

Probing Green's Function Zeros by Cotunneling through Mott Insulators

Carl Lehmann,^{1,2,*} Lorenzo Crippa^{2,3,4}, Giorgio Sangiovanni^{2,3} and Jan Carl Budich^{1,2,5,†}

¹*Institute of Theoretical Physics, Technische Universität Dresden, 01069 Dresden, Germany*

²*Würzburg-Dresden Cluster of Excellence ct.qmat, 97074 Würzburg, Germany*

³*Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg, Germany*

⁴*I. Institute of Theoretical Physics, University of Hamburg, Notkestrasse 9, 22607 Hamburg, Germany*

⁵*Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Strasse 38, 01187 Dresden, Germany*



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Quantum tunneling experiments have provided deep insights into basic excitations occurring as Green's function poles in the realm of complex quantum matter. However, strongly correlated quantum materials also allow for Green's functions zeros (GFZs) that may be seen as an antidote to the familiar poles and have so far largely eluded direct experimental study. Here, we propose and investigate theoretically how cotunneling through Mott insulators enables direct access to the shadow band structure of GFZs. In particular, we derive an effective Hamiltonian for the GFZ that is shown to govern the cotunneling amplitude and reveal fingerprints of many-body correlations clearly distinguishing the GFZ structure from the underlying free Bloch band structure of the system. Our perturbative analytical results are corroborated by numerical data in the framework of both exact diagonalization and matrix product state simulations for a one-dimensional model system consisting of a Su-Schrieffer-Heeger-Hubbard model coupled to two single-level quantum dots.

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Quantum tunneling and transport probes are among the most versatile diagnostic tools for gaining insight into the microscopic structure of quantum matter [1–4]. In the realm of strongly correlated systems [5–8], experimental breakthroughs along these lines range from single electron control in cotunneling experiments through quantum dots in the Coulomb blockade regime [9–14] to probing the fractional statistics of anyonic quasiparticles in topological phases [15–18]. However, despite this remarkable progress, the complexity of correlated many-body systems still retains a plethora of secrets, thus promising novel physical phenomena yet to be revealed. As an exciting example, Green's function zeros (GFZs) in Mott insulators [19–24] have recently been predicted to appear as a shadow of the underlying Bloch band structure [25–34], i.e., of the poles in the single-particle Green's function (GF) of a quantum material. Owing to Cauchy's argument principle, such GFZs and poles play a reciprocal role reminiscent of matter and antimatter in particle physics, and their cancellation at material interfaces has been recently discussed

in the context of topological edge modes [33]. Despite recent progress regarding the possibility of detecting GFZs either by exploiting zero-pole annihilation mechanisms [33–36] or through transport signatures [27], it is fair to say that a direct experimental probe of GFZs has largely remained elusive.

Here, we study cotunneling through Mott insulators as a sharp diagnostic tool to fully reveal the shadow band structure of GFZs. As a setting (see Fig. 1 for an illustration), we propose a reinterpretation and generalization of the

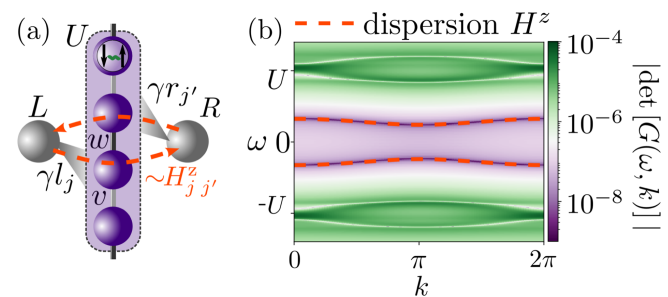


FIG. 1. Cotunneling reveals GFZ-Hamiltonian H^z : (a) two spinful auxiliary sites (gray, $\{L, R\}$), weakly coupled by tunneling amplitudes $\{\gamma l_j, \gamma r_{j'}\}$ to a Hubbard system in Mott regime (violet). Elastic cotunneling establishes an effective coupling between L and R (red, dashed line). (b) Numerical results (matrix product state methods) on the GF-determinant $|\det[G(\omega, k)]|$: SSH-Hubbard model at half filling with $N = 60$ spinful sites, $v = 0.75$, $w = 1.0$, $U = 10$, and analytic prediction of the in-gap zero dispersion of H^z (red, dashed line).

*Contact author: Carl.Lehmann1@tu-dresden.de

†Contact author: jan.budich@tu-dresden.de

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well-established experimental platform of cotunneling measurements through quantum dots [9,14,37–43] by replacing a quantum dot in the Coulomb-blockade regime with a many-body system in a Mott phase, which may even be engineered as a synthetic quantum material consisting of an array of coupled quantum dots [9–11,44]. We pinpoint two fundamental differences between our strongly correlated scenario and a tunneling probe for an uncorrelated band insulator. First, the band structure of GFZs appears in the numerator of the cotunneling amplitude, contrary to an energy denominator for an uncorrelated insulator. Second, genuine correlation effects decisively modify the zero bands compared to the underlying free band structure of the Mott insulator. Using the striking example of topological distinction between zero bands and the corresponding pole bands, we demonstrate how these subtle fingerprints of many-body correlations can be directly observed through the cotunneling amplitude in mesoscopic quantum transport experiments.

Zero-band structure through perturbation theory—To describe how to probe a solid-state system spectroscopically, we use the formalism of Green’s functions. At the one-particle level, this allows us to quantify the response of the system upon adding or removing an electron, taking into account correlation effects. The single-particle electronic Green’s function in the Källén-Lehmann representation at zero temperature is explicitly dependent on the spectrum of excitations of the system [45,46]:

$$G_{j,\sigma;j',\sigma'}(\omega) = \langle GS | [c_{j,\sigma}(\omega + E_{GS} - H_H)^{-1} c_{j',\sigma'}^\dagger + c_{j',\sigma'}^\dagger(\omega - E_{GS} + H_H)^{-1} c_{j,\sigma}] | GS \rangle, \quad (1)$$

where $c_{j,\sigma}^{(\dagger)}$ denotes the annihilation and creation operators for site j and spin σ . In the noninteracting limit, the Hamiltonian and $G(\omega)$ are readily diagonalizable in a single-particle basis. The determination of the spectral and geometrical properties of the system then amounts to the study of the poles of $G(\omega)$, each of which represents an infinitely long-lived single-particle eigenmode. However, in the presence of correlations, a large number of amplitudes in the numerator become nonzero, reflecting the multitude of scattering events promoted by the many-body interaction term. As a result, the spectral weight distribution is broadened in the frequency-momentum plane. There is, however, a remarkable consequence of this scenario: In the spectral distribution, a set of isolated GFZs can emerge. Their presence has been linked to peculiar thermodynamic [47] and topological properties [25–34], and the study of their dispersion is, therefore, an intriguing, if nontrivial, endeavor.

The GFZs are defined as zero eigenvalues of G or, equivalently, as the points at which its determinant vanishes [25]. In the noninteracting limit, there are no isolated zeros. In the opposite case, where the system is deep in the Mott

phase, two incoherent Hubbard bands form at high frequency, which contain the totality of the poles of the Green’s function and a large number of zeros. However, inside the hard Mott gap between the two Hubbard bands, no poles are present. By contrast, GFZs can, and do, manifest at low energy, irrespective of the system size. The focus of this Letter lies on how to detect these isolated in-gap GFZs, which are entirely responsible for the low-energy properties of the GF of Mott insulators [19–34].

As a first step in our discussion, we derive a remarkably simple and intuitive expression for G at low energies ($\omega \ll U$) deep in the Mott regime at half filling and with a paramagnetic ground state. Our noninteracting Hamiltonian $H_0 = \sum h_{j,j'} c_{j,\sigma}^\dagger c_{j',\sigma}$ consists of a linear combination of on-site terms, which we denote by M , and nonlocal hopping terms (W). The interaction term is of the Hubbard type $UH_{\text{int}} = 2U \sum_j (n_{j,\downarrow} - \frac{1}{2})(n_{j,\uparrow} - \frac{1}{2})$, where j labels the lattice site and $\sigma = \uparrow, \downarrow$ is the spin. The two competing energy scales are the bandwidth of H_0 , $2D$, and the local Coulomb interaction strength U , where $U \gg D$ for a Mott insulator. For convenience, we introduce the rescaled noninteracting Hamiltonian term $H'_0 = (1/D)H_0$ as well as the small parameter $\phi = (D/U)$. The Hamiltonian can, therefore, be rewritten as

$$H_H = U(\phi H'_0 + H_{\text{int}}). \quad (2)$$

In this form, H_H naturally suggests a perturbative analysis in ϕ : Indeed, by applying degenerate perturbation theory [48] up to first order in ϕ , we determine its perturbed eigenenergies E_ν^p and eigenstates $|E_\nu^p\rangle$, which we can then conveniently insert in Eq. (1) to obtain the perturbed Mott Green’s function. It is finally a matter of collecting all the lowest terms in ϕ and expanding the denominator at low energies, to arrive at a key expression for the Green’s function, which is valid for $\phi \ll 1$ and $\omega \ll U$ [49]:

$$G_{j,\sigma;j',\sigma'}(\omega) \approx \frac{1}{U^2} [-\omega \mathbb{I} + H^z]_{j,\sigma;j',\sigma'} + \mathcal{O}(\phi^3). \quad (3)$$

This expression is intuitively consistent with the strongly suppressed in-gap spectral distribution of a Mott insulator. More than that, it immediately and clearly highlights the presence, inside of the Mott gap, of points where the determinant of the Green’s function is exactly zero. These are the roots of the expression $H^z - \omega \mathbb{I}$. In other words, and in line with [33], we find that the low-energy isolated zeros of a Mott insulator are described by an effective Hamiltonian H^z . The detailed derivation of Eq. (3) can be found in Supplemental Material [50], including a general discussion of SU(2)-breaking bare Hamiltonians and ground states.

Our approach is able to precisely characterize the effective Hamiltonian and leads to a second interesting result about the GFZs: In this limit, H^z has, modulo some

exactly quantifiable renormalization, the same form as the noninteracting term H_0 of the original Hamiltonian Eq. (2).

For strong Coulomb repulsion U and at half filling, the Hubbard model at low energies is well described by an effective spin-12 model [5–8]. We can, therefore, rewrite the lowest-order terms in G in the spin basis, thereby obtaining an expression linking the approximated Green's function to spin-spin correlators, as derived in detail in [50]. For the bare Hamiltonian $h_{jj'} = (M + W)_{jj'}$, we find a remarkably elegant expression for the effective Hamiltonian of the GFZ:

$$H_{jj'}^z = M_{jj'}\delta_{jj'} + 4\langle\vec{S}_j \cdot \vec{S}_{j'}\rangle_{j \neq j'} W_{jj'}, \quad (4)$$

where j and j' are lattice sites. Here, expectation values are evaluated with respect to the ground-state eigenvector $|GS^0\rangle$ of the corresponding effective spin-12 model [55] and are, hence, accessible for a large variety of Hubbard models. The effective zeros Hamiltonian can then be decomposed into two terms, in a striking analogy with the on-site and hopping terms of the bare Hamiltonian H_0 : (i) The on-site terms of the noninteracting Hamiltonian, described by M , are carried over in the dispersion of the zeros without renormalization, while (ii) the hopping terms, described by W , are rescaled by the spin correlation function $\langle\vec{S}_j \cdot \vec{S}_{j'}\rangle$ [56]. This follows naturally from the combination of our perturbative approach around the atomic limit and the nature of competing energy scales in the system: Any quadratic on-site term commutes with H in the atomic limit, and the perturbed energy is just shifted by M without renormalization. On the contrary, hopping and interaction strength are in direct competition: Treating the first order perturbatively results in a lowest-order correction to the atomic limit Hamiltonian, which famously depends on the spin-spin correlation function, as in the derivation of the superexchange [8,57–59]. These antiferromagnetic correlations characterize paramagnetic Mott insulators beyond mean field and are responsible for the sign flip in the nearest-neighbor hopping in Eq. (4).

Probing the zeros—As clearly evidenced by Eqs. (3) and (4), the knowledge of the zeros dispersion is sufficient to determine the spectral properties of the Mott system at low frequency. Obtaining a clear hint of the zeros behavior from experimental observations is instead less straightforward, since any spectral measurement (e.g., via photoemission) would just confirm the presence of a gap, without being able to resolve the elusive zeros within. We propose a novel approach to the problem, which is, at the same time, surprisingly simple to implement: Instead of directly performing spectroscopic measurements on the Mott insulator, we employ it as the potential barrier in a cotunneling experiment and study the effective coupling between the leads. We illustrate the setup via a minimal example, which is a convenient adaption of already existing quantum dot experimental setups [9–11,38]. This is sketched in Fig. 1(a)

and described by $H_{\text{tot}} = H_H + \gamma C + H_D$. The system consists of two quantum dots, henceforth L and R , and a central tunneling medium. The Hamiltonian of the quantum dots, H_D , is that of a Hubbard atom with Coulomb repulsion $2U$. In order to reveal fingerprints of the GFZ, the central element is a spin-isotropic Hubbard model in the Mott phase, described by the previously discussed Eq. (2). The chemical potential of the quantum dots is increased by U in relation to the central Hubbard model and independently adjustable by μ_L, μ_R . The system-dot coupling C is given by arbitrary hopping amplitudes $\{l_i\}$ and $\{r_i\}$ between the i th site of the central Mott insulator and the L and R quantum dots. For simplicity, we will, from now on, omit the spin index σ and restrict ourselves to the case where $l_i = \delta_{i,j}$ and $r_i = \delta_{i,j'}$ for two different sites $j \neq j'$. The full derivation for the general case with arbitrary hopping array is provided in [50].

In a cotunneling experiment, only the leads are directly probed. This amounts to tracing out the degrees of freedom associated to the central system and considering only the overall propagation amplitude of excitation leaving (entering) the two leads via the quantum dots. These processes are, in our proposed setting, exactly described by the one-particle Green's function of the central tunneling medium. In short, by applying a Schrieffer-Wolff transformation [60–62] in the limit of weak system-dot coupling γ with small dot potentials $\mu_{L/R}$ [63] and assuming a large lead-dot interaction $\sim U$, we derive an effective spin-isotropic Hamiltonian $\bar{h}$ in the low-energy subspace. It describes the dynamics of a single particle cotunneling between the left and right quantum dots through the central medium:

$$\bar{h} = \begin{pmatrix} \mu_L + u_L(\mu_L, \mu_R) & t_{\text{co}}^*(\bar{\mu}) \\ t_{\text{co}}(\bar{\mu}) & \mu_R + u_R(\mu_L, \mu_R) \end{pmatrix}, \quad (5)$$

where $\bar{\mu}$ is an “average” chemical potential $\frac{1}{2}(\mu_L + \mu_R)$. The presence of the central tunneling medium gives rise to a renormalization to the on-site energies, given by $u_{L/R} \sim \mathcal{O}(\gamma^2)$, which can be conveniently reabsorbed by tuning the quantum dot chemical potentials. The most relevant quantity in Eq. (5) is the cotunneling amplitude

$$t_{\text{co}}(\bar{\mu}, l_j, r_{j'}) = \gamma^2 G_{j,j'}(\bar{\mu}), \quad (6)$$

which describes the coupling between the left and right quantum dot mediated via the central barrier (see Fig. 1 for an illustration). Since we are interested in a Mott insulator at half filling as the tunneling barrier, we can make use of the previously derived approximation for the Green's function in Eq. (3). We immediately notice how, through Eq. (3), the cotunneling amplitude t_{co} is directly related to the GFZ-Hamiltonian H^z of Eq. (4). Explicitly, for l_j and $r_{j'}$ (cf. Fig. 1) chosen such that $j \neq j'$ (see Ref. [50] for general tunnel couplings l, r):

$$t_{\text{co}} = \frac{\gamma^2}{U^2} (H^z)_{j,j'}. \quad (7)$$

As a central result, Eq. (7) clarifies the correspondence between the Mott Green's function and the cotunneling amplitude: Instead of directly probing the features of the vanishing spectral function inside the Mott gap, a nearly impossible task, we are now recasting the same information into what is effectively a potential barrier for the evanescent wave of the cotunneling experiment. Its features, and, in particular, the spectroscopically undetectable zeros, have a macroscopic effect on the measured occupations of the leads. As a further benefit, we can now take advantage of the well-established theoretical tools and experimental techniques employed in the study of quantum tunneling, such as charge stability diagrams [11,64–67] and time-resolved charge detection of single tunneling events [38,68–73].

Numerical results—We now provide numerical evidence of our key findings by considering the paradigmatic case of the one-dimensional Su-Schrieffer-Heeger (SSH)-Hubbard model [33,74], consisting of a bipartite chain with alternating hoppings v and w , studied with both open boundary conditions (OBC) and periodic boundary conditions (PBC). We numerically solve the Hamiltonian of the cotunneling setup by using density matrix renormalization group (DMRG) [75,76] in combination with the time-dependent variational principle [77–79] and exact diagonalization (ED) methods. We first compute the real-time GF and then transform it into the frequency domain, thereby gaining access to the GFZs.

We first prove that our analytical formula for the zeros Hamiltonian is an adequate approximation of the in-gap spectral features of a Mott insulator. Figure 1(b) shows a comparison between the determinant of the Green's function of the SSH-Hubbard model, obtained via DMRG, and the approximated formula for the GFZ Hamiltonian in Eq. (4). We note that the isolated zeros (dark purple regions of the color plot), which appear in the Mott gap, are in perfect agreement with the eigenvalues of H^z , already at the intermediate value of $\phi \approx 1/10$. In Supplemental Material [50], we provide a more detailed quantitative analysis.

We then turn our attention to the cotunneling setup, numerically simulated by supplementing the quantum dots and coupling terms, H_D and C , to the SSH-Hubbard Hamiltonian.

In Fig. 2, we show the emergent cotunneling amplitude t_{co} for the experimental setup in Fig. 1(a) between two interacting auxiliary quantum dots, as a function of the bandwidth D . We compare its behavior in the case of a Mott insulator and a conventional noninteracting insulator and plot the two resulting curves (red and gray) as a function of D . The numerically obtained curves are to be compared with the two dashed lines, which show the two different behaviors in the noninteracting and Mott limits, and can be extracted from Eq. (6). In the noninteracting limit, the behavior of the Green's function G , as defined in Eq. (1), is

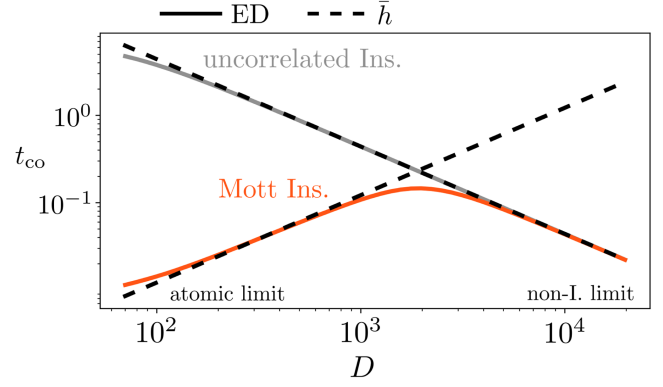


FIG. 2. Cotunneling amplitude t_{co} as function of bandwidth D (fixed $U = 2000$, $N = 16$, $\gamma = 20$, $l_i = \delta_{i,2}$, $r_i = \delta_{i,3}$, $v = 0.9w$, PBC). SSH-Hubbard model (solid, red line) shows linear D dependence within the Mott regime ($D/U < 1$), due to the energy nominator in GF Eq. (3). Noninteracting insulator (solid, gray line) with energy denominator (parameters as above but $U = 0$). Analytical results, Eq. (6) (dashed line).

determined by a single energy scale, the noninteracting bandwidth appearing at the denominator [45,46]. Hence, $t_{\text{co}} \sim D^{-1}$, and the two solid lines are on top of each other and agree with the noninteracting behavior (negative slope in the logarithmic plot). At around $(D/U) \approx 1$, i.e., near the Mott transition, the behavior of the interacting system changes: Now, the dominant energy scale of the system is the Coulomb interaction U , and approximation Eq. (3) holds. H^z , though renormalized as in Eq. (4), has an $\sim D$ dependence on the bandwidth, and the Mott cotunneling amplitude indeed agrees with the positive-slope dashed line. The general agreement between the approximated value of t_{co} and the numerically determined ones is remarkable, confirming the robustness of Eq. (6). Only at small bandwidth D , where $\gamma \approx D$, does our cotunneling approximation break down and higher-order tunneling processes become relevant.

Our cotunneling approach to detecting Green's function zeros can be nicely illustrated with the well-established tool of charge-stability diagrams [11,64–67,80], which are commonly used to describe the behavior of quantum dots as a function of control voltages. In Fig. 3(a), we show the charge-stability diagram of our cotunneling setup, by plotting the derivative of the charge occupation $N_{L/R}$ with respect to the detuning $\delta\mu = \mu_L - \mu_R$, at varying chemical potentials μ_L and μ_R . Because of the finite tunneling amplitude t_{co} , the boundaries of the characteristic checkerboard structure of the uncoupled system ($\gamma = 0$) are smeared out, and the localization of a single particle can be tuned smoothly from the left dot (1,0) to the right dot (0,1). Figure 3(b) shows a diagonal cut through Fig. 3(a) at a fixed average potential $\bar{\mu} = \frac{1}{2}(\mu_L + \mu_R)$ (red line). At zero temperature, the FWHM of the Lorentzian dispersion is directly proportional to the cotunneling amplitude. An alternative way of probing the cotunneling amplitude is

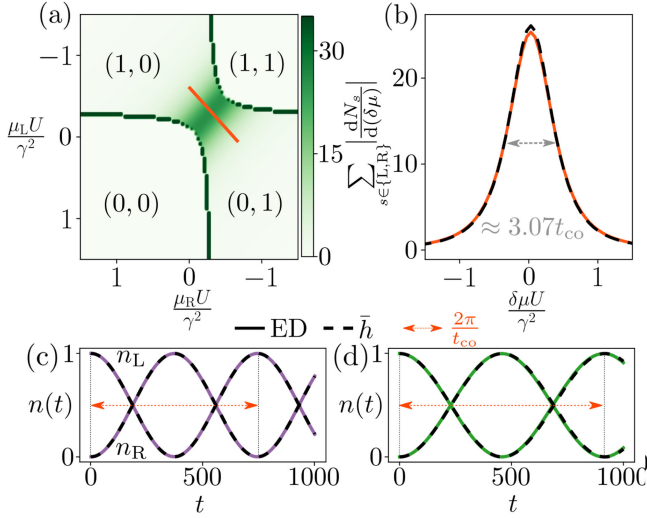


FIG. 3. Charge stability diagram (ED, $U = 200$, $N = 20$, $\gamma = 4$, $l_i = \delta_{i,2}$, $r_i = \delta_{i,3}$, $v = 18$, $w = 20$, PBC): (a) derivative of the particle number N_L (N_R) on left (right) dot for varying potentials μ_L and μ_R . In (b), cut through (a) (red line), FWHM is proportional to cotunneling t_{co} . (c),(d) Charge oscillations between aux dots (initial localization left dot), the same parameter as (a), but OBC, $l_i = \delta_{i,1}$, $r_i = \delta_{i,2}$ in (c) and $l_i = \delta_{i,3}$, $r_i = \delta_{i,4}$ in (d). Analytical results (dashed line) from Eq. (6).

to measure the frequency of Rabi-charge oscillations between the dots [38,70,72,73]. It can be extracted by the time evolution of a localized state and compared with the theoretical value $\Omega \approx \sqrt{|t_{co}|^2 + \omega_D^2}$, where $\omega_D \approx \frac{1}{2}\delta\mu + \mathcal{O}(\gamma^2/U)$ is a shifted detuning between the two quantum dots, which is easily controllable via μ_L and μ_R . In Figs. 3(c) and 3(d), we plot the numerically calculated time-dependent charge occupation values of the two quantum dots on resonance $\omega_D = 0$ [at peak maximum in Fig. 3(b)], when the system is initialized in the completely localized (1,0) state. The data are in perfect agreement with the predicted oscillation frequency, which can be easily extracted by Eq. (5).

The proposed probing scheme applies to generic Mott insulators, and so far our discussion has been generally applicable. As a particularly promising experimental realization, we now elaborate on a specific Hubbard system synthetically realizing a Mott insulator with coupled quantum dots. In a real experiment on quantum dot arrays, the perturbative limit $(\gamma/D) \ll (D/U) \ll 1$ may not be perfectly accessible and is further inherently tied to a small cotunneling amplitude, making it experimentally challenging. Despite this limitation, macroscopic values of t_{co} ($\geq 0.5 \mu\text{eV}$) can still be achieved for a broad range of typical parameters U , D , and γ , within an acceptable quantitative deviation ($\leq 10\%$; see Ref. [50] for details). Interestingly, we also find that the striking rescaling in Eq. (4) by spin-spin correlations can be probed qualitatively, without requiring fine-tuning of the dots. More

specifically, we find a notable amplification of the tunneling amplitude as a function of varying boundary conditions, a characteristic signature of this renormalization (see Ref. [50] for further details).

Conclusion—Starting from a degenerate perturbation theory around the atomic limit, we have derived a simple yet highly accurate approximation for the low-frequency features of a Mott Green’s function, which can be completely described by a dispersion relation for the Green’s function zeros. This situation is reminiscent of a noninteracting system, with the important distinction that the effective dispersion of zeros appears in the numerator of the Green’s functions and is renormalized compared to the underlying free band structure by means of spin-spin correlators, as we have quantified. Our main result is the establishment of a direct link between the dispersion of zeros and the transmission amplitude naturally probed in a cotunneling experiment, which drastically simplifies the task of observing and characterizing Green’s function zeros. Moreover, our approach allows, in principle, a reconstruction of the spectroscopically inaccessible GF determinant from its individual matrix elements. We have provided extensive numerical proof of the correctness and resilience of our approximation and suggested a feasible experimental setup for the verification of our key findings. Numerical simulations suggest that the fingerprints of the zeros dispersion and renormalization are observable already for small systems: Specifically, an ensemble of six quantum dots (two leads and four in the central Hubbard tunneling medium) is already sufficient to quantify an interesting correlation-induced renormalization of band parameters.

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Data availability—The data supporting this study’s findings are available within the Letter.

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