The channel-irreducible vertex of the Hubbard atom away from half filling: derivation

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1 Overview

The irreducible vertex Γ_r of the Hubbard atom is known in closed form at half filling [1]. Here we derive it at arbitrary filling (zero magnetic field) in all four channels $r \in \{\mathrm{d}, \mathrm{m}, \mathrm{s}, \mathrm{t}\}$. By definition $\Gamma_r = \beta^2\big(\chi_r^{-1} - \eta_r \chi_{0,r}^{-1}\big)$, where χ_r is the generalized susceptibility, an infinite matrix in two fermionic Matsubara frequencies. So the task is to invert χ_r in closed form.

At half filling χ_r is a diagonal matrix plus a mirror term plus a matrix of rank at most two, and the inversion is elementary. Away from half filling the mirror term becomes a dense *Cauchy matrix* $C_{nm} = \rho/(z_n + z_m)$ (Figure 1). The particle–hole susceptibility is then no longer a finite-rank perturbation of an easily invertible matrix. Two properties of C still allow a closed-form inverse:

1. $C^2 = h^2 \mathbb{1}$ for a number h: like the mirror it replaces, C is a scaled involution.
2. C maps a simple pole to a simple pole: $\sum_m C_{nm}/(z_m - x) = \alpha(x)/(z_n + x)$, with a thermal factor obeying $\alpha(x)\alpha(-x) = h^2$.

After multiplication by a polynomial, χ_r is a diagonal matrix plus λC plus a matrix of rank two. Each column of χ_r^{-1} is then built from a diagonal entry, one Cauchy column, a constant, and two pole pairs with one thermal denominator each. All coefficients follow from 2×2 linear systems whose determinants are given by a single quartic.

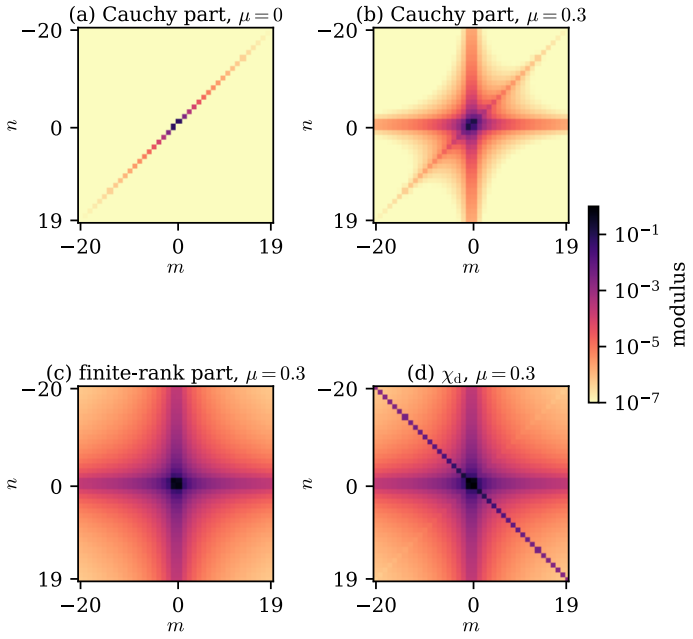


Figure 1: Structure of χ_d at $U = 2$, $\beta = 3$, $\omega = 0$, as moduli of matrix elements in the fermionic indices n, m. (a) At half filling the pair term is a mirror, nonzero only for $m = -n - 1$. (b) Away from half filling it becomes the dense Cauchy matrix C. (c) The remaining finite-rank part. (d) The full χ_d; the diagonal dominates.

Results.

- **Triplet:** Γ_t is a diagonal-minus-mirror term (Theorem 2).

- **Singlet:** Γ_s is a diagonal-plus-mirror term, the constant $2U$, and one separable term with a single thermal denominator (Theorem 3).
- **Density and magnetic:** Γ_d, Γ_m have the same anatomy: a diagonal term, the constant $\pm U$, a dense term without thermal factors, and two separable terms with one thermal denominator each (Theorem 4). At half filling the dense term becomes a mirror term and one separable term remains (Corollary 5).

The inverses are two-sided and agree with the limit of inverses on finite frequency boxes, i.e. with what numerical inversion converges to (Proposition 6).

Roadmap.
- Section 2 defines all quantities; Section 3 states the input, the susceptibility from the Lehmann representation.
- Section 4 states all results. The rest of the note proves them.
- Section 5 evaluates the Matsubara sums; Section 6 proves the particle–particle results, which need no Cauchy matrix.
- Section 7 develops the algebra of C, which Section 8 uses for the particle–hole channels. The limit $\mu \to 0$ and the finite-box statement are proved in Appendix B.

What is assumed. Everything is proved from the input Eqs. 13–15 (Ref. [2]) and the rational identities of Appendix A (checked by computer algebra). The Mathematica notebook `mathematica/doped_gamma.nb` derives the input from the Hamiltonian and replays the proofs step by step (Appendix D). Independent numerical checks are listed in Appendix D. Numerical stability in floating point is not discussed here.

Implementation. The results are implemented as `DopedHubbardAtom` in the Julia package HubbardAtoms.jl, which also evaluates them stably at low temperatures and near the removable singularities, and is tested against exact diagonalization and finite-box inversion.

2 Setup

2.1 Model and thermal weights

$$\mathcal{H} = U\left(n_\uparrow - \frac{1}{2}\right)\left(n_\downarrow - \frac{1}{2}\right) - \mu\big(n_\uparrow + n_\downarrow - 1\big), \quad a := \frac{U}{2}, \tag{1}$$

with real U, μ (the chemical potential measured from half filling, $\mu = 0$) and inverse temperature $\beta > 0$. The four states $|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle$ have energies $\frac{U}{4} + \mu$, $-\frac{U}{4}$, $-\frac{U}{4}$, $\frac{U}{4} - \mu$ and Boltzmann weights p_0, p_1, p_1, p_2 (p_1 is the weight of *each* singly occupied state). Hence

$$p_0 + 2p_1 + p_2 = 1, \qquad \frac{p_2}{p_0} = e^{2\beta\mu}, \qquad \frac{p_1}{p_0} = e^{\beta(a+\mu)}, \qquad \frac{p_1}{p_2} = e^{\beta(a-\mu)}. \tag{2}$$

Define

$$\rho := p_2 - p_0 = \langle n_\uparrow + n_\downarrow \rangle - 1, \qquad h := \beta\sqrt{p_0 p_2}, \qquad \overline{c} := \beta(p_0 + p_2)/2. \tag{3}$$

From Eq. 2, $p_1 + p_2 = (1+\rho)/2$, $p_0 + p_1 = (1-\rho)/2$, and

$$\rho^2 + 4p_0p_2 = (p_0 + p_2)^2, \qquad \overline{c}^2 - h^2 = \beta^2\rho^2/4. \tag{4}$$

For $\mu \neq 0$, inserting $p_2 = p_0 e^{2\beta\mu}$:

$$\begin{aligned} &\rho = 2p_0 e^{\beta\mu}\sinh(\beta\mu), \quad p_0 + p_2 = 2p_0 e^{\beta\mu}\cosh(\beta\mu) \\ \Longrightarrow \quad &\rho\coth(\beta\mu) = p_0 + p_2, \quad \rho^2 = 4p_0p_2\sinh^2(\beta\mu). \end{aligned} \tag{5}$$

2.2 Frequencies and propagator

Fermionic and bosonic Matsubara frequencies are $\nu_n = (2n+1)\pi/\beta$ and $\Omega_\ell = 2\ell\pi/\beta$ ($n, \ell \in \mathbb{Z}$). The bosonic transfer $\omega_k \coloneqq \Omega_k$ is fixed throughout. Write

$$x_n \coloneqq \mu + i\nu_n, \qquad w \coloneqq i\omega_k, \qquad J(x) \coloneqq \frac{1}{x^2 - a^2}. \tag{6}$$

The propagator $G(\nu) \coloneqq -\int_0^\beta \mathrm{d}\tau\, e^{i\nu\tau}\langle T c_\uparrow(\tau) c_\uparrow^\dagger\rangle$ follows from the Lehmann representation: $c_\uparrow^\dagger$ maps $|0\rangle \to |\uparrow\rangle$ (energy change $-a-\mu$, weight p_0+p_1) and $|\downarrow\rangle \to |\uparrow\downarrow\rangle$ (energy change $a-\mu$, weight p_1+p_2). So

$$G(\nu_n) = \frac{p_0+p_1}{x_n + a} + \frac{p_1+p_2}{x_n - a} = G(x_n) \coloneqq \frac{x_n + a\rho}{x_n^2 - a^2}, \tag{7}$$

where we use the same letter for the rational function $G(x)$.

2.3 Susceptibilities and the irreducible vertex

Following Ref. [1], the generalized susceptibility is

$$\begin{aligned}\chi_{\sigma\sigma'}(\nu,\nu',\omega) \coloneqq \iiint_0^\beta \mathrm{d}\tau_1\,\mathrm{d}\tau_2\,\mathrm{d}\tau_3\, e^{-i\nu\tau_1 + i(\nu+\omega)\tau_2 - i(\nu'+\omega)\tau_3} \\ \times \Big[\langle T c_\sigma^\dagger(\tau_1) c_\sigma(\tau_2) c_{\sigma'}^\dagger(\tau_3) c_{\sigma'}(0)\rangle - \langle T c_\sigma^\dagger(\tau_1) c_\sigma(\tau_2)\rangle\langle T c_{\sigma'}^\dagger(\tau_3) c_{\sigma'}(0)\rangle\Big].\end{aligned} \tag{8}$$

Its particle–particle form is $\chi_{\mathrm{pp},\sigma\sigma'}(\nu,\nu',\omega) \coloneqq \chi_{\sigma\sigma'}(\nu,\nu',-\omega-\nu-\nu')$. The channels and bare susceptibilities are

$$\chi_\mathrm{d} = \chi_{\uparrow\uparrow} + \chi_{\uparrow\downarrow}, \quad \chi_\mathrm{m} = \chi_{\uparrow\uparrow} - \chi_{\uparrow\downarrow}, \quad \chi_\mathrm{s} = \frac{-\chi_{\mathrm{pp},\uparrow\uparrow} + 2\chi_{\mathrm{pp},\uparrow\downarrow} - 2\chi_{0,\,\mathrm{pp}}}{4}, \quad \chi_\mathrm{t} = \frac{\chi_{\mathrm{pp},\uparrow\uparrow} + 2\chi_{0,\,\mathrm{pp}}}{4}, \tag{9}$$

$$\chi_{0,r}(\nu,\nu',\omega) = \delta_{\nu\nu'} B(\nu), \qquad B(\nu) = \begin{cases} -\beta G(\nu) G(\nu+\omega) & (r = \mathrm{d},\mathrm{m}), \\ -\frac{\beta}{2} G(\nu) G(-\nu-\omega) & (r = \mathrm{s},\mathrm{t}), \end{cases} \tag{10}$$

with $\chi_{0,\,\mathrm{pp}} \coloneqq \chi_{0,\,\mathrm{s}}$. At fixed ω_k all of these are matrices indexed by (n,m) with $\nu = \nu_n$, $\nu' = \nu_m$; we write $B_n \coloneqq B(\nu_n)$ and $\boldsymbol{B} \coloneqq \mathrm{diag}(B_n)$. The channel-irreducible vertex is

$$\Gamma_r = \beta^2(\chi_r^{-1} - \eta_r \boldsymbol{B}^{-1}), \qquad \eta_\mathrm{d} = \eta_\mathrm{m} = \eta_\mathrm{t} = 1, \quad \eta_\mathrm{s} = -1. \tag{11}$$

2.4 Lattice and mirror

Define the centered lattice and the mirror index

$$\begin{gathered} z_n \coloneqq x_n + \frac{w}{2} = \mu + i\pi\frac{2n+1+k}{\beta}, \qquad \overline{n} \coloneqq -n-k-1, \\ z_{\overline{n}} = 2\mu - z_n, \qquad x_{\overline{n}} = 2\mu - w - x_n. \end{gathered} \tag{12}$$

The lattice lies on the line $\mathrm{Re}\, z = \mu$, and the mirror reflects it about the real axis (Figure 2). The mirror matrix is $\mathcal{M}_{nm} \coloneqq \delta_{m\overline{n}}$, with $\mathcal{M}^2 = \mathbb{1}$. Products of infinite matrices are taken entrywise. A sum $\sum_n$ is the limit of partial sums over the mirror-symmetric boxes $\{n : |2n+1+k| \le 2M+1\}$, $M \to \infty$; we write PV ("principal value") where it converges only in this sense. All transposes are ordinary, not Hermitian. Symbols introduced inside a proof are local to it. A function φ on $\mathbb{C}$ is *proper rational* if it is rational and $\varphi(t) \to 0$ for $t \to \infty$.

3 Input: the generalized susceptibility

The Lehmann representation of $\chi_{\sigma\sigma'}$ for the atom is evaluated in Ref. [2] [Eq. (D3)]. At zero field and in our notation it reads

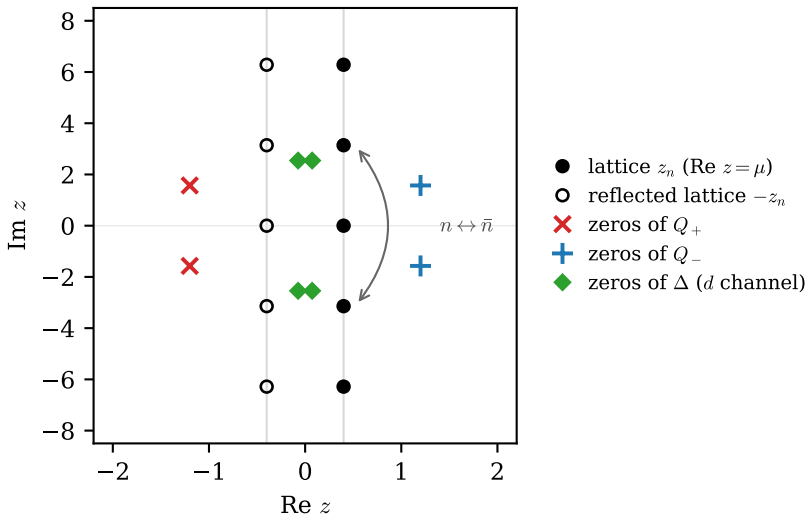


Figure 2: The complex plane for $U = 2.4$, $\beta = 2$, $\mu = 0.4$, $\omega = \omega_1$. The lattice z_n (filled) lies on Re $z = \mu$; the reflected lattice $-z_n$ (open), where the Cauchy kernel $1/(z + z_m)$ is singular, lies on Re $z = -\mu$. Crosses: zeros of $Q_\pm$ (Section 3); diamonds: zeros of e (Section 4.2). None lies on the lattice, so all lattice sums below reduce to finitely many residues.

$$\chi_{\uparrow\uparrow,nm} = -\beta G(x_n)G(x_n + w)\delta_{nm} + \beta a^2(1-\rho^2)J(x_n + w)J(x_m)(\delta_{k0} - \delta_{nm}), \tag{13}$$

$$\chi_{\uparrow\downarrow,nm} = -4\beta a^2 p_1 J(x_n)J(x_n + w)\delta_{nm} + 4\beta a^2(p_0 p_2 - p_1^2)J(x_n)J(x_m)\delta_{k0} + \mathcal{N}_{nm}, \tag{14}$$

$$\begin{aligned} \mathcal{N}_{nm} &:= c_{n+m+k+1}\Pi(x_n, x_m) + R_{\text{reg}}(x_n, x_m), \qquad c_\ell := \frac{\rho}{2\mu + i\Omega_\ell}, \\ \Pi(x, y) &:= \left(\frac{1}{x + w - a} + \frac{1}{y - a}\right)\left(\frac{1}{y + w - a} + \frac{1}{x - a}\right). \end{aligned} \tag{15}$$

The pair coefficient c_ℓ stems from the transition $|0\rangle \leftrightarrow |\uparrow\downarrow\rangle$. At $\mu = 0$ it is understood as its limit, $c_\ell = \beta p_0 \delta_{\ell 0}$ (by Eq. 5, $\rho/2\mu \to \beta p_0$). The regular part R_{reg} is a sum of twelve simple fractions, reproduced in Appendix C. We take Eqs. 13–15 as given; they follow exactly from the Lehmann representation (Appendix D).

Compact form. Define the **Cauchy matrix** $C_{nm} := c_{n+m+k+1}$. Since $2\mu + i\Omega_{n+m+k+1} = z_n + z_m$ by Eq. 12,

$$C_{nm} = \frac{\rho}{z_n + z_m} \quad (\mu \neq 0), \qquad C_{nm} = \beta p_0 \delta_{m\bar{n}} \quad (\mu = 0), \tag{16}$$

and $z_n + z_m = 2\mu + i(\cdots) \neq 0$ for $\mu \neq 0$. Further let

$$Q_\pm(z) := (z \pm a)^2 - \frac{w^2}{4}, \qquad q_0 := a^2 - \frac{w^2}{4} = (U^2 + \omega_k^2)/4. \tag{17}$$

Since $x_n = z_n - w/2$,

$$(x_n - a)(x_n + w - a) = Q_-(z_n), \qquad (x_n + a)(x_n + w + a) = Q_+(z_n), \qquad Q_\pm(-z) = Q_\mp(z). \tag{18}$$

Neither $Q_\pm(z_n)$ vanishes: its factors have imaginary parts ν_n and $\nu_n + \omega_k$, both nonzero.

> **Lemma 1** (compact input). With $z = z_n$ and $v = z_m$,
>
> $$\mathcal{N}_{nm} = \frac{4a^2 C_{nm} - 2a}{Q_-(z)Q_-(v)} + \frac{4a^2(1-\rho)(z + v + 2a)(zv + q_0)}{Q_+(z)Q_-(z)Q_+(v)Q_-(v)}. \tag{19}$$

Proof. Put $y := z + v = x_n + x_m + w$. The two factors of Π combine to

$$\Pi(x_n, x_m) = \frac{y - 2a}{(x_n + w - a)(x_m - a)} \cdot \frac{y - 2a}{(x_m + w - a)(x_n - a)} = \frac{(y - 2a)^2}{Q_-(z)Q_-(v)} \tag{20}$$

by Eq. 18. For $\mu \neq 0$, $(y - 2a)^2/y = y - 4a + 4a^2/y$, so $C_{nm}(y - 2a)^2 = \rho(y - 4a) + 4a^2 C_{nm}$. For $\mu = 0$ this holds too, because $\rho = 0$ and $C_{nm} \neq 0$ only where $y = 0$. Thus Eq. 19 is equivalent to

$$R_{\mathrm{reg}}\Big(z - \frac{w}{2}, v - \frac{w}{2}\Big) = \frac{-2a - \rho(z + v - 4a)}{Q_-(z)Q_-(v)} + \frac{4a^2(1 - \rho)(z + v + 2a)(zv + q_0)}{Q_+(z)Q_-(z)Q_+(v)Q_-(v)}, \tag{21}$$

which is the rational identity (A1) of Appendix A. □

4 Results

All lattice sums that occur below are expressed through

$$S_k(x) := \begin{cases} -\frac{\beta}{2}\tanh(\beta(x - \mu)/2) & k \text{ even} \\ -\frac{\beta}{2}\coth(\beta(x - \mu)/2) & k \text{ odd} \end{cases}, \tag{22}$$

which equals $\mathrm{PV}\sum_n (z_n - x)^{-1}$ for x off the lattice (Lemma 7).

4.1 Singlet and triplet

Let $b := 2\mu - w$ and $t_n := x_n(b - x_n)$; by Eq. 12, $x_{\overline{n}} = b - x_n$, so $t_{\overline{n}} = t_n$. Define

$$\mathcal{P}(t) := (t + a^2)^2 - a^2 b^2, \qquad \mathcal{G}(t) := t + a\rho b + a^2\rho^2, \qquad A_{\mathrm{s}} := a\rho b + a^2(1 - 8p_1), \tag{23}$$

$$\mathcal{T}_k(t) := -\frac{S_k(\mu + \xi)}{\xi}, \qquad \xi := \sqrt{b^2/4 - t}. \tag{24}$$

$\mathcal{T}_k$ is even in ξ, so either branch may be used (for $\xi = 0$ and even k, take the limit $\beta^2/4$). It equals $\sum_n (t_n - t)^{-1}$ (Lemma 9).

Theorem 2 (triplet). For $n \neq \overline{n}$, assuming $t_n + a\rho b + a^2 \neq 0$,

$$\Gamma_{\mathrm{t},nm} = \frac{\beta a^2(1 - \rho^2)\mathcal{P}(t_n)}{\mathcal{G}(t_n)(t_n + a\rho b + a^2)}(\delta_{nm} - \delta_{m\overline{n}}). \tag{25}$$

At a fixed point $n = \overline{n}$ (odd k, $n = -(k + 1)/2$), $\Gamma_{\mathrm{t},nm} = \Gamma_{\mathrm{t},mn} = 0$ for all m.

Theorem 3 (singlet). Assume

$$K_{\mathrm{s}} := 1 + \frac{2a}{\beta}\mathcal{T}_k(-A_{\mathrm{s}}) \neq 0. \tag{26}$$

Then

$$\Gamma_{\mathrm{s},nm} = \frac{\beta a^2(\rho^2 - 1 + 8p_1)\mathcal{P}(t_n)}{\mathcal{G}(t_n)(t_n + A_{\mathrm{s}})}(\delta_{nm} + \delta_{m\overline{n}}) + 4a - \frac{4a\,\mathcal{P}(-A_{\mathrm{s}})}{K_{\mathrm{s}}(t_n + A_{\mathrm{s}})(t_m + A_{\mathrm{s}})}. \tag{27}$$

If $t_n + A_{\mathrm{s}} = 0$ for some n, the entries in the rows and columns n and $\overline{n}$ are the limits of Eq. 27 as μ approaches its value; the divergent parts cancel.

At $\mu = 0$ both formulas reduce to Eq. 19 of Ref. [1] (Appendix D).

4.2 Density and magnetic

Let $\varepsilon := +1$ for $r = \mathrm{d}$ and $\varepsilon := -1$ for $r = \mathrm{m}$. Define

$$H(z) \coloneqq z^2 + 2a\rho z + q_1, \qquad q_1 \coloneqq q_0 + 4\varepsilon a^2 p_1, \qquad \lambda \coloneqq 4\varepsilon a^2,$$
$$P(z) \coloneqq Q_+(z)Q_-(z), \qquad G_2(z) \coloneqq (z + a\rho)^2 - \frac{w^2}{4}, \tag{28}$$

$$e(z) \coloneqq H(z)H(-z) - \lambda^2 h^2/\beta^2 = \left(z^2 + q_1\right)^2 - 4a^2\rho^2 z^2 - 16a^4 p_0 p_2 = (z^2 - s_1)(z^2 - s_2), \tag{29}$$

where $s_{1,2}$ are the roots of $s^2 + 2(q_1 - 2a^2\rho^2)s + q_1^2 - 16a^4 p_0 p_2$, and u_j is either square root of s_j. For $r = \mathrm{m}$ and $k = 0$, $q_1 = a^2(1 - 4p_1)$, so $H(a) = 4a^2 p_2$ and $H(-a) = 4a^2 p_0$ by Eq. 2. Then $e(a) = 0$: one root is $s_1 = a^2$, at the double zeros $\pm a$ of P. We call this root pair *atomic*. With the thermal function

$$\alpha_k(x) \coloneqq \rho\, S_k(x) - \overline{c}, \tag{30}$$

define

$$F(z) \coloneqq \frac{P(z)}{e(z)}, \qquad g_j(z) \coloneqq \frac{1}{z^2 - s_j},$$
$$\mathbb{D}(z, v) \coloneqq \frac{zF(z) - vF(v)}{z^2 - v^2}, \qquad \mathbb{D}(z, z) \coloneqq \frac{F(z) + zF'(z)}{2z}, \tag{31}$$

$$K_j \coloneqq \beta H(-u_j) + \lambda\alpha_k(u_j), \qquad Z_j \coloneqq \frac{u_j P(u_j)\left[\beta H(-u_j) - \lambda\alpha_k(u_j)\right]}{K_j}, \qquad \gamma_j \coloneqq \frac{\lambda\rho Z_j}{s_j - s_\ell}, \tag{32}$$

with $\ell \neq j$.

Theorem 4 (density and magnetic). Let $\mu \neq 0$, $e(z_n) \neq 0$ for all n, and $K_j \neq 0$. Then

$$\Gamma_{r,nm} = \beta P(z_n)\left[\frac{1}{G_2(z_n)} - \frac{H(-z_n)}{e(z_n)}\right]\delta_{nm} + 2\varepsilon a - \lambda\rho\mathbb{D}(z_n, z_m) + \sum_{j=1}^{2} \gamma_j\, g_j(z_n) g_j(z_m). \tag{33}$$

If $s_1 = s_2$, the sum over j is replaced by its limit $\lambda\rho\,\partial_s[Z(s)/((z_n^2 - s)(z_m^2 - s))]$ at $s = s_1$, where $Z(s) \coloneqq [Z(u) + Z(-u)]/2$ with $u^2 = s$, and $Z(u)$ is Z_j with u_j replaced by u. For $r = \mathrm{m}$ and $k = 0$ the atomic pair is omitted, both from the sum and from the assumption $K_j \neq 0$. The formula does not depend on the sign chosen for u_j, and the inverse χ_r^{-1} it represents is two-sided.

So Γ_d and Γ_m have the same anatomy as Γ_s: a diagonal term, the constant $\pm U$, a dense term without thermal factors, and two separable terms with one thermal denominator K_j each. Only $\alpha_k(u_j)$, i.e. tanh or coth at the two roots, has to be evaluated. The assumption $e(z_n) \neq 0$ is not essential either. As e has real coefficients and $z_{\overline{n}} = z_n^*$, lattice zeros of e come in mirror orbits $\{n, \overline{n}\}$. If e vanishes on one orbit, Eq. 33 still holds, with the entries in the rows and columns of the orbit taken as limits as μ approaches its value (Appendix B).

At $\mu = 0$, $\rho = 0$ and Theorem 4 does not apply literally. Here the Cauchy matrix is the mirror, $C = h\mathcal{M}$ with $h = \overline{c} = \beta p_0$, $H(z) = z^2 + q_1$ is even and $e(z) = \left(z^2 + q_1\right)^2 - 16a^4 p_0^2 = (z^2 - \hat{s})(z^2 + 4\varepsilon a^2(p_0 + p_1) + q_0)$ with

$$\hat{s} \coloneqq 4\varepsilon a^2(p_0 - p_1) - q_0, \qquad \hat{g}(z) \coloneqq \frac{1}{z^2 - \hat{s}}, \qquad \hat{D} \coloneqq \beta - \frac{2\varepsilon a S_k(\hat{u})}{\hat{u}}, \tag{34}$$

where $\hat{u}$ is either square root of $\hat{s}$; $\hat{D}$ is even in $\hat{u}$. Explicitly, $\hat{D} = \beta[1 + \varepsilon a \tanh(\beta\hat{u}/2)/\hat{u}]$ for even k, with the value $\beta(1 + \varepsilon a\beta/2)$ at $\hat{u} = 0$; for odd k, coth replaces tanh, and $\hat{u} = 0$ means $e(0) = 0$ at the mirror fixed point $z_n = 0$ (see below).

Corollary 5 (half filling). Let $\mu = 0$, $e(z_n) \neq 0$ for all n, and $\hat{D} \neq 0$. Then

$$\Gamma_{r,nm} = \beta P(z_n)\left[\frac{1}{G_2(z_n)} - \frac{H(z_n)}{e(z_n)}\right]\delta_{nm} + 2\varepsilon a - \lambda h F(z_n)\delta_{m\overline{n}} - \frac{2\varepsilon a\beta P(\hat{u})}{\hat{D}}\hat{g}(z_n)\hat{g}(z_m), \tag{35}$$

and the inverse χ_r^{-1} it represents is two-sided.

This is Eq. 19 of Ref. [1] for $r = \mathrm{d}, \mathrm{m}$ (Appendix D). Compared with Eq. 33, the dense term has become a mirror term, and only one separable term with one thermal denominator remains. The corollary is the limit $\mu \to 0$ of Theorem 4 (proof in Appendix B). The assumption $e(z_n) \neq 0$ matters only for $\beta H(z_n) = -\lambda h$ with $n \neq \overline{n}$, a genuine divergence (Section 4.3). At all other zeros of $e(z_n)$, including both signs at a mirror fixed point (odd k, $z_n = 0$), Eq. 35 holds after taking limits (Appendix B).

4.3 Finite boxes and divergences

Proposition 6 (finite boxes). Under the assumptions of Theorem 2, Theorem 3, Theorem 4 or Corollary 5, the restrictions of χ_r to the boxes $|2n + 1 + k| \leq 2M + 1$ are invertible for all sufficiently large M, and their inverses converge entrywise to $\chi_r^{-1} = \Gamma_r/\beta^2 + \eta_r \boldsymbol{B}^{-1}$.

Divergences. An entry of Γ_r can diverge only where a denominator in its closed form vanishes. Removable are the zeros of $t_n + A_\mathrm{s}$ (Theorem 3), of $s_1 - s_2$, and the lattice zeros of e on one mirror orbit for $\mu \neq 0$ (Theorem 4); at $\mu = 0$, the zeros of $e(z_n)$ with $\beta H(z_n) = \lambda h$, and both kinds at a mirror fixed point (Appendix B). Away from intersections of these exceptional sets, the remaining zeros are genuine poles under the following nonvanishing conditions:

- $K_j = 0$ with $u_j P(u_j) \neq 0$ and $s_1 \neq s_2$ (d, m). Then $\gamma_j K_j = 2\lambda\rho\beta u_j P(u_j) H(-u_j)/(s_j - s_\ell) \neq 0$, as $\alpha_k(u_j) \neq 0$. At $u_j = 0$ the zero of K_j can cancel, as at $\hat{u} = 0$ in Corollary 5.
- $\hat{D} = 0$ with $P(\hat{u}) \neq 0$ (d, m at $\mu = 0$).
- $\beta H(z_n) = -\lambda h$ with $n \neq \overline{n}$ (d, m at $\mu = 0$). There $N(z, \cdot)/P$ is even, so by Eq. 61 $P(z)\chi_r(\boldsymbol{e}_n - \boldsymbol{e}_{\overline{n}}) = -(\beta H(z_n) + \lambda h)(\boldsymbol{e}_n - \boldsymbol{e}_{\overline{n}}) = 0$: the mirror-odd vector is a null vector. For $r = \mathrm{d}$, $k = 0$, $n = 0$ this is $\beta U = 2\pi/\sqrt{3}$.
- $K_\mathrm{s} = 0$ with $\mathcal{P}(-A_\mathrm{s}) \neq 0$ (s).
- $t_n + a\rho b + a^2 = 0$ with $n \neq \overline{n}$ (t); the numerator is $a^2(1 - \rho^2)\mathcal{P}(t_n) \neq 0$.

Example. *Closed form against finite boxes* ($r = \mathrm{d}$, $U = 2$, $\beta = 3$, $\mu = 0.3$, $k = 1$). The inverses of χ_d on the boxes of Proposition 6 ($2M + 1$ frequencies, as k is odd) converge like $1/M$; the extrapolation $2\Gamma^{(256)} - \Gamma^{(128)}$ removes the leading error.

(n, m)	$M = 128$	$M = 256$	extrapolated	Eq. 33
$(0, 0)$	$25.9568 + 33.8867i$	$25.9592 + 33.8867i$	$25.96155 + 33.88673i$	$25.96157 + 33.88673i$
$(0, \overline{0})$	-16.2893	-16.2870	-16.28460	-16.28459
$(2, -1)$	$2.2186 + 0.0612i$	$2.2210 + 0.0612i$	$2.22334 + 0.06123i$	$2.22336 + 0.06123i$

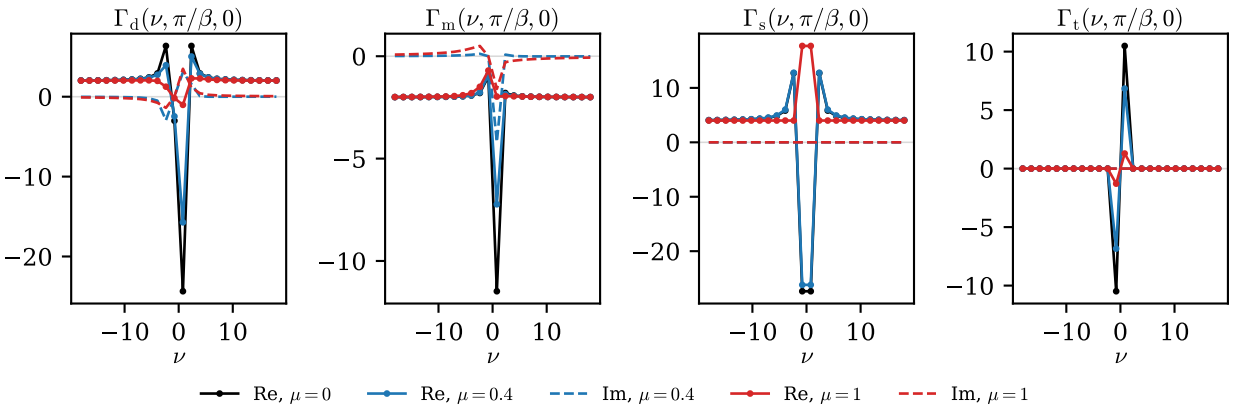


Figure 3: $\Gamma_r(\nu, \pi/\beta, 0)$ from Eq. 33 (Eq. 35 at $\mu = 0$), Eq. 27, Eq. 25 at $U = 2$, $\beta = 4$, for $\mu = 0$ (half filling, real), $\mu = 0.4$ and $\mu = 1$. Away from half filling Γ_d, Γ_m acquire imaginary parts; all Γ_r approach their bare values U, $-U$, $2U$, 0 at large $|\nu|$.

5 Matsubara sums

Lemma 7 (basic sum). For x off the lattice, $\mathrm{PV}\sum_n (z_n - x)^{-1} = S_k(x)$ (Eq. 22), and for $j \geq 2$, $\sum_n (z_n - x)^{-j} = S_k^{(j-1)}(x)/(j-1)!$, absolutely convergent. Moreover, for all k,

$$S_k(x \pm w/2) = -\frac{\beta}{2}\tanh(\beta(x-\mu)/2). \tag{36}$$

In particular, S_k takes the value $S_\pm := \pm(\beta/2)\tanh(\beta(a \pm \mu)/2)$ at both zeros $\mp a \pm w/2$ of $Q_\pm$; by Eq. 2, $S_+ = \beta(p_1 - p_0)/(2(p_1 + p_0))$ and $S_- = \beta(p_2 - p_1)/(2(p_1 + p_2))$.

Proof. For even k, $2n + 1 + k = 2n' + 1$ with $n' = n + k/2$, so $z_n - x = i\nu_{n'} - (x - \mu)$. For odd k, $2n + 1 + k = 2n''$, so $z_n - x = i\Omega_{n''} - (x - \mu)$. In both cases the box is symmetric in n' (resp. n''). The symmetric Mittag-Leffler expansions $\tanh y = \sum_j \big(y - i\pi\big(j + \tfrac{1}{2}\big)\big)^{-1}$ and $\coth y = \sum_j (y - i\pi j)^{-1}$ at $y = \beta(x - \mu)/2$ read $\tanh(\beta(x-\mu)/2) = (2/\beta)\sum_j \big(x - \mu - i\nu_j\big)^{-1}$ and $\coth(\beta(x-\mu)/2) = (2/\beta)\sum_j \big(x - \mu - i\Omega_j\big)^{-1}$, which is Eq. 22. For $j \geq 2$ the $(j-1)$-fold x-derivative of the series converges absolutely and uniformly on compact sets away from the lattice, so it may be differentiated term by term. For Eq. 36: $w/2 = i\pi k/\beta$ shifts the argument of tanh or coth by $\pm i\pi k/2$. For even k this is a multiple of the period $i\pi$; for odd k, $\coth(y \pm i\pi/2) = \tanh y$. □

Lemma 8 (residue rule). Let φ be proper rational without poles on the lattice. Then

$$\sum_n \varphi(z_n) = \sum_{x \in \text{ poles}(\varphi)} \operatorname*{Res}_{t=x}[\varphi(t)S_k(t)], \tag{37}$$

absolutely convergent if $\varphi = O(t^{-2})$, and as a PV sum if $\varphi \sim t^{-1}$. ($\mathrm{Res}_{t=x}$ of a function is the coefficient of $(t-x)^{-1}$ in its Laurent expansion at x.)

Proof. Partial fractions write φ as a finite sum of constants times $(t-x)^{-j}$, $j \geq 1$, over its poles x. By Lemma 7 each $(t-x)^{-j}$ sums to $S_k^{(j-1)}(x)/(j-1)!$, which is the residue of $(t-x)^{-j}S_k(t)$ at x, since S_k is analytic there. □

Lemma 9 (particle–particle sum). For $t \neq t_n$ $(\forall n)$, $\sum_n (t_n - t)^{-1} = \mathcal{T}_k(t)$ (Eq. 24), absolutely convergent. At the two points $t_\pm := -a^2 \pm ab$,

$$\mathcal{T}_k(t_+) = -\frac{2S_-}{2a - b}, \qquad \mathcal{T}_k(t_-) = \frac{2S_+}{2a + b}. \tag{38}$$

Proof. Since $x_n = z_n - w/2$ and $b/2 = \mu - w/2$, $t_n = b^2/4 - (z_n - \mu)^2$, so $(t_n - t)^{-1} = \big[(z_n - \mu + \xi)^{-1} - (z_n - \mu - \xi)^{-1}\big]/(2\xi)$. By Lemma 7 and the oddness of tanh and coth, the sum is $(S_k(\mu - \xi) - S_k(\mu + \xi))/(2\xi) = -S_k(\mu + \xi)/\xi$; it converges absolutely, as $t_n \sim n^2$. At $t_\pm$, $\xi^2 = (a \mp b/2)^2$. At t_+ take $\xi = a - b/2$: then $\mu + \xi = a + w/2$, and $S_k(\mu + \xi) = S_-$ by Eq. 36. At t_- take $\xi = -a - b/2$: then $\mu + \xi = -a + w/2$, and $S_k(\mu + \xi) = S_+$. □

6 Proofs for the singlet and triplet channels

6.1 Variables

With $t_\pm$ from Lemma 9, $\mathcal{P}(t) = (t - t_+)(t - t_-)$. Define

$$d_\pm := A_\mathrm{s} + t_\pm, \qquad c := c_{-k} = \begin{cases} \rho/b & (\mu, k) \neq (0,0) \\ \beta p_0 & \mu = k = 0 \end{cases}. \tag{39}$$

Then $d_+ d_- = \mathcal{P}(-A_\mathrm{s})$. For $t = x(b - x)$, direct expansion gives

$$(x-a)(b-x-a)=t-t_+,\qquad (x+a)(b-x+a)=t-t_-,$$
$$(x+a\rho)(b-x+a\rho)=\mathcal{G}(t), \tag{40}$$

and the product of the first two is $(x^2-a^2)((b-x)^2-a^2)=\mathcal{P}(t)$. Hence, by Eq. 10,

$$B_n=-\frac{\beta}{2}\frac{\mathcal{G}(t_n)}{\mathcal{P}(t_n)}=B_{\overline{n}}. \tag{41}$$

The pp entry (n,m) at transfer k is the ph entry at bosonic index $k':=-k-n-m-1$, with frequency $w':=i\omega_{k'}=b-x_n-x_m$. Then $\delta_{k'0}=\delta_{m\overline{n}}$, and the pair coefficient becomes $c_{n+m+k'+1}=c$. In the variables of Lemma 1 at transfer w', $z+v=x_n+x_m+w'=b$. By Eq. 18 and Eq. 40,

$$Q_-(z)Q_-(v)=(x_n-a)(b-x_n-a)(x_m-a)(b-x_m-a)=(t_n-t_+)(t_m-t_+), \tag{42}$$

and likewise $Q_+(z)Q_+(v)=(t_n-t_-)(t_m-t_-)$.

6.2 Structure

Let $\mathcal{M}_\pm:=(\mathbb{1}\pm\mathcal{M})/2$ be the projectors onto mirror-even and mirror-odd vectors. A diagonal matrix whose entries depend on n only through t_n commutes with the mirror $\mathcal{M}$. Define

$$L_{\mathrm{t}}(t):=-\frac{\beta}{2}\frac{t+a\rho b+a^2}{\mathcal{P}(t)},\quad L_{\mathrm{s}}(t):=\frac{\beta}{2}\frac{t+A_{\mathrm{s}}}{\mathcal{P}(t)},\quad g_\pm(t):=\frac{1}{t-t_\pm},\quad \gamma_\pm:=\frac{a(\rho\pm1)(2a\mp b)}{2b}, \tag{43}$$

and $\boldsymbol{L}_{\mathrm{s,\,t}}:=\mathrm{diag}\big(L_{\mathrm{s,\,t}}(t_n)\big)$.

Proposition 10.

$$\chi_{\mathrm{t}}=\boldsymbol{B}\mathcal{M}_++\boldsymbol{L}_{\mathrm{t}}\mathcal{M}_-,\qquad \chi_{\mathrm{s}}=\boldsymbol{L}_{\mathrm{s}}\mathcal{M}_+-\boldsymbol{B}\mathcal{M}_-+\chi_{\mathrm{s,\,reg}}, \tag{44}$$

where

$$\big(\chi_{\mathrm{s,\,reg}}\big)_{nm}=\frac{a(2ac-1)(t_n-t_-)(t_m-t_-)+a^2(1-\rho)(b+2a)(t_n+t_m+2a^2)}{\mathcal{P}(t_n)\mathcal{P}(t_m)}, \tag{45}$$

which for $b\neq0$ equals

$$\big(\chi_{\mathrm{s,\,reg}}\big)_{nm}=\gamma_+g_+(t_n)g_+(t_m)+\gamma_-g_-(t_n)g_-(t_m). \tag{46}$$

Proof. Insert $w\to w'$ into Eq. 13 and Eq. 14. In the δ_{nm} terms, $x_n+w'=b-x_m=x_{\overline{n}}$; in the $\delta_{k'0}=\delta_{m\overline{n}}$ terms, $x_m=x_{\overline{n}}$ and $x_n+w'=x_n$. With Eq. 40 (abbreviating $\mathcal{P}:=\mathcal{P}(t_n)$),

$$\begin{aligned}\chi_{\mathrm{pp},\uparrow\uparrow}&=2B_n\delta_{nm}-\frac{\beta a^2(1-\rho^2)}{\mathcal{P}}(\delta_{nm}-\delta_{m\overline{n}}),\\ \chi_{\mathrm{pp},\uparrow\downarrow}&=-\frac{4\beta a^2p_1}{\mathcal{P}}\delta_{nm}+\frac{4\beta a^2(p_0p_2-p_1^2)}{\mathcal{P}}\delta_{m\overline{n}}+\mathcal{N}|_{w=w'}.\end{aligned} \tag{47}$$

Triplet. $\big(\chi_{\mathrm{pp},\uparrow\uparrow}+2\boldsymbol{B}\big)/4$ has δ_{nm} coefficient $B_n-\beta a^2(1-\rho^2)/(4\mathcal{P})$ and $\delta_{m\overline{n}}$ coefficient $\beta a^2(1-\rho^2)/(4\mathcal{P})$. Using Eq. 41, these equal $(B+L_{\mathrm{t}})/2$ and $(B-L_{\mathrm{t}})/2$. As B and L_{t} commute with $\mathcal{M}$, $\frac{1}{2}(B+L_{\mathrm{t}})+\frac{1}{2}(B-L_{\mathrm{t}})\mathcal{M}=B\mathcal{M}_++L_{\mathrm{t}}\mathcal{M}_-$.

Singlet, delta terms. The δ_{nm} coefficient of $\big(-\chi_{\mathrm{pp},\uparrow\uparrow}+2\chi_{\mathrm{pp},\uparrow\downarrow}-2\boldsymbol{B}\big)/4$ is $-B_n+\beta a^2(1-\rho^2-8p_1)/(4\mathcal{P})=(L_{\mathrm{s}}-B)/2$. The $\delta_{m\overline{n}}$ coefficient is $\beta a^2[-(1-\rho^2)+8(p_0p_2-p_1^2)]/(4\mathcal{P})$. By Eq. 4 and $p_0+p_2=1-2p_1$, the bracket is $1-8p_1-\rho^2$, and the coefficient is $(L_{\mathrm{s}}+B)/2$. Together: $L_{\mathrm{s}}\mathcal{M}_+-B\mathcal{M}_-$.

Singlet, remaining terms: $(2/4)\mathcal{N}|_{w=w'}$. Insert into Eq. 19: $4a^2C\to4a^2c$, $z+v=b$, $zv+q_0=a^2+(t_n+t_m)/2$ at transfer w' (identity (A3)), and Eq. 42. This gives Eq. 45; for $b\neq0$, its partial fractions in t_n and t_m are Eq. 46 (identity (A3)). □

6.3 Proofs

Proof of Theorem 2. χ_{t} and $\boldsymbol{B}$ act on each orbit $\{n,\overline{n}\}$ separately. For $n \neq \overline{n}$ the orbit carries a 2×2 block with eigenvalue B_n on the even vector and $L_{\mathrm{t}}(t_n)$ on the odd vector; $L_{\mathrm{t}}(t_n) \neq 0$ is the assumption $t_n + a\rho b + a^2 \neq 0$. So $\chi_{\mathrm{t}}^{-1} = \boldsymbol{B}^{-1}\mathcal{M}_+ + \boldsymbol{L}_{\mathrm{t}}^{-1}\mathcal{M}_-$, and $\Gamma_{\mathrm{t}} = \beta^2(\boldsymbol{L}_{\mathrm{t}}^{-1} - \boldsymbol{B}^{-1})\mathcal{M}_-$ by Eq. 11. Further, $(\beta^2/2)(1/L_{\mathrm{t}} - 1/B) = -\beta\mathcal{P}[\mathcal{G} - (t + a\rho b + a^2)]/((t + a\rho b + a^2)\mathcal{G})$ with $\mathcal{G} - (t + a\rho b + a^2) = -a^2(1-\rho^2)$. At a fixed point the orbit is $\{n\}$ with $\mathcal{M}_- = 0$; then $\chi_{\mathrm{t},nn} = B_n$, $\Gamma_{\mathrm{t},nn} = 0$, and $L_{\mathrm{t}}(t_n)$ does not enter. □

Proof of Theorem 3. Idea. χ_{s} is an easily invertible matrix plus the rank-two term Eq. 46, so the Woodbury formula applies. Its 2×2 matrix becomes diagonal in a suitable basis.

For $U = 0$ both sides vanish ($L_{\mathrm{s}} = -B$, $\chi_{\mathrm{s,\,reg}} = 0$). Let $U \neq 0$, and first assume $b \neq 0$, $b \neq \pm 2a$, $d_\pm \neq 0$ and $t_n + A_{\mathrm{s}} \neq 0$ for all n. Then $\gamma_\pm \neq 0$, since $|\rho| < 1$.

Woodbury. Let $\boldsymbol{g}$ be the $\infty \times 2$ matrix with rows $(g_+(t_n), g_-(t_n))$ and $\gamma := \mathrm{diag}(\gamma_+, \gamma_-)$, so $\chi_{\mathrm{s,\,reg}} = \boldsymbol{g}\gamma\boldsymbol{g}^\top$ and $\mathcal{M}_+\boldsymbol{g} = \boldsymbol{g}$. The matrix $\boldsymbol{X} := \boldsymbol{L}_{\mathrm{s}}\mathcal{M}_+ - \boldsymbol{B}\mathcal{M}_-$ has inverse $\boldsymbol{X}^{-1} = \boldsymbol{L}_{\mathrm{s}}^{-1}\mathcal{M}_+ - \boldsymbol{B}^{-1}\mathcal{M}_-$ (all products are finite sums). Set $\boldsymbol{V}_{\mathrm{s}} := \boldsymbol{X}^{-1}\boldsymbol{g} = \boldsymbol{L}_{\mathrm{s}}^{-1}\boldsymbol{g}$ and $\Psi := \boldsymbol{g}^\top\boldsymbol{V}_{\mathrm{s}} = \sum_n (g_+, g_-)^\top(g_+, g_-)(t_n)/L_{\mathrm{s}}(t_n)$, absolutely convergent (terms $O(t_n^{-1}) = O(n^{-2})$). If $\gamma^{-1} + \Psi$ is invertible, then

$$Y := \boldsymbol{X}^{-1} - \boldsymbol{V}_{\mathrm{s}}(\gamma^{-1} + \Psi)^{-1}\boldsymbol{V}_{\mathrm{s}}^\top \tag{48}$$

satisfies $\chi_{\mathrm{s}}Y = \mathbb{1} + \boldsymbol{g}\Big[\gamma - (\mathbb{1} + \gamma\Psi)(\gamma^{-1} + \Psi)^{-1}\Big]\boldsymbol{V}_{\mathrm{s}}^\top = \mathbb{1}$. Y is symmetric, so also $Y\chi_{\mathrm{s}} = \mathbb{1}$. By Eq. 11 ($\eta_{\mathrm{s}} = -1$),

$$\Gamma_{\mathrm{s}} = \beta^2(\boldsymbol{L}_{\mathrm{s}}^{-1} + \boldsymbol{B}^{-1})\mathcal{M}_+ - \beta^2\boldsymbol{V}_{\mathrm{s}}(\gamma^{-1} + \Psi)^{-1}\boldsymbol{V}_{\mathrm{s}}^\top. \tag{49}$$

The first term gives the first term of Eq. 27: $(\beta^2/2)(1/L_{\mathrm{s}} + 1/B) = \beta\mathcal{P}[1/(t + A_{\mathrm{s}}) - 1/\mathcal{G}]$ and $\mathcal{G} - t - A_{\mathrm{s}} = a^2(\rho^2 - 1 + 8p_1)$.

Change of basis. Let $\kappa_n := 1/(t_n + A_{\mathrm{s}})$. Since $\mathcal{P} = (t - t_+)(t - t_-)$ and $t - t_\mp = (t + A_{\mathrm{s}}) - d_\mp$,

$$\frac{g_\pm(t_n)}{L_{\mathrm{s}}(t_n)} = \frac{2}{\beta}(1 - d_\mp\kappa_n), \quad \text{i.e.} \quad (\boldsymbol{V}_{\mathrm{s}})^\top_{n,:} = \frac{2}{\beta}\,\Theta^\top(1, \kappa_n)^\top, \quad \Theta := \begin{pmatrix} 1 & 1 \\ -d_- & -d_+ \end{pmatrix}. \tag{50}$$

Hence $\Big(\boldsymbol{V}_{\mathrm{s}}(\gamma^{-1} + \Psi)^{-1}\boldsymbol{V}_{\mathrm{s}}^\top\Big)_{nm} = (2/\beta)^2(1, \kappa_n)\Xi^{-1}(1, \kappa_m)^\top$ with $\Xi := \Theta^{-\top}(\gamma^{-1} + \Psi)\Theta^{-1}$. Inserting $\Psi = \sum_n (2/\beta)^2 L_{\mathrm{s}}(t_n)\Theta^\top(1, \kappa_n)^\top(1, \kappa_n)\Theta$ and $(2/\beta)^2 L_{\mathrm{s}} = (2/\beta)(t + A_{\mathrm{s}})/\mathcal{P}$,

$$\Xi = \Theta^{-\top}\gamma^{-1}\Theta^{-1} + \frac{2}{\beta}\sum_n \frac{1}{\mathcal{P}(t_n)}\begin{pmatrix} t_n + A_{\mathrm{s}} & 1 \\ 1 & 1/(t_n + A_{\mathrm{s}}) \end{pmatrix}. \tag{51}$$

By partial fractions over $t_+, t_-, -A_{\mathrm{s}}$, the three sums are combinations of $\mathcal{T}_k(t_+)$, $\mathcal{T}_k(t_-)$ and $\mathcal{T}_k(-A_{\mathrm{s}})$. Inserting Eq. 38, the off-diagonal entries of the two terms cancel, and (identity (A4))

$$\Xi = \mathrm{diag}\left(-\frac{1}{a}, \frac{K_{\mathrm{s}}}{a d_+ d_-}\right). \tag{52}$$

So $\gamma^{-1} + \Psi$ is invertible iff $K_{\mathrm{s}} \neq 0$, and

$$-\beta^2\left(\frac{2}{\beta}\right)^2(1, \kappa_n)\Xi^{-1}(1, \kappa_m)^\top = -4\left[-a + \frac{a d_+ d_- \kappa_n\kappa_m}{K_{\mathrm{s}}}\right] = 4a - \frac{4a\,\mathcal{P}(-A_{\mathrm{s}})}{K_{\mathrm{s}}(t_n + A_{\mathrm{s}})(t_m + A_{\mathrm{s}})}. \tag{53}$$

Excluded cases. Fix k. The values of μ where $b = 0$, $b = \pm 2a$, $d_\pm = 0$ or $t_n + A_{\mathrm{s}} = 0$ for some n are isolated, since these are nonconstant analytic functions of μ. Eq. 27 contains no b, $2a \pm b$ or $d_\pm$ in a denominator, and its divergent parts at $q := t_n + A_{\mathrm{s}} \to 0$ cancel. Indeed, the orbit $\{n, \overline{n}\}$ has $r \in \{1, 2\}$ elements, so $\mathcal{T}_k(-A_{\mathrm{s}}) = r/q + O(1)$ and $K_{\mathrm{s}} = 2ar/(\beta q) + O(1)$. Since $a^2(\rho^2 - 1 + 8p_1) = \mathcal{G}(t_n) - q$ and $\mathcal{G}(t_n) \neq 0$ (Eq. 40), the first term of Eq. 27 is $\beta\mathcal{P}(-A_{\mathrm{s}})(\delta_{nm} + \delta_{m\overline{n}})/q + O(1)$, and

the last one is $-2\beta\mathcal{P}(-A_{\mathrm{s}})/(rq)+O(1)$ for $m\in\{n,\overline{n}\}$ and $O(1)$ otherwise. For $m\in\{n,\overline{n}\}$, $\delta_{nm}+\delta_{m\overline{n}}=2/r$, so the $1/q$ terms cancel. Near all these values, $(\chi_{\mathrm{s}})_{nl}=O(|t_l|^{-1})$ and Y_{lm} is bounded for $l\notin\{n,\overline{n},m,\overline{m}\}$, uniformly, where $Y=\Gamma_{\mathrm{s}}/\beta^2-\boldsymbol{B}^{-1}$ with Eq. 27. As $|t_l|\sim l^2$, Lemma 17 extends $\chi_{\mathrm{s}}Y=\mathbb{1}$ to these values. □

7 The Cauchy matrix

Throughout this section $\mu\neq 0$.

Lemma 11 (values on the reflected lattice). For every n,

$$S_k(-z_n)=\frac{\beta}{2}\coth(\beta\mu),\qquad S_k'(-z_n)=\frac{\beta^2}{4\sinh^2(\beta\mu)},\qquad \rho\,S_k(-z_n)=\overline{c}. \tag{54}$$

Proof. Write $-z_n=x-w/2$ with $x:=-\mu-i\pi(2n+1)/\beta$. By Eq. 36, $S_k(-z_n)=-(\beta/2)\tanh(-\beta\mu-i\pi(2n+1)/2)=(\beta/2)\coth(\beta\mu)$, as tanh has period $i\pi$ and $\tanh(y-i\pi/2)=\coth y$. Differentiating Eq. 36 in x gives $S_k'(-z_n)=-(\beta^2/4)\cosh^{-2}(-\beta\mu-i\pi(2n+1)/2)=\beta^2/(4\sinh^2(\beta\mu))$. The last identity is Eq. 5. □

So S_k is *constant* on the reflected lattice (Figure 2). This is the source of all simplifications below.

Lemma 12 (square). $\sum_l C_{nl}C_{lm}=h^2\delta_{nm}$, absolutely convergent.

Proof. $C_{nl}C_{lm}=O(|z_l|^{-2})$. For $n\neq m$, partial fractions $[(z_n+z_l)(z_l+z_m)]^{-1}=(z_m-z_n)^{-1}\left[(z_l+z_n)^{-1}-(z_l+z_m)^{-1}\right]$ and Lemma 7 give $\rho^2[S_k(-z_n)-S_k(-z_m)]/(z_m-z_n)=0$ by Lemma 11. For $n=m$, $\rho^2\sum_l(z_l+z_n)^{-2}=\rho^2S_k'(-z_n)=h^2$ by Lemma 11 and Eq. 5. □

The action of C on rational functions is governed by the thermal function α_k of Eq. 30.

Lemma 13 (thermal function). With $y_\pm:=\beta(x\pm\mu)/2$,

$$\alpha_k(x)=\begin{cases}-h\cosh(y_+)/\cosh(y_-) & k \text{ even}\\ -h\sinh(y_+)/\sinh(y_-) & k \text{ odd}\end{cases},\qquad \alpha_k(x)\alpha_k(-x)=h^2. \tag{55}$$

Proof. For even k, insert $S_k(x)=-(\beta/2)\tanh y_-$, $p_2=p_0e^{2\beta\mu}$ and $h=\beta p_0e^{\beta\mu}$:

$$\alpha_k(x)=-\frac{\beta}{2}\frac{p_2e^{y_-}+p_0e^{-y_-}}{\cosh y_-}=-h\frac{\cosh(y_-+\beta\mu)}{\cosh y_-},\quad y_-+\beta\mu=y_+. \tag{56}$$

Under $x\to-x$, $y_\pm\to-y_\mp$, so the two quotients multiply to 1. Odd k: replace tanh, cosh by coth, sinh. □

Let $\mathcal{C}$ be the action of C on functions sampled on the lattice, $(\mathcal{C}\,\varphi)(z_m):=\sum_n C_{mn}\varphi(z_n)$.

Lemma 14 (Cauchy calculus). For x with x and $-x$ off the lattice, and every lattice point z,

$$\mathcal{C}[(t-x)^{-1}](z)=\frac{\alpha_k(x)}{z+x},\qquad \mathcal{C}[1](z)=\overline{c}\quad(\mathrm{PV}). \tag{57}$$

Higher poles follow by applying $(1/j!)\partial_x^j$; so $\mathcal{C}$ maps every proper rational function whose poles x satisfy this condition to an explicit proper rational function.

Proof. Partial fractions and Lemma 7 give

$$\sum_n\frac{\rho}{(z+z_n)(z_n-x)}=\frac{\rho[S_k(x)-S_k(-z)]}{z+x}=\frac{\alpha_k(x)}{z+x} \tag{58}$$

by Lemma 11. The constant rule is $\mathrm{PV}\sum_n C_{mn} = \rho S_k(-z_m) = \overline{c}$. The sums of x-derivatives converge uniformly near any admissible x, so Eq. 57 may be differentiated. □

8 Proofs for the density and magnetic channels

8.1 Structure

Let $\delta := \delta_{k0}$ and

$$\zeta_r := \beta a^2[1-\rho^2+4\varepsilon(p_0p_2-p_1^2)], \qquad N_2(v) := -2\varepsilon a(v^2+2a\rho v+q_0)+\delta\zeta_r(v^2-a^2), \tag{59}$$

$$N_0(v) := (v^2+2q_0-4a^2)N_2(v)+(2\varepsilon a-\delta\zeta_r)P(v), \qquad N(z,v) := N_0(v)+z^2N_2(v). \tag{60}$$

P is even by Eq. 18 and has no zeros on the lattice. In N_0 the terms of degree four cancel, so $N_0(v)/P(v) = O(v^{-1})$ and $N_2(v)/P(v) = O(v^{-2})$. We identify a function φ on the lattice with the vector $(\varphi(z_n))_n$ and write $(\chi_r\varphi)(z_n) := \sum_m \chi_{r,nm}\varphi(z_m)$.

Proposition 15 (structure).

$$P(z_n)\chi_{r,nm} = -\beta H(z_n)\delta_{nm} + \lambda C_{nm} + \frac{N(z_n,z_m)}{P(z_m)}. \tag{61}$$

Proof. Write $z := z_n$, $v := z_m$, and collect the terms of $\chi_r = \chi_{\uparrow\uparrow} + \varepsilon\chi_{\uparrow\downarrow}$ (Eq. 13, Eq. 14).

(a) δ_{nm} terms: $-\beta[G(x_n)G(x_n+w)+a^2(1-\rho^2+4\varepsilon p_1)J(x_n)J(x_n+w)]$. By Eq. 7 and Eq. 18, $G(x_n)G(x_n+w) = [(z+a\rho)^2-w^2/4]/P(z)$ and $J(x_n)J(x_n+w) = 1/P(z)$. The numerators add up to $(z+a\rho)^2 - w^2/4 + a^2(1-\rho^2) + 4\varepsilon a^2 p_1 = H(z)$.

(b) δ_{k0} terms (only for $k=0$, where $w=0$, $x_n=z$ and $P(z) = (z^2-a^2)^2$): $\zeta_r J(z)J(v)$, and $P(z)J(z)J(v) = (z^2-a^2)(v^2-a^2)/P(v)$.

(c) Remaining terms: $\varepsilon\mathcal{N}_{nm}$ with Eq. 19. Since $C_{nm}(z+v) = \rho$ and $Q_+(z)-Q_-(v) = (z+v)(z-v+2a)$, we have $Q_+(z)C_{nm} = Q_-(v)C_{nm} + \rho(z-v+2a)$. With $1/Q_-(v) = Q_+(v)/P(v)$ this gives

$$\begin{aligned} P(z)\mathcal{N}_{nm} = 4a^2C_{nm} + \frac{1}{P(v)}[&4a^2\rho(z-v+2a)Q_+(v) - 2aQ_+(z)Q_+(v) \\ &+4a^2(1-\rho)(z+v+2a)(zv+q_0)]. \end{aligned} \tag{62}$$

The numerator is quadratic in z. Its z coefficient is $4a^2Q_+(v)[\rho-1+(1-\rho)] = 0$, because $v^2+2av+q_0 = Q_+(v)$. Its z^2 coefficient is $-2aQ_+(v)+4a^2(1-\rho)v = -2a(v^2+2a\rho v+q_0)$, and its z^0 coefficient is $-2a(v^2+2q_0-4a^2)(v^2+2a\rho v+q_0)+2aP(v)$ (identity (A2)). Times ε, this is the part of Eq. 60 without ζ_r. The term (b) is the rest, since $(v^2-2a^2)(v^2-a^2)-P(v) = -a^2(v^2-a^2)$ at $k=0$. □

So, after multiplication by P, the finite-rank part of χ_r has only two output directions, 1 and z^2.

8.2 Rank-two sums

Lemma 16 (rank-two sums). For x off the lattice with $P(x)\neq 0$, and every z,

$$\mathcal{I}(z;x) := \sum_l \frac{N(z,z_l)}{P(z_l)(z_l-x)} = \overline{\mathcal{I}}(z;x) + \alpha_k(x)\frac{N(z,x)}{\rho P(x)}, \tag{63}$$

absolutely convergent, where

$$\overline{\mathcal{I}}(z;x) := \frac{\overline{c}N(z,x)}{\rho P(x)} + \sum_{y:P(y)=0}\operatorname*{Res}_{t=y}\frac{S_k(t)N(z,t)}{P(t)(t-x)}. \tag{64}$$

$\overline{\mathcal{I}}$ depends on the temperature only through β, $\overline{c}$ and $S_\pm$ (Lemma 7), and $P(x)\overline{\mathcal{I}}(z;x)$ is a polynomial in z and x.

Proof. At the zeros of P, $S_k = S_\pm$ (Lemma 7); for $k = 0$ they are double, and there $S_0' = S_0^2 - \beta^2/4$ by Eq. 36. The summand of $\mathcal{I}$ is $O(z_l^{-2})$, since N_0 has degree at most three. Lemma 8 gives the residue $S_k(x)N(z,x)/P(x)$ at $t = x$, plus the residues at the zeros of P; insert $\rho S_k(x) = \overline{c} + \alpha_k(x)$ (Eq. 30). In x, $\overline{\mathcal{I}}$ has poles only at the zeros of P, of at most their multiplicity. □

8.3 The proof of Theorem 4

Strategy. For $U = 0$, $\chi_r = \boldsymbol{B}$ and $\Gamma_\mathrm{d} = \Gamma_\mathrm{m} = 0$; let $U \neq 0$. Fix a lattice point $v = z_m$. We construct a bounded function y_v on the lattice with $\chi_r y_v = \boldsymbol{e}_m$, the m-th unit vector. By Eq. 61 this means, for every lattice point z,

$$-\beta H(z) y_v(z) + \lambda(\mathcal{C}\, y_v)(z) + \sum_l \frac{N(z,z_l)}{P(z_l)} y_v(z_l) = P(v)\delta_{zv}. \tag{65}$$

For $l \neq n$, $\chi_{r,nl} = O(|z_l|^{-2})$ by Eq. 13, Eq. 14 and Eq. 19, so $\sum_l \chi_{r,nl} y_v(z_l)$ converges absolutely. Its parts in Eq. 65 converge at least as PV sums (Lemma 14, Lemma 8), so they may be evaluated separately. We use Lemma 16 at $x = -v$, and Lemma 14 and Lemma 16 at $x = \pm u_j$. These points are off the lattice ($\mu \neq 0$, $e(z_n) \neq 0$), and $P(-v) = P(v) \neq 0$. We first assume that $u_j \neq 0$ and $P(u_j) \neq 0$ for the non-atomic pairs; Step 5 removes this assumption.

Step 1 (the Cauchy column). Through C, a unit vector at v produces the column $\lambda\rho/(z+v)$. Conversely, C maps $1/(t+v)$ back to a unit vector: $\mathcal{C}[(t+v)^{-1}](z) = \rho^{-1}\sum_l C(z,z_l)C(z_l,v) = (h^2/\rho)\delta_{zv}$ by Lemma 12. So try $y = D_v\delta_{zv} + E_v/(z+v)$. Insert it into the left side of Eq. 65. Use $H(z) = H(-v) + (z+v)(z-v+2a\rho)$, and Eq. 63 at $x = -v$, where $\alpha_k(-v) = 0$ (Lemma 11). The left side becomes

$$\begin{aligned}&\left[-\beta H(v) D_v + \frac{\lambda h^2}{\rho} E_v\right]\delta_{zv} + \frac{\lambda\rho D_v - \beta H(-v) E_v}{z+v} \\ &-\beta E_v(z-v+2a\rho) + D_v\frac{N(z,v)}{P(v)} + E_v\overline{\mathcal{I}}(z;-v).\end{aligned} \tag{66}$$

We choose D_v, E_v such that the first term is $P(v)\delta_{zv}$ and the second vanishes. The determinant of these two linear equations is $\beta^2 H(v)H(-v) - \lambda^2 h^2 = \beta^2 e(v) \neq 0$, and the solution is

$$D_v = -\frac{H(-v)P(v)}{\beta e(v)}, \qquad E_v = -\frac{\lambda\rho F(v)}{\beta^2}. \tag{67}$$

With these values the remaining terms are $1/(\beta e(v))$ times the left side of the identity (A7),

$$\begin{aligned}&\lambda\rho(z-v+2a\rho)P(v) - H(-v)N(z,v) - \frac{\lambda\rho}{\beta}P(v)\overline{\mathcal{I}}(z;-v) \\ &\quad = -e(v)N_2(z) + \lambda\rho z[P(v) - e(v)] + \lambda W(z;v^2).\end{aligned} \tag{68}$$

Here $W(z;s) \coloneqq W_0(s) + z^2 W_2(s)$ with polynomials W_0, W_2 of degree one in s, given in Appendix A. Both sides of Eq. 68 are polynomials in z and v (Lemma 16). So the remaining terms are the polynomial

$$\frac{1}{\beta}\left[-N_2(z) + \lambda\rho z(F(v) - 1) + \lambda\frac{W(z;v^2)}{e(v)}\right]. \tag{69}$$

Step 2 (the constant). For $y = 1$ the left side of Eq. 65 is $-\beta H(z) + \lambda\overline{c} + \mathrm{PV}\sum_l N(z,z_l)/P(z_l) = \beta N_2(z)/(2\varepsilon a)$, by $\mathcal{C}[1] = \overline{c}$ (Lemma 14) and identity (A6). So adding the constant $2\varepsilon a/\beta^2$ to y removes the first term of Eq. 69.

Step 3 (pole pairs). The rest of Eq. 69 must be removed by functions that are mapped to polynomials. A simple pole $1/(t-x)$ is mapped by $-\beta H + \lambda\,\mathcal{C}$ to poles at x and at $-x$ (Lemma 14). So consider $\varphi = f_+/(t-x) + f_-/(t+x)$. For it, the left side of Eq. 65 is a polynomial plus

$$\frac{-\beta H(x) f_+ + \lambda\alpha_k(-x) f_-}{z-x} + \frac{\lambda\alpha_k(x) f_+ - \beta H(-x) f_-}{z+x}. \tag{70}$$

Both residues vanish for some $(f_+, f_-) \neq 0$ iff the determinant $\beta^2 H(x)H(-x) - \lambda^2\alpha_k(x)\alpha_k(-x) = \beta^2 e(x)$ vanishes (Eq. 55), i.e. iff $x = \pm u_j$. For $x = u_j$ we take

$$\varphi_j(t) \coloneqq \frac{\beta H(-u_j)}{t-u_j} + \frac{\lambda\alpha_j}{t+u_j} = \frac{K_j t + u_j\big[\beta H(-u_j) - \lambda\alpha_j\big]}{t^2 - s_j}, \qquad \alpha_j \coloneqq \alpha_k(u_j). \tag{71}$$

With $H(z) - H(\pm u_j) = (z \mp u_j)(z \pm u_j + 2a\rho)$, the polynomial part is

$$-\beta\big[K_j(z+2a\rho) + u_j(\beta H(-u_j) - \lambda\alpha_j)\big] + \beta H(-u_j)\mathcal{I}(z;u_j) + \lambda\alpha_j\mathcal{I}(z;-u_j). \tag{72}$$

To evaluate it, set $v = \mp u_j$ in Eq. 68, where $e(v) = 0$ and $P(v) = P(u_j)$:

$$\frac{\lambda\rho}{\beta}P(u_j)\overline{\mathcal{I}}(z;\pm u_j) = \lambda\rho(\pm u_j + 2a\rho)P(u_j) - H(\pm u_j)N(z,\mp u_j) - \lambda W(z;s_j). \tag{73}$$

Insert this into Eq. 63 for $\mathcal{I}(z;\pm u_j)$, with $\alpha_k(-u_j) = h^2/\alpha_j$ (Eq. 55):

- The terms with $N(z,-u_j)$ carry the factor $\lambda^2 h^2 - \beta^2 H(u_j)H(-u_j) = -\beta^2 e(u_j) = 0$.
- The terms with $N(z,u_j)$ cancel.
- The terms with $\lambda\rho P(u_j)$ cancel the constant part of the first bracket.

What remains is

$$P(z)(\chi_r\varphi_j)(z) = -\beta K_j\left[z + \frac{W(z;s_j)}{\rho P(u_j)}\right]. \tag{74}$$

Step 4 (solving). P and e are monic and even of degree four, and $W(z;s)$ has degree one in s. Partial fractions in v^2 therefore give

$$F(v) - 1 = \sum_j F_j g_j(v), \qquad \frac{W(z;v^2)}{e(v)} = \sum_j \frac{W(z;s_j)}{s_j - s_\ell} g_j(v), \qquad F_j \coloneqq \frac{P(u_j)}{s_j - s_\ell}. \tag{75}$$

So the last two terms of Eq. 69 are $\beta^{-1}\sum_j \lambda\rho F_j g_j(v)\big[z + W(z;s_j)/\big(\rho P(u_j)\big)\big]$. By Steps 1–3 and Eq. 74,

$$y_v(z) \coloneqq D_v\delta_{zv} + \frac{E_v}{z+v} + \frac{1}{\beta^2}\left[2\varepsilon a + \lambda\rho\sum_j \frac{F_j g_j(v)}{K_j}\varphi_j(z)\right] \tag{76}$$

solves Eq. 65. To read off Γ_r, note that $\lambda\rho F_j g_j(v)\varphi_j(z)/K_j = \lambda\rho F_j z g_j(z) g_j(v) + \gamma_j g_j(z) g_j(v)$ by Eq. 71. Further, $F(z) - F(v) = -(z^2 - v^2)\sum_j F_j g_j(z) g_j(v)$ gives

$$\mathbb{D}(z,v) = \frac{F(v)}{z+v} - z\sum_j F_j g_j(z) g_j(v). \tag{77}$$

Hence

$$y_v(z) = -\frac{H(-z)P(z)}{\beta e(z)}\delta_{zv} + \frac{1}{\beta^2}\left[2\varepsilon a - \lambda\rho\mathbb{D}(z,v) + \sum_j \gamma_j g_j(z) g_j(v)\right]. \tag{78}$$

By Eq. 7 and Eq. 18, $B_n = -\beta G_2(z_n)/P(z_n)$; so by Eq. 11, $\beta^2\big[y_{z_m}(z_n) - \delta_{nm}/B_n\big]$ is the right side of Eq. 33.

Step 5 (two-sidedness, branches, special cases).

- Let $Y_{nm} \coloneqq y_{z_m}(z_n)$, so that $\chi_r Y = \mathbb{1}$. Y is symmetric because $\mathbb{D}$ is, and so is χ_r (Eq. 13, Eq. 14, Eq. 19). Hence $(Y\chi_r)_{nm} = \sum_l \chi_{r,ml} Y_{ln} = (\chi_r Y)_{mn} = \delta_{nm}$, the same absolutely convergent series.
- Let $K(u) \coloneqq \beta H(-u) + \lambda\alpha_k(u)$. Since $\alpha_k(u)\alpha_k(-u) = h^2$ (Eq. 55), for every u

$$\frac{\beta H(-u) - \lambda\alpha_k(u)}{K(u)} + \frac{\beta H(u) - \lambda\alpha_k(-u)}{K(-u)} = \frac{2\beta^2 e(u)}{K(u)K(-u)}. \tag{79}$$

  At a root the right side vanishes, so Z_j and γ_j do not depend on the sign of u_j.
- *Confluent roots.* By Eq. 79, the odd part $[Z(u) - Z(-u)]/2 = \beta^2 u P(u) e(u)/(K(u)K(-u))$ vanishes at the roots, so $Z(s_j) = Z_j$ for the even part $Z(s)$ of Theorem 4. Hence the sum over j in Eq. 33 is $\lambda\rho$ times the divided difference of $s \mapsto Z(s)/((z_n^2 - s)(z_m^2 - s))$ at s_1, s_2. Near a double root $u_\star^2$, $Z(u)$ is analytic in u at $\pm u_\star$: $K(u_\star) \neq 0$, and at a root $K(u) = 0$ iff $K(-u) = 0$ (Eq. 55, Eq. 29). So $Z(s)$, an even analytic function of u, is analytic in s, also for $u_\star = 0$. As μ approaches a value where $s_1 = s_2$ (a zero of the discriminant of e, a nonconstant analytic function of μ), the divided difference converges to the derivative stated in Theorem 4, and Lemma 17 extends $\chi_r Y = \mathbb{1}$.
- For $r = \mathrm{m}$ and $k = 0$ the atomic pair has $F_1 = P(a)/(a^2 - s_2) = 0$ and $W(z; a^2) = 0$ (Appendix A). So its terms in Step 4 vanish, and Step 3 is needed only for the non-atomic pair.
- *Excluded cases.* Steps 1–4 assumed $u_j \neq 0$ and $P(u_j) \neq 0$ for the non-atomic pairs. For $r = \mathrm{m}$, $k = 0$, $P(u_2) = 0$ would mean $s_2 = a^2 = s_1$, which is excluded. Otherwise, fix k: the values of μ where an assumption fails are zeros of $e(0) = s_1 s_2$ or of the resultant of e and P. These are nonconstant analytic functions of μ, so such values are isolated. Eq. 33 has neither u_j nor $P(u_j)$ in a denominator and depends on s_j only. Near such a value, $\chi_{r,nl} = O(|z_l|^{-2})$ for $l \neq n$ and Y_{lm} is bounded, uniformly; so Lemma 17 extends $\chi_r Y = \mathbb{1}$.
- *Lattice roots.* The case $e(z_n) = 0$ is treated in Appendix B. □

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Bibliography

[1] P. Thunström, O. Gunnarsson, S. Ciuchi, and G. Rohringer, Analytical investigation of singularities in two-particle irreducible vertex functions of the Hubbard atom, Physical Review B **98**, 235107 (2018).

[2] H. Eßl, M. Reitner, G. Sangiovanni, and A. Toschi, General Shiba mapping for on-site four-point correlation functions, Physical Review Research **6**, 033061 (2024).

A Rational identities

Each identity is checked exactly with SymPy: (A1)–(A5) by `doped-gamma/verify_identities.py`, (A6) and (A7) by `doped-gamma/verify_dm.py` (both channels, $k \neq 0$ and $k = 0$, all parameters free).

(A1) the twelve terms of Appendix C equal the two-term form in the proof of Lemma 1; and $\Pi(x_n, x_m) = (z + v - 2a)^2/(Q_-(z)Q_-(v))$.

(A2) the z^0 coefficient in the proof of Proposition 15: $4a^2\rho(2a - v)Q_+(v) - 2aq_0Q_+(v) + 4a^2(1 - \rho)q_0(v + 2a) = -2a(v^2 + 2q_0 - 4a^2)(v^2 + 2a\rho v + q_0) + 2aP(v)$.

(A3) Eq. 40; $zv + q_0 = a^2 + (t_n + t_m)/2$ at transfer $w' = b - x_n - x_m$; Eq. 45 and Eq. 46 from the twelve terms of Appendix C at w' with $c = \rho/b$.

(A4) $\Xi = \mathrm{diag}(-1/a, K_\mathrm{s}/(ad_+d_-))$ in the proof of Theorem 3, and $d_+d_- = \mathcal{P}(-A_\mathrm{s})$.

(A5) the δ_{nm} and δ_{k0} identities in the proof of Proposition 15, and $H(a) = 4a^2p_2$, $H(-a) = 4a^2p_0$ for $r = \mathrm{m}$, $k = 0$.

(A6) Step 2 of the proof of Theorem 4: $-\beta H(z)+\lambda\overline{c}+\mathrm{PV}\sum_l N(z,z_l)/P(z_l)=\beta N_2(z)/(2\varepsilon a)$, the sum evaluated by Lemma 8 and Lemma 16.

(A7) Eq. 68, where $\overline{\mathcal{I}}$ is evaluated by Lemma 16 and, with $\varpi := 4(p_0p_2-p_1^2)$,

$$\begin{aligned} W_0(s) &:= \varepsilon a q_0\big[\varpi-2\varepsilon(1-\rho^2)\big](s+q_0+2\varepsilon a^2)+\delta\beta a^4\psi(s),\\ W_2(s) &:= \varepsilon a\varpi(s+q_0+2\varepsilon a^2)-\delta\beta a^2\psi(s),\\ \psi(s) &:= -4\varepsilon p_1(p_0+p_2-\rho^2)\big[s+(1+2\varepsilon)a^2\big]+(1+\varepsilon)\rho^2\varpi(s-a^2). \end{aligned} \tag{80}$$

For $r=\mathrm{m}$ and $k=0$ ($\varepsilon=-1$, $q_0=a^2$) this shows $W_0(a^2)=W_2(a^2)=0$.

B Analytic details

Lemma 17 (continuity). Let $\chi(p)$ and $Y(p)$ be matrices indexed by the lattice, depending on a real parameter p (μ or β) near p_0, with entries continuous at p_0. Suppose that for all n, m there are c_{nm} and a finite set of indices l outside of which $|\chi(p)_{nl}Y(p)_{lm}|\le c_{nm}(1+l^2)^{-1}$ for all these p. If $\chi(p)Y(p)=\mathbb{1}$ for $p\ne p_0$, then also $\chi(p_0)Y(p_0)=\mathbb{1}$.

Proof. For fixed n, m, the finitely many exceptional terms of $\sum_l \chi_{nl}Y_{lm}$ are continuous at p_0, and the sum of the others is continuous by dominated convergence. □

Zeros of $e(z_n)$ at $\mu\ne 0$. Since e has real coefficients and $z_{\overline{n}}=z_n^*$, $e(z_{\overline{n}})=e(z_n)^*$: lattice zeros of e come in mirror orbits $O=\{n,\overline{n}\}$, with one element if $n=\overline{n}$. Let e vanish on one orbit O at $\mu=\mu_0\ne 0$, the other assumptions of Theorem 4 holding (with $s_1\ne s_2$ at μ_0). As $e(z_n)$ is a nonconstant analytic function of μ, Theorem 4 holds for $\mu\ne\mu_0$ near μ_0. Each root u_j that tends to a point z_c, $c\in O$, has $(z_c-u_j)\alpha_j\to\rho\ne 0$ and $K_j\to\infty$, since $(z_c-u)S_k(u)\to 1$ as $u\to z_c$ (Lemma 7). In the column y_v of Step 4 with $v=z_m$, $m\notin O$, the coefficients D_v, E_v and $F_jg_j(v)$ stay bounded. By Eq. 71, for $c\in O$,

$$\frac{\varphi_j(z_c)}{K_j}=\frac{\beta H(-u_j)/(z_c-u_j)+\lambda\alpha_j/(z_c+u_j)}{\beta H(-u_j)+\lambda\alpha_j}\to\frac{\beta H(-z_c)}{\lambda\rho}+\frac{1}{2z_c}\quad(u_j\to z_c), \tag{81}$$

it tends to $1/(z_c+z_{c'})$ if $u_j\to z_{c'}$ with $c'\ne c$, and it stays bounded otherwise. So $Y_{cm}=y_{z_m}(z_c)=Y_{mc}$ converges for $c\in O$, $m\notin O$, boundedly in m. For the block $(Y_{cc'})_{c,c'\in O}$, row $l\notin O$ of $\chi_rY=\mathbb{1}$ gives $\sum_{c\in O}\chi_{r,lc}Y_{cc'}=-\sum_{l'\notin O}\chi_{r,ll'}Y_{l'c'}$, whose right side converges by dominated convergence. The columns $P(z_l)\chi_{r,lc}=\lambda\rho/(z_l+z_c)+N(z_l,z_c)/P(z_c)$, $c\in O$ (Eq. 61), are linearly independent rational functions of z_l, with distinct poles at $-z_c$. So $|O|$ rows $l\notin O$ can be chosen for which the matrix $\big(\chi_{r,lc}(\mu_0)\big)$ is invertible, and the block converges. All entries of Y converge, boundedly off the diagonal, and Lemma 17 gives $\chi_rY=\mathbb{1}$ at μ_0.

Zeros of $e(z_n)$ at $\mu=0$. Let $\beta H(z_n)=\lambda h$ with $n\ne\overline{n}$ at $\beta=\beta_0$, so that $z_n^2=\hat{s}$ and $e(z)=(z^2-\hat{s})(z^2-\hat{s}+2\lambda h/\beta)$. As $\beta\to\beta_0$, $\hat{u}\to z_n$. The diagonal and mirror terms of Eq. 35 contribute $-\lambda hP(z_n)/e(z_n)+O(1)=-\beta P(z_n)/(2(z_n^2-\hat{s}))+O(1)$ to each of the entries (n,n) and $(n,\overline{n})$. Since $S_k(\hat{u})=1/(z_n-\hat{u})+O(1)$, $\hat{D}=2\varepsilon a/(\hat{u}(\hat{u}-z_n))+O(1)$, so the separable term contributes $\beta P(z_n)/(2(z_n^2-\hat{s}))+O(1)$ to the same entries and $O(1)$ to the others. The singular parts cancel.

At a mirror fixed point $n=\overline{n}$ (odd k, $z_n=0$), let $e(0)=0$ at $\beta=\beta_0$. The diagonal and mirror terms of Eq. 35 act on the same entry (n,n). As $\beta^2e(0)=(\beta H(0)-\lambda h)(\beta H(0)+\lambda h)$, they combine to $\beta P(0)/G_2(0)-\beta^2P(0)/(\beta H(0)-\lambda h)$. If $\beta H(0)=-\lambda h$ at β_0, this stays finite, and under the remaining assumptions of Corollary 5 nothing else is singular. If $\beta H(0)=\lambda h$, then $s:=\hat{s}\to 0$, and the combination is $\beta P(0)/s+O(1)$, as $\beta H(0)-\lambda h=-\beta s$. For odd k, $\coth(\beta\hat{u}/2)/\hat{u}=2/(\beta s)+O(1)$, so $\hat{D}=2\varepsilon a/s+O(1)$, and the separable term is $-2\varepsilon a\beta P(\hat{u})\hat{g}(0)^2/\hat{D}=-\beta P(0)/s+O(1)$ at (n,n) and $O(1)$ elsewhere. The singular parts cancel again.

In all these cases Eq. 35 extends continuously, and Lemma 17 (with $p = \beta$) gives $\chi_r Y = \mathbb{1}$ at β_0.

Proof of Corollary 5. Take $\mu \to 0$ at fixed k in Eq. 33. Then $\rho \to 0$, $\overline{c} \to h$ and $C_{nm} \to h\delta_{m\overline{n}}$ (Eq. 16). One root s_j of e tends to $\hat{s}$, the other, s_ℓ, to $-4\varepsilon a^2(p_0 + p_1) - q_0$. At a root u_j put $X_\pm := \beta H(\pm u_j)$. Then $X_+X_- = \lambda^2 h^2$ (Eq. 29) and $X_+ - X_- = 4a\beta\rho u_j$. With $\overline{c}^2 = h^2 + \beta^2\rho^2/4$ (Eq. 4) this gives

$$(X_- - \lambda\overline{c})(X_- + \lambda\overline{c}) = -\rho\big(4a\beta u_j X_- + \lambda^2\beta^2\rho/4\big). \tag{82}$$

By Eq. 30, $K_j = X_- - \lambda\overline{c} + \lambda\rho S_k(u_j)$ and $X_- - \lambda\alpha_k(u_j) = X_- + \lambda\overline{c} - \lambda\rho S_k(u_j)$.

- *The pair j.* Here $X_\pm \to \lambda h$, so the identity gives $(X_- - \lambda\overline{c})/\rho \to -2a\beta\hat{u}$. Hence $K_j/\rho \to \lambda S_k(\hat{u}) - 2a\beta\hat{u} = -2a\hat{u}\hat{D}$, $X_- - \lambda\alpha_k(u_j) \to 2\lambda h$ and $s_j - s_\ell \to 2\lambda h/\beta$. So $\gamma_j \to -2\varepsilon a\beta P(\hat{u})/\hat{D}$ if $\hat{u} \neq 0$.
- *The pair ℓ.* Here $X_\pm \to -\lambda h$, so $K_\ell \to -2\lambda h$, $X_- - \lambda\alpha_k(u_\ell) \to 0$ and $\gamma_\ell \to 0$. (For $r = \mathrm{m}$, $k = 0$ this is the atomic pair, absent anyway.)
- *The dense term.* By Eq. 77, $\lambda\rho\mathbb{D}(z_n, z_m) = \lambda C_{nm}F(z_m) - \lambda\rho z_n \sum_j F_j g_j(z_n) g_j(z_m) \to \lambda h F(z_n)\delta_{m\overline{n}}$, since $z_{\overline{n}} = -z_n$ at $\mu = 0$ and F is even.

So Eq. 33 tends entrywise to Eq. 35. For small $\mu \neq 0$ the assumptions of Theorem 4 hold: $e(z_n) \neq 0$ by continuity (automatically for large $|n|$), $s_1 \neq s_2$, $K_\ell \neq 0$, and $K_j \neq 0$ because $K_j/\rho \to -2a\hat{u}\hat{D} \neq 0$ (for $\hat{u} \neq 0$). The entries of C are bounded uniformly near $\mu = 0$ (by $\beta\rho/(2\pi)$ for $m \neq \overline{n}$, and $\rho/(2\mu) \to \beta p_0$). So $\chi_{r,nl} = O(|z_l|^{-2})$ for $l \neq n$, and the entries of $Y = \Gamma_r/\beta^2 + \boldsymbol{B}^{-1}$, with Γ_r from Eq. 33, are bounded off the diagonal, uniformly near $\mu = 0$. So Lemma 17 gives $\chi_r Y = \mathbb{1}$ at $\mu = 0$; Y stays symmetric. Finally, for even k, $\hat{u} = 0$ occurs at isolated β, where Eq. 35 is continuous in β (as $\hat{D} \neq 0$); Lemma 17 with $p = \beta$ covers it. For odd k, $\hat{u} = 0$ means $e(0) = 0$ at the mirror fixed point, treated above. □

Proof of Proposition 6. Let $\vartheta_n := (1 + |z_n - \mu|^2)^{1/2}$, $\boldsymbol{\vartheta} := \mathrm{diag}(\vartheta_n)$, and $\hat{\chi} := \boldsymbol{\vartheta}\chi_r\boldsymbol{\vartheta}$ on ℓ^2.

- $\hat{\chi} = \kappa_r\mathbb{1} + \hat{\chi}_c$ *with* $\hat{\chi}_c$ *compact*, where $\kappa_\mathrm{d} = \kappa_\mathrm{m} = \beta$ and $\kappa_\mathrm{s} = -\kappa_\mathrm{t} = \beta/2$.
  - $r = \mathrm{d}, \mathrm{m}$: by Eq. 61, $\chi_{r,nn} = -\beta H(z_n)/P(z_n) + O(z_n^{-4})$, so $\vartheta_n^2\chi_{r,nn} \to \beta$. Off the diagonal, $\chi_{r,nm} = O(|z_n|^{-2}\,|z_m|^{-2})$ by Eq. 13, Eq. 14 and Eq. 19. So these entries of $\hat{\chi}$ are square-summable, i.e. Hilbert–Schmidt.
  - $r = \mathrm{s}, \mathrm{t}$: $t_n/\vartheta_n^2 \to 1$, so $\vartheta_n^2 B_n \to -\beta/2$, $\vartheta_n^2 L_\mathrm{s}(t_n) \to \beta/2$ and $\vartheta_n^2 L_\mathrm{t}(t_n) \to -\beta/2$ (Eq. 41). By Eq. 44, $\hat{\chi} - \kappa_r\mathbb{1}$ is a matrix supported on the diagonal and the mirror with entries tending to zero, which is compact, plus (for $r = \mathrm{s}$) $\boldsymbol{\vartheta}\chi_{\mathrm{s,\,reg}}\boldsymbol{\vartheta}$, which is Hilbert–Schmidt by Eq. 45.
- $\hat{\chi}$ *is invertible.* For each m, $\hat{\chi}$ maps $\boldsymbol{\vartheta}^{-1}\chi_r^{-1}\boldsymbol{e}_m$ to $\vartheta_m\boldsymbol{e}_m$: the n-th entry of the image is $\vartheta_n\sum_l \chi_{r,nl}(\chi_r^{-1})_{lm} = \vartheta_n\delta_{nm}$, an absolutely convergent series. The vector $\boldsymbol{\vartheta}^{-1}\chi_r^{-1}\boldsymbol{e}_m$ lies in ℓ^2, because by the explicit formulas $(\chi_r^{-1})_{nm}$ is bounded in n for $n \notin \{m, \overline{m}\}$. So the range of $\hat{\chi}$ contains all basis vectors; being closed (a compact perturbation of $\kappa_r\mathbb{1}$ has closed range), it is all of ℓ^2. A compact perturbation of $\kappa_r\mathbb{1}$ that is onto is also injective (Fredholm alternative), hence invertible.

Convergence. Let $\mathbb{1}_M$ be the projection onto the box. Then $\hat{\chi}_M := \mathbb{1}_M\hat{\chi}\mathbb{1}_M + \kappa_r(\mathbb{1} - \mathbb{1}_M)$ converges to $\hat{\chi}$ in norm, since $(\mathbb{1} - \mathbb{1}_M)\hat{\chi}_c \to 0$ and $\hat{\chi}_c(\mathbb{1} - \mathbb{1}_M) \to 0$ for compact $\hat{\chi}_c$. So $\hat{\chi}_M$ is invertible for all sufficiently large M, and $\hat{\chi}_M^{-1} \to \hat{\chi}^{-1}$ in norm. On the box, $\hat{\chi}_M^{-1} = \boldsymbol{\vartheta}^{-1}(\mathbb{1}_M\chi_r\mathbb{1}_M)^{-1}\boldsymbol{\vartheta}^{-1}$. □

C The regular part

The regular part in Eq. 15 is [Ref. [2], Eq. (D3), at zero field]

$$\begin{aligned} R_{\mathrm{reg}}(x,y) = (p_0+p_1)\Big[&-\frac{1}{(y+w+a)(y+a)(x-a)}+\frac{1}{(x+w-a)(x-a)(y+a)} \\ &+\frac{1}{(x+w+a)(y-a)(x-a)}-\frac{1}{(x+w+a)(x-a)(y+w+a)} \\ &+\frac{1}{(y+a)(x+w+a)(y+w+a)}+\frac{1}{(y+a)(x+w+a)(x+a)} \\ &+\frac{1}{(y-a)(x+a)(y+w-a)}-\frac{1}{(y-a)(x+w+a)(x+a)} \\ &+\frac{1}{(x+w-a)(x+a)(y+w-a)}-\frac{1}{(y+a)(x+w-a)(x+a)}\Big] \\ -(p_1+p_2)\Big[&\frac{1}{(y-a)(x+w-a)(y+w-a)}+\frac{1}{(y-a)(x+w-a)(x-a)}\Big]. \end{aligned} \tag{83}$$

D Numerical checks

- **Mathematica:** `mathematica/doped_gamma.nb` derives Eqs. 13–15 exactly from the Lehmann representation of Eq. 1, checks Lemma 1, Proposition 10, Proposition 15, the lemmas of Section 5 and Section 7, Theorem 2, Theorem 3, Steps 1–4 of the proof of Theorem 4 and (A2)–(A4), (A6), (A7) symbolically, and compares Theorem 4, Theorem 3, Theorem 2 and Corollary 5 with finite-box inversion (62 checks).
- **Vertices** (`doped-gamma/check_vertices.jl`): Eq. 25 and Eq. 27 agree with an independent residue-based BigFloat evaluator (`doped-gamma/doped_gamma.jl`) to 3×10^{-15}, Eq. 33 at 256 bits to 10^{-65} (300 entries, $k=0,1,2,-3,5$, $|\mu|\le 2\,|U|$); at $\mu=0$, Eq. 25, Eq. 27 and Eq. 35 agree with `HubbardAtoms.jl` (Eq. 19 of Ref. [1]) to 3×10^{-14}.
- **Implementation:** the test suite of `HubbardAtoms.jl` compares `DopedHubbardAtom` with exact diagonalization, with finite-box inversion and with `BigFloat` evaluation, including the removable singularities listed under *Divergences*.