Unified role of Green's function poles and zeros in correlated topological insulators

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Green's function zeros, which can emerge only if correlation is strong, have been for long overlooked and believed to be devoid of any physical meaning, unlike Green's function poles. Here, we prove that Green's function zeros instead contribute on the same footing as poles to determine the topological character of an insulator. The key to the proof, worked out explicitly in 2D but easily extendable in 3D, is to express the topological invariant in terms of a *quasiparticle* thermal Green's function matrix $G_*(i\epsilon,\mathbf{k}) = 1/\big(i\epsilon - H_*(\epsilon,\mathbf{k})\big)$, with hermitian $H_*(\epsilon,\mathbf{k})$, by filtering out the positive definite *quasiparticle* residue. In that way, the topological invariant is easily found to reduce to the TKNN formula for quasiparticles described by the non-interacting Hamiltonian $H_*(0,\mathbf{k})$. Since the poles of the quasiparticle Green's function $G_*(\epsilon,\mathbf{k})$ on the real frequency axis correspond to poles and zeros of the physical-particle Green's function $G(\epsilon,\mathbf{k})$, both of them equally determine the topological character of an insulator.

I. INTRODUCTION

The determinant of the retarded Green's function $G_0(\epsilon,\mathbf{k})$, with ϵ the frequency and $\mathbf{k}$ the momentum, for periodic models of non-interacting electrons have poles whenever ϵ hits the dispersion energy $\epsilon_n(\mathbf{k})$ of a band n, i.e., a single-particle excitation. Similarly, the poles of the determinant of the fully-interacting $G(\epsilon,\mathbf{k})$ can be associated to coherent, i.e., with infinite lifetime, single-particle excitations, which thus have a clear physical meaning. The manifold in the Brillouin zone where these poles are at $\epsilon = 0$ defines the Fermi surface, in which case the system is metallic.

However, the determinant of $G(\epsilon,\mathbf{k})$ in presence of interaction may also develop zeros [1], whose manifold at $\epsilon = 0$ defines the so-called Luttinger surface [2]. For long time, these zeros have not been given any physical significance, despite Volovik [3] early on recognised that a Luttinger surface bears the same non-trivial topological content of a Fermi surface. Only recently, the Green's function zeros started to attract growing physical interest. For instance, it has been shown that a Luttinger surface defined by the simple roots of $\det\big(G(0,\mathbf{k})\big)$ does sustain Landau's quasiparticles [4], even in non-symmetry breaking Mott insulators [5]. Those quasiparticles have the same physical properties as conventional ones at a Fermi surface, with the major difference that they are incompressible [6] and do not contribute to charge transport [5]. Elaborating on Volovik's observation [3], Gurarie [7] and Essin and Gurarie [8] have proposed that, upon increasing electron correlations, topological edge modes, i.e., edge poles of the Green's function, may transform into edges zeros without making the topological insulator a trivial one or closing the single-particle gap. More recently, this intriguing scenario has been further explored in Ref. [9], whose authors show that model topological insulators turn, upon rising interaction strength, into Mott insulators with topologically trivial lower and upper Hubbard bands, but with ingap valence and conduction bands of Green's function zeros that are topological and yield Green's function edge zeros. This result suggests that an edge-bulk correspondence exists also for Green's function zeros, thus clarifying the mechanism underlying the transformation of edge poles into edge zeros [7, 8].

All these small pieces of evidence suggest that Green's function zeros, that may arise only in strongly correlated systems, do have a physical meaning as important as that of Green's function poles. This connection has been uncovered when the zeros cross the chemical potential, thus in the presence of a Luttinger surface [3–5]. However, despite the supporting evidences [7–9], the direct role of Green's function zeros in assessing the topological character of an insulator has not been explicitly demonstrated. That is precisely the goal of the present work.

II. TKNN FORMULA FOR INTERACTING INSULATORS

The expression of the topological invariant of two dimensional periodic insulators in presence of interaction, which coincides with the zero temperature Hall conductance in units of $e^2/2\pi\hbar$ [10, 11] at least when perturbation theory is valid, see Appendix B, reads

$$W(G) = \frac{1}{24\pi^2}\int d\epsilon\, d\mathbf{k}\, \epsilon_{\mu\nu\rho}\, \mathrm{Tr}\Big(G(i\epsilon,\mathbf{k})\,\partial_\mu G(i\epsilon,\mathbf{k})^{-1}\, G(i\epsilon,\mathbf{k})\,\partial_\nu G(i\epsilon,\mathbf{k})^{-1}\, G(i\epsilon,\mathbf{k})\,\partial_\rho G(i\epsilon,\mathbf{k})^{-1}\Big)\,, \tag{1}$$

where $G(i\epsilon,\mathbf{k}) = G(-i\epsilon,\mathbf{k})^\dagger$ is the interacting Green's functions in the Matsubara formalism, see Appendix A, with ϵ the Matsubara frequency, and it is a matrix represented in a generic basis of single-particle wavefunctions.

We hereafter assume that $G(i\epsilon,\mathbf{k})$ is invertible, which implies that the system is an insulator without any Luttinger surface. It can be easily demonstrated that the winding number $W(G_1\,G_2) = W(G_1) + W(G_2)$ and that $W(G) = 0$ if G is hermitian, see Appendix C.

Zhong and Zhang have shown [12] that the topological invariant (1) reduces to the TKNN expression of the quantised Hall conductance [13] in which the role of the Bloch waves of the occupied bands is played by the eigenstates of the hermitian matrix $-G(0,\mathbf{k})^{-1}$ with negative eigenvalues. The proof is based on the observation that the two maps $(\epsilon,\mathbf{k}) \to G(i\epsilon,\mathbf{k})^{-1}$ and $(\epsilon,\mathbf{k}) \to i\epsilon + G(0,\mathbf{k})^{-1}$ are homotopic, and thus the winding number (1) of the former map coincides with that of the latter, which, in turns, reduces to the TKNN formula.

Here, we would like to prove explicitly the equivalence relation but using a different map $(\epsilon,\mathbf{k}) \to G_*(i\epsilon,\mathbf{k})^{-1}$, which, we believe, has the more transparent physical meaning of the inverse of the *quasiparticle* Green's function, which we discuss more extensively at the end of the section. Specifically, following [5, 6] we write the interacting Green's function matrix as, see also Appendix A,

$$\begin{aligned} G(i\epsilon,\mathbf{k}) &= \frac{1}{i\epsilon - H_0(\mathbf{k}) - \Sigma(i\epsilon,\mathbf{k})} \\ &= \sqrt{Z(\epsilon,\mathbf{k})}\;\frac{1}{i\epsilon - H_*(\epsilon,\mathbf{k})}\;\sqrt{Z(\epsilon,\mathbf{k})} \\ &\equiv \sqrt{Z(\epsilon,\mathbf{k})}\;G_*(i\epsilon,\mathbf{k})\;\sqrt{Z(\epsilon,\mathbf{k})}\;, \end{aligned} \tag{2}$$

where $H_0(\mathbf{k})$ is the non-interacting Hamiltonian represented in the chosen basis of single-particle wavefunctions,

$$\begin{aligned} \Sigma(i\epsilon,\mathbf{k}) &= \Sigma(-i\epsilon,\mathbf{k})^\dagger \equiv \Sigma_1(i\epsilon,\mathbf{k}) + i\,\Sigma_2(i\epsilon,\mathbf{k}) \\ \Sigma_1(i\epsilon,\mathbf{k}) &= \Sigma_1(i\epsilon,\mathbf{k})^\dagger = \Sigma_1(-i\epsilon,\mathbf{k}) \\ &= \frac{\Sigma(i\epsilon,\mathbf{k}) + \Sigma(-i\epsilon,\mathbf{k})}{2} \\ \Sigma_2(i\epsilon,\mathbf{k}) &= \Sigma_2(i\epsilon,\mathbf{k})^\dagger = -\Sigma_2(-i\epsilon,\mathbf{k}) \\ &= \frac{\Sigma(i\epsilon,\mathbf{k}) - \Sigma(-i\epsilon,\mathbf{k})}{2i} \end{aligned}$$

the self-energy matrix in that same basis, which accounts for all interaction effects,

$$Z(\epsilon,\mathbf{k}) = Z(-\epsilon,\mathbf{k}) = \left(1 - \frac{\Sigma_2(i\epsilon,\mathbf{k})}{\epsilon}\right)^{-1}, \tag{3}$$

a positive definite matrix if the system is insulating without a Luttinger surface, see Appendix A, which can be regarded as the *quasiparticle* residue, and

$$\begin{aligned} &H_*(\epsilon,\mathbf{k}) = H_*(-\epsilon,\mathbf{k}) \\ &= \sqrt{Z(\epsilon,\mathbf{k})}\,\Big(H_0(\mathbf{k}) + \Sigma_1(i\epsilon,\mathbf{k})\Big)\,\sqrt{Z(\epsilon,\mathbf{k})}\;, \end{aligned} \tag{4}$$

is the hermitian *quasiparticle* Hamiltonian. It follows that the winding number (1) can be written as

$$\begin{aligned} W\big(G\big) &= W\Big(\sqrt{Z}\;G_*\,\sqrt{Z}\Big) = W\big(G_*\big) + W\big(Z\big) \\ &= W\big(G_*\big)\,, \end{aligned}$$

since the winding number of the positive definite matrix Z vanishes.
A further reason for choosing the map $(\epsilon,\mathbf{k}) \to G_*(i\epsilon,\mathbf{k})^{-1}$ is that, under the analytic continuation on the real axis from above, $i\epsilon \to \epsilon + i0^+$, i.e., for the retarded components of Green's function and self-energy, the poles of $G_*(\epsilon,\mathbf{k})$ correspond to both poles and zeros of $G(\epsilon,\mathbf{k})$, i.e., the vanishing eigenvalues of the quasiparticle residue matrix (3) on the real axis, thus making more explicit their deep connection.

In the basis that diagonalises $H_*(\epsilon,\mathbf{k})$, i.e.,

$$H_*(\epsilon,\mathbf{k})\mid\alpha(\epsilon,\mathbf{k})\rangle = \epsilon_\alpha(\epsilon,\mathbf{k})\;\mid\alpha(\epsilon,\mathbf{k})\rangle\,,$$

where one can choose $\mid\alpha(\epsilon,\mathbf{k})\rangle = \mid\alpha(-\epsilon,\mathbf{k})\rangle$,

$$\begin{aligned} W\big(G\big) &= \frac{1}{24\pi^2}\int d\epsilon\,d\mathbf{k}\,\epsilon_{\mu\nu\rho} \\ &\sum_{\alpha\beta\gamma}\frac{1}{i\epsilon-\epsilon_\alpha(\epsilon,\mathbf{k})}\,\frac{1}{i\epsilon-\epsilon_\beta(\epsilon,\mathbf{k})}\,\frac{1}{i\epsilon-\epsilon_\gamma(\epsilon,\mathbf{k})} \\ &\qquad \partial_\mu G_*(i\epsilon,\mathbf{k})^{-1}_{\alpha\beta}\,\partial_\mu G_*(i\epsilon,\mathbf{k})^{-1}_{\beta\gamma}\,\partial_\mu G_*(i\epsilon,\mathbf{k})^{-1}_{\gamma\alpha}\;, \end{aligned} \tag{5}$$

having defined

$$\begin{aligned} \partial_\mu G_*(i\epsilon,\mathbf{k})^{-1}_{\alpha\beta} &\equiv \langle\alpha(\epsilon,\mathbf{k})\mid\partial_\mu G_*(i\epsilon,\mathbf{k})^{-1}\mid\beta(\epsilon,\mathbf{k})\rangle \\ &= i\,\delta_{\mu0}\,\delta_{\alpha\beta} - \langle\alpha(\epsilon,\mathbf{k})\mid\partial_\mu H_*(\epsilon,\mathbf{k})\mid\beta(\epsilon,\mathbf{k})\rangle \\ &\equiv i\,\delta_{\mu0}\,\delta_{\alpha\beta} - F^\mu_{\alpha\beta}(\epsilon,\mathbf{k})\,. \end{aligned}$$

The term in (5) with $\alpha=\beta=\gamma$ vanishes because of the antisymmetric tensor, so that we are left with the cases of either two states equal and different from the third, or of all states different, which we denote as $W^{(1)}(G)$ and $W^{(2)}(G)$, respectively. Specifically,

$$\begin{aligned} W^{(1)}(G) &= -\frac{1}{8\pi^2}\int d\epsilon\,d\mathbf{k}\,\epsilon_{\mu\nu\rho} \\ &\sum_{\alpha\beta}{}'\,\frac{1}{i\epsilon-\epsilon_\beta(\epsilon,\mathbf{k})}\,\partial_\mu\left(\frac{1}{i\epsilon-\epsilon_\alpha(\epsilon,\mathbf{k})}\right) \\ &\qquad\qquad \Big\{F^\nu_{\alpha\beta}(\epsilon,\mathbf{k})\,F^\rho_{\beta\alpha}(\epsilon,\mathbf{k})\Big\}\,, \\ W^{(2)}(G) &= -\frac{1}{24\pi^2}\int d\epsilon\,d\mathbf{k}\,\epsilon_{\mu\nu\rho} \\ &\sum_{\alpha\beta\gamma}{}'\,\frac{1}{i\epsilon-\epsilon_\alpha(\epsilon,\mathbf{k})}\,\frac{1}{i\epsilon-\epsilon_\beta(\epsilon,\mathbf{k})}\,\frac{1}{i\epsilon-\epsilon_\gamma(\epsilon,\mathbf{k})} \\ &\qquad\qquad \Big\{F^\mu_{\alpha\beta}(\epsilon,\mathbf{k})\,F^\nu_{\beta\gamma}(\epsilon,\mathbf{k})\,F^\rho_{\gamma\alpha}(\epsilon,\mathbf{k})\Big\}\,, \end{aligned} \tag{6}$$

where Σ' means the summation over different indices. Let us begin by analysing $W^{(1)}(G)$ in Eq. (6). We note that, for $\alpha \neq \beta$,

$$\begin{aligned} F^{\nu}_{\alpha\beta}(\epsilon,\mathbf{k}) &= \langle \alpha(\epsilon,\mathbf{k}) \mid \partial_\nu H_*(\epsilon,\mathbf{k}) \mid \beta(\epsilon,\mathbf{k})\rangle \\ &= \Big(\epsilon_\alpha(\epsilon,\mathbf{k}) - \epsilon_\beta(\epsilon,\mathbf{k})\Big) \langle \partial_\nu \alpha(\epsilon,\mathbf{k}) \mid \beta(\epsilon,\mathbf{k})\rangle \\ &= \Big(\epsilon_\beta(\epsilon,\mathbf{k}) - \epsilon_\alpha(\epsilon,\mathbf{k})\Big) \langle \alpha(\epsilon,\mathbf{k}) \mid \partial_\nu \beta(\epsilon,\mathbf{k})\rangle\,, \end{aligned} \tag{7}$$

so that

$$\begin{aligned} W^{(1)}(G) &= -\frac{1}{8\pi^2}\int d\epsilon\, d\mathbf{k}\, \epsilon_{\mu\nu\rho} \\ &\sum_{\alpha\beta} \frac{\big(\epsilon_\alpha(\epsilon,\mathbf{k}) - \epsilon_\beta(\epsilon,\mathbf{k})\big)^2}{i\epsilon - \epsilon_\beta(\epsilon,\mathbf{k})}\, \partial_\mu\left(\frac{1}{i\epsilon - \epsilon_\alpha(\epsilon,\mathbf{k})}\right) \\ &\langle \partial_\nu \alpha(\epsilon,\mathbf{k}) \mid \beta(\epsilon,\mathbf{k})\rangle\langle \beta(\epsilon,\mathbf{k}) \mid \partial_\rho \alpha(\epsilon,\mathbf{k})\rangle \\ &= -\frac{1}{16\pi^2}\int d\epsilon\, d\mathbf{k}\, \epsilon_{\mu\nu\rho} \sum_{\alpha\beta} \partial_\mu\, S_{\alpha\beta}(\epsilon,\mathbf{k}) \\ &\langle \partial_\nu \alpha(\epsilon,\mathbf{k}) \mid \beta(\epsilon,\mathbf{k})\rangle\langle \beta(\epsilon,\mathbf{k}) \mid \partial_\rho \alpha(\epsilon,\mathbf{k})\rangle\,, \end{aligned} \tag{8}$$

where the constraint $\alpha \neq \beta$ is automatically fulfilled and one can readily demonstrate that

$$\begin{aligned} S_{\alpha\beta}(\epsilon,\mathbf{k}) = 2\,\ln\frac{i\epsilon - \epsilon_\alpha(\epsilon,\mathbf{k})}{i\epsilon - \epsilon_\beta(\epsilon,\mathbf{k})} - \frac{i\epsilon - \epsilon_\alpha(\epsilon,\mathbf{k})}{i\epsilon - \epsilon_\beta(\epsilon,\mathbf{k})} \\ + \frac{i\epsilon - \epsilon_\beta(\epsilon,\mathbf{k})}{i\epsilon - \epsilon_\alpha(\epsilon,\mathbf{k})}\,, \end{aligned}$$

which has a discontinuous imaginary part crossing $\epsilon = 0$ if $\epsilon_\alpha(0,\mathbf{k})\,\epsilon_\beta(0,\mathbf{k}) < 0$. We can write

$$\begin{aligned} S_{\alpha\beta}(\epsilon,\mathbf{k}) &= K_{\alpha\beta}(\epsilon,\mathbf{k}) \\ &+ 2\pi i\,\mathrm{sign}(\epsilon)\left[\theta\big(\epsilon_\alpha(\epsilon,\mathbf{k})\big) - \theta\big(\epsilon_\beta(\epsilon,\mathbf{k})\big)\right], \end{aligned}$$

where $K_{\alpha\beta}(\epsilon,\mathbf{k})$ is now continuous at $\epsilon = 0$, so that, since $S_{\alpha\beta}(\epsilon,\mathbf{k})$ is antisymmetric, and $\epsilon_\alpha(\epsilon,\mathbf{k}) \neq 0$, $\forall\, \alpha,\epsilon,\mathbf{k}$, then

$$\begin{aligned} W^{(1)}(G) = \frac{i}{2\pi}\int d\mathbf{k}\,\epsilon_{ij} \sum_\alpha \theta\big(-\epsilon_\alpha(0,\mathbf{k})\big) \\ \langle \partial_i \alpha(0,\mathbf{k}) \mid \partial_j \alpha(0,\mathbf{k})\rangle \\ - \frac{1}{16\pi^2}\int d\epsilon\, d\mathbf{k}\,\epsilon_{\mu\nu\rho} \sum_{\alpha\beta} \partial_\mu\, K_{\alpha\beta}(\epsilon,\mathbf{k}) \\ \langle \partial_\nu \alpha(\epsilon,\mathbf{k}) \mid \beta(\epsilon,\mathbf{k})\rangle\langle \beta(\epsilon,\mathbf{k}) \mid \partial_\rho \alpha(\epsilon,\mathbf{k})\rangle\,, \end{aligned} \tag{9}$$

where $i,j = 1,2$. The second term, which we denote as I, is only contributed by $\mathrm{Im}\, K_{\alpha\beta}(\epsilon,\mathbf{k})$, which is odd in ϵ, vanishes at $\epsilon \to \pm\infty$ and, by definition, is continuous at $\epsilon = 0$. That allows partial integration, which, through Eq. (7), leads to

$$\begin{aligned} I &= -\frac{1}{8\pi^2}\int d\epsilon\, d\mathbf{k}\,\epsilon_{\mu\nu\rho} \sum_{\alpha\beta} K_{\alpha\beta}(\epsilon,\mathbf{k}) \\ &\langle \partial_\mu \alpha(\epsilon,\mathbf{k}) \mid \partial_\nu \beta(\epsilon,\mathbf{k})\rangle\langle \beta(\epsilon,\mathbf{k}) \mid \partial_\rho \alpha(\epsilon,\mathbf{k})\rangle \\ &= -\frac{1}{8\pi^2}\int d\epsilon\, d\mathbf{k}\,\epsilon_{\mu\nu\rho} \sum_{\alpha\beta\gamma} \frac{K_{\alpha\beta}(\epsilon,\mathbf{k})}{\epsilon_\alpha(\epsilon,\mathbf{k}) - \epsilon_\gamma(\epsilon,\mathbf{k})} \\ &\frac{1}{\epsilon_\beta(\epsilon,\mathbf{k}) - \epsilon_\gamma(\epsilon,\mathbf{k})}\,\frac{1}{\epsilon_\alpha(\epsilon,\mathbf{k}) - \epsilon_\beta(\epsilon,\mathbf{k})} \\ &\left\{F^{\mu}_{\alpha\gamma}(\epsilon,\mathbf{k})\, F^{\nu}_{\gamma\beta}(\epsilon,\mathbf{k})\, F^{\rho}_{\beta\alpha}(\epsilon,\mathbf{k})\right\}. \end{aligned} \tag{10}$$

Since I is real, we can take the complex conjugate, send $\epsilon \to -\epsilon$ and then either exchange β and γ as well as μ and ρ, thus getting

$$\begin{aligned} I &= -\frac{1}{8\pi^2}\int d\epsilon\, d\mathbf{k}\,\epsilon_{\mu\nu\rho} \sum_{\alpha\beta\gamma} \frac{-K_{\alpha\gamma}(\epsilon,\mathbf{k})}{\epsilon_\alpha(\epsilon,\mathbf{k}) - \epsilon_\gamma(\epsilon,\mathbf{k})} \\ &\frac{1}{\epsilon_\beta(\epsilon,\mathbf{k}) - \epsilon_\gamma(\epsilon,\mathbf{k})}\,\frac{1}{\epsilon_\alpha(\epsilon,\mathbf{k}) - \epsilon_\beta(\epsilon,\mathbf{k})} \\ &\left\{F^{\mu}_{\alpha\gamma}(\epsilon,\mathbf{k})\, F^{\nu}_{\gamma\beta}(\epsilon,\mathbf{k})\, F^{\rho}_{\beta\alpha}(\epsilon,\mathbf{k})\right\}, \end{aligned} \tag{11}$$

or, instead, exchange α and γ as well as ν and ρ, in that way obtaining

$$\begin{aligned} I &= -\frac{1}{8\pi^2}\int d\epsilon\, d\mathbf{k}\,\epsilon_{\mu\nu\rho} \sum_{\alpha\beta\gamma} \frac{-K_{\gamma\beta}(\epsilon,\mathbf{k})}{\epsilon_\alpha(\epsilon,\mathbf{k}) - \epsilon_\gamma(\epsilon,\mathbf{k})} \\ &\frac{1}{\epsilon_\beta(\epsilon,\mathbf{k}) - \epsilon_\gamma(\epsilon,\mathbf{k})}\,\frac{1}{\epsilon_\alpha(\epsilon,\mathbf{k}) - \epsilon_\beta(\epsilon,\mathbf{k})} \\ &\left\{F^{\mu}_{\alpha\gamma}(\epsilon,\mathbf{k})\, F^{\nu}_{\gamma\beta}(\epsilon,\mathbf{k})\, F^{\rho}_{\beta\alpha}(\epsilon,\mathbf{k})\right\}. \end{aligned} \tag{12}$$

Therefore, recalling that $K_{\alpha\beta}(\epsilon,\mathbf{k}) = -K_{\beta\alpha}(\epsilon,\mathbf{k})$ is antisymmetric, we can rewrite I as one third of the sum of (10), (11) and (12), thus

$$
\begin{aligned}
I &= \frac{1}{24\pi^2}\int d\epsilon\, d\mathbf{k}\,\epsilon_{\mu\nu\rho}\sum_{\alpha\beta\gamma}\frac{K_{\alpha\beta}(\epsilon,\mathbf{k})+K_{\beta\gamma}(\epsilon,\mathbf{k})+K_{\gamma\alpha}(\epsilon,\mathbf{k})}{\big(\epsilon_\alpha(\epsilon,\mathbf{k})-\epsilon_\beta(\epsilon,\mathbf{k})\big)\big(\epsilon_\beta(\epsilon,\mathbf{k})-\epsilon_\gamma(\epsilon,\mathbf{k})\big)\big(\epsilon_\gamma(\epsilon,\mathbf{k})-\epsilon_\alpha(\epsilon,\mathbf{k})\big)} \\
&\qquad\qquad \left\{F^\mu_{\alpha\gamma}(\epsilon,\mathbf{k})\,F^\nu_{\gamma\beta}(\epsilon,\mathbf{k})\,F^\rho_{\beta\alpha}(\epsilon,\mathbf{k})\right\} \\
&= \frac{1}{24\pi^2}\int d\epsilon\, d\mathbf{k}\,\epsilon_{\mu\nu\rho}\sum_{\alpha\beta\gamma}{}'\,\frac{1}{i\epsilon-\epsilon_\alpha(\epsilon,\mathbf{k})}\,\frac{1}{i\epsilon-\epsilon_\beta(\epsilon,\mathbf{k})}\,\frac{1}{i\epsilon-\epsilon_\gamma(\epsilon,\mathbf{k})}\left\{F^\mu_{\alpha\beta}(\epsilon,\mathbf{k})\,F^\nu_{\beta\gamma}(\epsilon,\mathbf{k})\,F^\rho_{\gamma\alpha}(\epsilon,\mathbf{k})\right\} \\
&= -W^{(2)}(G)\,,
\end{aligned}
$$

where the equivalence between the first and the second equations can be readily worked out.

In conclusion, we have proved that the winding number (1) can be written, not unexpectedly, as

$$
\begin{aligned}
W(G) = -\frac{1}{16\pi^2}\int d\epsilon\, d\mathbf{k}\,\epsilon_{\mu\nu\rho}\,\partial_\mu\Bigg\{\sum_{\alpha\beta} S_{\alpha\beta}(\epsilon,\mathbf{k}) \\
\langle\partial_\nu\alpha(\epsilon,\mathbf{k})\mid\beta(\epsilon,\mathbf{k})\rangle\langle\beta(\epsilon,\mathbf{k})\mid\partial_\rho\alpha(\epsilon,\mathbf{k})\rangle\Bigg\}\,,
\end{aligned}
$$

namely, as the integral of a full derivative of a function that has a discontinuity at $\epsilon = 0$, for which reason the integral does not vanish and yields

$$
\begin{aligned}
W(G) = \frac{i}{2\pi}\int d\mathbf{k}\,\epsilon_{ij}\sum_\alpha \theta\big(-\epsilon_\alpha(0,\mathbf{k})\big) \\
\langle\partial_i\alpha(0,\mathbf{k})\mid\partial_j\alpha(0,\mathbf{k})\rangle\,,
\end{aligned}
\tag{13}
$$

i.e., the TKNN expression [13] for *quasiparticles* described by the non-interacting Hamiltonian $H_*(0,\mathbf{k})$. Since $H_*(\epsilon,\mathbf{k})$ includes by definition both poles and zeros of the retarded Green's function, we conclude that both of them contribute on equal footing to the topological invariant $W(G)$.

We emphasise that only through the representation (2) of the Green's function $G(i\epsilon,\mathbf{k})$ we have been able to straightforwardly derive the simple expression of $W(G)$ in Eq. (13). Since that same representation is also the key to the proof that Landau's quasiparticles exist at Luttinger as well as Fermi surfaces [4, 5], we suspect it is not just a mathematical trick but hints at a deeper physical meaning. Indeed, we are convinced that the bands of $H_*(0,\mathbf{k})$ lying inside the single-particle gap of a Mott insulator describe *fractionalised* quasiparticles not carrying all electron's quantum numbers, for instance neutral but spinful, even when they do not cross the chemical potential. Moreover, since those fractionalised quasiparticles cannot have any weight in the physical single-particle excitations, it is reasonable to expect that they are associated to the existence of ingap bands of zeros of the physical retarded Green's function.

Finally, we remark that all above results has been obtained in two dimensions (2D). However, the expression of topological invariants in 3D insulators [12, 14–18] also involve winding numbers that generalise (1) in higher dimensions [12], or describe other invariants like polarisation [17]. Therefore, it remains true that the quasiparticle residue (3) disappears from the expression of the topological invariant, which is therefore only determined by the quasiparticle Green's function $G_*(i\epsilon,\mathbf{k})$, see Eq. (2), exactly like in 2D. For instance, we can readily show, simply following [19], that the parity of the eigenvalues of $H_*(0,\mathbf{k})$ at time-reversal invariant momenta determine the topological invariant [14] of interacting Z_2 topological insulators with inversion symmetry.

III. A TOY EXAMPLE

We now analyse a toy model inspired by Ref. [9]. Specifically, we consider an interacting BHZ model [20], whose inverse Green's function for a fixed spin reads

$$
\begin{aligned}
\hat{G}(i\epsilon,\mathbf{k})^{-1} &= i\epsilon-\epsilon(\mathbf{k})\,\hat{\tau}_3-\lambda\,\sin k_1\,\hat{\tau}_1 \\
&\quad+\lambda\,\sin k_2\,\hat{\tau}_2-\hat{\Sigma}(i\epsilon,\mathbf{k}) \\
&= i\epsilon-\hat{H}(\mathbf{k})-\hat{\Sigma}(i\epsilon,\mathbf{k})\,,
\end{aligned}
\tag{14}
$$

where $\epsilon(\mathbf{k}) = M-\cos k_1-\cos k_2$, a hat is introduced to distinguish matrices from scalars, and $\hat{\tau}_a$, $a=1,2,3$, are the Pauli matrices in the two-orbital subspace. Without interaction, the model describes a topological insulator if $\epsilon(\mathbf{\Gamma})\,\epsilon(\mathbf{M})<0$, with $\mathbf{M}=(\pi,\pi)$, which occurs if $0<|M|<2$.

We assume that [9]

$$
\hat{\Sigma}(i\epsilon,\mathbf{k}) = \frac{\Delta^2}{i\epsilon+\hat{H}'(\mathbf{k})}\,,
\tag{15}
$$

with $\Delta>0$ and where $\hat{H}'(\mathbf{k})$ has the same form as $\hat{H}(\mathbf{k})$ in (14) but with renormalised parameters, thus $\epsilon(\mathbf{k})\to\epsilon'(\mathbf{k}) = M'-t'\big(\cos k_1+\cos k_2\big)$ and $\lambda\to\lambda'$. It follows that $\hat{H}'(\mathbf{k})$ is topological if $0<|M'|<2$, which we take for granted.

We also assume that the model is deep inside the Mott insulating regime, which implies that Δ is in magnitude much larger than all the other parameters in (14). In this case, the poles of the retarded Green's function, $\hat{G}(\epsilon+i0^+,\mathbf{k})$, describes two lower and two upper Hubbard bands, with dispersion,

respectively, $\epsilon_{\rm LHB}(\mathbf{k}) \simeq -\Delta + \delta\epsilon_{1(2)}(\mathbf{k}) \ll 0$ and $\epsilon_{\rm UHB}(\mathbf{k}) \simeq +\Delta + \delta\epsilon_{1(2)}(\mathbf{k}) \gg 0$, where $\delta\epsilon_{1(2)}(\mathbf{k})$ are the eigenvalues of $\hat{H}(\mathbf{k}) - \hat{H}'(\mathbf{k})$. The occupied lower Hubbard bands have opposite Chern numbers so that, from the point of view of the Green's function poles, the system is a trivial Mott insulator, as noted in [9].
However, besides those poles, the retarded Green's function also has valence and conduction bands of zeros with dispersion the eigenvalues of $-\hat{H}'(\mathbf{k})$ in Eq. (15), which are therefore topological [9].

The obvious question is whether the non-trivial topology of the Green's function zeros has any physical significance. For that, we follows the analysis of the previous section. Upon defining $E'(\mathbf{k})^2 = \epsilon'(\mathbf{k})^2 + \lambda'^2 \left(\sin^2 k_1 + \sin^2 k_2\right)$ one readily finds that the quasiparticle residue (3) reads in this case

$$\hat{Z}(\epsilon, \mathbf{k}) = \frac{\epsilon^2 + E'(\mathbf{k})^2}{\epsilon^2 + E'(\mathbf{k})^2 + \Delta^2} = Z(\epsilon, \mathbf{k})\, \hat{I}\,, \qquad (16)$$

and is proportional to the identity matrix $\hat{I}$, and thus

$$\hat{H}_*(\epsilon, \mathbf{k}) = Z(\epsilon, \mathbf{k}) \left(\hat{H}(\mathbf{k}) + \frac{\Delta^2}{\epsilon^2 + E'(\mathbf{k})^2}\, \hat{H}'(\mathbf{k}) \right),$$

which has exactly the same form as $\hat{H}$ with frequency dependent parameters $\epsilon_*(\epsilon, \mathbf{k})$ and $\lambda_*(\epsilon, \mathbf{k})$ that can be easily determined. At $\epsilon = 0$ and for large Δ,

$$\hat{H}_*(0, \mathbf{k}) = Z(0, \mathbf{k}) \left(\hat{H}(\mathbf{k}) + \frac{\Delta^2}{E'(\mathbf{k})^2}\, \hat{H}'(\mathbf{k}) \right) \simeq \hat{H}'(\mathbf{k})\,,$$

explicitly showing that only the Green's function zeros contribute to the topological invariant (13) in this toy example, and with opposite sign respect to the topology of the valence band of zeroes that are described by $-\hat{H}'$. We emphasise that the exact correspondence between the ingap quasiparticle bands, eigenvalues of the Hamiltonian $\hat{H}_*(0, \mathbf{k})$, and the inverted bands of zeros of the retarded physical Green's function holds only in the limit of infinite Mott-Hubbard gap.

IV. CONCLUDING REMARKS

The winding number $W(G)$ of the physical electron Green's function $G(i\epsilon, \mathbf{k}) \in \mathrm{GL}(n, \mathbb{C})$ can be written as the winding number $W(G_*)$ of a quasiparticle Green's function $G_*(i\epsilon, \mathbf{k}) = 1/\big(i\epsilon - H_*(\epsilon, \mathbf{k})\big)$, see Eq. (2), whose poles on the real frequency axis are associated to both poles and zero of $G(\epsilon, \mathbf{k})$. We have shown explicitly that $W(G_*)$ reduces to the famous TKNN formula for free electrons, here the quasiparticles, described by the Hamiltonian $H_*(0, \mathbf{k})$.

This result implies that, against all expectations, the zeros of the real frequency Green's function do have a topological relevance, which is consistent with earlier studies [3–9], and nonetheless striking. Indeed, one would naïvely argue that the position of the ingap zeros could be easily changed from the positive to the negative side of the real frequency axis, or vice versa, by slightly modifying the Hamiltonian parameters, e.g., moving the chemical potential inside the insulating gap. However, if one accepts our viewpoint that ingap bands of zeros, or, more correctly, ingap bands of the quasiparticle Hamiltonian $H_*(0, \mathbf{k})$, may describe genuine excitations that do not carry all electron's quantum numbers, then their response to a shift in chemical potential is expected to differ substantially from that of non-interacting bands.
An enlightening example is in our opinion offered by a Hubbard atom with Hamiltonian $U(n-1)^2/2$, the simplest realisation of a Mott insulator. Its Green's function on the real frequency axis,

$$G(\epsilon) = \frac{1}{2} \left(\frac{1}{\epsilon + U/2} + \frac{1}{\epsilon - U/2} \right),$$

has poles at $\epsilon = \pm U/2$ and a zero at $\epsilon = 0$. Through equations (2) and (3) one finds that, for imaginary frequencies,

$$Z(\epsilon) = \frac{\epsilon^2}{\epsilon^2 + U^2/4}\,, \quad G_*(i\epsilon) = \frac{1}{i\epsilon}\,.$$

It is tempting to associate the zero-frequency pole of the quasiparticle $G_*(i\epsilon)$ and the vanishing quasiparticle residue $Z(0) = 0$ to the free spin-1/2 of the isolated atom. In contrast, a non-interacting atom, $U = 0$, has

$$G(i\epsilon) = G_*(i\epsilon) = \frac{1}{i\epsilon}\,, \quad Z(\epsilon) = 1\,,$$

consistently with the fact that the zero frequency excitations are physical single-particle ones, $Z(0) = 1$. We now imagine to couple the atom to a metallic reservoir with which it exchanges electrons, as one would do in statistical mechanics to fix the chemical potential, and assume that the atomic level is at energy ϵ_d with respect to the chemical potential of the reservoir. The atom plus the reservoir thus describe a conventional Anderson impurity model. In the case of the Hubbard atom with $\epsilon_d \ll U$, one expects that the zero-frequency pole of the quasiparticle Green's function is immediately promoted to a Kondo resonance pinned at the bath chemical potential, thus

$$G_*(i\epsilon) = \frac{1}{i\epsilon} \to \frac{1}{i\epsilon + i\, T_K\, \mathrm{sign}(\epsilon)}\,, \quad Z(\epsilon) \to \frac{T_K}{\Gamma}\,,$$

where Γ is the *bare* hybridisation width and T_K the Kondo temperature. In other words, the coupling to the bath allows revealing the hidden physical meaning of the zero, i.e., its being a free spin prompt to Kondo screening. On the contrary, in the case of the non-interacting

atom

$$G_*(i\epsilon) = \frac{1}{i\epsilon} \to \frac{1}{i\epsilon - \epsilon_d + i\,\Gamma\,\mathrm{sign}(\epsilon)} \ ,$$

which describes a resonant level centred at ϵ_d. It is remarkable that, while the non-interacting atom simply inherits the chemical potential of the bath, the Hubbard atom does not; the Kondo resonance is always pinned at the chemical potential even though the atomic level is offset by ϵ_d.
This very simple example not only supports our interpretation that ingap quasiparticle bands in Mott insulators may describe fractionalised excitations, but also suggests that these bands respond very differently from conventional ones to a change in chemical potential induced by the contact with a charge reservoir, in contrast to a recent claim [21].

Our analysis also extends the notion of topological transitions and adiabatic transformations for strongly interacting electrons. Indeed, it was already known that some topological invariants are contributed by zero-frequency roots of the Green function [3]. That, however, seems at odds with the expected behaviour of topological invariants under adiabatic transformations, since neither a closure of the charge gap nor any symmetry breaking occurs when Green's function zeros cross the chemical potential. In light of our results, this phenomenon acquires a straightforward physical explanation: Green's function zeros crossing the chemical potential form a Luttinger surface that hosts gapless excitations [4, 5] despite the finite charge gap, thus providing the non-adiabaticity required to change topology.

Finally, our results raise several questions worth being addressed in the future. The correspondence between topological bands and edge modes of Green's function zeros [7–9] suggests that, similarly to the conventional case of edge poles, the edge zeros are ultimately responsible of the quantised Hall conductance (13), although the surface is charge insulating. In the model quantum spin-Hall insulator of Sec. III, that puzzling prediction can be explained by noticing that, according to Ref. [5], the edge quasiparticles at the Luttinger surface, actually a point, can carry a spin current, thus a quantised spin-Hall conductance. However, that simple explanation would not work for a hypothetical Chern Mott insulator with edge zeros crossing the chemical potential. Therefore, even though the results of Sec. II prove that bulk bands of Green's function zeros contributes to the topological invariant (1), the actual role of edge zeros remains unclear.
A further question regards fractional Chern insulators. Indeed, if the winding number (1) does correspond to the Hall conductance, which may not always be the case, see Appendix B, one may wonder how it may ever be fractional since the TKNN formula should yield an integer value. In view of the similar issue that arises in the fractional quantum Hall effect [22], we believe that the ground state degeneracy, also expected in a fractional Chern insulator [23], is the key ingredient. Specifically, we suspect that $H_*(0,\mathbf{k})$ calculated over each ground state has valence bands with ill-defined Chern number, because, e.g., they touch the zone boundaries with finite slope. However, assuming, for simplicity, that the ground state is threefold degenerate, the Hall conductance is better defined as [22]

$$\begin{aligned}\sigma_{\mathrm{H}} &= \frac{1}{3}\Big(W(G_1) + W(G_2) + W(G_3)\Big) \\ &= \frac{1}{3}\,W\big(G_1\,G_2\,G_3\big)\,,\end{aligned}$$

where G_n is the Green's function calculated over the ground state $\mid n\rangle$, $n = 1, 2, 3$. The sum of the three winding numbers corresponds to the TKNN formula applied to the quasiparticles valence bands of all three ground states. We speculate, see, e.g., Ref. [24], that all these bands as a whole correspond to a well-behaved single band once unfolded into a threefold larger Brillouin zone, whose Chern number is therefore an integer ℓ, thus $\sigma_{\mathrm{H}} = \ell/3$, a fractional value. Incidentally, it is suggestive that the sum of the winding numbers is just the winding number of $G = G_1\,G_2\,G_3$, which is still a complex invertible matrix. The above is just a speculation that we believe worth investigating.

We conclude by emphasising that the winding number (1) in two dimensions, although being a topological invariant, not necessarily coincides with the quantised Hall conductance when perturbation theory breaks down, see Appendix B. Similarly, we cannot exclude that the extensions of the Green's function winding number in three dimensions [12, 14, 17, 19] might be unrelated to the physical observables they are supposed to reproduce when there is no adiabatic connection between the interacting system and the non-interacting one. That leaves open the question about the actual physical meaning of those winding numbers [25, 26].

ACKNOWLEDGMENTS

We are very grateful to Adriano Amaricci, Elio König Michel Ferrero, Giorgio Sangiovanni and, especially, Roberto Percacci for helpful discussions and comments.

Appendix A: Properties of thermal Green's functions

Hereafter, we consider a generic basis of Bloch wavefunctions $\phi_{a\mathbf{k}}(\mathbf{k})$, where a include also the spin label, with associated creation, $c^\dagger_{a\mathbf{k}}$, and annihilation, $c_{a\mathbf{k}}$, operators. We assume that lattice translational symmetry is not broken. The Green's function matrix in imaginary

time $\tau \in [-\beta, \beta]$, where $\beta = 1/T$, is defined through its components, diagonal in momentum,

$$G_{ab}(\tau, \mathbf{k}) = -\big\langle\, T_\tau \Big(c_{a\mathbf{k}}(\tau)\, c^\dagger_{b\mathbf{k}} \Big)\, \big\rangle\,, \tag{A1}$$

where T_τ is the time-ordering operator and $c_{a\mathbf{k}}(\tau) = \mathrm{e}^{H\tau}\; c_{a\mathbf{k}}\; \mathrm{e}^{-H\tau}$ the imaginary time evolution of the operator. The Fourier transform of (A1) in Matsubara frequencies $i\epsilon_\ell = (2\ell+1)\pi T$ is readily found to be

$$G_{ab}(i\epsilon_\ell, \mathbf{k}) = \frac{1}{\Omega} \sum_{n,m} \Big(\mathrm{e}^{-\beta E_n} + \mathrm{e}^{-\beta E_m} \Big) \frac{\langle n \mid c_{a\mathbf{k}} \mid m \rangle \langle m \mid c^\dagger_{b\mathbf{k}} \mid n \rangle}{i\epsilon_\ell - \big(E_m - E_n\big)}\,,$$

where $\Omega = \mathrm{Tr}\,\big(\mathrm{e}^{-\beta H}\big)$ is the partition function, $|n\rangle$ and $|m\rangle$ many-body eigenstates with eigenvalues E_n and E_m, respectively. We note that $G_{ab}(i\epsilon_\ell, \mathbf{k})^* = G_{ba}(-i\epsilon_\ell, \mathbf{k})$, and thus

$$G(i\epsilon_\ell, \mathbf{k})^\dagger = G(-i\epsilon_\ell, \mathbf{k})\,. \tag{A2}$$

This property must evidently hold true also for the inverse matrices. Therefore, using Dyson's equation

$$G(i\epsilon_\ell, \mathbf{k})^{-1} = i\epsilon_\ell - H_0(\mathbf{k}) - \Sigma(i\epsilon_\ell, \mathbf{k})\,,$$

where $H_0(\mathbf{k})$ is the non-interacting Hamiltonian that includes the chemical potential term $-\mu\, N$, and $\Sigma(i\epsilon_\ell, \mathbf{k})$ the self energy, both being matrices in the same basis of Bloch wavefunctions, one concludes that also

$$\Sigma(i\epsilon_\ell, \mathbf{k})^\dagger = \Sigma(-i\epsilon_\ell, \mathbf{k})\,. \tag{A3}$$

We can write $G(i\epsilon_\ell, \mathbf{k}) = G_1(i\epsilon_\ell, \mathbf{k}) + i\, G_2(i\epsilon_\ell, \mathbf{k})$ where

$$\begin{aligned} G_1(i\epsilon_\ell, \mathbf{k}) &= \frac{G(i\epsilon_\ell, \mathbf{k}) + G(i\epsilon_\ell, \mathbf{k})^\dagger}{2} \\ &= \frac{G(i\epsilon_\ell, \mathbf{k}) + G(-i\epsilon_\ell, \mathbf{k})}{2}\,, \\ G_2(i\epsilon_\ell, \mathbf{k}) &= \frac{G(i\epsilon_\ell, \mathbf{k}) - G(i\epsilon_\ell, \mathbf{k})^\dagger}{2i} \\ &= \frac{G(i\epsilon_\ell, \mathbf{k}) - G(-i\epsilon_\ell, \mathbf{k})}{2i}\,, \end{aligned}$$

are both hermitian, G_1 even and G_2 odd in ϵ_ℓ. Specifically, the matrix elements of G_2 read

$$G_{2\,ab}(i\epsilon_\ell, \mathbf{k}) = -\frac{\epsilon_\ell}{\Omega} \sum_{n,m} \Big(\mathrm{e}^{-\beta E_n} + \mathrm{e}^{-\beta E_m} \Big) \frac{\langle n \mid c_{a\mathbf{k}} \mid m \rangle \langle m \mid c^\dagger_{b\mathbf{k}} \mid n \rangle}{\epsilon_\ell^2 + \big(E_m - E_n\big)^2}\,.$$

Since G_2 is hermitian, it can be diagonalised by a unitary transformation $c_{a\mathbf{k}} \to c_{\alpha\mathbf{k}}$ that yields the eigenvalues

$$G_{2\,\alpha}(i\epsilon_\ell, \mathbf{k}) = -\frac{\epsilon_\ell}{\Omega} \sum_{n,m} \Big(\mathrm{e}^{-\beta E_n} + \mathrm{e}^{-\beta E_m} \Big) \frac{\big|\langle n \mid c_{\alpha\mathbf{k}} \mid m \rangle\big|^2}{\epsilon_\ell^2 + \big(E_m - E_n\big)^2}\,,$$

which are negative for $\epsilon_\ell > 0$ and positive otherwise. It follows that, once we write $\Sigma(i\epsilon_\ell, \mathbf{k}) = \Sigma_1(i\epsilon_\ell, \mathbf{k}) + i\,\Sigma_2(i\epsilon_\ell, \mathbf{k})$, where

$$\begin{aligned} \Sigma_1(i\epsilon_\ell, \mathbf{k}) &= \frac{\Sigma(i\epsilon_\ell, \mathbf{k}) + \Sigma(i\epsilon_\ell, \mathbf{k})^\dagger}{2} \\ &= \frac{\Sigma(i\epsilon_\ell, \mathbf{k}) + \Sigma(-i\epsilon_\ell, \mathbf{k})}{2}\,, \\ \Sigma_2(i\epsilon_\ell, \mathbf{k}) &= \frac{\Sigma(i\epsilon_\ell, \mathbf{k}) - \Sigma(i\epsilon_\ell, \mathbf{k})^\dagger}{2i} \\ &= \frac{\Sigma(i\epsilon_\ell, \mathbf{k}) - \Sigma(-i\epsilon_\ell, \mathbf{k})}{2i}\,, \end{aligned}$$

are also both hermitian, the former even in ϵ_ℓ and the latter odd, the eigenvalues of $\Sigma_2(i\epsilon_\ell, \mathbf{k})$ are negative for $\epsilon_\ell > 0$ and positive otherwise, just like those of $G_2(i\epsilon_\ell, \mathbf{k})$.

The quasiparticle residue matrix is defined by (3), i.e.,

$$Z(\epsilon_\ell, \mathbf{k}) = Z(-\epsilon_\ell, \mathbf{k}) = \left(1 - \frac{\Sigma_2(i\epsilon_\ell, \mathbf{k})}{\epsilon_\ell} \right)^{-1}\,,$$

and is therefore a semi-positive definite matrix that becomes strictly positive definite in insulators without Luttinger surfaces, where $\Sigma_2(0, \mathbf{k}) = 0$. Similarly, the quasiparticle Hamiltonian (4), i.e.,

$$\begin{aligned} &H_*(\epsilon_\ell, \mathbf{k}) = H_*(-\epsilon_\ell, \mathbf{k}) \\ &\quad = \sqrt{Z(\epsilon_\ell, \mathbf{k})}\; \Big(H_0(\mathbf{k}) + \Sigma_1(i\epsilon_\ell, \mathbf{k}) \Big)\; \sqrt{Z(\epsilon_\ell, \mathbf{k})}\,, \end{aligned}$$

is hermitian and even in ϵ_ℓ. Therefore, if $\mid \alpha(\epsilon_\ell, \mathbf{k})\rangle$ is eigenstate of $H_*(\epsilon_\ell, \mathbf{k})$ with eigenvalue $\epsilon_\alpha(\epsilon_\ell, \mathbf{k})$, we can always define $\mid \alpha(-\epsilon_\ell, \mathbf{k})\rangle = \mid \alpha(\epsilon_\ell, \mathbf{k})\rangle$ the eigenstate of $H_*(-\epsilon_\ell, \mathbf{k})$ with the same eigenvalue $\epsilon_\alpha(\epsilon_\ell, \mathbf{k})$. We end emphasising that the representation (2) of the Green's function in terms of the quasiparticle one,

$$G_*(i\epsilon, \mathbf{k}) = \frac{1}{i\epsilon - H_*(\epsilon, \mathbf{k})}\,,$$

with hermitian $H_*(\epsilon, \mathbf{k})$ is a rigorous result that remains valid also when $H_*(0, \mathbf{k})$ has zero eigenvalues, i.e., when Fermi and/or Luttinger surfaces are present.

Appendix B: Topological invariant in two dimensions

The Hall conductance in non-interacting insulators is quantized in units $e^2/2\pi\hbar$, where the integer quantum is a topological invariant known as the first Chern number. This is calculated upon the occupied bands and is robust under any smooth deformation of the Hamiltonian. On the other hand, in the case of interacting electrons, band theory of independent electrons does not hold and yet a quantized topological invariant, which reduces to the Chern number if the interaction is switched off, can be still defined. However, while the expression of this

invariant, the winding number (1), could be well anticipated by algebraic topology arguments, we believe that the most accepted derivation, see, e.g., Refs. [10, 11], is not formally correct. Therefore, we here rederive the Hall conductance by standard quantum many-body theory [27].

Hereafter, we consider a periodic model of interacting electrons and use units in which $\hbar = 1$. The off-diagonal component σ_{ij}, $i \neq j$, of the conductivity tensor is related to the current-current response function $\chi_{ij}(\omega)$ through

$$\sigma_{ij} = -\lim_{\omega\to 0} \frac{e^2}{i\omega}\, \chi_{ij}(\omega)\,,$$

where, in the basis of the Hamiltonian eigenstates $\mid n\rangle$, with eigenvalues E_n,

$$\chi_{ij}(\omega) = \chi_{ji}(-\omega) = \frac{1}{Z}\sum_{nm} \frac{\mathrm{e}^{-\beta E_n} - \mathrm{e}^{-\beta E_m}}{\omega - E_m + E_n} \int d\mathbf{x}\, d\mathbf{y}\, \langle n \mid J_i(\mathbf{x}) \mid m\rangle\langle m \mid J_j(\mathbf{y}) \mid n\rangle\,,$$

with $J_i(\mathbf{x})$ the i-the component of the current density operator at position $\mathbf{x}$. Therefore, the antisymmetric component of the current-current tensor is, for small ω,

$$\frac{\chi_{ij}(\omega) - \chi_{ji}(\omega)}{2} \simeq -\omega\, \frac{1}{Z}\sum_{nm} \frac{\mathrm{e}^{-\beta E_n} - \mathrm{e}^{-\beta E_m}}{\left(E_m + E_n\right)^2} \int d\mathbf{x}\, d\mathbf{y}\, \langle n \mid J_i(\mathbf{x}) \mid m\rangle\langle m \mid J_j(\mathbf{y}) \mid n\rangle = \omega\, \frac{\partial \chi_{ij}(\omega)}{\partial \omega}\Big|_{\omega=0}\,,$$

which is imaginary, and thus, switching to Matsubara frequencies and for $i \neq j$,

$$\frac{\sigma_{ij} - \sigma_{ji}}{2} = i\, e^2\, \frac{\partial \chi_{ij}(i\omega)}{\partial i\omega}\Big|_{\omega=0}\,,$$

where now

$$\chi_{ij}(i\omega) = -\int_0^\beta d\tau\, \mathrm{e}^{i\omega\tau} \int d\mathbf{x}\, d\mathbf{y}\, \langle\, T_\tau \Big(J_i(\mathbf{x},\tau)\, J_j(\mathbf{y},0)\Big)\,\rangle\,,$$

is the correlation function in the Matsubara formalism, with τ the imaginary time. Fig. 1 shows the representation of $\chi_{ij}(i\omega)$ in skeleton diagrams. It is worth noticing that only one of the two current vertices is fully interacting, otherwise we would double count interaction effects as mistakenly done in Ref. [11].

We are interested in the derivative of $\chi_{ij}(i\omega)$ with respect to $i\omega$ calculated at $\omega = 0$, which, by inspection of Fig. 1, can be represented as in Fig. 2, where, only because of the derivative, the current vertices are now both fully interacting. Through the Ward-Takahashi identity

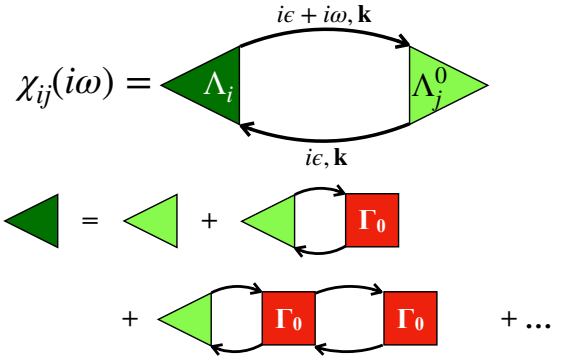

FIG. 1. Top panel: current-current correlation function $\chi_{ij}(i\omega)$ in skeleton diagrams. Black arrow lines are interacting single-particle Green's functions G, whose Matsubara frequency and momentum are explicitly shown; green triangle represents the non-interacting current vertex Λ_j^0, while dark green triangle the fully interacting one Λ_i. Bottom panel: Bethe-Salpeter equation satisfied by the interacting Λ_i in terms of the interaction vertex Γ_0 irreducible in the particle-hole channel.

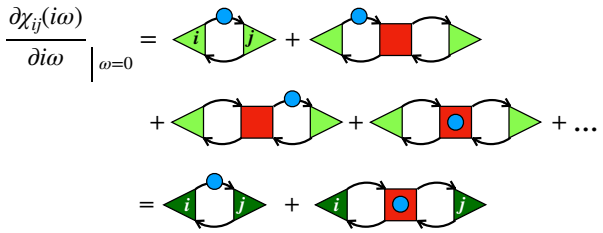

FIG. 2. Diagrammatic representation of $\partial\chi_{ij}(i\omega)/\partial i\omega$ up to first order in the skeleton expansion. The cyan circle represents $\partial/\partial i\omega$. Note that all diagrams must be evaluated at $\omega = 0$ after taking the derivative.

the fully interacting current vertex at $\omega = 0$ is simply $\Lambda_i = -\partial G^{-1}/\partial k_i$, and, since $\partial G = -G\,\partial G^{-1}\,G$, we can write in 2D and for $T = 0$

$$\begin{aligned}\frac{\sigma_{12}-\sigma_{21}}{2} &= \frac{e^2}{2\pi}\,\nu_{\rm H}\\ &= \frac{e^2}{(2\pi)^3}\int d\epsilon\, d\mathbf{k}\,{\rm Tr}\Big(G(i\epsilon,\mathbf{k})\,\partial_{k_1}G(i\epsilon,\mathbf{k})^{-1}\,G(i\epsilon,\mathbf{k})\,\partial_\epsilon G(i\epsilon,\mathbf{k})^{-1}\,G(i\epsilon,\mathbf{k})\,\partial_{k_2}G(i\epsilon,\mathbf{k})^{-1}\Big)+\frac{e^2}{2\pi}\,K_L\\ &= \frac{e^2}{2\pi}\left\{\frac{1}{24\pi^2}\int d\epsilon\, d\mathbf{k}\,\epsilon_{\mu\nu\rho}\,{\rm Tr}\Big(G(i\epsilon,\mathbf{k})\,\partial_\mu G(i\epsilon,\mathbf{k})^{-1}\,G(i\epsilon,\mathbf{k})\,\partial_\nu G(i\epsilon,\mathbf{k})^{-1}\,G(i\epsilon,\mathbf{k})\,\partial_\rho G(i\epsilon,\mathbf{k})^{-1}\Big)+K_L\right\}\\ &= \frac{e^2}{2\pi}\Big[W(G)+K_L\Big]\,,\end{aligned} \tag{B1}$$

where ν_H is the quantised Hall conductance, $\epsilon_{\mu\nu\rho}$, with indices running from 0 to 2, the antisymmetric tensor, $\partial_0=\partial_\epsilon$ and $\partial_{1(2)}=\partial_{k_{1(2)}}$, and $W(G)$, see (1), is the winding number of the map $(\epsilon,\mathbf{k})\to G(i\epsilon,\mathbf{k})\in {\rm GL}(n,\mathbb{C})$, assuming that the Green's function $G(i\epsilon,\mathbf{k})$ is an $n\times n$ invertible matrix, with n the dimension of the single-particle wavefunction basis, which is true provided the system is insulating and has no Luttinger surface.
The additional term besides the winding number involves the derivative of the irreducible vertex Γ_0 and reads explicitly

$$K_L=\frac{i\pi}{(2\pi)^6}\sum\int d\epsilon\, d\mathbf{k}\, d\epsilon'\, d\mathbf{k}'\;\epsilon_{ij}\;\partial_i G_{ba}(i\epsilon,\mathbf{k})\;F_{ab;a'b'}\big(i\epsilon,\mathbf{k};i\epsilon',\mathbf{k}'\big)\;\partial_j G_{b'a'}(i\epsilon',\mathbf{k}')\,, \tag{B2}$$

where

$$\begin{aligned}F_{ab;a'b'}\big(i\epsilon,\mathbf{k};i\epsilon',\mathbf{k}'\big)=\lim_{\omega\to0}\frac{1}{2i\omega}\Big\{&\Gamma_0\big(i\epsilon+i\omega\,\mathbf{k}\,a,i\epsilon'\,\mathbf{k}'\,a';i\epsilon'+i\omega\,\mathbf{k}'\,b',i\epsilon\,\mathbf{k}\,b\big)\\ &-\Gamma_0\big(i\epsilon\,\mathbf{k}\,a,i\epsilon'+i\omega\,\mathbf{k}'\,a';i\epsilon'\,\mathbf{k}'\,b',i\epsilon+i\omega\,\mathbf{k}\,b\big)\Big\}=-F_{a'b';ab}\big(i\epsilon',\mathbf{k}';i\epsilon,\mathbf{k}\big)\,,\end{aligned} \tag{B3}$$

with

$$\begin{aligned}&\Gamma_0\big(i\epsilon+i\omega\,\mathbf{k}\,a,i\epsilon'\,\mathbf{k}'\,a';i\epsilon'+i\omega\,\mathbf{k}'\,b',i\epsilon\,\mathbf{k}\,b\big)\\ &\quad=\Gamma_0\big(i\epsilon'\,\mathbf{k}'\,a',i\epsilon+i\omega\,\mathbf{k}\,a;i\epsilon\,\mathbf{k}\,b,i\epsilon'+i\omega\,\mathbf{k}'\,b'\big)\,,\end{aligned}$$

the irreducible vertex in the particle-hole channel with transferred frequency ω. Since

$$\begin{aligned}&\Gamma_0\big(i\epsilon+i\omega\,\mathbf{k}\,a,i\epsilon'\,\mathbf{k}'\,a';i\epsilon'+i\omega\,\mathbf{k}'\,b',i\epsilon\,\mathbf{k}\,b\big)^*\\ &\quad=\Gamma_0\big(-i\epsilon\,\mathbf{k}\,b,-i\epsilon'-i\omega\,\mathbf{k}'\,b';-i\epsilon'\,\mathbf{k}'\,a',-i\epsilon-i\omega\,\mathbf{k}\,a\big)\,,\end{aligned}$$

and $G_{ba}(i\epsilon,\mathbf{k})^*=G_{ab}(-i\epsilon,\mathbf{k})$, one can readily show that K_L in (B2) is indeed real. We observe that F in (B3) is odd under $(i\epsilon,\mathbf{k},ab)\leftrightarrow(i\epsilon,\mathbf{k}',a'b')$, unlike what claimed in [10, 11], which compensates the change of sign of the antisymmetric tensor ϵ_{ij} under $i\leftrightarrow j$. Therefore, K_L may well be finite in principle. Nonetheless, one may still argue that F could vanish. Indeed, the irreducibility in the particle-hole channel suggests that Γ_0 depends on $i\omega$ only through the frequency carried by the particle-particle channel, as can be verified by inspection of few orders in the skeleton expansion. That frequency remains invariant if in the top panel of Fig. 1 we change the frequency of the upper Green's function from $i\epsilon+i\omega$ to $i\epsilon$, and that of the lower one from $i\epsilon$ to $i\epsilon+i\omega$, thus $\omega\to-\omega$ in the particle-hole channel. If that is true, Γ_0 is even in ω, and since it must also be smooth, then its derivative at $\omega=0$ has to vanish, as also argued by Ref. [17] on the basis of the skeleton expansion. However, once perturbation theory breaks down, one cannot exclude that the full series develops odd contributions, and thus that K_L becomes non zero.

Further insight in that direction can be gained through the Streda formula [28, 29]

$$\frac{\partial\rho}{\partial B}\Big|_{B=0}=\frac{e}{2\pi c}\,\nu_{\rm H}\,, \tag{B4}$$

where ρ is the electron density. The spin-Hall conductance is defined similarly provided ρ is replaced by the spin density [30]. The electron density at $T=0$ can be

calculated through [6]

$$\begin{aligned}\rho &= \frac{n}{2} + \int \frac{d\epsilon\, d\mathbf{k}}{(2\pi)^3}\, \mathrm{Tr}\Big(G(i\epsilon,\mathbf{k})\Big) \\ &= \frac{n}{2} - \int \frac{d\epsilon\, d\mathbf{k}}{(2\pi)^3}\, \frac{\partial \ln\det G(i\epsilon,\mathbf{k})}{\partial i\epsilon} + I_L \\ &= \frac{n}{2} - \int \frac{d\epsilon\, d\mathbf{k}}{(2\pi)^3}\, \frac{\partial \ln\det G_*(i\epsilon,\mathbf{k})}{\partial i\epsilon} + I_L \\ &= \int \frac{d\mathbf{k}}{(2\pi)^2}\, \theta\big(-\epsilon_\alpha(0,\mathbf{k})\big) + I_L\,,\end{aligned} \tag{B5}$$

where n is the number of bands, including spin, we used the fact that

$$\ln\det G(i\epsilon,\mathbf{k}) = \ln\det G_*(i\epsilon,\mathbf{k}) + \ln\det Z(\epsilon,\mathbf{k})\,,$$

and $\ln\det Z(\epsilon,\mathbf{k})$ gives no contribution to the integral since its derivative is odd, and, finally,

$$\begin{aligned}I_L &= \int \frac{d\epsilon\, d\mathbf{k}}{(2\pi)^3}\, \mathrm{Tr}\bigg(G(i\epsilon,\mathbf{k})\, \frac{\partial\Sigma(i\epsilon,\mathbf{k})}{\partial i\epsilon}\bigg) \\ &= \frac{1}{\pi}\int \frac{d\mathbf{k}}{(2\pi)^2}\, \mathrm{Im}\,\mathcal{I}(i0^+,\mathbf{k})\,.\end{aligned}$$

The function $\mathcal{I}(i\epsilon,\mathbf{k}) = \mathcal{I}(-i\epsilon,\mathbf{k})^*$ is defined as [6]

$$\mathcal{I}(i\epsilon,\mathbf{k}) = \Phi(i\epsilon,\mathbf{k}) - \mathrm{Tr}\Big(\Sigma(i\epsilon,\mathbf{k})\, G(i\epsilon,\mathbf{k})\Big)\,,$$

having written the Luttinger-Ward functional, which can be constructed fully non-perturbatively [31], as

$$\Phi[G] = T\sum_\ell \int \frac{d\mathbf{k}}{(2\pi)^2}\, \mathrm{e}^{i\epsilon_\ell 0^+}\, \Phi(i\epsilon_\ell,\mathbf{k})\,.$$

In the perturbative regime, $\mathrm{Im}\,\mathcal{I}(i\epsilon,\mathbf{k}) \sim \epsilon$ for small ϵ and thus $I_L = 0$, in which case (B5) reduces to the well known statement of Luttinger's theorem [32]. However, when perturbation theory breaks down, I_L is generally nonzero [6].

In presence of a magnetic field B, the derivative of the first term in (B5) with respect to B and calculated at $B = 0$ yields the Streda formula for non-interacting electrons described by the quasiparticle Hamiltonian $H_*(0,\mathbf{k})$, which is just the TKNN expression (13). It follows that

$$\frac{\partial I_L}{\partial B}\Big|_{B=0} \equiv \frac{e}{2\pi c}\, K_L\,, \tag{B6}$$

namely that the winding number (1) may not correspond to the quantised Hall conductance when perturbation theory breaks down and $I_L \neq 0$, in accordance, e.g., with the results of [25, 26].

Appendix C: Properties of the winding number

Using the property of the antisymmetric tensor, the equivalence $G(i\epsilon,\mathbf{k})^\dagger = G(-i\epsilon,\mathbf{k})$, and the fact that one of the derivatives in the winding number (1) is $\partial_\epsilon = -\partial_{-\epsilon}$, one finds that

$$\begin{aligned}W(G)^* &= \frac{1}{24\pi^2}\int d\epsilon\, d\mathbf{k}\, \epsilon_{\mu\nu\rho}\, \mathrm{Tr}\Big(G(-i\epsilon,\mathbf{k})\, \partial_\rho G(-i\epsilon,\mathbf{k})^{-1}\, G(-i\epsilon,\mathbf{k})\, \partial_\nu G(-i\epsilon,\mathbf{k})^{-1}\, G(-i\epsilon,\mathbf{k})\, \partial_\mu G(-i\epsilon,\mathbf{k})^{-1}\Big) \\ &= -\frac{1}{24\pi^2}\int d\epsilon\, d\mathbf{k}\, \epsilon_{\mu\nu\rho}\, \mathrm{Tr}\Big(G(i\epsilon,\mathbf{k})\, \partial_\rho G(i\epsilon,\mathbf{k})^{-1}\, G(i\epsilon,\mathbf{k})\, \partial_\nu G(i\epsilon,\mathbf{k})^{-1}\, G(i\epsilon,\mathbf{k})\, \partial_\mu G(i\epsilon,\mathbf{k})^{-1}\Big) \\ &= \frac{1}{24\pi^2}\int d\epsilon\, d\mathbf{k}\, \epsilon_{\rho\nu\mu}\, \mathrm{Tr}\Big(G(i\epsilon,\mathbf{k})\, \partial_\rho G(i\epsilon,\mathbf{k})^{-1}\, G(i\epsilon,\mathbf{k})\, \partial_\nu G(i\epsilon,\mathbf{k})^{-1}\, G(i\epsilon,\mathbf{k})\, \partial_\mu G(i\epsilon,\mathbf{k})^{-1}\Big) = W(G)\,,\end{aligned}$$

thus that $W(G)$ is real, as expected. Now suppose that the function $G(i\epsilon,\mathbf{k})$, beside satisfying (A2), which guarantees that $W(G)$ is real, is also hermitian. It follows that $G(i\epsilon,\mathbf{k}) = G(i\epsilon,\mathbf{k})^\dagger = G(-i\epsilon,\mathbf{k})$, thus $G(i\epsilon,\mathbf{k})$ is even in ϵ, hence its derivative is odd. As a consequence, the winding number trivially vanishes being an integral over $\epsilon \in [-\infty,\infty]$ of an odd function. This is precisely the reason why $W(Z) = 0$, since the quasiparticle residue matrix $Z(\epsilon,\mathbf{k})$, Eq. (3) of the main text, is hermitian and even in ϵ.

1. Proof of $W(G_1\, G_2) = W(G_1) + W(G_2)$

We shortly write

$$W(G) = \frac{1}{24\pi^2}\int d\mathbf{x}\, \epsilon_{\mu\nu\rho}\, \mathrm{Tr}\Big(G(\mathbf{x})\, \partial_\mu G(\mathbf{x})^{-1}\, G(\mathbf{x})\, \partial_\nu G(\mathbf{x})^{-1}\, G(\mathbf{x})\, \partial_\rho G(\mathbf{x})^{-1}\Big)\,,$$

where $\mathbf{x} = \big(x_0, x_1, x_2\big)$ is a three component vector. Assume that $G(\mathbf{x}) = G_1(\mathbf{x})\, G_2(\mathbf{x})$, then, since the winding number of the product can be written as, defining, for simplicity, $G \equiv G(\mathbf{x})$,

$$\begin{aligned} G\,\partial_\mu G &= G_1\, G_2\, \partial_\mu \left(G_2^{-1}\, G_1^{-1}\right) \\ &= G_1 \left(G_2\, \partial_\mu G_2^{-1} + \partial_\mu G_1^{-1}\, G_1\right) G_1^{-1}\,, \end{aligned}$$

$$\begin{aligned} W(G_1 G_2) &= \frac{1}{24\pi^2} \int d\mathbf{x}\, \epsilon_{\mu\nu\rho}\, \mathrm{Tr}\Big[\left(G_2\, \partial_\mu G_2^{-1} + \partial_\mu G_1^{-1}\, G_1\right) \left(G_2\, \partial_\nu G_2^{-1} + \partial_\nu G_1^{-1}\, G_1\right) \left(G_2\, \partial_\rho G_2^{-1} + \partial_\rho G_1^{-1}\, G_1\right) \Big] \\ &= W(G_1) + W(G_2) \\ &\quad + \frac{3}{24\pi^2} \int d\mathbf{x}\, \epsilon_{\mu\nu\rho}\, \mathrm{Tr}\Big[G_2\, \partial_\mu G_2^{-1}\, G_2\, \partial_\nu G_2^{-1}\, \partial_\rho G_1^{-1}\, G_1 \,+\, \partial_\mu G_1^{-1}\, G_1\, \partial_\nu G_1^{-1}\, G_1\, G_2\, \partial_\rho G_2^{-1} \Big]\,. \end{aligned} \tag{C1}$$

Since $G\,\partial_\mu G^{-1} = -\partial_\mu G\, G^{-1}$ and $\epsilon_{\mu\nu\rho}\Big(\partial_\mu\partial_\nu G\Big) = 0$ if G is smooth, we find that

$$\begin{aligned} I &\equiv \epsilon_{\mu\nu\rho}\, \mathrm{Tr}\Big[G_2\, \partial_\mu G_2^{-1}\, G_2\, \partial_\nu G_2^{-1}\, \partial_\rho G_1^{-1}\, G_1 \,+\, \partial_\mu G_1^{-1}\, G_1\, \partial_\nu G_1^{-1}\, G_1\, G_2\, \partial_\rho G_2^{-1} \Big] \\ &= -\epsilon_{\mu\nu\rho}\, \mathrm{Tr}\Big[\partial_\mu G_2\, \partial_\nu G_2^{-1}\, \partial_\rho G_1^{-1}\, G_1 \,+\, \partial_\mu G_1^{-1}\, \partial_\nu G_1\, G_2\, \partial_\rho G_2^{-1} \Big] \\ &= -\epsilon_{\mu\nu\rho}\, \mathrm{Tr}\Big[\partial_\mu\Big(G_2\, \partial_\nu G_2^{-1}\Big)\, \partial_\rho G_1^{-1}\, G_1 \,+ \partial_\nu\Big(\partial_\mu G_1^{-1}\, G_1\Big)\, G_2\, \partial_\rho G_2^{-1} \Big]\,. \end{aligned} \tag{C2}$$

Integrating by part the first term, and then switching the indexes $\mu \leftrightarrow \nu$ in the first term and $\mu \leftrightarrow \rho$ in the second one, we obtain

$$\begin{aligned} I &= -\epsilon_{\mu\nu\rho}\, \mathrm{Tr}\Big[-\, G_2\, \partial_\nu G_2^{-1}\, \partial_\mu\Big(\partial_\rho G_1^{-1}\, G_1\Big) + \, G_2\, \partial_\rho G_2^{-1}\, \partial_\nu\Big(\partial_\mu G_1^{-1}\, G_1\Big) \Big] \\ &= -\epsilon_{\mu\nu\rho}\, \mathrm{Tr}\Big[G_2\, \partial_\mu G_2^{-1}\, \partial_\nu\Big(\partial_\rho G_1^{-1}\, G_1\,\Big) - G_2\, \partial_\mu G_2^{-1}\, \partial_\nu\Big(\partial_\rho G_1^{-1}\, G_1\Big) \Big] = 0\,, \end{aligned} \tag{C3}$$

which proves that

$$W\big(G_1\, G_2\big) = W(G_1) + W(G_2)\,. \tag{C4}$$

[1] Equivalently, in the basis that diagonalises $G(\epsilon, \mathbf{k})$ for strictly real ϵ, there may be elements along the diagonal that vanish at certain ϵ and $\mathbf{k}$. That is evidently different from the case in which the Green's function, represented in a basis in which it is not diagonal, has diagonal terms that may cross zero. This circumstance has been discussed in [33]. In particular, the diagonal elements of the non-interacting Green's function have only poles in the diagonal basis, while they may have also zeros in a generic non-diagonal basis, whose role has been analysed, e.g., in [34–36].

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