MODELING AND COMPUTATION OF KUBO CONDUCTIVITY FOR 2D INCOMMENSURATE BILAYERS

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Abstract. This paper presents a unified approach to the modeling and computation of the Kubo conductivity of incommensurate bilayer heterostructures at finite temperature.

Firstly, we derive an expression for the large-body limit of Kubo-Greenwood conductivity in terms of an integral of the conductivity function with respect to a current-current correlation measure. We then observe that the incommensurate structure can be exploited to decompose the current-current correlation measure into local contribution and deduce an approximation scheme which is exponentially convergent in terms of domain size.

Secondly, we analyze the cost of computing local conductivities via Chebyshev approximation. Our main finding is that if the inverse temperature β is sufficiently small compared to the inverse relaxation time η, namely $\beta \lesssim \eta^{-1/2}$, then the dominant computational cost is $\mathcal{O}(\eta^{-3/2})$ inner products for a suitably truncated Chebyshev series, which significantly improves on the $\mathcal{O}(\eta^{-2})$ inner products required by a naive Chebyshev approximation.

Thirdly, we propose a rational approximation scheme for the low temperature regime $\eta^{-1/2} \lesssim \beta$, where the cost of the polynomial method increases up to $\mathcal{O}(\beta^2)$, but the rational scheme scales much more mildly with respect to β.

1. Introduction

Periodic bilayer 2D heterostructures are typically studied using Bloch Theory [14]. This technique breaks down in the case of *incommensurate* heterostructures, where the ensemble is not periodic, though each individual sheet may maintain its own periodicity. Previous work introduced a configuration space representation of incommensurate materials, where incommensurate systems are classified by local configurations [4, 5, 16], motivated by concepts introduced in [1, 17]. The configuration space approach proved to be useful for numerical simulation of the density of states [5]. In the present paper, we consider conductivity, which proves to be significantly more challenging to compute numerically, especially in the low temperature and long dissipation time regime. We shall restrict ourselves to the tight-binding model, which has the advantage of being designed for large systems while maintaining accurate quantum information.

Our first main result will be to prove that the Kubo conductivity is well defined in the thermodynamic limit, as was done for the density of states in [16], and has a similar formulation in terms of configuration space integrals. For each local configuration, we compute a local conductivity using the classical current-current correlation

formulation [14] and then integrate over a compact parametrization of all local configurations. Specifically, in Theorem 2.1, we obtain an exponential rate of convergence of the averaged local conductivities to the thermodynamic limit. Related results have also been obtained within the framework of C* algebras [4] and for a disordered lattice gas [17], whereas our approach uses the direct matrix framework developed in [16].

Our second main result will be the cost analysis of a linear-scaling conductivity algorithm based on Chebyshev approximation, which is the direct analogue of the Fermi Operator Expansion (FOE) for the density matrix [11, 12] and the Kernel Polynomial Method (KPM) for the density of states [16, 21]. Both of these methods expand their respective quantity of interest q in terms of some functionals c_k of the Chebyshev polynomials $T_k(E)$ of the hamiltonian matrix H,

$$q = \sum_{k=0}^{\infty} c_k\big(T_k(H)\big),$$

and then truncate this series to a finite set of indices $K = \{0, \ldots, k_{max}\}$ to allow for numerical evaluation. This truncation is well justified since in both cases it can be shown that the contributions from large matrix powers k decay exponentially. However, unlike the density matrix and the density of states, the conductivity σ requires an expansion in terms of pairs of Chebyshev polynomials,

$$(1.1) \qquad \sigma = \sum_{k_1,k_2=0}^{\infty} c_{k_1,k_2}\big(T_{k_1}(H), T_{k_2}(H)\big),$$

which allows for more complex decay behavior and hence necessitates a more careful analysis of how to choose the truncation indices $K \subset \mathbb{N}^2$. Indeed, we will see in Section 3 that the shape of the large terms in (1.1) depends heavily on the values of the inverse temperature β and inverse relaxation time η and changes from "wedge along the diagonal" for $\beta \lesssim \eta^{-1/2}$ to "equilateral triangle" for $\beta \gtrsim \eta^{-1}$, see Figure 3, and the number of significant coefficients changes correspondingly from $\mathcal{O}\big(\eta^{-3/2}\big)$ for $\beta \lesssim \eta^{-1/2}$ to $\mathcal{O}\big(\beta^2\big)$ for $\beta \gtrsim \eta^{-1}$, see Table 1.

In the high-temperature regime $\beta \lesssim \eta^{-1/2}$, this implies that the cost of our algorithm, which is asymptotically proportional to the number of terms in (1.1), is significantly lower than the $\mathcal{O}\big(\eta^{-2}\big)$ which would result if we ignored the special form of the decay in (1.1). In the low-temperature regime $\beta \gtrsim \eta^{-1}$, however, the $\mathcal{O}\big(\beta^2\big)$ scaling of the polynomial algorithm is rather restrictive but can be overcome by a rational approximation as we will demonstrate in Subsection 3.3.

The new algorithms we propose represent a significant first step towards reliable and efficient simulation of conductivity in incommensurate heterostructures at low temperatures and long relaxation times.

1.1. **Notation.**
- We denote the L^2 norm, the operator norm, and the Frobenius norm over discrete space as $\|\cdot\|_2, \|\cdot\|_{\ell^2}, \|\cdot\|_{\mathrm{op}}, \|\cdot\|_{\mathrm{F}}$. The supremum norm of a function $f : X \to Y$ on a domain $\Omega \subset X$ is denoted by $\|f\|_\Omega$.
- $B_r = \{x \in \mathbb{R}^2 : |x| < r\}$.
- For vectors $v, w \in \mathbb{R}^N$ and $A \in \mathbb{R}^{N \times N}$, we have $\langle v|w \rangle = \sum_{i=1}^{N} v_i w_i^*$ and $\langle v|A|w \rangle = \sum_{i,j=1}^{N} A_{ij} v_i w_j^*$.
- $\mathcal{L}(\ell^2(\Omega))$ are the bounded operators from $\ell^2(\Omega)$ to itself.
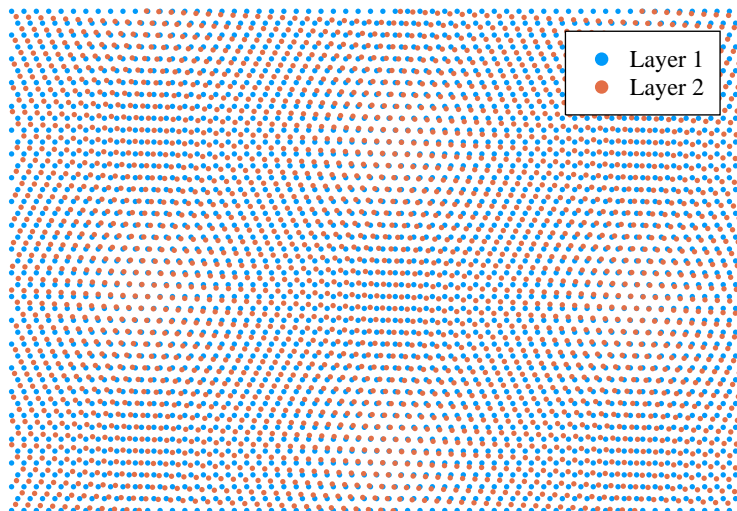
FIGURE 1. Hexagonal bilayer lattices with a 2.5° relative twist.

- We write "$f(x) = \mathcal{O}\big(g(x)\big)$ for $x \to x_0$" if $\lim_{x \to x_0} \frac{|f(x)|}{|g(x)|} \in [0, \infty)$, and "$f(x) = \Theta\big(g(x)\big)$ for $x \to x_0$" if $\lim_{x \to x_0} \frac{|f(x)|}{|g(x)|} \in (0, \infty)$.

2. CONDUCTIVITY IN INCOMMENSURATE BILAYERS

2.1. **Incommensurate bilayer.** Informally, an *incommensurate bilayer* is a union of two infinite sheets of material, which are individually periodic, but when joined together become aperiodic (see Fig. 1 for an example). To formalize this concept, let

$$\mathcal{R}_\ell := \{A_\ell m \,:\, m \in \mathbb{Z}^2\},$$

with non-singular $A_\ell \in \mathbb{R}^{2 \times 2}$, be two Bravais lattices defining the periodicity of the two sheets indexed by $\ell \in \{1, 2\}$. For future reference, let $\tau(1) = 2, \tau(2) = 1$ denote the transposition operator, and let

$$\Gamma_\ell = \{A_\ell \beta \,:\, \beta \in [0, 1)^2\}$$

denote the unit cell for $\mathcal{R}_\ell$. In terms of the reciprocal lattices

$$\mathcal{R}_\ell^* := \{2\pi A_\ell^{-T} n \,:\, n \in \mathbb{Z}^2\},$$

we can state the assumption of incommensurability as follows:

Assumption 2.1. *The bilayer $\mathcal{R}_1 \cup \mathcal{R}_2$ is* incommensurate, *that is,*

$$v + \mathcal{R}_1^* \cup \mathcal{R}_2^* = \mathcal{R}_1^* \cup \mathcal{R}_2^* \quad \Leftrightarrow \quad v = (0, 0).$$

As shown in [4, 13, 16], incommensurability leads to a form of ergodicity that allows us to replace sampling over bilayer sites with sampling over bilayer shifts or disregistry (henceforth called *configurations*; cf. Remark 2.1).

Lemma 2.1. *Let $\mathcal{R}_1$ and $\mathcal{R}_2$ satisfy Assumption 2.1, and $g \in C_{\mathrm{per}}(\Gamma_{\tau(\ell)})$, then*

$$\lim_{r \to \infty} \frac{1}{\#\mathcal{R}_\ell \cap B_r} \sum_{R_\ell \in \mathcal{R}_\ell \cap B_r} g(R_\ell) = \frac{1}{|\Gamma_{\tau(\ell)}|} \int_{\Gamma_{\tau(\ell)}} g(b) db,$$

where $B_r = \{x \in \mathbb{R}^2 \,:\, |x| \leq r\}$.

Lemma 2.1 is the basis of an efficient algorithm for computing the density of states in incommensurate bilayers [16]. In the present work, it plays a similar role in the computation of transport properties.

Remark 2.1. *The relative shift b between the layers parameterizes the local environment of sites uniquely. For example, if we let $R \in \mathcal{R}_1$, we have*

$$\mathcal{R}_1 \cup \mathcal{R}_2 + R = \mathcal{R}_1 \cup (\mathcal{R}_2 + R) = \mathcal{R}_1 \cup (\mathcal{R}_2 + \mathrm{mod}_2(R)),$$

where $\mathrm{mod}_2(R) = R + R' \in \Gamma_2$ for an appropriately chosen $R' \in \mathcal{R}_2$. The shift $b = \mathrm{mod}_2(R)$ therefore selects the new environment of site R, $\mathcal{R}_1 \cup (\mathcal{R}_2 + \mathrm{mod}_2(R))$.

As a consequence of this observation, we will from now on refer to the shift b as a configuration, *and the space of configurations (Γ_1, Γ_2) as* configuration space.

2.2. **Tight-binding model.**

The tight-binding model [14] is an electronic structure model, that has been successfully employed in the modeling of two-dimensional heterostructures [5, 9, 10]. For the purpose of the present work, it will be sufficient to formulate it at an abstract and slightly simplified level.

Let $\mathcal{A}_\ell$ denote the index set of atomic orbitals for each lattice site of sheet ℓ, then the degree of freedom space for the entire bilayer is given by

$$(2.1) \qquad \Omega = (\mathcal{R}_1 \times \mathcal{A}_1) \cup (\mathcal{R}_2 \times \mathcal{A}_2).$$

(Note that the orbital set $\mathcal{A}_\ell$ also accounts for multi-lattice structures in the configuration of atomic nuclei.) The tight-binding model is described by an operator (or, more intuitively, an infinite matrix) $H \in \mathcal{L}(\ell^2(\Omega))$,

$$(2.2) \qquad H_{R\alpha, R'\alpha'} = h_{\alpha\alpha'}(R - R').$$

Assumption 2.2. *We assume $h_{\alpha\alpha'} \in C^n(\mathbb{R}^2)$ for some $n > 0$, and is exponentially localized for $R = (R_1, R_2) \in \mathbb{R}^2$:*

$$(2.3) \qquad \begin{aligned} |h_{\alpha\alpha'}(R)| &\lesssim e^{-\gamma_0|R|}, \\ |\partial_{R_1}^{m'} \partial_{R_2}^m h_{\alpha\alpha'}(R)| &\lesssim e^{-\gamma_{m'm}|R|}, \end{aligned}$$

for $\gamma_{m'm} > 0$ and $\gamma_0 > 0$, $m + m' \leq n$. Further, we assume

$$h_{\alpha\alpha'}(R) = h_{\alpha'\alpha}(-R).$$

Note that H is symmetric. Since the infinite-dimensional electronic structure problem (diagonalizing H) cannot be solved directly, we first consider a projection to a finite subset of the degree of freedom space

$$(2.4) \qquad \Omega^r = \left[\left[\mathcal{R}_1 \cap B_r \right] \times \mathcal{A}_1 \right] \cup \left[\left[\mathcal{R}_2 \cap B_r \right] \times \mathcal{A}_2 \right], \qquad \text{for } r > 0.$$

Let the projected Hamiltonian be the matrix $H^r = H|_{\Omega^r}$, then we can solve the corresponding eigenvalue problem

$$(2.5) \qquad H^r v_i = \varepsilon_i v_i,$$

with $\|v_i\|_{\ell^2} = 1$. A wide range of physical quantities of interest can be inferred from the eigenpairs (ε_i, v_i), including electronic conductivity which we discuss next.

Under Assumption 2.2, the spectrum of H^r is uniformly bounded as $r \to \infty$. Upon shifting and rescaling the Hamiltonian, we may therefore assume, without loss of generality, that $\|H\|_{\mathrm{op}} < 1$.

2.3. **Current-current correlation measure.** The conductivity tensor will be defined in terms of the *current-current correlation measure*. To introduce it, let $p \in \{1, 2\}$, and $A \in \mathbb{R}^{\Omega^r \times \Omega^r}$ be a Hamiltonian. Then the *velocity operator* $\partial_p A \in \mathbb{R}^{\Omega^r \times \Omega^r}$ is given by

$$(2.6) \qquad [\partial_p A]_{R\alpha, R'\alpha'} = i(R' - R)_p A_{R\alpha, R'\alpha'}, \qquad R\alpha, R'\alpha' \in \Omega^r.$$

Equivalently, we can define $\partial_p A$ in terms of a commutator, $\partial_p A = i[A, \mathbf{R}_p] = i(A\mathbf{R}_p - \mathbf{R}_p A)$, where $\mathbf{R}_p$ is understood as a diagonal matrix

$$[\mathbf{R}_p]_{R\alpha, R'\alpha'} = \delta_{\alpha\alpha'} \delta_{RR'} R_p.$$

The matrix-valued current-current correlation measure $\bar{\mu}^r$ on the finite system Ω^r, is defined by [7]

$$(2.7) \qquad \begin{aligned} &\int_{\mathbb{R}^2} \phi(E_1, E_2) d\bar{\mu}^r(E_1, E_2) \\ &= \left[\frac{1}{|\Omega^r|} \sum_{i,i'} \phi(\varepsilon_i, \varepsilon_{i'}) \operatorname{Tr}\left[|v_i\rangle \langle v_i | \partial_p H^r | v_{i'} \rangle \langle v_{i'} | \partial_{p'} H^r | \right] \right]_{p,p'=1,2} \end{aligned}$$

where (ε_i, v_i) denote the eigenpairs of the Hamiltonian H^r, and E_1, E_2 are integration variables. (In particular, the indices in E_1, E_2 are unrelated to the indices of the layers.)

We note that (2.7) is the current-current correlation measure since the current operator $i[\mathbf{R}_p, A]$ is the negative of the velocity operator $\partial_p A = i[A, \mathbf{R}_p]$. For the sake of simplicity of notation, we will henceforth simply drop the brackets $[\bullet]_{p,p'}$ on the right-hand side of (2.7). In numerical computations, we will approximate general functions $\phi(E_1, E_2)$ by sums of products of univariate functions

$$\phi(E_1, E_2) \approx \tilde{\phi}(E_1, E_2) := \sum_{(k_1, k_2) \in K} \phi_{k_1}(E_1) \phi_{k_2}(E_2),$$

where K is a finite index-set. In this case, we can rewrite (2.7) (with ϕ replaced with $\tilde{\phi}$) as

$$(2.8) \qquad \int_{\mathbb{R}^2} \tilde{\phi}(E_1, E_2) \, d\bar{\mu}^r(E_1, E_2) = \frac{1}{|\Omega^r|} \sum_{(k_1, k_2) \in K} \operatorname{Tr}\left[\phi_{k_1}(H_r) \partial_p H^r \phi_{k_2}(H_r) \partial_{p'} H^r \right].$$

For brevity we collect the set of conductivity parameters $\zeta = (\beta, \eta, \omega, E_F) \in \mathcal{P} = \mathbb{R}_+^2 \times \mathbb{R}^2$. The conductivity tensor for the finite system Ω^r can now be defined by

$$(2.9) \qquad \bar{\sigma}^r = \int_{\mathbb{R}^2} F_\zeta(E_1, E_2) d\bar{\mu}^r(E_1, E_2),$$

where the *conductivity function* F_ζ is defined as follows: if e is the elementary charge, $\hbar$ the Planck constant, E_F the Fermi-level of the system, and $f_\beta(E) = (1 + e^{\beta(E-E_F)})^{-1}$ the Fermi-Dirac distribution, then

$$(2.10) \qquad F_\zeta(E_1, E_2) = \frac{ie^2}{\hbar^2} \frac{f_\beta(E_1 - E_F) - f_\beta(E_2 - E_F)}{(E_1 - E_2)(E_1 - E_2 + \omega + i\eta)}.$$

We note that for any reasonable model, it holds that $E_F \in (-1, 1)$ since otherwise the Hamiltonian would only involve either valence or conductance band states.

Our aim throughout the remainder of Section 2 is to show that the thermodynamic limit $\sigma := \lim_{r \to \infty} \bar{\sigma}^r$ exists, and to establish a configuration space representation with an exponential convergence rate.

Remark 2.2. *The formulation* (2.9) *is consistent with the formulation for periodic systems* [14] *and with the* C* *algebra formulation of a generalized Kubo formula for incommensurate bilayers* [4]. *We will obtain a definition through a thermodynamic limit argument using a direct matrix formulation, thus giving this formulation additional justification. Here we focus on the thermodynamic limit taken as a sequence of circular domains, though we observe that this could be extended to a more general class of limit sequences. In particular, as long as the sequence does not generate a proportionally imbalanced boundary relative to bulk, the sequence will converge to the same limit. We restrict ourselves to the circular domain limit to avoid distraction from the key points of this paper.*

Implicitly, $\bar{\sigma}^r$ and later σ depend on the model parameters $\zeta = (\beta, \eta, \omega, E_F)$, but for the sake of brevity of notation, this dependence is suppressed. However, we emphasize that for a quantitative convergence analysis the parameters β, η are in fact crucial since they characterize the region of analyticity of the conductivity function F_ζ.

2.4. **Local current-current correlation measure.** In order to pass to the limit as $r \to \infty$, we follow the ideas in [16] and define a local (or, projected) conductivity, which will later take the role of g in Lemma 2.1. To motivate, we first observe that the expression in (2.7) can be written as

$$\int_{\mathbb{R}^2} \phi(E_1, E_2) \, d\bar{\mu}^r(E_1, E_2) = \frac{1}{|\Omega^r|} \sum_{i,i'} \phi(\varepsilon_i, \varepsilon_{i'}) \mathrm{Tr}\big[|v_i\rangle\langle v_i|\partial_p H^r|v_{i'}\rangle \langle v_{i'}|\partial_{p'} H^r|\big]$$

$$= \frac{1}{|\Omega^r|} \sum_{R\alpha \in \Omega^r} \left[\sum_{i,i'} \phi(\varepsilon_i, \varepsilon_{i'}) \langle e_{R\alpha}|v_i\rangle\langle v_i|\partial_p H^r|v_{i'}\rangle \langle v_{i'}|\partial_{p'} H^r|e_{R\alpha}\rangle \right].$$

Here we have defined $e_{R\alpha} \in \ell^2(\Omega_r)$ via

$$[e_{R\alpha}]_{R'\alpha'} = \delta_{\alpha\alpha'}\delta_{RR'}, \quad R'\alpha' \in \Omega_r,$$

and (ε_i, v_i) are the eigenpairs of H^r. We see that the trace is decomposed into projections onto diagonal elements. We further observe that the left-most sum, normalized by $\frac{1}{|\Omega_r|}$, looks remarkably similar to a discretized integral. The crucial step then is how to realize the thermodynamic limit as an integral. We will formalize this with the help of Lemma 2.1, which will convert this expression into an integral over configuration space. To that end, we define the Hamiltonian for a shifted configuration,

$$(2.11) \qquad [H_\ell(b)]_{R\alpha, R'\alpha'} = h_{\alpha\alpha'}\big(b(\delta_{\alpha \in \mathcal{A}_{\tau(\ell)}} - \delta_{\alpha' \in \mathcal{A}_{\tau(\ell)}}) + R - R'\big), \quad R\alpha, R'\alpha' \in \Omega.$$

Likewise, we have $H_\ell^r(b) = H_\ell(b)|_{\Omega^r}$. Since $H_\ell^r(b)$ is symmetric, we can define the local current-current correlation measure $\mu_\ell^r[b]$ for a finite system Ω^r, at configuration b, in layer ℓ, via

$$(2.12) \quad \int_{\mathbb{R}^2} \phi(E_1, E_2) \, d\mu_\ell^r[b] = \sum_{\substack{i,i' \\ \alpha \in \mathcal{A}_\ell}} \phi(\varepsilon_i, \varepsilon_{i'}) \langle e_{0\alpha}|v_i\rangle\langle v_i|\partial_p H_\ell^r(b)|v_{i'}\rangle \langle v_{i'}|\partial_{p'} H_\ell^r(b)|e_{0\alpha}\rangle,$$

where (ε_i, v_i) are the eigenpairs of $H_\ell^r(b)$ (and thus implicitly depend on r, ℓ, and b).

Our next result states that $\lim_{r\to\infty} \mu_\ell^r[b]$ is well-defined. To that end, we first define a strip in the complex plane

$$S_a = \{z \mid \mathrm{Re}(z) \in [-a-1, a+1], \mathrm{Im}(z) \in [-a, a]\}.$$

Lemma 2.2. *Under Assumptions 2.1 and 2.2, there exist unique measures $\mu_\ell[b], \ell = 1, 2$, such that for all F that are analytic on $S_a \times S_a$,*

$$\int_{\mathbb{R}^2} F(E_1, E_2) d\mu_\ell^r[b](E_1, E_2) \to \int_{\mathbb{R}^2} F(E_1, E_2) d\mu_\ell[b](E_1, E_2)$$

with the rate

$$\left| \int_{\mathbb{R}^2} F(E_1, E_2) d\mu_\ell^r[b](E_1, E_2) - \int_{\mathbb{R}^2} F(E_1, E_2) d\mu_\ell[b](E_1, E_2) \right|$$
$$\lesssim \sup_{z,z' \in S_a \setminus S_{a/2}} |F(z, z')| e^{-\gamma ar - c \log(a)},$$

for some $c, \gamma > 0$. Furthermore, we have that the maps

$$b \mapsto \int_{\mathbb{R}^2} F(E_1, E_2) d\mu_\ell^r[b](E_1, E_2) \in C^n(\Gamma_{\tau(\ell)}), \qquad and$$

$$b \mapsto \int_{\mathbb{R}^2} F(E_1, E_2) d\mu_\ell[b](E_1, E_2) \in C_{per}^n(\Gamma_{\tau(\ell)}),$$

Combining Lemma 2.2 and Lemma 2.1, we are now ready to define the thermodynamic limit of the current-current correlation measure and associated conductivity tensor by

$$\mu = \nu \left(\int_{\Gamma_2} \mu_1[b] \, db + \int_{\Gamma_1} \mu_2[b] \, db \right) \qquad and$$

(2.13)
$$\sigma = \int F_\zeta \, d\mu(E_1, E_2),$$

where

$$\nu = \frac{1}{|\Gamma_1| \cdot |\mathcal{A}_1| + |\Gamma_2| \cdot |\mathcal{A}_2|}.$$

Moreover, we propose an alternative approximation to μ that exploits the configuration integrals, and the corresponding approximation of the conductivity,

$$\mu^r = \nu \left(\int_{\Gamma_2} \mu_1^r[b] \, db + \int_{\Gamma_1} \mu_2^r[b] \, db \right), \qquad and$$

(2.14)
$$\sigma^r = \int F_\zeta \, d\mu^r(E_1, E_2).$$

With these definitions, we can state our first main result.

Theorem 2.1. *Let Assumptions 2.1 and 2.2 be satisfied, then*

$$\bar{\sigma}^r \to \sigma \qquad and \qquad \sigma^r \to \sigma \qquad as \ r \to \infty.$$

More precisely, if $\lambda = \min\{\eta, \beta^{-1}\}$, then there exist constants $c, \gamma > 0$, independent of λ and r, such that

$$|\sigma - \sigma^r| \lesssim e^{-\gamma \lambda r - c \log(\lambda)}.$$

Remark 2.3. *Although we prove convergence of $\bar{\sigma}^r \to \sigma$, we do not obtain a rate. Indeed, as a supercell-like approximation of an incommensurate system this sequence is expected to converge slowly [6]. Here, $\bar{\sigma}^r$ has error proportional to $(\eta r)^{-1}$ from the boundary effects, as the error of the domain edge site contributions do not decay. This is poor decay compared to the exponential convergence found in the σ^r scheme (2.14). For the development of a numerical algorithm (see Section 3), we therefore*

use the expression for σ^r as a starting point, where large domain sizes r are replaced by an (embarrassingly parallel) integration over local configurations.

3. LINEAR SCALING ALGORITHM FOR LOCAL CONDUCTIVITIES

The numerical evaluation of the approximate conductivity (2.14) splits into two orthogonal subproblems, namely the evaluation of the local conductivity

$$(3.1) \qquad \sigma_\ell^r[b] := \int F_\zeta(E_1, E_2) \, d\mu_\ell^r[b](E_1, E_2)$$

and the integration over local configurations b. In most applications, the interlayer coupling functions h are smooth, and thus Lemma 2.2 implies that $b \mapsto \sigma^r[b]$ is also smooth. The periodic trapezoidal rule (uniformly distributed quadrature points with uniform quadrature weights) applied to (3.1) hence converges superalgebraically. In the present section, we therefore focus solely on the approximation of the local conductivity at a fixed configuration b, and to this end we simplify the notation by setting

$$\sigma_{\mathrm{loc}} := \sigma_\ell^r[b], \qquad H_{\mathrm{loc}} := H_\ell(b), \qquad M_p^{\mathrm{loc}} := \partial_p H_\ell(b).$$

3.1. Algorithm outline.
The local conductivity formula (3.1) is easily evaluated once the eigenpairs (ε_i, v_i) of the hamiltonian H_r are available, however computing these eigenpairs takes $\mathcal{O}(|\Omega_r|^3)$ floating-point operations which is prohibitively expensive in many applications. Alternatively, let us consider an approximate conductivity function $\tilde{F}_\zeta$ obtained by truncating the Chebyshev series of F_ζ,

$$(3.2) \qquad \begin{aligned} \tilde{F}_\zeta(E_1, E_2) &:= \sum_{(k_1, k_2) \in K} c_{k_1 k_2} \, T_{k_1}(E_1) \, T_{k_2}(E_2) \\ &\approx \sum_{k_1, k_2 = 0}^{\infty} c_{k_1 k_2} \, T_{k_1}(E_1) \, T_{k_2}(E_2) = F_\zeta(E_1, E_2) \end{aligned}$$

where $K \subset \mathbb{N}^2$ is a finite set of indices and $T_k(E)$ denotes the kth Chebyshev polynomial defined through the three-term recurrence relation

$$(3.3) \qquad T_0(x) = 1, \quad T_1(x) = x, \quad T_{k+1}(x) = 2x \, T_k(x) - T_{k-1}(x).$$

Inserting (3.2) into (2.8), we obtain an approximate local conductivity

$$\begin{aligned} \tilde{\sigma}_{\mathrm{loc}} &:= \sum_{i_1, i_2} \tilde{F}_\zeta(\varepsilon_{i_1}, \varepsilon_{i_2}) \, \langle v_{i_1} | M_p^{\mathrm{loc}} | v_{i_2} \rangle \, \langle v_{i_2} | M_{p'}^{\mathrm{loc}} | e_{0,\alpha} \rangle \langle e_{0,\alpha} | v_{i_1} \rangle \\ &= \sum_{i_1, i_2} \sum_{(k_1, k_2) \in K} c_{k_1 k_2} \, \langle e_{0,\alpha} | v_{i_1} \rangle \, T_{k_1}(\varepsilon_{i_1}) \, \langle v_{i_1} | M_p^{\mathrm{loc}} | v_{i_2} \rangle \, T_{k_2}(\varepsilon_{i_2}) \, \langle v_{i_2} | M_{p'}^{\mathrm{loc}} | e_{0,\alpha} \rangle \\ (3.4) \qquad &= \sum_{(k_1, k_2) \in K} c_{k_1 k_2} \left(T_{k_1}(H_{\mathrm{loc}}) \, M_p^{\mathrm{loc}} \, T_{k_2}(H_{\mathrm{loc}}) \, M_{p'}^{\mathrm{loc}} \right)_{0,\alpha;0,\alpha} \end{aligned}$$

which can be evaluated without computing the eigendecomposition as follows.

Algorithm 1 Local conductivity via Chebyshev approximation

1: $|v_{k_1}\rangle := M_p^{\mathrm{loc}} T_{k_1}(H_{\mathrm{loc}}) |e_{0,\alpha}\rangle$ for all $k_1 \in K_1 := \{k_1 \mid \exists k_2 : (k_1, k_2) \in K\}$.

2: $|w_{k_2}\rangle := T_{k_2}(H_{\mathrm{loc}}) M_{p'}^{\mathrm{loc}} |e_{0,\alpha}\rangle$ for all $k_2 \in K_2 := \{k_2 \mid \exists k_1 : (k_1, k_2) \in K\}$.

3: $\tilde{\sigma}_{\mathrm{loc}} := \displaystyle\sum_{(k_1,k_2)\in K} c_{k_1 k_2} \langle v_{k_1} | w_{k_2} \rangle.$

Lines 1 and 2 of Algorithm 1 take $|K_1|$ and $|K_2|$, respectively, matrix-vector products when evaluated using the recurrence relation (3.3), while Line 3 requires $|K|$ inner products. Due to the sparsity of H_{loc}, both types of products take $\mathcal{O}(|\Omega_r|)$ floating-point operations, thus we conclude that Algorithm 1 scales linearly in the matrix size $|\Omega_r|$. Furthermore, the error in the computed local conductivity $\tilde{\sigma}_{\mathrm{loc}}$ can be estimated in terms of the dropped Chebyshev coefficients $c_{k_1 k_2}$ as follows.

Lemma 3.1. *It holds that*

$$\left|\tilde{\sigma}_{\mathrm{loc}} - \sigma_{\mathrm{loc}}\right| \lesssim \sum_{(k_1,k_2)\in\mathbb{N}^2\setminus K} |c_{k_1 k_2}|.$$

Proof. The bound follows immediately from (3.4) after noting that M_p^{loc} and $T_k(H_{\mathrm{loc}})$ are bounded for $a \in \{1, 2\}$ and all $k \in \mathbb{N}$. $\square$

A more careful analysis of Algorithm 1 reveals that since $|K_1|, |K_2| \leq |K|$ and both matrix-vector and inner products take $\mathcal{O}(|\Omega_r|)$ floating-point operations, the computational cost of this algorithm is dominated by the cost of Line 3 which is $|K|$ inner products. In the light of Lemma 3.1, the sets K achieving the smallest error bound for a given size $|K|$ are of the form

$$K(\tau) := \left\{(k_1, k_2) \in \mathbb{N}^2 \mid |c_{k_1 k_2}| \geq \tau\right\}$$

for some truncation tolerance τ, thus $|K|$ is linked to the decay of the Chebyshev coefficients which in turn depends on the analyticity properties of F_ζ. To analyze these, it is convenient to split the conductivity function $F_\zeta(E_1, E_2) = f_{\mathrm{temp}}(E_1, E_2) f_{\mathrm{relax}}(E_1, E_2)$ into the two factors

(3.5)
$$f_{\mathrm{temp}}(E_1, E_2) := \frac{f_\beta(E_1 - E_F) - f_\beta(E_2 - E_F)}{E_1 - E_2}$$

and

(3.6)
$$f_{\mathrm{relax}}(E_1, E_2) := \frac{1}{E_1 - E_2 + \omega + \iota\eta},$$

which are easily seen to be analytic[1] everywhere except, respectively, on the sets

(3.7) $S_{\mathrm{temp}} := \left(S_{\mathrm{temp}}^{(1)} \times \mathbb{C}\right) \cup \left(\mathbb{C} \times S_{\mathrm{temp}}^{(1)}\right)$ with $S_{\mathrm{temp}}^{(1)} := \left\{E_F + \frac{\iota\pi k}{\beta} \mid k \text{ odd}\right\}$

and

$$S_{\mathrm{relax}} := \left\{(E_2, E_2) \in \mathbb{C}^2 \mid E_1 - E_2 + \omega + \iota\eta = 0\right\}.$$

The conductivity function F_ζ is thus analytic except on the union of these two sets.

---

[1]A precise definition of analyticity in two dimensions will be provided in Definition B.1.

TABLE 1. Classification of conductivity parameters ζ and number of significant terms in the Chebyshev series of F_ζ.

Constraint	Parameter range	# significant terms
Relaxation	$\beta \lesssim \eta^{-1/2}$	$\mathcal{O}\big(\eta^{-3/2}\big)$
Mixed	$\eta^{-1/2} \lesssim \beta \lesssim \eta^{-1}$	$\mathcal{O}\big(\beta\eta^{-1}\big)$
Temperature	$\eta^{-1} \lesssim \beta$	$\mathcal{O}\big(\beta^2\big)$

In one dimension, it is well known that the Chebyshev coefficients c_k of a function $f(x)$ analytic on a neighborhood of $[-1, 1]$ decay exponentially, $|c_k| \leq C \exp(-\alpha\, k)$, and the decay rate α is equal[2] to the parameter α of the largest Bernstein ellipse

$$(3.8) \qquad E(\alpha) := \Big\{ \cosh(\tilde\alpha)\cos(\theta) + \iota\,\sinh(\tilde\alpha)\sin(\theta)) \mid \tilde\alpha \in [0,\alpha), \theta \in [0, 2\pi) \Big\}$$

which can be inscribed into the domain of analyticity of f. In two dimensions, we have two decay rates α_1, α_2 and in the case of the conductivity function F_ζ we have two sets of singularities $S_{\text{temp}}, S_{\text{relax}}$ limiting the possible values of α_1 and α_2. This suggests to partition the space of parameters ζ into *relaxation-constrained*, *mixed-constrained*, and *temperature-constrained* depending on whether two, one, or zero of the decay rates are constrained by the singularities S_{relax} rather than S_{temp}. In Subsection 3.2, we will characterize these parameter regimes more precisely and present asymptotic estimates regarding the number of significant Chebyshev coefficients in each case, a summary of which is provided in Table 1. We see that for fixed η, the cost of Algorithm 1 gradually increases from $\mathcal{O}\big(\eta^{-3/2}\big)$ to $\mathcal{O}\big(\beta^2\big)$ for increasing inverse temperature β which renders conductivity calculations at low temperatures (i.e., large β) particularly expensive. In Subsection 3.3, we present an alternative algorithm based on a pole expansion of F_ζ which provably reduces the cost of evaluating the local conductivity to $\mathcal{O}\big(\beta^{1/2}\eta^{-5/4}\big)$ inner products for all $\beta \gtrsim \eta^{-1/2}$ and whose actual scaling was empirically found to be $\mathcal{O}\big(\beta^{1/2}\eta^{-1.05}\big)$ inner products (see (3.15)).

3.2. **Chebyshev coefficients of the conductivity function.** Let us denote by α_{relax} the parameter of the ellipse penetrating the line $\omega + \iota\eta + [-1, 1]$ up to the endpoints, and by y_ζ half the width of this ellipse $E(\alpha_{\text{relax}})$ along the line $\{z \mid \text{Re}(z) = E_F\}$; see Figure 2. The partition into temperature-, mixed-, and relaxation-constrained conductivity parameters depends on whether and to what extent the Fermi-Dirac poles $S_{\text{temp}}^{(1)} = \big\{E_F + \frac{\iota\pi k}{\beta} \mid k \text{ odd}\big\}$ penetrate this ellipse $E(\alpha_{\text{relax}})$.

- Relaxation-constrained: $\beta \in \big(0, \frac{\pi}{y_\zeta}\big]$. The Fermi-Dirac poles do not penetrate $E(\alpha_{\text{relax}})$.
- Mixed-constrained: $\beta \in \big[\frac{\pi}{y_\zeta}, \frac{\pi}{\eta}\big]$. The Fermi-Dirac poles penetrate $E(\alpha_{\text{relax}})$ but do not extend beyond the line $\omega + \iota\eta + [-1, 1]$.
- Temperature-constrained: $\beta \in \big[\frac{\pi}{\eta}, \infty\big)$. The Fermi-Dirac poles penetrate $E(\alpha_{\text{relax}})$ beyond the line $\omega + \iota\eta + [-1, 1]$.

This partition allows us to formulate the following result.

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[2]More precisely, it is the *asymptotic* rate of decay which is equal to the parameter of the ellipse of analyticity. Further details are provided in Appendix B.
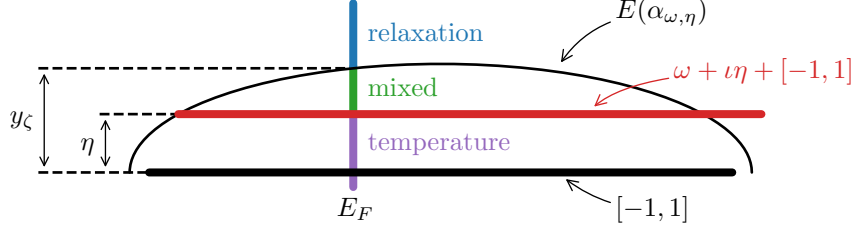
FIGURE 2. Partitioning of the conductivity parameters ζ depending on the location of the Fermi-Dirac poles.

Theorem 3.1. *There exist $\alpha_{\mathrm{diag}}(\zeta)$ and $\alpha_{\mathrm{anti}}(\zeta) > 0$ such that the Chebyshev coefficients $c_{k_1 k_2}$ of F_ζ are bounded by*

$$(3.9) \qquad |c_{k_1,k_2}| \le C(\zeta) \exp\big[-\alpha_{\mathrm{diag}}(\zeta)\,(k_1 + k_2) - \alpha_{\mathrm{anti}}(\zeta)\,|k_1 - k_2|\big]$$

for some $C(\zeta) < \infty$ independent of k_1, k_2. In the limit $\beta \to \infty$ and $\omega, \eta \to 0$ with $|\omega| \le C\eta$ for some $C > 0$ and assuming $E_F \in (-1, 1)$, it holds that $y_\zeta = \Theta\big(\sqrt{\eta}\big)$,

$$\alpha_{\mathrm{diag}}(\zeta) = \begin{cases} \Theta(\eta) & \text{if } \zeta \text{ is relaxation- or mixed-constrained,} \\ \Theta(\beta^{-1}) & \text{if } \zeta \text{ is temperature-constrained,} \quad \text{and} \end{cases}$$

$$\alpha_{\mathrm{anti}}(\zeta) = \begin{cases} \Theta(\sqrt{\eta}) & \text{if } \zeta \text{ is relaxation-constrained,} \\ \Theta(\beta^{-1}) & \text{if } \zeta \text{ is mixed- or temperature-constrained.} \end{cases}$$

A proof of Theorem 3.1 as well as exact formulae for α_{relax}, $\alpha_{\mathrm{diag}}(\zeta)$, and $\alpha_{\mathrm{anti}}(\zeta)$ are provided in Appendix B. Figures 3b to 3d show Chebyshev coefficients matching the predictions of Theorem 3.1 perfectly, and we note that Table 1 follows easily from Theorem 3.1.

We numerically observed the bound (3.9) to describe the correct decay behavior and the decay rates of $\alpha_{\mathrm{diag}}(\zeta)$ and $\alpha_{\mathrm{anti}}(\zeta)$ to be quantitatively accurate for temperature- and mixed-constrained parameters as well for relaxation-constrained parameters with β close to the critical value $\frac{\pi}{y_\zeta}$. For relaxation-constrained parameters far away from this critical value, however, the level lines of $c_{k_1 k_2}$ are piecewise concave rather than piecewise straight as predicted by Theorem 3.1, see Figure 3a, and this extra concentration reduces the number of significant Chebyshev coefficients from $\mathcal{O}\big(\eta^{-3/2}\big)$ to $\mathcal{O}\big(\eta^{-1.1}\big)$, see Figure 4. Since we do not have an explanation for this phenomenon, we will continue with the theoretically asserted scaling of $\mathcal{O}\big(\eta^{-3/2}\big)$ for clarity of exposition.

Theorem 3.1 suggests to truncate the Chebyshev series (3.2) using

$$(3.10) \qquad K(\tau) := \Big\{ (k_1, k_2) \in \mathbb{N}^2 \mid \exp\big(-\alpha_{\mathrm{diag}}\,|k_1 + k_2| - \alpha_{\mathrm{anti}}\,|k_1 - k_2|\big) \ge \tau \Big\},$$

where here and in the following we no longer explicitly mention the dependence of $\alpha_{\mathrm{diag}}(\zeta), \alpha_{\mathrm{anti}}(\zeta)$ on ζ. The following theorem analyzes the error incurred by this approximation.

Theorem 3.2. *It holds that*

$$(3.11) \qquad \big|\tilde{\sigma}_{\mathrm{loc}} - \sigma_{\mathrm{loc}}\big| = \mathcal{O}\Big(\alpha_{\mathrm{diag}}^{-1}\,\alpha_{\mathrm{anti}}^{-1}\,\tau\,|\log(\tau)|\Big).$$

Proof. See Appendix C.1. □

(A) $\beta = \frac{\pi}{5y_\zeta}$ (far relaxation)

(B) $\beta = \frac{\pi}{y_\zeta}$ (relaxation)

(C) $\beta = \frac{\pi}{2\eta}$ (mixed)
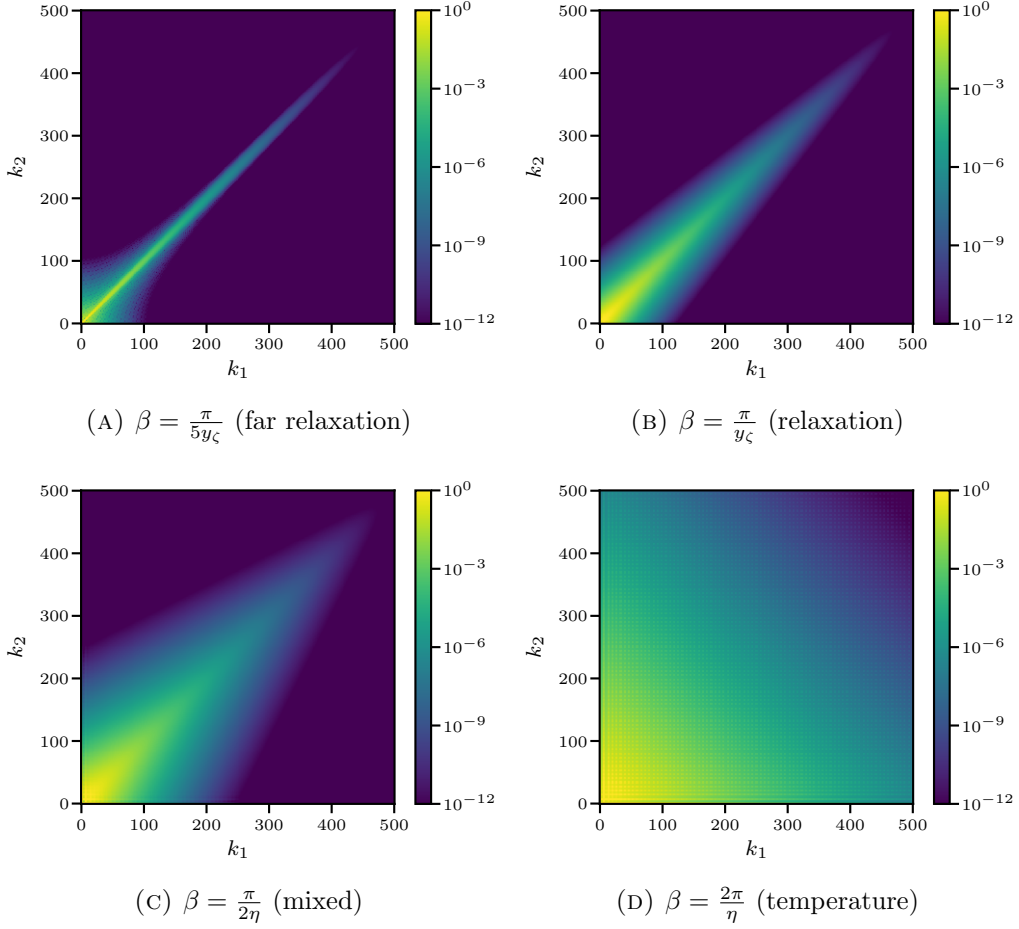
(D) $\beta = \frac{2\pi}{\eta}$ (temperature)

FIGURE 3. Normalized Chebyshev coefficients $\hat{c}_{k_1k_2} := |c_{k_1k_2}|/|c_{00}|$ of the conductivity function F_ζ with $E_F = \omega = 0$, $\eta = 0.06$, and β as indicated.
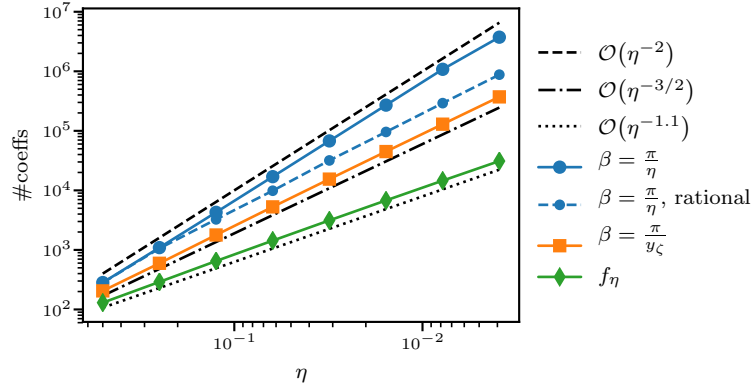

FIGURE 4. Number of normalized Chebyshev coefficients $\hat{c}_{k_1k_2} := |c_{k_1k_2}|/|c_{00}|$ larger than 10^{-3} for F_ζ with $E_F = \omega = 0$ and $f_\eta(E_1, E_2) := \frac{1}{E_1-E_2+\iota\eta}$. The "rational" line refers to the total number of Chebyshev coefficients in the pole expansion from Theorem 3.3 as described in Figure 5.

It is shown in Appendix C.2 that if $\varepsilon = \tau \, |\log \tau|$, then $\tau = \frac{\varepsilon}{|\log \varepsilon|}\big(1 + o(1)\big)$ in the limit $\varepsilon \to 0$. Combining this estimate with Theorem 3.2, we conclude that we need to choose the truncation tolerance $\tau_\varepsilon := \frac{\alpha_{\mathrm{diag}} \, \alpha_{\mathrm{anti}} \, \varepsilon}{|\log(\alpha_{\mathrm{diag}} \, \alpha_{\mathrm{anti}} \, \varepsilon)|}$ to guarantee an error $\big|\tilde{\sigma}_{\mathrm{loc}} - \sigma_{\mathrm{loc}}\big| \lesssim \varepsilon$, which in turn yields

$$|K(\tau_\varepsilon)| = \mathcal{O}\left(\frac{|\log(\alpha_{\mathrm{diag}} \, \alpha_{\mathrm{anti}} \, \varepsilon)|^2}{\alpha_{\mathrm{diag}} \, \alpha_{\mathrm{anti}}} \right)$$

according to (3.10).

3.3. Pole expansion for low-temperature calculations.

We have seen in the previous subsection that for increasing β, the sparsity in the Chebyshev coefficients of F_ζ induced by the factor $\frac{1}{E_1 - E_2 + \omega + \iota\eta}$ decreases and the number of coefficients eventually scales as $\mathcal{O}(\beta^2)$ such that Algorithm 1 becomes expensive at low temperatures. To avoid this poor low-temperature scaling, we propose to expand F_ζ into a sum over the poles in S_{temp} as described in Theorem 3.3 below and apply Algorithm 1 to each term separately.

Theorem 3.3. *Let $k \in \mathbb{N}$ and denote by α_{k,β,E_F} the parameter of the ellipse through the Fermi-Dirac poles $E_F \pm \frac{(2k+1)\,\pi\iota}{\beta}$. There exists a function $R_{k,\beta,E_F}(E_1, E_2)$ analytic on the biellipse $E\big(\alpha_{k,\beta,E_F}\big)^2 \supset E\big(\alpha_{0,\beta,E_F}\big)^2$ such that*

$$(3.12) \qquad F_\zeta(E_1, E_2) = \frac{1}{E_1 - E_2 + \omega + \iota\eta} \left(\sum_{z \in Z_k} \frac{1}{\beta} \frac{1}{(E_1 - z)\,(E_2 - z)} + R_{k,\beta,E_F}(E_1, E_2) \right),$$

where

$$Z_k := \left\{ E_F + \frac{\ell\pi\iota}{\beta} \ \Big| \ \ell \in \{-2k+1, -2k+3, \ldots, 2k-3, 2k-1\} \right\} \subset S_{\beta,E_F}.$$

Proof. See Appendix C.3. $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\square$

For k large enough, the remainder term (the last term in (3.12)) becomes relaxation constrained such that Algorithm 1 becomes fairly efficient. For the pole terms, on the other hand, we propose to employ Algorithm 1 using the weighted Chebyshev approximation

$$\frac{1}{(E_1 - z)\,(E_2 - z)\,(E_1 - E_2 + \omega + \iota\eta)} \approx \sum_{k_1 k_2 \in K_z} c(z)_{k_1 k_2} \frac{T_{k_1}(E_1)}{E_1 - z} \frac{T_{k_2}(E_2)}{E_2 - z}$$

where the weight $(E - z)^{-1}$ is chosen such that two factors $(E_1 - z)^{-1}$ and $(E_2 - z)^{-1}$ on the left- and right-hand side cancel. The coefficients $c(z)_{k_1 k_2}$ are therefore again the Chebyshev coefficients of a relaxation-constrained function

$$\frac{1}{E_1 - E_2 + \omega + \iota\eta} \approx \sum_{k_1 k_2 \in K_z} c(z)_{k_1 k_2} T_{k_1}(E_1)\, T_{k_2}(E_2)$$

and exhibit the concentration described in Theorem 3.1. This leads us to the following algorithm.

Algorithm 2 Local conductivity via pole expansion

1: $\tilde{\sigma}_{\text{loc}} := \int \frac{R_{k,\beta,E_F}(E_1,E_2)}{E_1-E_2+\omega+\iota\eta} \, d\mu_\ell^r(E_1,E_2)$, evaluated using Algorithm 1.
2: **for** $z \in Z_{k,\beta,E_F}$ **do**
3:     $\tilde{\sigma}_{\text{loc}} := \tilde{\sigma}_{\text{loc}} + \frac{1}{\beta} \int \frac{1}{(E_1-z)(E_2-z)(E_1-E_2+\omega+\iota\eta)} \, d\mu_\ell^r(E_1,E_2)$, evaluated using
     Algorithm 1 with the weighted Chebyshev polynomials $(E-z)^{-1} T_k(E)$.
4: **end for**

Theorem 3.4. *The dominant computational cost of Algorithm 2 is*

$$(3.13) \qquad \#\text{IP} = \mathcal{O}\big(k\,\eta^{-3/2}\big) + \begin{cases} \mathcal{O}\big(\eta^{-3/2}\big) & \text{if } \beta\,\eta^{1/2} \lesssim k, \\ \mathcal{O}\big(\frac{\beta\eta^{-1}}{k}\big) & \text{if } \beta\eta \lesssim k \lesssim \beta\,\eta^{1/2}, \\ \mathcal{O}\big(\frac{\beta^2}{k^2}\big) & \text{if } k \lesssim \beta\eta, \end{cases}$$

inner products if we assume that solving a single linear system of the form $(H - zI)^{-1}\,v$ is less expensive than $\mathcal{O}(\eta^{-3/2})$ inner products (see Remark 3.2). This cost is minimized if we choose

$$(3.14) \qquad k = \begin{cases} \Theta(1) & \text{if } \beta \lesssim \eta^{-1/2}, \\ \Theta\big(\beta^{1/2}\,\eta^{1/4}\big) & \text{if } \eta^{-1/2} \lesssim \beta \lesssim \eta^{-3/2}, \\ \Theta\big(\beta^{2/3}\,\eta^{1/2}\big) & \text{if } \eta^{-3/2} \lesssim \beta, \end{cases}$$

which yields

$$\#\text{IP} = \begin{cases} \mathcal{O}\big(\eta^{-3/2}\big) & \text{if } \beta \lesssim \eta^{-1/2}, \\ \mathcal{O}\big(\beta^{1/2}\,\eta^{-5/4}\big) & \text{if } \eta^{-1/2} \lesssim \beta \lesssim \eta^{-3/2}, \\ \mathcal{O}\big(\beta^{2/3}\,\eta^{-1}\big) & \text{if } \eta^{-3/2} \lesssim \beta. \end{cases}$$

Proof. It follows from Theorem 3.1 that the first term in (3.13) describes the cost of the for-loop in Algorithm 2 while the second term describes the cost of Line 1. Since the first term is strictly increasing while the second is decreasing, the sum of the two terms is minimized by the unique k such that the first term equals the second term which one can readily verify to be given by (3.14). $\qquad\square$

We note that Algorithm 2 reduces to Algorithm 1 if $\beta \lesssim \eta^{-1/2}$, but scales better than Algorithm 1 for larger values of β, e.g., for $\beta \sim \eta^{-1} \sim \chi$ we have $\#\text{IP} = \mathcal{O}\big(\chi^{7/4}\big)$ in the case of Algorithm 2 while $\#\text{IP} = \mathcal{O}\big(\chi^2\big)$ for Algorithm 1. The first term in (3.12) further reduces to $\mathcal{O}\big(k\,\eta^{-1.1}\big)$ if we assume the improved $\mathcal{O}\big(\eta^{-1.1}\big)$-scaling for the number of significant Chebyshev coefficients of $f(E_1,E_2) = \frac{1}{E_1-E_2+\omega+\iota\eta}$ suggested by Figure 4. In this case, the optimal choice of k and the corresponding costs are

$$(3.15) \quad k = \begin{cases} \Theta(1) \\ \Theta\big(\beta^{1/2}\,\eta^{0.05}\big) \\ \Theta\big(\beta^{2/3}\,\eta^{0.37}\big) \end{cases} \quad \text{and} \quad \#\text{IP} = \begin{cases} \mathcal{O}\big(\eta^{-1.1}\big) & \text{if } \beta \lesssim \eta^{-1/2}, \\ \mathcal{O}\big(\beta^{1/2}\,\eta^{-1.05}\big) & \text{if } \eta^{-1/2} \lesssim \beta \lesssim \eta^{-3/2}, \\ \mathcal{O}\big(\beta^{2/3}\,\eta^{-0.73}\big) & \text{if } \eta^{-3/2} \lesssim \beta. \end{cases}$$

These predictions are compared against numerical results in Figure 5 where we observe good qualitative agreement between the theory and the experiment. For $\beta \sim \eta^{-1} \sim \chi$, equation (3.15) yields $\#\text{IP} = \mathcal{O}\big(\chi^{1.55}\big)$ which is only marginally more expensive than the $\mathcal{O}\big(\chi^{1.5}\big)$ cost of Algorithm 1 in the case of relaxation-constrained parameters $\beta^2 \sim \eta^{-1} \sim \chi$. This is empirically demonstrated by the "rational" line in Figure 4.
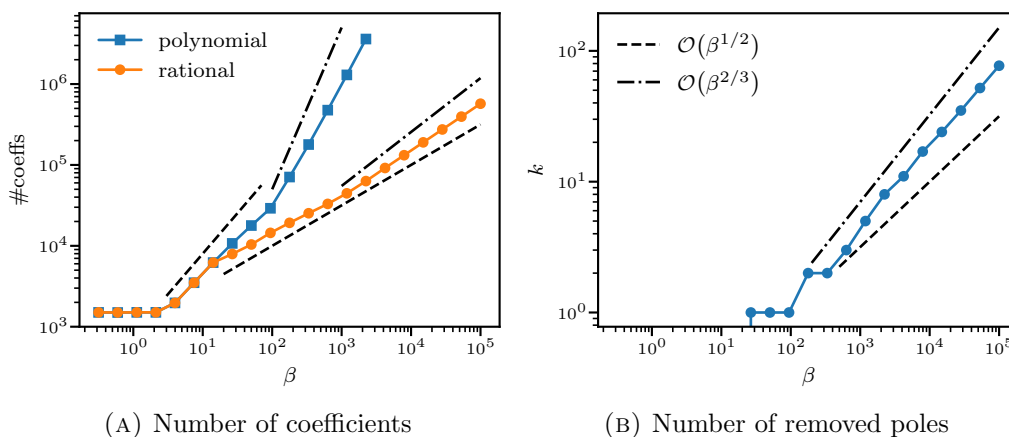
(A) Number of coefficients

(B) Number of removed poles

FIGURE 5. (a) Number of normalized Chebyshev coefficients $\hat{c}_{k_1 k_2} := |c_{k_1 k_2}|/|c_{00}|$ larger than 10^{-3} for F_ζ with $\eta = 0.06$ and $E_F = \omega = 0$. The "polynomial" line counts the number of significant coefficients in the Chebyshev expansion from (3.2), while the "rational" line counts the sum of the Chebyshev coefficients of all the terms in the pole expansion from (3.12). The dashed lines denote $\mathcal{O}(\beta)$ and $\mathcal{O}(\beta^{1/2})$, respectively, and the dash-dotted lines denote $\mathcal{O}(\beta^2)$ and $\mathcal{O}(\beta^{2/3})$, respectively, cf. (3.15). (b) Index k for the set of poles Z_k from Theorem 3.3. This number was determined by increasing k starting from 0 until the number of coefficients reported in (a) stopped decreasing.

Remark 3.1. *Instead of running Algorithm 1 for each pole $z \in Z_{k,\beta,E_F}$ separately, we can apply Algorithm 1 to a group of poles $\tilde{Z} \subset Z_{k,\beta,E_F}$ if we weigh the Chebyshev polynomials $T_k(E)$ with $q(E) := \prod_{z \in \tilde{Z}} (E - z)^{-1}$, and the same idea can also be used to improve the concentration of the Chebyshev coefficients of R_{k,β,E_F}. Grouping the poles in this manner reduces the computational cost of Algorithm 2, but amplifies the round-off errors by a factor $r := \max_{E \in [-1,1]} |q(E)| / \min_{E \in [-1,1]} |q(E)|$ such that the result is fully dominated by round-off errors if this ratio exceeds 10^{16}. Since $|q(E_F)| \sim \beta^{|\tilde{Z}|}$ while $|q(\pm 1)| \sim 1$, this means that we have to keep the group size rather small (e.g. $|\tilde{Z}| \leq 4$ for $\beta = 10^4$) to maintain numerical stability. We therefore conclude that grouping poles reduces the prefactor, but does not change the asymptotics of the computational cost of Algorithm 2.*

Remark 3.2. *One can show as a corollary of (3.4) that the radius r of the local configurations Ω^r must grow linearly with the maximal degree $k_{\max} := \max\{k_1 + k_2 \mid (k_1, k_2) \in K(\tau)\}$ of the polynomial approximation from (3.2) to achieve a constant error for all $k_{\max}$, and according to Theorem 3.1 the asymptotic scaling of $k_{\max}$ is given by*

$$k_{\max} = \begin{cases} \mathcal{O}(\eta^{-1}) & \text{if } \zeta \text{ is relaxation- or mixed-constrained,} \\ \mathcal{O}(\beta) & \text{if } \zeta \text{ is temperature-constrained.} \end{cases}$$

Solving a linear system $(H_{\mathrm{loc}} - z)^{-1} v$ associated with the two-dimensional configuration Ω^r using a direct solver takes

$$(3.16) \qquad \mathcal{O}\big((\Omega^r)^{3/2}\big) = \mathcal{O}\big(r^3\big) = \mathcal{O}\big(k_{\max}^3\big)$$

$$(3.17) \qquad = \begin{cases} \mathcal{O}(\eta^{-3}) & \text{if } \zeta \text{ is relaxation- or mixed-constrained,} \\ \mathcal{O}(\beta^3) & \text{if } \zeta \text{ is temperature-constrained,} \end{cases}$$

floating-point operations, see e.g. [8, §7.6], while approximating $p(E) \approx 1/(E - z)$ and evaluating $p(H_{\mathrm{loc}}) \approx (H_{\mathrm{loc}} - z)^{-1}$ (or equivalently, using an iterative linear solver like conjugate gradients) takes

$$\mathcal{O}\big(\mathrm{degree}(p)\, m\big) = \begin{cases} \mathcal{O}\big(\beta\, \eta^{-2}\big) & \text{if } \zeta \text{ is relaxation- or mixed-constrained,} \\ \mathcal{O}\big(\beta^3\big) & \text{if } \zeta \text{ is temperature-constrained,} \end{cases}$$

floating-point operations where we used that $\mathrm{degree}(p) = \mathcal{O}\big(|\operatorname{Im}(z)|^{-1}\big) = \mathcal{O}(\beta)$ according to fundamental results in approximation theory, see e.g. [19]. We conclude that iterative solvers scale slightly better than direct ones in the relaxation- and mixed-constrained cases and scale as well as direct ones in the temperature-constrained case.

Similarly, we find that the cost of computing $\mathcal{O}\big(\eta^{-3/2}\big)$ inner products is

$$\mathcal{O}\big(\eta^{-3/2}\, m\big) = \begin{cases} \mathcal{O}\big(\eta^{-7/2}\big) & \text{if } \zeta \text{ is relaxation- or mixed-constrained,} \\ \mathcal{O}\big(\eta^{-3/2}\, \beta^2\big) & \text{if } \zeta \text{ is temperature-constrained,} \end{cases}$$

floating-point operations, hence the assumption in Theorem 3.4 is satisfied if $\beta \lesssim \eta^{-3/2}$.

3.4. Remarks Regarding Implementation.
We conclude this section by pointing out two features of the proposed algorithms which are relevant when one considers their practical implementation.

3.4.1. *Memory Requirements.* Algorithm 1 as formulated above suggests that we precompute and store both the vectors $|v_{k_1}\rangle$ for all $k_1 \in K_1$ and $|w_{k_2}\rangle$ for all $k_2 \in K_2$, but this requires more memory than needed since we can rewrite the algorithm as follows.

Algorithm 3 Memory-optimised version of Algorithm 1

1: Precompute $|v_{k_1}\rangle$ for all $k_1 \in K_1$ as in Algorithm 1.
2: **for** $k_2 \in K_2$ in ascending order **do**
3:     Evaluate $|w_{k_2}\rangle$ using the recurrence relation (3.3).
4:     Discard $|w_{k_2-2}\rangle$ as it will no longer be needed.
5:     Compute the inner products $\langle v_{k_1}|w_{k_2}\rangle$ for all k_1 such that $(k_1, k_2) \in K$, and accumulate the results as in Algorithm 1.
6: **end for**

Furthermore, even caching all the vectors $|v_{k_1}\rangle$ is not needed if the function to be evaluated is relaxation-constrained: it follows from the wedge-like shape of the Chebyshev coefficients of such functions shown in Figure 3b that in every iteration of the loop in Algorithm 3, we only need vectors $|v_{k_1}\rangle$ with index k_1 within some fixed distance from k_2. The vectors $|v_{k_1}\rangle$ can hence be computed and discarded on the fly just like $|w_{k_2}\rangle$, albeit with a larger lag between computing and discarding. Quantitatively, this reduces the memory requirements from $\mathcal{O}\big(\eta^{-1} |\Omega^r|\big)$ for both

Algorithms 1 and 3 to $\mathcal{O}\big(\eta^{-1/2}\,|\Omega^r|\big)$ for the final version described above, assuming the function to be evaluated is relaxation-constrained.

3.4.2. *Choosing the Approximation Scheme.* Algorithms 1 and 2 involve three basic operations, namely matrix-vector products, inner products and linear system solves, and a fundamental assumption in their derivation was that matrix-vector and inner products are approximately equally expensive and linear system solves are not significantly more expensive than that (see Theorem 3.4 for the precise condition). The former assumption is true in the sense that both matrix-vector and inner products scale linearly in the matrix size m, but their prefactors are very different: the inner product $\langle w \,|\, v \rangle$ takes $2m - 1$ floating-point operations, while the cost of the matrix-vector product $H \,|v\rangle$ is approximately equal to twice the number of nonzeros in H. Even in the simplest case of a single triangular lattice and a tight-binding Hamiltonian H involving only nearest-neighbour terms as well as s and p orbitals, the number of nonzeros per column of H is about 6 (number of neighbours) times 4 (number of orbitals), hence the cost of evaluating $H \,|v\rangle$ is approximately $48m$ which is 24 times more expensive than the inner product. Similarly, the assumption regarding the costs of linear system solves holds true in the asymptotic sense as discussed in Remark 3.2, but the situation may look very different once we include the prefactors. This observation has two practical implications.

- Rather than choosing the number of removed poles k in Theorem 3.3 solely to minimise the number of coefficients, one should benchmark the runtimes of inner products, matrix-vector products and linear system solves and choose the k which yields the smallest overall runtime.
- Fairly small values of η are required before the wedge shown in Figure 3b becomes thin enough that the savings due to a smaller number of inner products make a significant difference compared to the cost of the matrix vector products, and even smaller η are required to compensate for the additional costs of solving the linear systems introduced by the pole expansion in Theorem 3.3.

We have seen in Remark 3.2 that the matrix size m must scale with η^{-2} in order to achieve a constant error in the local conductivities σ_{loc}, hence the latter point implies that demonstrating the savings brought about by the sparsity of the Chebyshev coefficients in a physically meaningful setting requires large-scale computations which are beyond the scope of this paper and will be the topic of a future publication.

4. Conclusion

We have demonstrated in this paper how to construct numerical algorithms for conductivity in incommensurate heterostructures where classical Bloch theory is unavailable. Our construction is based on two key observations:

- The ergodicity property of incommensurate bilayers allows to replace conductivity calculations on the infinite system with an integral over the two unit cells. The resulting formula presented in Section 2 is similar to Bloch's theorem and extends an analogous construction for the density of states in [16].
- Unlike in Bloch's theorem, the two unit cells require padding with a buffer region which may involve tens of thousands of atoms which is far beyond the reach of the diagonalization algorithm. We therefore proposed an alternative, linearly scaling algorithm in the spirit of the Kernel Polynomial Method and Fermi Operator Expansion which lead us to consider the two-dimensional

Chebyshev approximation of the conductivity function F_ζ in Section 3. Our main finding is that for relaxation-constrained parameters $\beta \lesssim \eta^{-1/2}$, only $\mathcal{O}(\eta^{-3/2})$ inner products are required to compute local conductivities, and we presented a rational approximation scheme which effectively allows to reduce arbitrary parameter regimes to the relaxation-constrained case.

The present work lays the theoretical foundations for the direct simulation of conductivity in incommensurate heterostructures. An effective implementation of our proposed algorithms, briefly outlined in Subsection 3.4, will be the purpose of future work.

Acknowledgement

Appendix A. Proofs: Conductivity

A.1. **Notation.** Throughout several of the following proofs it will become necessary to compare resolvent matrices $(z - H^r)^{-1}$ and $(z - H^{r'})^{-1}$ of different size r, r'. To that end, it is convenient to implicitly extend all matrices to be defined over Ω. Specifically: if A is usually defined over Ω^r, then we use the implicit extension to Ω given by

$$[A]_{R\alpha, R'\alpha'} = \begin{cases} A_{R\alpha, R'\alpha'}, & \text{if } R\alpha \in \Omega_r, R'\alpha' \in \Omega_r, \\ 0, & \text{otherwise.} \end{cases}$$

A.2. **Proof of Lemma 2.2.** We let $\Lambda = [-1, 1]$ and recall that this interval contains the spectrum for all Hamiltonians H^r, $r > 0$. Letting $r > 0$ and $a > 0$, then following the same argument as [16, Lemma 4.2] we have the existence of $\tilde\gamma > 0$ such that, for $z \in \mathbb{C}$ with $d(z, \Lambda) > a/2$, and $\Omega' \subset \Omega$ such that $\Omega_r \subset \Omega'$,

$$
\begin{aligned}
(A.1) \quad & \left| \left[(z - H^r_\ell(b))^{-1} \right]_{R\alpha, R'\alpha'} - \left[(z - H_\ell(b)|_{\Omega'})^{-1} \right]_{R\alpha, R'\alpha'} \right| \\
& \qquad \lesssim a^{-6} \min \left\{ e^{-a\tilde\gamma |R - R'|}, e^{-a\tilde\gamma(r - \max\{|R|, |R'|\})} \right\}.
\end{aligned}
$$

We have the following Lemma:

Lemma A.1. *Using Assumption 2.2, we have*

$$(z - H_\ell(b))^{-1} := \lim_{r \to \infty} (z - H^r_\ell(b))^{-1}$$

is defined over $\mathcal{L}(\ell^2(\Omega))$. Further, $(z - H_\ell(b))^{-1}$ is periodic over $\Gamma_{\tau(\ell)}$.

Proof. From (A.1), we have that $(z - H^r_\ell(b))^{-1}$ is Cauchy over $\mathcal{L}(\ell^2(\Omega))$, and hence has a well defined limit $(z - H_\ell(b))^{-1}$. $\|H^r_\ell(b + 2\pi A_{\tau(\ell)} n) - H^r_\ell(b)\|_{\text{op}} \to 0$ for $n \in \mathbb{Z}^2$ as $r \to \infty$, and hence $(z - H_\ell(b))^{-1}$ is periodic over $\Gamma_{\tau(\ell)}$. $\qquad \square$

Let $P_r : \ell^2(\Omega) \to \ell^2(\Omega)$ be the projection defined by

$$[P_r \psi]_{R\alpha} = \delta_{|R| < r} \psi_{R\alpha}.$$

We now introduce two lemmas we will use for the convergence estimates. The matrix A in Lemma A.2 corresponds to resolvent differences as in (A.1), while the second lemma will be applied to resolvents and localized Hamiltonian operators.

Lemma A.2. *For $A \in \mathcal{L}(\ell^2(\Omega))$ satisfying (for $r > 1$)*

$$|A_{R\alpha,R'\alpha'}| \lesssim e^{-\tilde{c}\log(a)} \min\{e^{-a\gamma_c|R-R'|}, e^{-a\gamma_c(r-\max\{|R|,|R'|\})}\},$$

it holds that

$$\|P_{r/2}^* A P_{r/2}\|_{\text{op}} \lesssim e^{-\gamma_c ar/2 - c\log(a) + c\log(r)}.$$

Proof. We estimate

$$\begin{aligned}
\|P_{r/2}^* A P_{r/2}\|_{\text{op}}^2 &\leq \|P_{r/2}^* A P_{r/2}\|_F^2 \\
&\lesssim e^{-\gamma_c ar - 2\tilde{c}\log(a)} |\Omega_{r/2}|^2 \\
&\lesssim r^4 e^{-\gamma_c ar - 2\tilde{c}\log(a)} \\
&\lesssim e^{-\gamma_c ar - 2\tilde{c}\log(a) + 4\log(r)}
\end{aligned}$$

for $c = \max\{2\tilde{c}, 4\}$, so we then have

$$\|P_{r/2}^* A P_{r/2}\|_{\text{op}} \lesssim e^{-\gamma_c ar/2 - c\log(a) + c\log(r)}.$$

$\square$

Recall $e_{0\alpha} \in \ell^2(\Omega)$ such that $[e_{0\alpha}]_{R\alpha'} = \delta_{0R}\delta_{\alpha\alpha'}$.

Lemma A.3. *If $A, A^{(1)}, A^{(2)} \in \mathcal{L}(\ell^2(\Omega))$ satisfies*

$$|A_{R\alpha,R'\alpha'}^{(j)}| \lesssim e^{-\gamma_c a|R-R'| - \tilde{c}\log(a)}$$

for some $\gamma_c > 0$, then there exist $\gamma_d, c > 0$ such that

(A.2) $$\||(1 - P_{r/2})^* A|e_{0\alpha}\rangle\|_{\ell^2} \lesssim e^{-\gamma_d ar - c\log(a)} \qquad \text{and}$$

(A.3) $$|[A^{(1)} A^{(2)}]_{R\alpha,R'\alpha'}| \lesssim e^{-\gamma_d a|R-R'| - c\log(a)}.$$

Proof. The two estimates result follows from straightforward direct estimations of the individual vector or matrix entries of, respectively, $Ae_{0\alpha}$ and $[A^{(1)} A^{(2)}]_{R\alpha,R'\alpha'}$. $\square$

To proceed with the proof of Lemma 2.2, we recognize that we can rewrite the current-current correlation measure in terms of a contour integral.

Lemma A.4. *Let ϕ be analytic on $S_a \times S_a$ and $\mathcal{C}_a \subset S_a - S_{a/2}$ a complex contour encircling the spectrum of $H_\ell^r(b)$, then*

$$\int_{\mathbb{R}^2} \phi(E_1, E_2) d\mu_\ell^r[b](E_1, E_2)$$

(A.4)
$$= -\frac{1}{4\pi^2} \oint_{z' \in \mathcal{C}_a} \oint_{z \in \mathcal{C}_a} \phi(z, z')$$
$$\sum_{\alpha \in \mathcal{A}_\ell} \langle e_{0\alpha}|(z - H_\ell^r(b))^{-1} \partial_p H_\ell^r(b)(z' - H_\ell^r(b))^{-1} \partial_{p'} H_\ell^r(b)|e_{0\alpha}\rangle dz dz'.$$

Proof. Inserting the spectral decomposition of $H_\ell^r(b)$ into the right-hand side of (A.4) and then applying Cauchy's integral formula twice yields the definition (2.12) of the local current-current correlation measure $\mu_\ell^r[b]$. $\square$

For the remainder of this proof, we denote $P = P_{r/2}$ for the sake of brevity. Then,

$$\langle e_{0\alpha}|(z - H_\ell^r(b))^{-1} \partial_p H_\ell^r(b)(z' - H_\ell^r(b))^{-1} \partial_{p'} H_\ell^r(b)|e_{0\alpha}\rangle$$
$$= \sum_{U_i \in \{P, 1-P\}} \langle e_{0\alpha}|(z - H_\ell^r(b))^{-1} U_1 \partial_p H_\ell^r(b) U_2 (z' - H_\ell^r(b))^{-1} U_3 \partial_{p'} H_\ell^r(b)|e_{0\alpha}\rangle$$
$$= S_1^r + S_2^r,$$

where $S_1^r = S_1^r(z, z')$, $S_2^r = S_2^r(z, z')$ are given by

$$S_1^r = \langle e_{0\alpha}|(z - H_\ell^r(b))^{-1}P\partial_p H_\ell^r(b)P(z' - H_\ell^r(b))^{-1}P\partial_{p'} H_\ell^r(b)|e_{0\alpha}\rangle \qquad \text{and}$$

$$S_2^r = \sum_{\substack{U_i \in \{P, 1-P\} \\ (U_1, U_2, U_3) \neq (P, P, P)}} \langle e_{0\alpha}|(z - H_\ell^r(b))^{-1}U_1\partial_p H_\ell^r(b)U_2(z' - H_\ell^r(b))^{-1}U_3\partial_{p'} H_\ell^r(b)|e_{0\alpha}\rangle.$$

Using Lemma A.1 and the resolvent formulation above, we can see that the limits $\mu_\ell[b] := \lim_{r\to\infty} \mu_\ell^r[b]$ and $S_j := \lim_{r\to\infty} S_j^r$ exist. However, we wish to obtain an error estimate. We can estimate

$$\left| \int_{\mathbb{R}^2} F(E_1, E_2) d\mu_\ell^r[b](E_1, E_2) - \int_{\mathbb{R}^2} F(E_1, E_2) d\mu_\ell[b](E_1, E_2) \right|$$

$$\lesssim \oint_{z' \in \mathcal{C}_a} \oint_{z \in \mathcal{C}_a} |F(z, z')| \left| S_1^r + S_2^r - S_1 - S_2 \right| dz dz'$$

$$\lesssim \sup_{z, z' \in \mathcal{C}_a} |F(z, z')| \cdot \sup_{z, z' \in \mathcal{C}_a} \left| S_1^r + S_2^r - S_1 - S_2 \right|$$

(A.5)
$$\leq \sup_{z, z' \in \mathcal{C}_a} |F(z, z')| \cdot \sup_{z, z' \in \mathcal{C}_a} \left(|S_1^r - S_1| + |S_2^r| + |S_2| \right).$$

Applying Lemma A.3, we readily obtain

(A.6)
$$|S_2^r| \lesssim e^{-\gamma_a r a - c' \log(a)}$$

for some constants $\gamma_a, c' > 0$.

Next, we claim that there exist constants γ_b, c'' such that

(A.7)
$$|S_1^r - S_1| \lesssim e^{-\gamma_b r a - c'' \log(a) + c'' \log(r)}.$$

Proof of (A.7). We define two sets of operators,

$$\Delta\mathcal{B}_r = \big\{ P[(z - H_\ell^r(b))^{-1} - (z - H_\ell(b))^{-1}]P,$$
$$\qquad P[\partial_p H_\ell^r(b) - \partial_p H_\ell(b)]P,$$
$$\qquad P[(z' - H_\ell^r(b))^{-1} - (z' - H_\ell(b))^{-1}]P,$$
$$\qquad P[\partial_p H_\ell^r(b) - \partial_{p'} H_\ell(b)]P \big\}, \qquad \text{and}$$

$$\mathcal{B}_r = \big\{ P(z - H_\ell^r(b))^{-1}P, P\partial_p H_\ell^r(b)P, P(z' - H_\ell^r(b))^{-1}P, P\partial_{p'} H_\ell^r(b)P$$
$$\qquad P(z - H_\ell(b))^{-1}P, P\partial_p H_\ell(b)P, P(z' - H_\ell(b))^{-1}P, P\partial_{p'} H_\ell(b)P \big\}.$$

Then, we can decompose

(A.8)
$$S_1^r - S_1 = \langle \sum_j e_{0\alpha}|A_1^{(j)} A_2^{(j)} A_3^{(j)} A_4^{(j)}|e_{0\alpha}\rangle,$$

where each of the operators $A_i^{(j)} \in \mathcal{B}_r \cup \Delta\mathcal{B}_r$ and for every j at least one $A_i^{(j)} \in \Delta\mathcal{B}_r$.
Using Lemma A.2, it is straightforward to see that

$$\|A\|_{\text{op}} \lesssim \max\{a^{-1}, 1\} \qquad \text{for } A \in \mathcal{B}_r \text{ and}$$
$$\|A\|_{\text{op}} \lesssim e^{-\gamma_b r a - c'' \log(a) + c'' \log(r)} \qquad \text{for } A \in \Delta\mathcal{B}_r,$$

which we apply to (A.8) to complete the proof. □

Combining (A.5), (A.6) and (A.7) we conclude that there exist $\gamma, c > 0$, such that

$$\left| \int_{\mathbb{R}^2} F(E_1, E_2) d\mu_\ell^r[b](E_1, E_2) - \int_{\mathbb{R}^2} F(E_1, E_2) d\mu_\ell^{r'}[b](E_1, E_2) \right|$$
$$\leq \sup_{z, z' \in \mathcal{C}_a} |F(z, z')| e^{-\gamma r a - c \log(a) + c \log(r)}.$$

In particular, it follows that $\int_{\mathbb{R}^2} F(E_1, E_2) d\mu_\ell^r[b](E_1, E_2)$ has a limit, which we denote by

$$\int_{\mathbb{R}^2} F(E_1, E_2) d\mu_\ell[b](E_1, E_2) := \lim_{r \to \infty} \int_{\mathbb{R}^2} F(E_1, E_2) d\mu_\ell^r[b](E_1, E_2).$$

As the limit of a bounded sequence of (matrix-valued) Radon measures, it is clear that $\mu_\ell[b]$ is again a Radon measure.

Finally, we establish the regularity of $\mu_\ell^r[b]$ and $\mu_\ell[b]$ as functions of $b \in \Gamma_{\tau(\ell)}$, where we recall that τ is the transposition operator, $\tau(1) = 2$ and $\tau(2) = 1$. The statement that

$$b \mapsto \int_{\mathbb{R}^2} F(E_1, E_2) d\mu_\ell^r[b](E_1, E_2) \in C^n(\Gamma_{\tau(\ell)})$$

follows immediately from the resolvent representation (A.4) and the fact that $(z - H_\ell^r(b))^{-1}$ is n times differentiable with respect to b (All operators involved here are finite-dimensional).

Thus, it remains only to show the regularity

(A.9) $$b \mapsto \int_{\mathbb{R}^2} F(E_1, E_2) d\mu_\ell[b](E_1, E_2) \in C_{\mathrm{per}}^n(\Gamma_{\tau(\ell)}).$$

To that end, we consider the operator $H_\ell(b) \in \mathcal{L}(\ell^2(\Omega))$. Using Lemma A.1, we have

$$\int_{\mathbb{R}^2} F(E_1, E_2) d\mu_\ell[b](E_1, E_2) = \frac{-1}{4\pi} \oint_{z' \in \mathcal{C}_a} \oint_{z \in \mathcal{C}_a}$$
$$F(z, z') \langle e_{0\alpha} | (z - H_\ell(b))^{-1} \partial_p H_\ell(b) (z' - H_\ell(b))^{-1} \partial_{p'} H_\ell(b) | e_{0\alpha} \rangle dz dz'.$$

We notice that differentiation of the resolvent $(z - H_\ell^r(b))^{-1}$ leads to products of the resolvent $(z - H_\ell^r(b))^{-1}$ and matrices of the form $\partial_{b_1}^{m_1} \partial_{b_2}^{m_2} H_\ell^r(b)$, all of which are well defined in the thermodynamic limit and have periodic limits with respect to $\Gamma_{\tau(\ell)}$. For an example, consider the derivative

$$\partial_{b_1}(z - H_\ell^r(b))^{-1} = (z - H_\ell^r(b))^{-1} \partial_{b_1} H_\ell^r(b)(z - H_\ell^r(b))^{-1}$$
$$\to (z - H_\ell(b))^{-1} \partial_{b_1} H_\ell(b)(z - H_\ell(b))^{-1}.$$

Hence $(z - H_\ell(b))^{-1}$ is a differentiable operator when acting on an element of the domain, and we trivially find $\int F \mu_\ell[b] \in C_{\mathrm{per}}^n(\Gamma_{\tau(\ell)})$.

A.3. **Proof of Theorem 2.1.** We recall that the current-current correlation measure for the finite system was defined through

(A.10) $$\int_{\mathbb{R}^2} F(E_1, E_2) d\bar{\mu}^r(E_1, E_2) = \sum_{ii'} F(\varepsilon_i, \varepsilon_{i'}) \frac{1}{|\Omega^r|} \mathrm{Tr}[|v_i\rangle \langle v_i | \partial_p H^r | v_{i'}\rangle \langle v_{i'} | \partial_{p'} H^r |].$$

We can decompose this into local current-current correlation measures of the finite system by defining $\mu_{R\alpha}^r$ via

$$\int_{\mathbb{R}^2} F(E_1, E_2) d\mu_{R\alpha}^r = \sum_{ii'} F(\varepsilon_i, \varepsilon_{i'}) [|v_i\rangle \langle v_i | \partial_p H^r | v_{i'}\rangle \langle v_{i'} | \partial_{p'} H^r |]_{R\alpha, R\alpha}.$$

Hence,

$$\int_{\mathbb{R}^2} F(E_1, E_2) d\bar{\mu}^r(E_1, E_2) = \frac{1}{|\Omega^r|} \sum_{R\alpha \in \Omega^r} \int_{\mathbb{R}^2} F(E_1, E_2) d\mu_{R\alpha}^r(E_1, E_2).$$

We will also reserve the notation for $\Omega' \subset \Omega$ finite

$$\int_{\mathbb{R}^2} F(E_1, E_2') d\mu_\ell^{\Omega'}[b] = \sum_{ii'} F(\varepsilon_i, \varepsilon_{i'}) \frac{1}{|\Omega'|} [|v_i\rangle\langle v_i|\partial_p H_\ell(b)|_{\Omega'}|v_{i'}\rangle\langle v_{i'}|\partial_{p'} H_\ell(b)|_{\Omega'}|]_{R\alpha, R\alpha}.$$

Here, (E_i, v_i) are the eigenpairs for $H_\ell(b)|_{\Omega'}$. We pick $D > 0$, and then consider $\bar{\sigma}^r$, where we wish to consider the limit $r \to \infty$. We have

$$\bar{\sigma}^r = \frac{1}{|\Omega^r|} \int_{\mathbb{R}^2} F_\zeta(E_1, E_2) d\bar{\mu}^r(E_1, E_2)$$

$$= \int_{\mathbb{R}^2} \frac{1}{|\Omega^r|} F_\zeta(E_1, E_2) \left(\sum_{R\alpha \in \Omega^{r-D}} d\mu_{R\alpha}^r(E_1, E_2) + \sum_{R\alpha \in \Omega^r \setminus \Omega_{r-D}} d\mu_{R\alpha}^r(E_1, E_2) \right).$$

We define the domain Ω_R^r for $R \in \mathcal{R}_\ell$ such that

$$\Omega_R^r = \left((\mathcal{R}_\ell \cap B_r - R) \times \mathcal{A}_\ell \right) \cup \left(\mathcal{R}_{\tau(\ell)} \cap B_r - R + \mathrm{mod}_{\tau(\ell)}(R) \right) \times \mathcal{A}_{\tau(\ell)} \right).$$

For $|R| < r - D$,

$$\left| \int_{\mathbb{R}^2} F_\zeta(E_1, E_2) \sum_{\alpha \in \mathcal{A}_\ell} d\mu_{R\alpha}^r(E_1, E_2) - \int_{\mathbb{R}^2} F_\zeta(E_1, E_2) d\mu_\ell^D[R](E_1, E_2) \right|$$

$$= \left| \int_{\mathbb{R}^2} F_\zeta(E_1, E_2) d\mu_\ell^{\Omega_R^r}[R](E_1, E_2) - \int_{\mathbb{R}^2} F_\zeta(E_1, E_2) d\mu_\ell^D[R](E_1, E_2) \right|$$

$$\lesssim e^{-\gamma\lambda D - c\log(\lambda)}.$$

The last line follows from (A.1), the fact that $\Omega_D \subset \Omega_R^r$, and $F_\zeta(E_1, E_2)$ is analytic on $S_\lambda \times S_\lambda$. Using Theorem 2.1, we have

$$\limsup_{r\to\infty} \left| \int_{\mathbb{R}^2} F_\zeta(E_1, E_2) \frac{1}{|\Omega^r|} \sum_{R\alpha \in \Omega_{r-D}} d\mu_{R\alpha}^r(E_1, E_2) \right.$$

$$\left. - \int_{\mathbb{R}^2} F_\zeta(E_1, E_2) \nu \sum_{\alpha \in \mathcal{A}_\ell} \int_{\Gamma_{p(\ell)}} d\mu_\ell^D[b](E_1, E_2) \right| \lesssim e^{-\gamma\lambda D - c\log(\lambda)}.$$

Further,

$$\frac{1}{|\Omega^r|} \int_{\mathbb{R}^2} F_\zeta(E_1, E_2) \sum_{R\alpha \in \Omega^r \setminus \Omega_{r-D}} d\mu_{R\alpha}^r(E_1, E_2) \to 0$$

as $r \to \infty$ since $\frac{|\Omega^r \setminus \Omega_{r-D}|}{|\Omega^r|} \to 0$. Hence we have, letting $D \to \infty$,

$$\frac{1}{|\Omega^r|} \int_{\mathbb{R}^2} F_\zeta(E_1, E_2) d\bar{\mu}^r(E_1, E_2) \to \int_{\mathbb{R}^2} F_\zeta(E_1, E_2) d\mu(E_1, E_2) = \sigma.$$

This is the desired global thermodynamic result. Finally,

$$|\sigma - \sigma^r| \lesssim e^{-\gamma\lambda r - c\log(\lambda) + c\log(r)}$$

is a trivial application of Lemma 2.2.

Appendix B. Proof of Theorem 3.1

B.1. **Approximation theory background.** This subsection briefly recalls some concepts from approximation theory and introduces the notation used in the remainder of this section. A textbook introduction to the topics discussed here can be found e.g., in [19].

Joukowsky map $\phi(z)$. The three-term recurrence relation (3.3) for the Chebyshev polynomials $T_k(x)$ implies the identity

(B.1) $$T_k\big(\phi(z)\big) := \frac{z^k + z^{-k}}{2} \qquad \text{where} \qquad \phi(z) := \frac{z + z^{-1}}{2}$$

as one can easily verify by induction, and the Bernstein ellipses (3.8) can be expressed in terms of the Joukowsky map $\phi(z)$ as

$$E(\alpha) = \{\phi(z) \mid z \in \mathbb{C},\, 0 \le \log|z| < \alpha\}.$$

Parameter function $\alpha_b(x)$. It will be convenient in the following to express $E(\alpha)$ in terms of the variable $x := \phi(z)$ which requires us to study the inverse Joukowsky map $\phi_\pm^{-1}(x) = x \pm \sqrt{x^2 - 1}$. Since $\phi(z) = \phi\big(z^{-1}\big)$, this inverse has two branches related by $\phi_\pm^{-1}(x) = \big(\phi_\mp^{-1}(x)\big)^{-1}$. Given any curve $b \subset \mathbb{C}$ connecting the two branch points $x = \pm 1$, we define

$$\phi_b^{-1}(x) := x + \sqrt[b]{x^2 - 1}$$

where $\sqrt[b]{x^2 - 1}$ denotes the branch of $\sqrt{x^2 - 1}$ with branch cut along b and sign such that $\phi_b^{-1}(\infty) = \infty$. The Bernstein ellipses $E(\alpha)$ then become the level sets

$$E(\alpha) = \{x \in \mathbb{C} \mid \alpha_{[-1,1]}(x) < \alpha\}$$

of the parameter function

$$\alpha_b(x) := \log|\phi_b^{-1}(x)|.$$

The following properties of $\alpha_b(x)$ follow immediately from the above discussion.

Lemma B.1. *It holds that*
- $\alpha_b(x) = 0$ *for all* $x \in [-1, 1]$ *and all branch cuts* b,
- $\alpha_{[-1,1]}(x) \ge 0$ *for all* $x \in \mathbb{C}$,
- $\alpha_b(x+0n) = -\alpha_b(x-0n)$ *for all* $x \in b$ *and all branch cuts* b, *where the notation* $x \pm 0n$ *indicates that we evaluate* $\alpha_b(x)$ *on different sides of the branch cut.*

Zero-width contours. In an abuse of notation, we define $\partial\gamma$ for curves $\gamma \subset \mathbb{C}$ as the counterclockwise contour around a domain of infinitesimal width, e.g.,

$$\partial[-1, 1] = \big([-1, 1] + 0\iota\big) \cup \big([-1, 1] - 0\iota\big),$$

where the signed zero in the imaginary part indicates which branch to evaluate for a function with branch cut along $[-1, 1]$.

Example 1. *Using the definition of* $\partial[-1, 1]$ *and* $\sqrt[{[-1,1]}]{\cdot}$, *we compute*

$$\int_{\partial[-1,1]} \sqrt[{[-1,1]}]{x^2 - 1}\, dx = \int_{1+0\iota}^{-1+0\iota} \iota\, \sqrt{1 - x^2}\, dx + \int_{-1-0\iota}^{1-0\iota} (-\iota)\, \sqrt{1 - x^2}\, dx$$

$$= -2\,\iota \int_{-1}^{1} \sqrt{1 - x^2}\, dx = -\pi\,\iota.$$

Exponential decay with asymptotic rate α. Following the $\mathcal{O}_\varepsilon$ notation of [20], we introduce $a_k \leq_\varepsilon C(\alpha) \exp(-\alpha k)$ as a shorthand notation for exponential decay with asymptotic rate α, i.e.,

$$a_k \leq_\varepsilon C(\alpha) \exp(-\alpha k) \quad : \Longleftrightarrow \quad \forall \tilde{\alpha} < \alpha : a_k \leq C(\tilde{\alpha}) \exp(-\tilde{\alpha} k),$$

and we also write $a_k \lesssim_\varepsilon \exp(-\alpha k)$ if the prefactor $C(\alpha)$ is irrelevant. Note that if $\lim_{\tilde{\alpha} \to \alpha} C(\tilde{\alpha})$ exists and is bounded, then $a_k \leq_\varepsilon C(\alpha) \exp(-\alpha k)$ is equivalent to $a_k \leq C(\alpha) \exp(-\alpha k)$. A typical example of a sequence $a_k \leq_\varepsilon C(\alpha) \exp(-\alpha k)$ is $a_k := k \exp(-\alpha k)$, in which case $C(\tilde{\alpha}) = \max_k k \exp(-(\alpha - \tilde{\alpha}) k)$ and $\lim_{\tilde{\alpha} \to \alpha} C(\tilde{\alpha}) = \infty$. For the purposes of this paper, the distinction between the two statements "$a_k \leq_\varepsilon C(\alpha) \exp(-\alpha k)$" and "$a_k \leq C \exp(-\alpha k)$ for some unspecified $C > 0$" is required for correctness, but it is of little practical relevance.

Analyticity in two dimensions. We extend the notion of analyticity to two-dimensional functions $f(z_1, z_2)$ as follows.

Definition B.1. *A function $f : \Omega \to \mathbb{C}$ with $\Omega \subset \mathbb{C}^2$ is called* analytic *if $f(z_1, z_2)$ is analytic in the one-dimensional sense in each variable z_1, z_2 separately for every $(z_1, z_2) \in \Omega$.*

By a well-known result due to Hartogs (see e.g. [15, Theorem 1.2.5]), a function $f(z_1, z_2)$ analytic in the above one-dimensional sense is continuous and differentiable in the two-dimensional sense. Furthermore, it is known that if $f(z_1, z_2)$ is analytic on the biannulus $A(r_1) \times A(r_2)$ with $A(r) := \{z \mid r^{-1} < |z| < r\}$, it can be expanded into a Laurent series

$$f(z_1, z_2) = \sum_{k_1, k_2 = -\infty}^{\infty} a_{k_1 k_2} \, z_1^{k_1} \, z_2^{k_2}$$

with coefficients given by

$$a_{k_1 k_2} = -\frac{1}{4\pi^2} \int_{\gamma_2} \int_{\gamma_1} f(z_1, z_2) \, z_1^{-k_1 - 1} \, z_2^{-k_2 - 1} \, dz_1 \, dz_2$$

for any bicontour $\gamma_1 \times \gamma_2$ where $\gamma_\ell \subset A(r_\ell)$ are two closed contours winding once around the origin, see [18, Theorem 1.5.26].

B.2. **Auxiliary results.** We next establish a contour-integral formula for the Chebyshev coefficients of analytic functions in Theorem B.1 and demonstrate in Theorem B.2 how this formula translates into a bound on the Chebyshev coefficients. Both results are straightforward generalizations of the one-dimensional results (see e.g., [19]) except that we allow for a general branch cut in Theorem B.2 which will be important in Subsection B.3.

Theorem B.1. *A function $f(x_1, x_2)$ analytic on $[-1, 1]^2$ can be expanded into a Chebyshev series*

$$(B.2) \qquad f(x_1, x_2) = \sum_{k_1, k_2 = 0}^{\infty} c_{k_1 k_2} \, T_{k_1}(x_1) \, T_{k_2}(x_2) \quad on \ [-1, 1]^2$$

with coefficients $c_{k_1 k_2}$ given by

$$c_{k_1 k_2} = -\frac{(2 - \delta_{k_1 0})(2 - \delta_{k_2 0})}{4\pi^2} \int_{\partial[-1,1]} \int_{\partial[-1,1]} f(x_1, x_2) \, \frac{T_{k_1}(x_1)}{\sqrt[{[-1,1]}]{x_1^2 - 1}} \, \frac{T_{k_2}(x_2)}{\sqrt[{[-1,1]}]{x_2^2 - 1}} \, dx_1 \, dx_2.$$

Proof. $f(x_1, x_2)$ is analytic on $[-1, 1]$ and $\phi(z)$ maps the unit circle $\{|z| = 1\}$ holomorphically onto $[-1, 1]$, thus $f(\phi(z_1), \phi(z_2))$ is analytic on $\{|z| = 1\}^2$ and can be expanded into a Laurent series

$$(B.3) \qquad f(\phi(z_1), \phi(z_2)) = \sum_{k_1, k_2 = -\infty}^{\infty} a_{k_1, k_2} z_1^{k_1} z_2^{k_2}$$

with coefficients $a_{k_1 k_2}$ given by

$$(B.4) \qquad a_{k_1 k_2} = -\frac{1}{4\pi^2} \int_{|z_2|=1} \int_{|z_1|=1} f(\phi(z_1), \phi(z_2)) z_1^{-k_1-1} z_2^{-k_2-1} \, dz_1 \, dz_2.$$

Since $\phi(z) = \phi(z^{-1})$, we conclude that $a_{k_1 k_2}$ is symmetric about the origin in both k_1 and k_2, i.e., $a_{k_1, k_2} = a_{-k_1, k_2}$ and $a_{k_1, k_2} = a_{k_1, -k_2}$. The terms in (B.3) can therefore be rearranged as a Chebyshev series in $\phi(z_{1,2})$,

$$f(\phi(z_1), \phi(z_2)) = \sum_{k_1, k_2 = 0}^{\infty} (2 - \delta_{k_1 0})(2 - \delta_{k_2 0}) a_{k_1 k_2} \frac{z_1^{k_1} + z_1^{-k_1}}{2} \frac{z_2^{k_2} + z_2^{-k_2}}{2}$$

$$= \sum_{k=0}^{\infty} c_{k_1 k_2} T_{k_1}(\phi(z_1)) T_{k_2}(\phi(z_2)),$$

which is (B.2) with $c_{k_1 k_2} := (2 - \delta_{k_1 0})(2 - \delta_{k_2 0}) a_{k_1 k_2}$. The formula for the coefficients follows by substituting

$$z_\ell \to \phi_{[-1,1]}^{-1}(x_\ell), \qquad dz_\ell \to \frac{\phi(x_\ell)}{\sqrt[{[-1,1]}]{x^2 - 1}} \, dx_\ell \quad \text{and} \quad \{|z_\ell| = 1\} \to \partial[-1, 1]$$

for both $\ell = 1$ and $\ell = 2$ in the integrals in (B.4). $\qquad \square$

Theorem B.2. *Let $\Omega_1, \Omega_2 \subseteq \mathbb{C}$ be two simply connected sets such that both sets contain -1 and 1. Then it holds that*

$$\left| \frac{(2 - \delta_{k_1 0})(2 - \delta_{k_2 0})}{4\pi^2} \int_{\partial\Omega_2} \int_{\partial\Omega_1} f(x_1, x_2) \frac{T_{k_1}(x_1)}{\sqrt[{b_1}]{x_1^2 - 1}} \frac{T_{k_2}(x_2)}{\sqrt[{b_2}]{x_2^2 - 1}} \, dx_1 \, dx_2 \right| \leq \dots$$

$$\leq C(\partial\Omega_1) C(\partial\Omega_2) \|f\|_{\partial\Omega_1 \times \partial\Omega_2} \exp(-\alpha_1 k_1 - \alpha_2 k_2)$$

for all $k_1, k_2 \in \mathbb{N}$ and all branch cuts $(b_\ell \subset \Omega_\ell)_{\ell \in \{1,2\}}$ connecting $-1, 1$, where

$$\left(\alpha_\ell := \min \alpha_{b_\ell}(\partial\Omega_\ell) \right)_{\ell \in \{1,2\}} \qquad \text{and} \qquad C(\partial\Omega) := \frac{1}{\pi} \int_{\phi_b^{-1}(\partial\Omega)} \frac{|dz|}{|z|}.$$

Proof. Reversing the substitutions in the proof of Theorem B.1 transforms the expression on the left-hand side to (B.4) up to a factor $(2 - \delta_{k_1 0})(2 - \delta_{k_2 0})$ and the integrals running over $\phi_b^{-1}(\partial\Omega_\ell)$ instead of $\{|z_\ell| = 1\}$ for $\ell \in \{1, 2\}$. The claim follows by bounding these integrals using Hölder's inequality. $\qquad \square$

We illustrate the application of Theorems B.1 and B.2 by proving the following corollary which can be found e.g., in [2, Theorem 11], [20, Lemma 5.1] and [3, Theorem 11].

Corollary B.1. *The Chebyshev coefficients of a function $f(x_1, x_2)$ analytic on $E(\alpha_1) \times E(\alpha_2)$ are bounded by*

$$(B.5) \qquad |c_{k_1 k_2}| \lesssim 4 \|f\|_{\partial E(\alpha_1) \times \partial E(\alpha_2)} \exp(-\alpha_1 k_1 - \alpha_2 k_2) \quad \text{for all } k_1, k_2 \in \mathbb{N}.$$

Proof. $f(x_1, x_2)$ is analytic on $[-1,1]^2 \subset E(\alpha_1) \times E(\alpha_2)$, thus Theorem B.1 says that we can expand $f(x_1, x_2)$ into a Chebsyhev series with coefficients given by

$$c_{k_1 k_2} = -\frac{(2 - \delta_{k_1 0})(2 - \delta_{k_2 0})}{4\pi^2} \int_{\partial\Omega_2} \int_{\partial\Omega_1} f(x_1, x_2) \frac{T_{k_1}(x_1)}{^{[-1,1]}\sqrt{x_1^2 - 1}} \frac{T_{k_2}(x_2)}{^{[-1,1]}\sqrt{x_2^2 - 1}} \, dx_1 \, dx_2$$

where $\Omega_1 = \Omega_2 = [-1, 1]$. Using Cauchy's integral theorem as well as the analyticity of $f(x_1, x_2)$, we can replace the two contour domains $\Omega_1 = \Omega_2 = [-1, 1]$ with $\Omega_\ell = E(\tilde{\alpha}_\ell)$ for any $\tilde{\alpha}_\ell < \alpha_\ell$ which by Theorem B.2 implies

$$|c_{k_1, k_2}| \leq 4 \, \|f\|_{\partial E(\tilde{\alpha}_1) \times \partial E(\tilde{\alpha}_2)} \exp\left(-\tilde{\alpha}_1 k_1 - \tilde{\alpha}_2 k_2\right)$$

where we used $C(\partial E(\alpha)) = \frac{1}{\pi} \int_{|z| = \exp(\alpha)} \frac{|dz|}{|z|} = 2$ and $\alpha_{[-1,1]}(\partial E(\alpha)) = \alpha$. This is precisely the bound (B.5). $\square$

B.3. Chebyshev coefficients of the conductivity function.

This subsection establishes the bound (3.9) with explicit formulae for $\alpha_{\mathrm{diag}}(\zeta)$ and $\alpha_{\mathrm{anti}}(\zeta)$, which will be done in two steps. First, we will prove Theorem B.3 below which bounds the Chebyshev coefficients of the factor $f(x_1, x_2) = \frac{1}{x_1 - x_2 + s}$ from (3.6) where we set $s := \omega + \iota\eta$ for notational convenience. The extension to the conductivity function F_ζ will then be an easy modification of Theorem B.3.

We note that $\frac{1}{x_1 - x_2 + s}$ is analytic at all $x_1 \in \mathbb{C}$ except $x_1 = x_2 - s$, and likewise $\frac{1}{x_1 - x_2 + s}$ is analytic at all $x_2 \in \mathbb{C}$ except $x_2 = x_1 + s$. The condition that $\frac{1}{x_1 - x_2 + s}$ be analytic on a domain $\Omega_1 \times \Omega_2$ is thus equivalent to $(\Omega_1 + s) \cap \Omega_2 = \{\}$ which is clearly the case for $\Omega_1 = \Omega_2 = [-1, 1]$ and $\mathrm{Im}(s) \neq 0$, see Figure 6a. By Theorem B.1, we can thus expand $\frac{1}{x_1 - x_2 + s}$ into a Chebyshev series with coefficients given by
(B.6)

$$c_{k_1 k_2} = -\frac{(2 - \delta_{k_1 0})(2 - \delta_{k_2 0})}{4\pi^2} \int_{\partial\Omega_2} \int_{\partial\Omega_1} \frac{1}{x_1 - x_2 + s} \frac{T_{k_1}(x_1)}{^{b_1}\sqrt{x_1^2 - 1}} \frac{T_{k_2}(x_2)}{^{b_2}\sqrt{x_2^2 - 1}} \, dx_1 \, dx_2$$

where for now $\Omega_1 = \Omega_2 = b_1 = b_2 = [-1, 1]$.

Like in the proof of Corollary B.1, we will next use Cauchy's integral theorem repeatedly to move the contour domains Ω_1, Ω_2 to appropriate shapes and then employ Theorem B.2 to bound the Chebyshev coefficients. To this end, let us introduce

$$\hat{\alpha}_{\max}(s) := \min\{\alpha_{[-1,1]}(\pm 1 - s)\} = \alpha_{[-1,1]}\left(1 - |\mathrm{Re}(s)| - \iota \, \mathrm{Im}(s)\right),$$

which is the parameter of the ellipse $E(\hat{\alpha}_{\max}(s))$ penetrating the line $[-1, 1] - s$ up to the endpoints $\pm 1 + s$, and let us denote by

$$\hat{D}(s) := \left(E(\hat{\alpha}_{\max}(s)) + s\right) \cap \{x \mid \mathrm{Im}(x) < 0\}$$

the portion of $E(\hat{\alpha}_{\max}(s)) + s$ penetrating $[-1, 1]$ (see Figure 6c). Arguing similarly as above, we see that $\frac{1}{x_1 - x_2 + s}$ is analytic on $[-1, 1] \times \left([-1, 1] \cup \overline{\hat{D}(s)}\right)$, thus we can replace $\Omega_2 = [-1, 1]$ with $\Omega_2 = [-1, 1] \cup \hat{D}(s)$ without changing the value of the integral. We next move the branch cut $b_2 = [-1, 1]$ to the lower boundary of Ω_2,

$$b_2 = \hat{b}^\star(s) := \left([-1, 1] \setminus \hat{D}(s)\right) \cup \{x \in \partial\hat{D}(s) \mid \mathrm{Im}(s) < 0\},$$

which allows us to replace $\Omega_2 = [-1, 1] \cup \hat{D}(s)$ with $\Omega_2 = \hat{b}^\star(s)$ and finally replace $\Omega_1 = [-1, 1]$ with $\Omega_1 = E(\tilde{\alpha}_1)$ for any $\tilde{\alpha}_1 < \hat{\alpha}_{\max}(s)$, see Figure 6b. By Theorem B.2, these final contours imply the bound
(B.7)

$$|c_{k_1 k_2}| \lesssim \exp\left(-\hat{\alpha}_{\max}(s) \, k_1 - \hat{\alpha}_{\min}(s) \, k_2\right)$$

with

(B.8) $$\hat{\alpha}_{\min}(s) := \min \alpha_{\hat{b}^\star(s)}\big(\partial\hat{b}^\star(s)\big) = -\max \alpha_{[-1,1]}\big(\hat{b}^\star(s)\big),$$

where for the second equality we used Lemma B.1. We note that the last expression in (B.8) may be interpreted as minus the parameter of the smallest ellipse containing $\hat{D}(s)$, see Figure 6c.

By the symmetry of $\frac{1}{x_1-x_2+s}$, the bound (B.7) also holds with the roles of k_1, k_2 interchanged, and since $\hat{\alpha}_{\max}(s) > 0$ but $\hat{\alpha}_{\min}(s) < 0$, we may summarize the two bounds with

(B.9) $$|c_{k_1 k_2}| \lesssim \begin{cases} \exp\big(-\hat{\alpha}_{\max}(s)k_1 - \hat{\alpha}_{\min}(s)\,k_2\big) & \text{if } k_1 \geq k_2, \\ \exp\big(-\hat{\alpha}_{\min}(s)\,k_1 - \hat{\alpha}_{\max}(s)k_2\big) & \text{if } k_1 \leq k_2. \end{cases}$$

Rewriting (B.9) in the form (B.10), we arrive at the following theorem.

Theorem B.3. *The Chebyshev coefficients $c_{k_1 k_2}$ of $f(x_1, x_2) := \frac{1}{x_1-x_2+s}$ with $\mathrm{Re}(s) \in [-1, 1]$ are bounded by*

(B.10) $$|c_{k_1,k_2}| \lesssim \exp\big(-\hat{\alpha}_{\mathrm{diag}}(s)\,(k_1 + k_2) - \hat{\alpha}_{\mathrm{anti}}(s)\,|k_1 - k_2|\big)$$

where

$$\hat{\alpha}_{\mathrm{diag}}(s) := \frac{1}{2}\big(\hat{\alpha}_{\max}(s) + \hat{\alpha}_{\min}(s)\big) \quad \text{and} \quad \hat{\alpha}_{\mathrm{anti}}(s) := \frac{1}{2}\big(\hat{\alpha}_{\max}(s) - \hat{\alpha}_{\min}(s)\big).$$

A closer inspection of the above argument reveals that the bound (B.10) applies to any function $f(x_1, x_2) = \frac{g(x_1,x_2)}{x_1-x_2+s}$ as long as $g(x_1, x_2)$ is analytic on $E\big(\hat{\alpha}_{\max}(s)\big)^2$, and in particular it applies to the conductivity function $F_\zeta(E_1, E_2) = \frac{g_{\beta, E_F}(E_1,E_2)}{E_1-E_2+\omega+\iota\eta}$ if the singularities S_{temp} of g_{β, E_F} from (3.7) satisfy

$$E\big(\alpha_{\omega,\eta}\big)^2 \cap S_{\mathrm{temp}} = \{\} \iff E\big(\alpha_{\omega,\eta}\big) \cap S_{\mathrm{temp}}^{(1)} = \{\} \iff \beta \leq \frac{\pi}{y_\zeta},$$

i.e., if ζ is relaxation-constrained (note that $\alpha_{\omega,\eta} = \hat{\alpha}_{\max}(\omega + \iota\eta)$). Furthermore, the argument and hence the bound (B.10) can be extended to the non-relaxation-constrained case $\beta \geq \frac{\pi}{y_\zeta}$ if we replace $\hat{\alpha}_{\max}(\zeta)$ with

$$\alpha_{\max}(\zeta) = \min\big\{\hat{\alpha}_{\max}(\omega + \iota\eta),\, \alpha_{[-1,1]}\big(E_F + \tfrac{\pi\iota}{\beta}\big)\big\},$$

see Figure 6d. This leads to new variables $D(\zeta), b^\star(\zeta)$ and $\alpha_{\min}(\zeta)$ defined analogously to, respectively, $\hat{D}(\zeta), \hat{b}^\star(\zeta)$ and $\hat{\alpha}_{\min}(\zeta)$ but starting from $\alpha_{\max}(\zeta)$ instead of $\hat{\alpha}_{\max}(s)$.

B.4. **Asymptotics.** To complete the proof of Theorem 3.1, it remains to show the asymptotic scaling of y_ζ as well as $\alpha_{\mathrm{diag}}(\zeta)$ and $\alpha_{\mathrm{anti}}(\zeta)$, which we will do using the following auxiliary result.

Lemma B.2. *It holds that*

(B.11) $\alpha_{[-1,1]}(x) = \Theta\big(|\mathrm{Im}(x)|\big)$ *for $x \to x^\star$ with $x^\star \in (-1, 1)$,*

(B.12) $\alpha_{[-1,1]}(x) = \Theta\big(\sqrt{|x \mp 1|}\big)$ *for $x \to \pm 1$ with $\pm\,\mathrm{Re}(x) - 1 \geq C|\mathrm{Im}(x)|$.*

Proof. (B.11): $\alpha_{[-1,1]}(x) = \mathrm{Re}\big(\log \phi_{[-1,1]}^{-1}(x)\big)$ is harmonic on either side of the branch cut and can thus be expanded into a Taylor series around any $x^\star \in (-1, 1) \pm 0\iota$.
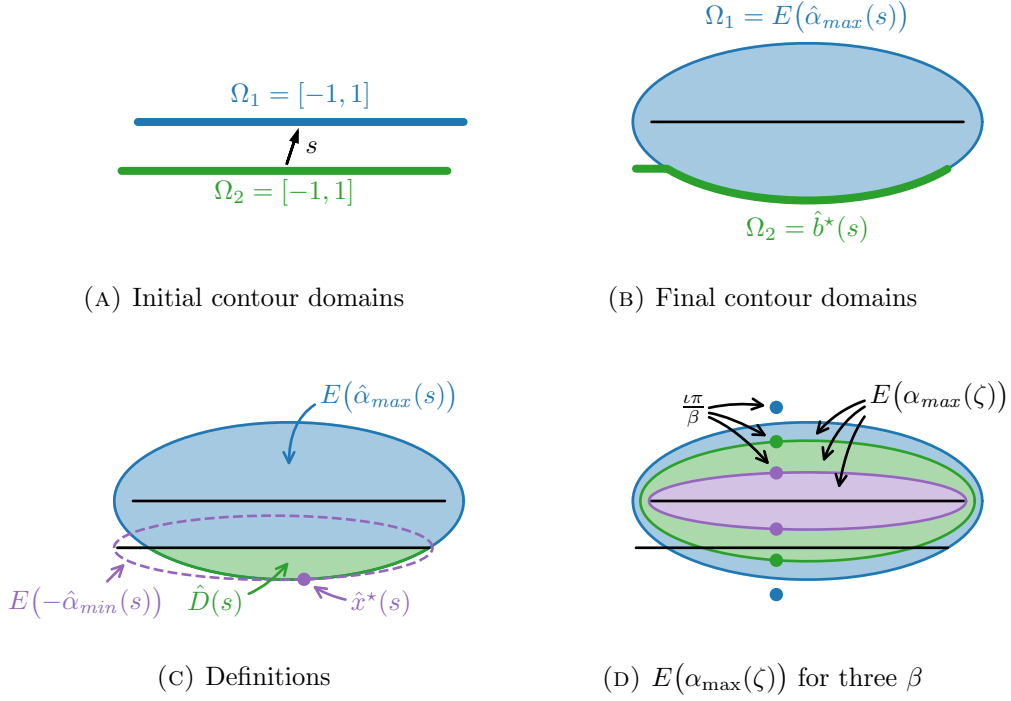
(A) Initial contour domains

(B) Final contour domains

(C) Definitions

(D) $E\big(\alpha_{\max}(\zeta)\big)$ for three β

FIGURE 6. Illustration of the various definitions in Subsection B.3.

Since $\alpha_{[-1,1]}(x^\star) = 0$ for all $x^\star \in (-1,1) \pm 0\iota$, the constant term vanishes, and writing $\alpha_{[-1,1]}(x) = \big(\varphi^{-1}(\mathrm{Re}(x), \mathrm{Im}(x))\big)_1$ with

$$\varphi(\alpha, \theta) := \begin{pmatrix} \mathrm{Re}\big(\phi\big(\exp(\alpha + \iota\,\theta)\big)\big) \\ \mathrm{Im}\big(\phi\big(\exp(\alpha + \iota\,\theta)\big)\big) \end{pmatrix}, \qquad \nabla\varphi(0, \theta) = \begin{pmatrix} 0 & \cos(\theta) \\ \sin(\theta) & 0 \end{pmatrix},$$

we conclude that

$$\frac{\partial \alpha_{[-1,1]}}{\partial \mathrm{Re}(x)}(x^\star) = \Big(\nabla\varphi(0, \theta^\star)^{-1}\Big)_{11} = 0,$$

$$\frac{\partial \alpha_{[-1,1]}}{\partial \mathrm{Im}(x)}(x^\star) = \Big(\nabla\varphi(0, \theta^\star)^{-1}\Big)_{12} = \sin(\theta^\star)^{-1} \neq 0$$

where $\theta^\star = \mathrm{acos}\big(\mathrm{Re}(x^\star)\big)$.

(B.12): We compute

$$\alpha\big(w^2 \pm 1\big) = \mathrm{Re}\bigg(\log\Big(w^2 \pm 1 + \sqrt{(w^2 \pm 1)^2 - 1}\,\Big)\bigg)$$

$$= \mathrm{Re}\bigg(\log\Big(1 \mp w\,\sqrt{w^2 \pm 2 \mp w^2}\,\Big)\bigg)$$

$$= \mathrm{Re}\Big(\mp \sqrt{\pm 2}\,w + \mathcal{O}(w^2)\Big) \quad \text{for } w \to 0,$$

where by $\sqrt{(w^2 \pm 1)^2 - 1}$ we mean a w-dependent combination of the two branches of the square-root function such that $\alpha\big(w^2 \pm 1\big)$ is harmonic around $w = 0$. The claim follows by substituting $w = \sqrt{x \mp 1}$ and noting that $\sqrt{\pm 2}\,\sqrt{x \mp 1}$ is bounded away from the imaginary axis as long as x is bounded away from $[-1, 1]$. □

Lemma B.2 immediately yields $\alpha_{\mathrm{relax}} = \alpha_{[-1,1]}\big(1 - |\omega| + \iota\eta\big) = \Theta\big(\sqrt{\eta}\big)$ which in turn implies $y_\zeta = \Theta\big(\sqrt{\eta}\big)$ as one can verify by Taylor-expanding the formula

$$y_\zeta = \sinh(\alpha_{\omega,\eta}) \sqrt{1 - \frac{E_F^2}{\cosh(\alpha_{\omega,\eta})^2}}$$

which follows easily from the geometric definition given in Figure 2.

For temperature-constrained parameters $\beta \geq \frac{\pi}{\eta}$ corresponding to the innermost ellipse in Figure 6d, it holds that $D(\zeta) = \emptyset$, $b^\star(\zeta) = [-1,1]$, $\alpha_{\min}(\zeta) = 0$ and thus

$$\alpha_{\mathrm{diag}}(\zeta) = \alpha_{\mathrm{anti}}(\zeta) = \alpha_{\max}(\zeta) = \Theta\big(\beta^{-1}\big)$$

where for the last equality we again employed Lemma B.2. It hence remains to analyze the asymptotics of $\alpha_{\mathrm{diag}}(\zeta)$ and $\alpha_{\mathrm{anti}}(\zeta)$, to which end we introduce

(B.13)
$$x^\star(\zeta) := \arg\min_{x \in \partial b^\star(\zeta)} \alpha_{b^\star(\zeta)}(x) = \arg\max_{x \in b^\star(\zeta)} \alpha_{[-1,1]}(x),$$

which is the point where $D(\zeta)$ and $E\big(-\alpha_{\min}(\zeta)\big)$ touch, see Figure 6c for an illustration of the analogous variable $\hat{x}^\star(s)$. We observe the following.

Lemma B.3. $x^\star(\zeta)$ is unique for $|\omega|$ small enough, and $\lim_{\omega\to 0} \mathrm{Re}\big(x^\star(\zeta)\big) = 0$.

Proof. One easily verifies from the geometric interpretation of $x^\star(\zeta)$ that $x^\star(\zeta)$ is unique and satisfies $\mathrm{Re}\big(x^\star(\zeta)\big) = 0$ if $\omega = 0$. The uniqueness and limit then follow from the continuity of $\alpha_{[-1,1]}(x)$ and $b^\star(\zeta)$. $\square$

Lemma B.4. $\alpha_{\min}(\zeta) = -\alpha_{[-1,1]}\big(x^\star(\zeta)\big)$ and $\alpha_{\max}(\zeta) = \alpha_{[-1,1]}\big(x^\star(\zeta) - \omega - \iota\eta\big)$.

Proof. The claim follows directly from (B.13). $\square$

Lemma B.5. In the limit considered in Theorem 3.1, it holds that

$$\big|\mathrm{Im}\big(x^\star(\zeta)\big)\big| = \begin{cases} \Theta\big(\eta^{1/2}\big) & \text{if } \beta \leq \frac{\pi}{y_\zeta}, \\ \Theta\big(\beta^{-1}\big) & \text{if } \beta \geq \frac{\pi}{y_\zeta}. \end{cases}$$

and thus $\eta = \mathcal{O}\big(|x^\star(\zeta)|^2\big)$

Proof. We conclude from Lemma B.3 that for small ω, $x^\star(\zeta)$ is near the imaginary axis where $b^\star(\zeta) \ni x^\star(\zeta)$ satisfies

$$\mathrm{Im}\big(b^\star(\zeta)\big) = \big\{ \sinh\big(\alpha_{\max}(\zeta)\big) \sin(\theta) - \eta \mid \theta \approx \tfrac{3\pi}{2} \big\}.$$

The claim then follows from the asymptotics for $\alpha_{\max}(\zeta)$ which are easily obtained using Lemma B.2. $\square$

Using the above results as well as the shorthand notation $s = \omega + \iota\eta$, we get for the diagonal decay rate

$$\alpha_{\mathrm{diag}}(\zeta) = \tfrac{1}{2}\big(\alpha_{\max}(\zeta) + \alpha_{\min}(\zeta)\big)$$

$$= \tfrac{1}{2}\Big(\alpha_{[-1,1]}\big(x^\star(\zeta) - s\big) - \alpha_{[-1,1]}\big(x^\star(\zeta)\big)\Big)$$

$$= \frac{\partial \alpha_{[-1,1]}}{\partial \mathrm{Im}(x)}(0)\, \mathrm{Im}\big(x^\star(\zeta) - s - x^\star(\zeta)\big) + \ldots$$

$$\mathrm{Re}\left(\frac{\partial^2}{\partial x^2} \log \phi_{[-1,1]}^{-1}(x)\Big|_{x=0} \Big(\big(x^\star(\zeta) - s\big)^2 - x^\star(\zeta)^2\Big)\right) + \mathcal{O}\big(|x^\star(\zeta)|^{3/2}\big)$$

$$= \frac{\partial \alpha_{[-1,1]}}{\partial \mathrm{Im}(x)}(0)\, \eta + \mathcal{O}\big(|x^\star(\zeta)|^{3/2}\big) = \Theta\big(\eta\big).$$

For the anti-diagonal decay rate $\alpha_{\mathrm{anti}}(\zeta)$, on the other hand, we repeat the above calculations with a negative sign for $\alpha_{\min}(\zeta)$, which means that the $x^\star(\zeta)$ in the linear term and the $x^\star(\zeta)^2$ in the quadratic term on the third line add up rather than cancel and thus

$$\alpha_{\mathrm{anti}}(\zeta) = \frac{\partial \alpha_{[-1,1]}}{\partial \operatorname{Im}(x)}(0) \operatorname{Im}\big(x^\star(\zeta)\big) + \mathcal{O}\big(|x^\star(\zeta)|^2\big) = \begin{cases} \Theta\big(\eta^{1/2}\big) & \text{if } \beta \leq \frac{\pi}{y_\zeta}, \\ \Theta\big(\beta^{-1}\big) & \text{if } \beta \geq \frac{\pi}{y_\zeta}. \end{cases}$$

This completes the proof of Theorem 3.1.

Appendix C. Other Proofs: Numerics

C.1. **Proof of Theorem 3.2.** Let us introduce

$$b_{k_1 k_2} := \exp\big(-\alpha_{\max}(\zeta)\, k_1 - \alpha_{\min}(\zeta)\, k_2\big)$$

with

$$\alpha_{\max}(\zeta) := \alpha_{\mathrm{diag}}(\zeta) + \alpha_{\mathrm{anti}}(\zeta), \qquad \alpha_{\min}(\zeta) := \alpha_{\mathrm{diag}}(\zeta) - \alpha_{\mathrm{anti}}(\zeta).$$

Using Lemma 3.1 as well as the bound (3.9), we obtain

$$\begin{aligned}
\big|\tilde{\sigma}_{\mathrm{loc}} - \sigma_{\mathrm{loc}}\big| &\lesssim \sum_{(k_1,k_2)\in\mathbb{N}^2\setminus K(\tau)} |c_{k_1 k_2}| \\
&\leq 2\, C(\zeta) \sum_{(k_1,k_2)\in\mathbb{N}^2\setminus K(r)\wedge k_1\geq k_2} b_{k_1 k_2} \\
&= 2\, C(\zeta) \Bigg(\underbrace{\sum_{k_2=0}^{K_2(\tau)-1} \sum_{k_1=K_1(\tau,k_2)}^{\infty} b_{k_1 k_2}}_{A} + \underbrace{\sum_{k_2=K_2(\tau)}^{\infty} \sum_{k_1=k_2}^{\infty} b_{k_1 k_2}}_{B}\Bigg)
\end{aligned}$$

where

$$K_2(\tau) := \left\lceil \frac{-\log(\tau)}{2\,\alpha_{\mathrm{diag}}(\zeta)} \right\rceil, \qquad K_1(\tau,k_2) := \left\lceil -\frac{\log(\tau) + \alpha_{\min}(\zeta)\, k_2}{\alpha_{\max}(\zeta)} \right\rceil.$$

For the two terms A and B, we obtain using $\alpha_{\mathrm{diag}}(\zeta) = \mathcal{O}\big(\alpha_{\mathrm{anti}}(\zeta)\big)$ and hence $\alpha_{\max}(\zeta) = \Theta\big(\alpha_{\mathrm{anti}}(\zeta)\big)$,

$$\begin{aligned}
A &= \sum_{k_2=0}^{K_2(\tau)-1} \exp\big(-\alpha_{\min}(\zeta)\, k_2\big) \sum_{k_1=K_1(\tau,k_2)}^{\infty} \exp\big(-\alpha_{\max}(\zeta)\, k_1\big) \\
&\leq \sum_{k_2=0}^{K_2(\tau)-1} \exp\big(-\alpha_{\min}(\zeta)\, k_2\big) \frac{\tau \exp\big(\alpha_{\min}(\zeta)\, k_2\big)}{1 - \exp\big(-\alpha_{\max}(\zeta)\big)} \\
&= \frac{K_2(\tau)}{1 - \exp\big(-\alpha_{\max}(\zeta)\big)}\, \tau \\
&= \mathcal{O}\Big(\alpha_{\mathrm{diag}}(\zeta)^{-1}\, \alpha_{\mathrm{anti}}(\zeta)^{-1}\, \tau \log(\tau)\Big)
\end{aligned}$$

and

$$B = \sum_{k_2=K_2(\tau)}^{\infty} \exp\big(-\alpha_{\min}(\zeta)\,k_2\big) \sum_{k_1=k_2}^{\infty} \exp\big(-\alpha_{\max}(\zeta)\,k_1\big)$$

$$= \sum_{k_2=K_2(\tau)}^{\infty} \exp\big(-\alpha_{\mathrm{diag}}(\zeta)\,k_2\big)\, \frac{1}{1-\exp\big(-\alpha_{\max}(\zeta)\big)}$$

$$\leq \frac{\tau}{1-\exp\big(-\alpha_{\mathrm{diag}}(\zeta)\big)}\, \frac{1}{1-\exp\big(-\alpha_{\max}(\zeta)\big)}$$

$$= \mathcal{O}\bigg(\alpha_{\mathrm{diag}}(\zeta)^{-1}\,\alpha_{\mathrm{anti}}(\zeta)^{-1}\,\tau\bigg).$$

C.2. **Inverse of $\varepsilon = \tau\,|\log(\tau)|$.** This subsection establishes the following result.

Theorem C.1. *Let $\varepsilon,\tau \in (0,\infty)$ be such that $\varepsilon = \tau\,|\log\tau|$. It then holds*

$$\tau = \frac{\varepsilon}{|\log\varepsilon|}\,\big(1 + o(1)\big) \qquad for \qquad \varepsilon \to 0.$$

Proof. Dividing $\varepsilon = \tau\,|\log\tau|$ by $|\log\varepsilon| = \big|\log\tau + \log\log\tau\big|$, we obtain

$$\frac{\varepsilon}{|\log\varepsilon|} = \tau\,\frac{1}{\big|1 + \frac{\log\log\tau}{|\log\tau|}\big|} \qquad \Longleftrightarrow \qquad \tau = \frac{\varepsilon}{|\log\varepsilon|}\,\big|1 + \tfrac{\log\log\tau}{|\log\tau|}\big|.$$

The claim follows after noting that $\tau\,|\log(\tau)|$ is monotonically increasing in τ and hence $\tau \to 0$ for $\varepsilon \to 0$. $\qquad\square$

C.3. **Proof of Theorem 3.3.** According to Riemann's removable singularity theorem in higher dimensions (see e.g. [18, Thm. 4.2.1]), the function

(C.1) $$R(E_1, E_2) = \big(E_1 - E_2 + \omega + \iota\eta\big)\,F_\zeta(E_1, E_2) - \frac{1}{\beta}\,\frac{1}{(E_1 - z)\,(E_2 - z)}$$

with $z := \frac{\pi\iota}{\beta}$ can be analytically continued to

$$\mathcal{S}_z := \Big(\{z\} \times \big(\mathbb{C} \setminus \mathcal{S}_{\beta,E_F}\big)\Big) \cup \Big(\big(\mathbb{C} \setminus \mathcal{S}_{\beta,E_F}\big) \times \{z\}\Big)$$

if $R(E_1, E_2)$ is bounded on this set, or equivalently if

(C.2) $$\lim_{E_1 \to z} (E_1 - z)\,R(E_1, E_2) = 0$$

for some arbitrary $E_2 \in \mathbb{C} \setminus \mathcal{S}_{\beta,E_F}$ and likewise with the roles of E_1 and E_2 interchanged. In order to verify (C.2), we compute

(C.3) $$\lim_{E_1 \to z} (E_1 - z)\,f_{\mathrm{temp}}(E_1, E_2) = \lim_{E_1 \to z} (E_1 - z)\,\frac{f_{\beta,E_F}(E_1) - f_{\beta,E_F}(E_2)}{E_1 - E_2}$$

(C.4) $$= \frac{1}{z - E_2}\,\lim_{E_1 \to z} \frac{E_1 - z}{1 + \exp\big(\beta\,(E_1 - E_F)\big)}$$

(C.5) $$= \frac{1}{\beta}\,\frac{1}{E_2 - z}$$

where on the last line we used L'Hôpital's rule to determine the limit. It follows from (C.5) that for $E_1 \to z$, the first and second term in (C.1) cancel and hence (C.2) holds. The transposed version of (C.2) follows from the symmetry of (C.1), thus we conclude that $R(E_1, E_2)$ can indeed be analytically continued to $\mathcal{S}_z$. Theorem 3.3

then follows by rewriting (3.12) in the form (C.1) and applying the above argument to each of the terms in the sum over Z_k.

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