidean geodesics between network nodes) are then added.

**Statement of the result:** The functions $\Gamma_i^{(n)}(\omega)$ of equation (10) are $O(\omega^{-4})$ in the large-$\omega$ limit, and can be written as the local traces

$$\Gamma_i^{(n)}(\omega) = \text{Tr}_i \left( \hat{\Gamma}^{(n)}(\omega) \right); \quad \Gamma^{(n)} \equiv \sum_i \Gamma_i^{(n)},$$

where the operators $\hat{\Gamma}^{(n)}(\omega)$ are explicitly gauge-invariant, and under Hermitian conjugation have the symmetry

$$\left( \hat{\Gamma}^{(n)}(\omega) \right)^\dagger = \hat{\Gamma}^{(n)}(\omega^*) \quad (12)$$

The first two of these operators can be written in terms of $\hat{G}(\omega) = (\omega - \hat{h})^{-1}$ to give the principal result of this paper as

$$\hat{\Gamma}^{(1)}(\omega) = -f_{ab} \hat{G} \hat{h}_a^i \hat{G} \hat{h}_b^i \hat{G}, \quad (13)$$

$$\hat{\Gamma}^{(2)}(\omega) = \frac{1}{2} f_{ab} f_{cd} \hat{G} \hat{h}_a^i \hat{G} \hat{h}_b^j \hat{G} \hat{h}_c^k \hat{G} \hat{h}_d^l \hat{G} + f_{ab} f_{cd} \hat{G} \hat{h}_a^i \hat{G} \hat{h}_b^j \hat{G} \hat{h}_c^k \hat{G} \hat{h}_d^l \hat{G}, \quad (14)$$

$$f_{ab} \equiv -\frac{i}{2} (e/\hbar) F_{ab}; \quad (15)$$

here $\hat{h}_a^i$ and $\hat{h}_2^{ab} = \hat{h}_2^{ba}$ are members of a set of embedding-dependent gauge-invariant locallytraceless Hermitian operators recursively defined for $m \geq 1$ by

$$\hat{h}_1^a = [\hat{h}, iX^a], \quad h_{n+1}^{a...bc} = [\hat{h}_{m}^{a...b}, i\hat{X}^c], \quad (16)$$

where $\hat{h}_{m}^{a_1...a_m}$ is fully symmetric in its contravariant tensor indices, as a consequence of the property $[\hat{X}^a, \hat{X}^b] = 0$. One may also write

$$\hat{h}(q) \equiv \hat{U}(q)^{-1} \hat{h} \hat{U}(q) = \hat{h}^0 + \sum_{n=1}^{\infty} \frac{1}{n!} \hat{h}_{n}^{a_1...a_n} q_{a_1} \ldots q_{a_n},$$

$$\hat{U}(q) \equiv \exp(i q_a \hat{X}^a) = \sum_i e^{i q_a x_i} \hat{P}_i, \quad (17)$$
which remains well-defined even in the thermodynamic limit, when $\hat{X}^a$ itself becomes unbounded.

For $n > 1$, the expressions for $\hat{\Gamma}^{(n)}(\omega)$ are not unique, as there are locally-traceless gauge-invariant operators which can be added to them. For $n = 2$, this follows from the four linear relations

$$\text{Tr}_i \left( 2\hat{\Gamma}^{(2)}_{\{2,1,1\}} + \hat{\Gamma}^{(2)}_{\{2,1,2\}} - \hat{\Gamma}^{(2)}_{\{1,2,1\}} + \hat{\Gamma}^{(2)}_{\{1,1,2\}} \right) = 0,$$

$$\text{Tr}_i \left( \hat{\Gamma}^{(2)}_{\{2,1,1\}} - \hat{\Gamma}^{(2)}_{\{1,1,2\}} \right) = 0,$$

$$\text{Tr}_i \left( \hat{\Gamma}^{(2)}_{\{2,1,1\}} + 2\hat{\Gamma}^{(2)}_{\{1,1,2\}} + \hat{\Gamma}^{(2)}_{\{1,1,1,1\},2} + \hat{\Gamma}^{(2)}_{\{1,1,1,1\},3} \right) = 0,$$

$$\text{Tr}_i \left( \hat{\Gamma}^{(2)}_{\{1,1,1,1\},1} - \hat{\Gamma}^{(2)}_{\{1,1,1,1\},2} + \hat{\Gamma}^{(2)}_{\{1,1,1,1\},3} \right) = 0,$$

where a full set of seven gauge-invariant operators in terms of which $\hat{\Gamma}^{(2)}$ can be represented is

$$\hat{\Gamma}^{(2)}_{\{2,2\}} = \frac{1}{4} f_{ac} f_{bd} \hat{G} \hat{h}^{ab}_{2} \hat{G} \hat{h}^{cd}_{2} \hat{G},$$

$$\hat{\Gamma}^{(2)}_{\{2,1,1\}} = \frac{1}{2} f_{ac} f_{bd} \hat{G} \hat{h}^{ab}_{2} \hat{G} \hat{h}^{cd}_{3} \hat{G},$$

$$\hat{\Gamma}^{(2)}_{\{1,2,1\}} = \frac{1}{2} f_{ab} f_{cd} \hat{G} \hat{h}^{ab}_{2} \hat{G} \hat{h}^{cd}_{3} \hat{G},$$

$$\hat{\Gamma}^{(2)}_{\{1,1,2\}} = \frac{1}{2} f_{ac} f_{bd} \hat{G} \hat{h}^{ab}_{1} \hat{G} \hat{h}^{cd}_{2} \hat{G},$$

$$\hat{\Gamma}^{(2)}_{\{1,1,1,1\},1} = f_{abc} f_{def} \hat{G} \hat{h}^{ab}_{1} \hat{G} \hat{h}^{cd}_{1} \hat{G} \hat{h}^{ef}_{1} \hat{G},$$

$$\hat{\Gamma}^{(2)}_{\{1,1,1,1\},2} = f_{abc} f_{def} \hat{G} \hat{h}^{ab}_{1} \hat{G} \hat{h}^{cd}_{3} \hat{G} \hat{h}^{ef}_{1} \hat{G},$$

$$\hat{\Gamma}^{(2)}_{\{1,1,1,1\},3} = f_{abc} f_{def} \hat{G} \hat{h}^{ab}_{1} \hat{G} \hat{h}^{cd}_{3} \hat{G} \hat{h}^{ef}_{1} \hat{G}.$$

In view of (18a)-(18d), this basis can be said to have dimension $D = 7$ with rank $R = 3$. The expression (14) for $\hat{\Gamma}^{(2)}$ as $\hat{\Gamma}^{(2)}_{\{1,2,1\}} + \hat{\Gamma}^{(2)}_{\{1,1,1,1\}}$ is the unique solution to the problem of finding the operator $\hat{\Gamma}^{(2)}$ obeying $\text{Tr}(\hat{\Gamma}^{(2)}) = \Gamma^{(2)}$ as the “most economical” choice of a weighted sum of operators (19a)-(19g) (i.e., the one using the smallest number of terms, in this case 2, which is less than the rank of the basis, equal to 3).

Briet et al. have studied Landau diamagnetism in the continuum Schrödinger Hamiltonian given (in units $\hbar = m_e = 1$) as $\hat{H} = \frac{1}{2} \delta^{ab} \hat{p}_a \hat{p}_b + V(x)$, $\hat{p}_a \equiv -i \partial / \partial x^a$, for which $\hat{h}^{ab}_1 = \delta^{ab} \hat{p}_a$ and $\hat{h}^{ab}_2 = \delta^{ab} \mathbb{1}$. In this model $[\hat{h}^{ab}, \hat{h}^{bc}] = 0$, which is not generically true for the network model, and $\hat{h}^{ab}$ is in the center of the algebra, i.e., is a c-number. For this Schrödinger model, the authors of Ref. [1] give a formula for the quadratic term of a gauge-invariant expansion in
flux density, which they appear to attribute to Cornean and Nenciu, equivalent to
\[ \Gamma^{(2)} = \text{Tr} \left( \hat{\Gamma}^{(2)}_{\{1,1,1,1\}} \right) + \frac{1}{2} \delta^{ab} \delta^{cd} f_{ac} f_{bd} \text{Tr} \left( \hat{G} \hat{h}_{a}^{b} \hat{h}_{1}^{b} \right). \] (20)

The Schrödinger model can be considered as a continuum limit of the generic discrete network model considered here, and the formula (20) is the specialization to c-number \( \hat{h}_{2}^{ab} \rightarrow \delta^{ab} \) of an alternative form for \( \hat{\Gamma}^{(2)} \) where the traceless operator inside the trace (18a) has been added to (14), eliminating the operator (19c) with label \( \{1,2,1\} \), thus giving a “non-economical” expression for \( \hat{\Gamma}^{(2)} \) with 4 (rather than 2) terms, if (12) is respected.

It is noteworthy that the general result reported here was obtained purely algebraically, using simple associative-algebra methods which can be implemented in a finite-dimensional Hilbert space, without requiring any consideration of a thermodynamic limit, or functional analysis of the space of functions in continuous Euclidean space, which seems to be a central feature of the Schrödinger-differential-equation-based discussion in Refs. 1 and 2.

For most applications, expansions beyond quadratic order become impractical, and quadratic order is all that is needed for the diamagnetic susceptibility. However, some discussion of the higher order case of general \( n \) will be given.

A generic set of operators which can be linearly combined to represent \( \hat{\Gamma}^{(n)} \), has the form
\[ \hat{\Gamma}^{(n)}_{\{m_{1},\ldots,m_{k}\},\alpha} = \frac{f_{\bullet} \cdots f_{\bullet}}{m_{1}! \cdots m_{k}!} \hat{G} \hat{h}_{m_{1}}^{\bullet} \hat{G} \cdots \hat{G} \hat{h}_{m_{k}}^{\bullet} \hat{G}, \] (21)
where “\( \bullet \)” represents unspecified indices, and \( \alpha \) labels the way the contravariant indices on the \( 2 \leq k \leq 2n \) instances of the symmetric tensor operators \( h_{m}^{a_{1} \ldots a_{m}} \) with \( 1 \leq m \leq n \), and \( \sum_{i} m_{i} = 2n \), are paired by contraction with the covariant indices on the \( n \) instances of the antisymmetric tensors \( f_{ab} \) (indices on the same instance of \( \hat{h}_{m}^{\bullet} \) cannot be paired). Given an allowed pairing, the operators (21) are defined up to an arbitrary choice of sign, which will here be fixed so the left-right order of covariant indices in \( f_{ab} \) is the same is that of the contravariant indices in the operator product with which they are contracted.

The notation \( m_{k} = \{m_{1},\ldots,m_{k}\} \) will also be used, with \( \overline{m}_{k} = \{m_{k},\ldots,m_{1}\} \) denoting the reversed pattern. As will be seen, the structure of \( \Gamma^{(n)} \) shows that the expression for \( \hat{\Gamma}^{(n)} \) should be a weighted sum of operators (21) with real weights:
\[ \hat{\Gamma}^{(n)} = \sum_{m,\alpha} C_{m,\alpha} \hat{\Gamma}^{(n)}_{m,\alpha}, \quad C_{m,\alpha} = C^{*}_{m,\alpha}. \] (22)
The operators (21) have the conjugation property that

$$\left( \hat{\Gamma}^{(n)}_{m_k,\alpha}(\omega) \right)^\dagger = \hat{\Gamma}^{(n)}_{\overline{m}_k,\overline{\alpha}}(\omega^\ast),$$

which for \( \alpha \neq \overline{\alpha} \) is consistent with the chosen sign convention for the ordering of indices in \( f_{ab} \). Then, given that they are real,

$$C_{m,\alpha} = C_{\overline{m},\overline{\alpha}},$$

and the basis set of operators (21) can be grouped into pairs that are each other’s conjugates, or singles that are self-conjugate. Only a reduced basis set that consists of the singles, plus the sums \( \hat{\Gamma}^{(n)}_{m_k,\alpha} \pm \hat{\Gamma}^{(n)}_{\overline{m}_k,\overline{\alpha}} \) of the two members of each pair, is needed to represent \( \hat{\Gamma}^{(n)} \).

For \( n = 2 \), this reduced basis set has dimension \( D' = 6 \) with rank \( R' = 3 \). For \( n > 2 \), the number of operators (21) grows rapidly, and for \( n = 3 \) a numerical linear-algebra analysis reveals that the basis set of operators of type \( \hat{\Gamma}^{(3)}_{m_k,\alpha}(\omega) \) has \( D = 75 \) with \( R = 22 \), and the reduced basis set has dimension \( D' = 17 + 29 = 46 \) with 17 singles plus 29 pairs, and rank \( R' = 15 \) (so \( 17 + 2 \times 29 = 75 \)). If an expression for \( \hat{\Gamma}^{(n)} \) is found as a weighted linear combination of a subset of \( R' \) members of the reduced basis set, (so the set of their traces is a linearly-independent basis of functions of \( \omega \)) it will be unique, with real weights that are in general rational numbers when the choice of the subset is unstructured (randomly selected). However the normalization of the operators (21) has been chosen so that, by using a suitably-chosen subset, all the weights become integers, and less that \( R' \) of them are non-zero, as seen in the case \( n = 2 \), when (14) is expressed in terms of operators (21), and in detailed investigations of the case \( n = 3 \) using numerical linear-algebra methods described in the Appendix.

A principle of “maximum economy” suggests that the optimal choice of the subset of operators with linearly-independent traces is that which minimizes the number of non-zero integer weights \( C_{m_k,\alpha} \) when \( \hat{\Gamma}^{(n)} \) is expressed in the form (22) obeying (24), which is uniquely given once the choice of the subset is made. Based on the case \( n = 2 \), it is tempting to conjecture that such an optimal choice is unique, and provides a “canonical” form for \( \hat{\Gamma}^{(n)} \). However, the possible uniqueness of such a “most economical” choice has not been checked for the case \( n = 3 \), as an algorithm to search for it was not constructed.

In the absence of a canonical form for \( \hat{\Gamma}^{(n)} \), one generic feature perhaps worth mentioning is that, for \( n > 1 \), the linear relations between the traces always allow a form for \( \hat{\Gamma}^{(n)} \) to
be found that omits $\hat{\Gamma}^{(n)}_{\{n,n\}}$, so that $\hat{\Gamma}^{(n)}(\omega)$ is $O(\omega^{-4})$ for large $\omega$, like its trace. While this cannot be done in the case $n = 1$, the leading $O(\omega^{-3})$ behavior of $\hat{\Gamma}^{(1)}(\omega)$ given in [13] is easily seen to be traceless.

**Derivation of the result:** The vector potential of a uniform magnetic flux density in Euclidean space has the form

$$A_a(x) = -\frac{1}{2} F_{ab} x^b + \partial_a \chi(x), \quad (25)$$

where $F_{ab}$ is antisymmetric, and $\chi(x)$ is a gauge ambiguity. A network vector potential operator is defined by

$$\hat{A}_a = \sum_{i\sigma} A_a(x_i) |i\sigma\rangle\langle i\sigma|. \quad (26)$$

The Bohm-Aharonov phase factor is

$$U(x_1, x_2) = e^{i(e/\hbar)\chi(x_1)} e^{f_{ab} x_1^a x_2^b} e^{-i(e/\hbar)\chi(x_1)}. \quad (27)$$

The factors involving $\chi(x)$ can be eliminated by the gauge transformation

$$|i\sigma\rangle \mapsto e^{i(e/\hbar)\chi(x_1)} |i\sigma\rangle. \quad (28)$$

With this gauge choice (the “linear gauge”), $A_a(x) = -\frac{1}{2} F_{ab} x^b$ is a linear function of $x$, and $U(x_1, x_2)$ is simply given by $\exp(f_{ab} x_1^a x_2^b)$. The residual gauge-dependence is in the arbitrary choice of origin of the coordinate system: in this gauge, quantities that are invariant under a uniform translation of the network in Euclidean space, $\hat{X}^a \mapsto \hat{X}^a + \delta x^a \mathbb{1}$, are gauge-invariant.

In the linear gauge, the network vector potential operator is given by

$$\hat{A}_a = -\frac{1}{2} F_{ab} \hat{X}^b \quad (29)$$

with $[\hat{A}_a, \hat{A}_b] = 0$, $[\hat{A}_a, \hat{X}^b] = 0$, and

$$\hat{A}_a \hat{X}^a = 0. \quad (30)$$

A useful property in this gauge is

$$\hat{h}^{ab...c} \hat{A}_a = \hat{A}_a \hat{h}^{ab...c}. \quad (31)$$

For the change $\hat{h} \mapsto \hat{h} + \hat{\nabla}$, $\hat{G} \mapsto \hat{G}^V$, which is given by the infinite geometric series

$$\hat{G}^V \equiv (\omega - \hat{h} - \hat{\nabla})^{-1} \equiv \hat{G} + \hat{G} \hat{V} \hat{G} + \hat{G} \hat{V} \hat{G} \hat{V} \hat{G} + \ldots \quad (32)$$

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For the change $\hat{G} \mapsto \hat{G}^A$, in the linear gauge,

$$\langle i\sigma|\hat{V}|j\sigma' \rangle = \langle i\sigma|\hat{h}|j\sigma \rangle \sum_{n=1}^{\infty} \frac{1}{n!} (f_{ab} x_i^a x_j^b)^n.$$  \hspace{1cm} (33)

As an operator,

$$\hat{V} = \sum_{n=1}^{\infty} \frac{\hat{h}^{(n)}}{n!},$$  \hspace{1cm} (34)

$$\hat{h}^{(n)} = \left( \prod_{i=1}^{n} f_{a_i b_i} \right) \left( \prod_{i=1}^{n} \hat{X}^{a_i} \right) \hat{h} \left( \prod_{i=1}^{n} \hat{X}^{b_i} \right).$$  \hspace{1cm} (35)

Note that the substitution $\hat{h} \mapsto -\hat{G}^{-1}$ can be made in (35). With the supplementary definition $\hat{h}^{(0)} \equiv \hat{h}$,

$$f_{ab} \hat{X}^a \hat{h}^{(n)} \hat{X}^b = \hat{h}^{(n+1)}.$$  \hspace{1cm} (36)

Here $\hat{h}^{(n)}$ is a traceless Hermitian operator, which can also be written, for any $r$ in the range $[0, n]$, as

$$\hat{h}^{(n)} = \left( \prod_{i=1}^{r} \hat{A}_{a_i} \right) \hat{h}^{a_1...a_r} \left( \prod_{j=r+1}^{n} \hat{A}_{a_j} \right);$$  \hspace{1cm} (37)

because of the property (31), and mutual commutativity of the components $\hat{A}_a$, the product of operators in (37) can be written in any order.

The series for $\text{Tr}(\hat{G}^A)$ in powers of $(e/\hbar)$ has the form

$$\text{Tr}(\hat{G}^A) = \text{Tr}(\hat{G}) + \sum_{n=1}^{\infty} \Gamma^{(n)},$$  \hspace{1cm} (38)

$$\sum_{n=1}^{\infty} \lambda^n \Gamma^{(n)} = \sum_{k=1}^{\infty} \text{Tr} \left( \hat{G} \left( \sum_{n=1}^{\infty} \frac{1}{n!} \lambda^n \hat{h}^{(n)} \hat{G} \right)^k \right).$$  \hspace{1cm} (39)

The term $\Gamma^{(n)}$ is the trace of an operator $\hat{G} \hat{V}^{(n)} \hat{G}$ where $\hat{V}^{(n)}(\omega)$ is nominally a polynomial of degree $n - 1$ in $\hat{G}$:

$$\hat{V}^{(n)}(\omega) = \frac{1}{n!} \hat{h}^{(n)} + \left( \sum_{k=1}^{n-1} \frac{1}{k!(n-k)!} \hat{h}^{(k)} \hat{G}(\omega) \hat{h}^{(n-k)} \hat{G} \right) + \ldots + \hat{h}^{(1)}(\hat{G}(\omega) \hat{h}^{(1)})^{n-1}. \hspace{1cm} (40)$$

(The nominal polynomial degree in $\hat{G}$ ignores the “hidden” linear dependence of $\hat{h}^{(n)}$ on $\hat{G}^{-1}$.) It will be useful to examine the large-$\omega$ behavior of $\Gamma^{(n)}$. While the operator $\hat{G} \hat{V}^{(n)} \hat{G}$
is $O(\omega^{-2})$ in this limit, its trace $\Gamma^{(n)}$ is in fact $O(\omega^{-4})$. The expansion is developed using

$$
\hat{G} = \omega^{-1} \mathbb{1} + \sum_{k=1}^{\infty} \omega^{-k+1} (\hat{h})^k.
$$

(41)

The nominally-leading behavior of $\Gamma^{(n)}(\omega)$ at large $\omega$ is $(n! \omega^2)^{-1} \text{Tr}(\hat{h}^{(n)})$, which vanishes because $\hat{h}^{(n)}$ is traceless, so the apparently-leading term becomes

$$
\Gamma^{(n)}(\omega) = \frac{1}{n!} \frac{1}{\omega^3} \text{Tr}(\hat{O}_n) + O(\omega^{-4}),
$$

(42)

with

$$
\hat{O}_n = \hat{h}^{(0)} \hat{h}^{(n)} + \hat{h}^{(n)} \hat{h}^{(0)} + \sum_{k=1}^{n-1} \frac{n!}{k!(n-k)!} \hat{h}^{(k)} \hat{h}^{(n-k)}.
$$

(43)

Using (35), these terms can be combined to give

$$
\Gamma^{(n)}(\omega) = (1 - (-1)^n) \frac{1}{n!} \frac{1}{\omega^3} \text{Tr}(\hat{h}^{(n)}) + O(\omega^{-4}).
$$

(44)

While (because of the prefactor) this obviously vanishes for even $n$, it in fact vanishes for all $n > 0$ because for odd $n$ $\text{Tr}(\hat{h}^{(n)})$ vanishes:

$$
\text{Tr}(\hat{h}^{(n)}) = (\prod_i f_{ab_i}) \text{Tr}(\hat{h}(\prod_i \hat{X}^a_i) \hat{h}(\prod_i (\hat{X}^b_i)))
$$

$$
= (-1)^n \text{Tr}(\hat{h}^{(n)}),
$$

(45)

where the cyclic property of the trace and the antisymmetry of $f_{ab}$ have been used. (Note that here, wherever the cyclic property of the trace is invoked, it always only involves moving instances of $\hat{X}^a$ between the left and right side of the operator-product inside the trace; since $\hat{X}^a$ commutes with $\hat{P}_i$, results derived for the global trace apply equally to the local trace.) Further examination shows that the $O(\omega^{-4})$ term is generically non-vanishing, and this is the generic large-$\omega$ behavior of all terms $\Gamma^{(n)}(\omega)$.

The explicit expressions for the first three of the $\Gamma^{(n)}$ are

$$
\Gamma^{(1)} = \text{Tr}\left(\hat{G} \hat{h}^{(1)} \hat{G}\right),
$$

(46)

$$
\Gamma^{(2)} = \text{Tr}\left(\frac{1}{2} \hat{G} \hat{h}^{(2)} \hat{G} + \hat{G} \hat{h}^{(1)} \hat{G} \hat{h}^{(1)} \hat{G}\right),
$$

(47)

$$
\Gamma^{(3)} = \text{Tr}\left(\frac{1}{6} \hat{G} \hat{h}^{(3)} \hat{G} + \frac{1}{2} \hat{G} \hat{h}^{(2)} \hat{G} \hat{h}^{(1)} \hat{G} + \frac{1}{2} \hat{G} \hat{h}^{(1)} \hat{G} \hat{h}^{(1)} \hat{G} + \hat{G} \hat{h}^{(1)} \hat{G} \hat{h}^{(1)} \hat{G}\right).
$$

(48)
Features to note are (i) these expressions are invariant under reversing the order of the operator products inside the trace and (ii) the operators inside the trace can be represented as products of the $f \cdot$ times products of operators $\hat{G}, \hat{G}^{-1},$ and $i\hat{X}^\bullet$, added together with with real rational coefficients. The manipulations to bring them to explicitly gauge-invariant form, by using commutation relations $[\hat{X}^\bullet, \hat{X}^\bullet] = 0$ and $[\hat{h}^\bullet_m, i\hat{X}^\bullet] = \hat{h}^\bullet_{m+1}$ to eliminate all instances of $i\hat{X}^\bullet$ in favor of gauge-invariant operators $\hat{h}^\bullet_m$, together with use of the identity $\hat{G}^{-1}\hat{G} = \hat{G}\hat{G}^{-1} = \mathbb{I}$, can only produce linear combinations of operators (21) with real rational coefficients, plus traceless gauge-dependent remainder terms.

While these expressions are gauge invariant under $\hat{A}_a \mapsto \hat{A}_a + \delta A_a \mathbb{I}$, the operators $\hat{h}^{(n)}$ inside the trace depend explicitly on $\hat{A}$, and are not themselves gauge invariant. The difficulty with these expressions for $\Gamma^{(n)}$ is that, while they are gauge-invariant (which is easily verified using the numerical linear-algebra approach described in the Appendix), they are given as the trace of a sum of operators which individually do not have gauge-invariant traces.

The algebraic strategy for the manipulations to bring these expressions to explicitly gauge-invariant form is to reorder the gauge-dependent operator products inside the trace to produce a sum of products of gauge-invariant operators plus a discardable gauge-dependent remainder term which is traceless, so does not contribute to the function $\Gamma^{(n)}(\omega)$.

A key identity, is, for any operator $\hat{O}$,

$$[\hat{O}, \hat{G}] \equiv \hat{G}\hat{G}^{-1}\hat{O}\hat{G} - \hat{G}\hat{O}\hat{G}^{-1}\hat{G} \equiv \hat{G}[\hat{G}^{-1}, \hat{O}]\hat{G}. \quad (49)$$

Then, in particular,

$$\hat{G}h^a\hat{G} \equiv [\hat{G}, i\hat{X}^a], \quad (50)$$

which can be used to increase or decrease powers of $\hat{G}$ in a product of operators. For example, using this one obtains

$$h^{(1)} = if_{ab}\hat{h}^a\hat{X}_b = -if_{ab}\hat{X}^a\hat{h}^b, \quad (51)$$

$$\hat{G}h^{(1)}\hat{G} \equiv -f_{ab}\hat{G}h^a\hat{h}^b\hat{G} + f_{ab}\hat{X}^a\hat{G}\hat{X}^b. \quad (52)$$

The identity that (when $n > 1$) allows $\hat{\Gamma}^{(n)}_{\{n,n\}}$ to be eliminated from expressions for $\Gamma^{(n)}$
can be derived using (50). First note that

\[ \hat{\Gamma}^{(n)}_{\{n,n\}} = \frac{1}{n!n!} (\prod_i f_{a_i b_i} \hat{G} h_{a_1...a_n} \hat{G} h_{b_1...b_n} \hat{G} ) = \frac{1}{n!n!} (\prod_i f_{a_i b_i} \hat{G} [h_{a_1...a_n-1}, i \hat{X}^{a_n}] \hat{G} h_{b_1...b_n} \hat{G} ) \]

\[ = \frac{1}{n!n!} (\prod_i f_{a_i b_i} ) ( - \hat{G} i \hat{X}^{a_n} \hat{h}_{a_1...a_n-1} \hat{G} h_{b_1...b_n} \hat{G} ) \]

\[ + \hat{G} \hat{h}_{a_1...a_n-1} \hat{G} \hat{h}_{b_1...b_n} i \hat{X}^{a_n} \hat{G} ) . \]

Then, using (50), this gives the identity

\[ \text{Tr} \left( n \hat{\Gamma}^{(n)}_{\{n,n\}} + \hat{\Gamma}^{(n)}_{\{1,n-1,n\}} + \hat{\Gamma}^{(n)}_{\{n-1,1,n\}} - \hat{\Gamma}^{(n)}_{\{n-1,n,1\}} \right) = 0. \] (53)

Note that this is consistent with the property that, while \( \hat{\Gamma}^{(n)}_{\{n,n\}}(\omega) \) is \( O(\omega^{-3}) \) for large \( \omega \), its trace is \( O(\omega^{-4}) \). (The leading \( O(\omega^{-3}) \) term in its large-\( \omega \) expansion is

\[ \lim_{\omega \to \infty} \hat{\Gamma}^{(n)}_{\{n,n\}}(\omega) \to \left( \prod_{i=1}^n f_{a_i b_i} \right) \left( \sum_{a_1...a_n} \hat{G}_{n} a_1...a_n \hat{G}_{n} h_{b_1...b_n} \hat{G} \right) . \]

which is traceless by antisymmetry of \( f_{ab} \) and the cyclic property of the trace; tracelessness is only immediately obvious for odd \( n \), but for all \( n \geq 1 \) it is easily seen after after replacement of both instances of \( h^{\bullet}_{n} \) by \( [h^{\bullet}_{n-1}, i \hat{X}^{\bullet}] \), with \( "h_{0}^{\bullet} \equiv \hat{h}. \) For \( n = 2 \), (53) corresponds to (18a) minus (18b). The other \( n = 2 \) linear relations (18b)-(18d) can be obtained by similar manipulations, though they were in fact initially found using numerical linear-algebra methods.

The explicitly-gauge-invariant form for \( \Gamma^{(n)}(\omega) \) can be expressed in terms of the traces of operators of the form (21). However, the explicitly gauge-invariant functions defined by the traces of this set of operators are an overcomplete set of functions, with a high degree of linear dependence, so there is no unique solution to the problem of writing \( \Gamma^{(n)} \) as a sum of traces of gauge-invariant operators. An efficient approach to the problem, described in the Appendix, is to use numerical linear-algebra methods to obtain a linearly-independent reduced basis of the traces of operators (21), then numerically solve the linear-algebra problem of expanding \( \Gamma^{(n)}(\omega) \) in this basis, which is a floating-point numerical computation that produces recognizably rational-valued expansion coefficients up to machine rounding precision. However, to avoid just asserting that (13) and (14) “have been shown to be true”, they will now be derived algebraically using associative-algebra methods.
First examine $\Gamma^{(1)}$: the necessary work is already done in \eqref{eq:52}; since $f_{ab}\text{Tr}(\hat{X}^a\hat{G}\hat{X}^b)$ vanishes as a consequence of the cyclic property of the trace plus antisymmetry of $f_{ab}$,

$$\Gamma^{(1)} = \text{Tr}\left(\hat{G}\hat{h}^{(1)}\hat{G}\right) = -f_{ab}\text{Tr}\left(\hat{G}\hat{h}^a\hat{G}\hat{h}^b\hat{G}\right), \quad (54)$$

which immediately confirms \eqref{eq:13}.

Next, examine $\Gamma^{(2)}$, which is the main focus of this work, as it will be needed for a modern re-examination of formulas for Landau diamagnetism. The starting point is the presentation \eqref{eq:47} of $\Gamma^{(2)}(\omega)$ as the gauge-invariant sum $\Gamma^{(2a)} + \Gamma^{(2b)}$ of two terms which are not individually gauge invariant:

$$\Gamma^{(2a)} = \frac{1}{2}\text{Tr}\left(\hat{G}\hat{h}^{(2)}\hat{G}\right), \quad (55)$$

$$\Gamma^{(2b)} = \text{Tr}\left(\hat{G}\hat{h}^{(1)}\hat{G}\hat{h}^{(1)}\hat{G}\right) = f_{ab}f_{cd}\text{Tr}\left(\hat{G}\hat{h}^a\hat{X}^b\hat{G}\hat{X}^c\hat{h}^d\hat{G}\right), \quad (56)$$

where \eqref{eq:51} has been used symmetrically to replace both instances of $\hat{h}^{(1)}$, and begin the modification of the second term. Then symmetrically use $\hat{X}^a\hat{G} - \hat{G}\hat{X}^a \equiv i(\hat{G}\hat{h}^a\hat{G})$, and $\hat{X}^a\hat{h}^b - \hat{h}^b\hat{X}^a \equiv i\hat{h}^{ab}$, together with $f_{ab}f_{cd}\hat{X}^b\hat{X}^c = f_{db}f_{ca}\hat{X}^b\hat{X}^c$ and $f_{ab}\hat{X}^a\hat{h}^b = f_{ab}\hat{h}^b\hat{X}^a$, to get

$$\hat{X}^b\hat{G}\hat{X}^c \equiv \hat{G}\hat{h}^b\hat{G}\hat{h}^c\hat{G} + \frac{1}{2}\hat{G}\hat{h}^{bc}\hat{G} + \hat{\Delta}^{bc}_1 + \hat{\Delta}^{bc}_2, \quad (57)$$

$$\hat{\Delta}^{bc}_1 = \frac{1}{2}\left(\hat{G}\hat{X}^b\hat{X}^c + \hat{X}^b\hat{X}^c\hat{G}\right), \quad (58)$$

$$\hat{\Delta}^{bc}_2 = \frac{1}{2}i\hat{G}\left(\{\hat{h}^b, \hat{X}^c\} - \{\hat{h}^c, \hat{X}^b\}\right)\hat{G}, \quad (59)$$

where $\hat{\Delta}^{ab}_1$ is a symmetric tensor operator, and $\hat{\Delta}^{bc}_2$ is antisymmetric; here $\{A, B\} \equiv AB + BA$ is the anticommutator (symmetrized product). Now reassemble the full operator product in the expression for $\Gamma^{(2b)}$, and examine

$$\hat{\Delta}_1 \equiv f_{ab}f_{cd}\hat{G}\hat{h}^a\hat{\Delta}^{bc}_1\hat{h}^d\hat{G} = \frac{1}{2}f_{ab}f_{cd} \times \left((\hat{G}\hat{h}^a\hat{G})\hat{X}^b\hat{X}^c\hat{h}^d\hat{G} + \hat{G}\hat{h}^a\hat{X}^b\hat{X}^c\hat{G}\hat{h}^d\hat{G}\right).$$
Expanding \((\hat{G}\hat{h}^a\hat{G})\) as \(i(\hat{G}\hat{X}^a - \hat{X}^a\hat{G})\) then gives

\[
\hat{\Delta}_1 = -\frac{1}{2}f_{ab}f_{cd}\left(\hat{X}^a\hat{G}\hat{X}^b\hat{X}^c\hat{h}^d\hat{G} - \hat{G}\hat{h}^a\hat{X}^b\hat{X}^c\hat{G}\hat{X}^d\right) \\
= -\frac{1}{2}f_{ab}f_{cd}\left(\hat{X}^a\hat{G}\hat{X}^b\hat{X}^c\hat{h}^d\hat{G} - \hat{G}\hat{h}^d\hat{X}^c\hat{X}^b\hat{G}\hat{X}^a\right) \\
= -\frac{1}{4}f_{ab}f_{cd}\left(\{\hat{X}^a, \hat{G}\{\hat{X}^b\hat{X}^c, \hat{h}^d\}\hat{G}\}\right) \\
- \frac{1}{4}f_{ab}f_{cd}\left(\{\hat{X}^a, \hat{G}\{\hat{X}^b\hat{X}^c, \hat{h}^d\}\hat{G}\}\right).
\]

Using the identities \(\text{Tr}([\hat{A}, \hat{B}]) \equiv 0\), and \(\text{Tr}([\hat{A}, \hat{B}]) \equiv 2\text{Tr}(\hat{A}\hat{B})\), plus the cyclic property of the trace, gives

\[
\text{Tr}\left(\hat{\Delta}_1\right) = \frac{1}{2}f_{ab}f_{cd}\text{Tr}\left(\hat{X}^a\hat{G}\hat{X}^b\hat{X}^c\hat{h}^d\hat{G}\right). \tag{60}
\]

Next examine

\[
\hat{\Delta}_2 \equiv f_{ab}f_{cd}\hat{G}\hat{h}^a\hat{D}_2\hat{h}^d\hat{G} = \frac{1}{4}f_{ab}f_{cd} \times (\hat{G}\hat{h}^a\hat{G})(\{\hat{h}^b, \hat{X}^c\} - \{\hat{c}^b, \hat{X}^b\})(\hat{G}\hat{h}^d\hat{G}). \tag{61}
\]

Again expanding \((\hat{G}\hat{h}^a\hat{G})\) as \(i(\hat{G}\hat{X}^a - \hat{X}^a\hat{G})\) gives

\[
\hat{\Delta}_2 = \frac{1}{4}f_{ab}f_{cd}\hat{G}\hat{X}^a(\hat{X}^b\hat{h}^c - \hat{h}^c\hat{X}^b)\hat{G}\hat{X}^d \\
+ \frac{1}{4}f_{ab}f_{cd}\hat{G}\hat{X}^a(\{\hat{h}^b, \hat{X}^c\} - \{\hat{c}^b, \hat{X}^b\})\hat{G}\hat{X}^d \\
- \frac{1}{4}f_{ab}f_{cd}\left(\hat{G}\hat{X}^a(\{\hat{h}^b, \hat{X}^c\} - \{\hat{c}^b, \hat{X}^b\})\hat{G}\hat{X}^d \\
- \hat{X}^a\hat{G}(\{\hat{X}^c, \hat{h}^b\})\hat{G}\hat{X}^d\right).
\]

Use \(\hat{h}^b = [\hat{h}, i\hat{X}^b]\) to get

\[
\hat{\Delta}_2 = -\frac{1}{2}f_{ab}f_{cd}\hat{G}\hat{X}^a\hat{X}^c\hat{X}^b\hat{G} \\
+ \frac{1}{4}f_{ab}f_{cd}\hat{G}\hat{X}^a(\{\hat{h}^b, \hat{X}^c\} - \{\hat{c}^b, \hat{X}^b\})\hat{G}\hat{X}^d \\
+ \frac{1}{4}f_{ab}f_{cd}\left(\hat{G}\hat{X}^a(\{\hat{h}^b, \hat{X}^c\} - \{\hat{c}^b, \hat{X}^b\})\hat{G}\hat{X}^d \\
- \hat{X}^a\hat{G}(\hat{X}^c, \hat{h}^b)\hat{G}\hat{X}^d\right).
\]

Now take the trace; the third term is a commutator, so is traceless, and the second term vanishes using the result that if \(\hat{O}^{(ab)}\) is an antisymmetric tensor operator, \(f_{ab}f_{cd}\text{Tr}(\hat{X}^a\hat{O}^{(bc)}\hat{X}^d) = 0\). The remaining two terms survive:

\[
\text{Tr}\left(\hat{\Delta}_2\right) = -\frac{1}{2}\text{Tr}\left(\hat{G}\hat{h}^{(2)}\hat{G}\right) + \frac{1}{2}f_{ab}f_{cd}\text{Tr}\left(\hat{X}^a\hat{G}\hat{h}^{bc}\hat{X}^d\hat{G}\right).
\]
The second of these terms is equal to $-\text{Tr}(\hat{\Delta}_1)$. Then assembling the various parts together gives $\Gamma^{(2)}(\omega) = \text{Tr}(\hat{\Gamma}^{(2)}(\omega))$, with $\hat{\Gamma}^{(2)}$ given by (14), a representation of $\Gamma^{(2)}$ as the trace of a sum of gauge-invariant operators. This has been achieved at the expense of a rather onerous amount of algebraic manipulation, for which the “roadmap” was not obvious. In fact, the result (14) was initially obtained using numerical linear-algebra methods described in the Appendix, and the above exercise was carried out merely to demonstrate that the result can indeed be obtained algebraically.

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DATA AVAILABILITY STATEMENT

Data sharing is not applicable to this article as no new data were created or analyzed in this study.

Appendix A: Numerical linear-algebra methods

This Appendix on numerical linear-algebra techniques adapted to this problem is included for the possible guidance of any further explorations of the structure of $\hat{\Gamma}^{(n)}$ for $n \geq 3$, that might be undertaken.

Since the process of transforming gauge-invariant (but not explicitly gauge-invariant) expressions for $\Gamma^{(n)}$ in the form of (16)-(18) to the explicitly-gauge-invariant form (22) purely algebraic, it can be formulated in terms of the associative algebra of operators $\{\hat{X}^a, a = 1, \ldots d\}$ which obey $[\hat{X}^a, \hat{X}^b] = 0$, and operators $\hat{G}(\omega), \hat{G}^{-1}(\omega)$ which obey $\hat{G}\hat{G}^{-1} = \hat{G}^{-1}\hat{G} = 1$, with no other relations, (plus a set of antisymmetric c-number symbols $f_{ab} = -f_{ba}$).

The process can be carried using a generic $N \times N$ matrix representation of the algebra, provided $N$ is not so small that extra non-generic linear dependencies are introduced (for example, the choice $N = 1$ is clearly too small).

Furthermore, the algebraic structures are independent of $\omega$, which is the key to the nu-
merical linear-algebra approach that uses the data provided by multiple instances of representations of the algebra with different \( \omega \), to define an overcomplete set of linear equations, that can be numerically solved using a least-squares method, to produce (up to floating-point precision) a set of weights which are \textit{a priori} known to be rational if computed in exact arithmetic, and so can be recovered from the finite-precision complex floating-point numerical linear-algebra results, which are in the form of simple recognizable rationals plus small residual errors from finite machine precision.

First choose \( N \) and \( d \geq 2 \), and randomly populate the diagonal entries of real diagonal \( N \times N \) matrices \( ˆX^a, a = 1, \ldots, d \), and the \( \frac{1}{2}d(d-1) \) independent entries of the real antisymmetric covariant tensor \( F_{ab} \), and from it obtain \( f_{ab} \). The algebraic structure is independent of \( d \) provided an antisymmetric symbol \( f_{ab} \) exists, so the choice \( d = 2 \) suffices. The choice \( N \geq 12 \) worked for studying \( \Gamma^{(3)} \); failures were observed at smaller \( N \), but their origin was not investigated in any detail. Next generate a random complex Hermitian \( N \times N \) matrix \( ˆh \), and diagonalize it, to allow \( ˆG(\omega) = (\omega \mathbb{I} - ˆh)^{-1} \) to be obtained for any desired choice of \( \omega \) for which \( ˆG(\omega) \) is non-singular. (Since the result is algebraic, is is not necessary to insist that \( ˆh \) is Hermitian, but doing so guarantees \( ˆG(\omega) \) is non-singular if the imaginary part of \( \omega \) is non-vanishing.)

Then, for a treatment of \( \Gamma^{(n)}(\omega) \), compute the \( N \times N \) matrix representations of \( ˆh^{a_1 \ldots a_m}_m \) for all \( 1 \leq m \leq n \). Next, for any choice of the c-number covariant vector \( \delta A_a \) compute the diagonal matrices \( ˆA_a = -\frac{1}{2} F_{ab} ˆX^b + \delta A_a \mathbb{I} \), and compute the matrix representations of \( ˆh^{(1)}, \ldots, ˆh^{(n)} \). Use these, together with \( ˆG(\omega_i) \), to compute \( \Gamma^{(n)}(\omega_i) \), Repeating this with different choices of \( \delta A_a \) (and getting the same result, at least to the rounding accuracy of floating-point arithmetic) verifies the gauge invariance of the initial expression of type (46)-(48) for \( \Gamma^{(n)}(\omega) \).

Next catalog a complete set of the operators \( \hat{\Gamma}^{(n)}_{m_k, \alpha} \) that can be used to represent \( \hat{\Gamma}^{(n)} \). These can be classified by partitions of \( 2n \) into \( k \) parts equal to or smaller than \( n \), which is only possible for \( 2 \leq k \leq 2n \). For a given partition, the set of all distinct permutations of the parts gives the set of possible values of \( m_k = \{m_1, m_2, \ldots, m_k\} \). The operator product defined by a given \( m_k \) has \( 2n \) contravariant indices that need to be paired by contraction with the \( 2n \) covariant indices on the \( n \) instances of \( f_{ab} \). There are \( (2n - 1)!! \) possible pairings of \( 2n \) indices, but not all are allowed, as indices on the same instance of \( ˆh^{a_1 \ldots a_m}_m \) cannot be paired. When constructing a given operator specified by a distinct permutation of a
partition and an index pairing, the left-right ordering of the indices in a paring factor \(f_{ab}\) should match that of the indices in the operator product that it pairs. This set of operators is invariant under a conjugation that simultaneously reverses the order of the operator product (and hence the order of \(\{m_1, \ldots, m_k\}\)) and the indices of all factors \(f_{ab}\), which preserves the rule for the index ordering in \(f_{ab}\). Individual operators are either self-conjugate, of grouped into mutually-conjugate pairs by this operation. The reduced basis (with dimension \(D'\)) of functions of \(\omega\) consists of the traces of each self-conjugate operator, plus the sum of the traces of each mutually-conjugate pair. For each reduced-basis function, the operator inside the trace has the symmetry \((12)\).

Denote the set of functions just constructed by \(\{f_i(\omega), i = 1, \ldots, D'\}\). For \(n > 1\) there is linear dependence between these functions, and a linearly-independent set of \(R' < D'\) of these functions must be selected. This is done by evaluating them on \(D'\) distinct randomly-selected complex values \(\{\omega_i, i = 1, \ldots, D'\}\), and carrying out a rank-revealing procedure on the \(D' \times D'\) complex matrix \(A_{ij} = f_j(\omega_i)\). Linear dependence must be removed from the basis set by removing redundant functions. Once this reduction has been made, there is a unique expansion of \(\Gamma^{(n)}(\omega)\) in terms of the \(R'\) retained members of the reduced basis, as a weighted sum with rational weights. The recommended method of solution is to use a least-squares solution to a substantially overcomplete set of linear equations

\[
\Gamma^{(n)}(\omega_i) = \sum_{j=1}^{R'} f_j(\omega_i)C_j, \quad i = 1, \ldots, i_{\text{max}} > R',
\]  

(A1)

where the \(C_j\) will be recognizable rationals (up to floating-point precision). Increasing the overcompleteness of the data used for the least-squares fit seems to reduce the residual errors. The \(D' - R'\) omitted functions can also be obtained as weighted sums (with rational weights of the \(R'\) retained functions by the same method). Once the weights of \(\Gamma^{(n)}\) and the linear relations are obtained in rational form, they can be tested by numerical evaluation at randomly-chosen \(\omega\). All further manipulations to optimize the expressions, or find a “canonical” form, are done in exact integer arithmetic.

The arbitrariness in this procedure is in the selection of the linearly-independent basis of \(R'\) functions out of the full set of \(D'\) functions of the reduced basis. One possibly-optimal structured approach is to order the basis by the number of parts in \(m_k\) (a partial ordering), from \(k = 2\) to \(k = 2n\), and test for linear dependence among the traces of the first \(j\) operators in the list, sequentially for \(j = 2, 3, 4, \ldots\). Each time linear dependence is found, eliminate
the last operator or operator-pair. When the list is exhausted, $R'$ entries will remain. In such a chosen subset, for $n = 3$, the weights $C_{m_k,\alpha}$ were integers, and less than $R'$ of the basis functions were included in the expression for $\Gamma^{(3)}$ (2 out of $R' = 15$ integer weights were “unexpected” zeroes). A result obtained using this method is (for real $\omega$)

$$\hat{\Gamma}^{(3)} = 12\hat{\Gamma}^{(14|25|36)}_{\{3,3\}}$$

$$+ 12\hat{\Gamma}^{(14|25|36)}_{\{3,2,1\}} - 8\hat{\Gamma}^{(16|24|35)}_{\{1,2,2,1\}} - 12\hat{\Gamma}^{(14|25|36)}_{\{2,1,1,2\}}$$

$$+ 8\hat{\Gamma}^{(15|26|34)}_{\{2,1,1,2\}} - 4\hat{\Gamma}^{(13|25|46)}_{\{2,2,1,1\}} + \text{H.c.)}$$

$$+ 12\hat{\Gamma}^{(14|25|36)}_{\{3,1,1,1\}} + \text{H.c.)} + 4\hat{\Gamma}^{(13|26|45)}_{\{2,1,1,1,1\}} + \text{H.c.)}$$

$$- 4\hat{\Gamma}^{(12|34|56)}_{\{1,3,1,1,1\}} - 6\hat{\Gamma}^{(16|25|34)}_{\{1,1,1,1,1,1\}}.$$  \(\text{(A2)}\)

Here the superscripts on the operators on the RHS indicate how the six contravariant indices (numbered from left to right) in the operator product should be contracted in pairs using the three factors of $f_{ab}$; for example

$$\hat{\Gamma}^{(14|25|36)}_{\{3,2,1\}} = \frac{1}{3!2!} f_{a_1a_2} f_{a_3a_4} f_{a_5a_6}$$

$$\times \hat{G} h_{a_1} h_{a_2} h_{a_3} h_{a_4} h_{a_5} h_{a_6} \hat{G}.$$  \(\text{(A3)}\)

For complex $\omega$, the “Hermitian conjugate” (H.c.) should be reinterpreted so as not to include complex conjugation of $\omega$ (or as Hermitian conjugation of the operator followed by complex conjugation of $\omega$).

The integer forms of the linear relations (of which there are 31, for $n = 3$) could then be used to attempt to reduce the number of non-zero terms in the integer-weighted expression for $\Gamma^{(n)}$, leaving its trace unchanged, but this was left undone, in the absence of an obvious algorithm, as there was no immediate need for results with $n > 2$. In fact, the form (A2) may well be optimal for $n = 3$.

**REFERENCES**

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