Quantum Criticality Perspective on the Charging of Narrow Quantum-Dot Levels

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Understanding the charging of exceptionally narrow levels in quantum dots in the presence of interactions remains a challenge within mesoscopic physics. We address this fundamental question in the generic model of a narrow level capacitively coupled to a broad one. Using bosonization we show that for arbitrary capacitive coupling charging can be described by an analogy to the magnetization in the anisotropic Kondo model, featuring a low-energy crossover scale that depends in a power-law fashion on the tunneling amplitude to the level. Explicit analytical expressions for the exponent are derived and confirmed by detailed numerical and functional renormalization-group calculations.

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Introduction.—Confined nanostructures offer a unique arena for thoroughly interrogating the interplay between interference and interactions while holding the promise of future applications. Particularly appealing are semiconductor quantum dots (QDs), for which the manipulation of spin [1,2] and charge [3] has recently been demonstrated. The precise and rapid control of switchable gate voltages renders these devices attractive candidates for a solid-state qubit [4,5]. The accurate manipulation of QD setups requires, however, detailed understanding of how charging proceeds. Indeed, interactions can substantially modify the orthodox picture of charging, whether by renormalizing the tunneling rates or by introducing nonmonotonicities into the population of individual levels [6–8]. Even the simplest two-level device, where each level harbors only a single spinless electron, displays remarkably rich behavior [9].

We consider a situation in which the width of one narrow level is much smaller than the width of the other broad one. A disparity in widths is generic for QDs in the intermediate regime between integrable and chaotic [6]. It was reported in several artificial structures [10,11], and has been exploited for charge sensing [12,13]. As the energy ϵ_- of the narrow level is raised, its occupation varies from 1 to 0 over a characteristic width Ω. This energy scale, or the corresponding charge-fluctuation time scale $\hbar/\Omega$, manifests itself in charge sensing and transmission-phase measurements [14]. The effect of interlevel repulsion U on Ω has been explored only in the large-U limit, revealing novel correlation effects [15–18]. The physical mechanism determining Ω for moderate U remains unclear [9].

In this Letter we solve the fundamental question of the charging of a narrow QD level from a quantum-critical perspective. Because of the capacitative coupling U, every switching of the narrow level initiates restructuring of the broad level and its attached Fermi sea, in direct analogy with the x-ray edge singularity. For nonzero tunneling to the narrow level, coherent superpositions of these charge rearrangements lead to Kondo physics [19] with the charge state (0 or 1) acting as a pseudospin, and the energy of the narrow level acting as a Zeeman field. Using Abelian bosonization we show that Ω, being the Kondo scale in the pseudospin language, depends on the tunneling amplitudes in a power-law fashion. We derive explicit analytical expressions for the exponents encompassing all physical regimes of the model (at zero temperature T). In a second step we confirm our predictions by detailed numerical (NRG) [20] and functional (FRG) [21] renormalization-group (RG) calculations, thus resolving this challenging aspect of mesoscopic physics.

Model and objective.—Our specific model for charging is depicted schematically in the inset of Fig. 1, and is defined by the Hamiltonian (σ is the pseudospin index)

$$\mathcal{H} = \sum_{\sigma=\pm}\Big[\sum_k \epsilon_k c^\dagger_{k\sigma}c_{k\sigma} + V_\sigma\sum_k (c^\dagger_{k\sigma}d_\sigma + d^\dagger_\sigma c_{k\sigma}) + \epsilon_\sigma d^\dagger_\sigma d_\sigma\Big] + b/2(d^\dagger_+ d_- + d^\dagger_- d_+) + U\Delta\hat{n}_+\Delta\hat{n}_-. \quad (1)$$

Here, $d^\dagger_\pm$ ($c^\dagger_{k\pm}$) creates an electron on the dot (in the leads), and $\Delta\hat{n}_\pm$ equals $d^\dagger_\pm d_\pm - 1/2$. Equation (1) is a generalized Anderson impurity model with pseudo-spin-dependent tunneling amplitudes $V_+ \geq V_- \geq 0$ and a tilted magnetic field, whose components are $\epsilon_+ - \epsilon_-$ and the direct hopping amplitude b. This form follows from a generic model of spinless electrons with two dot levels and two leads by simultaneous unitary transformations in the dot and the lead space [16–18]. The Hamiltonian (1) has recently gained considerable attention in connection with phase lapses, population inversion, and many-body resonances

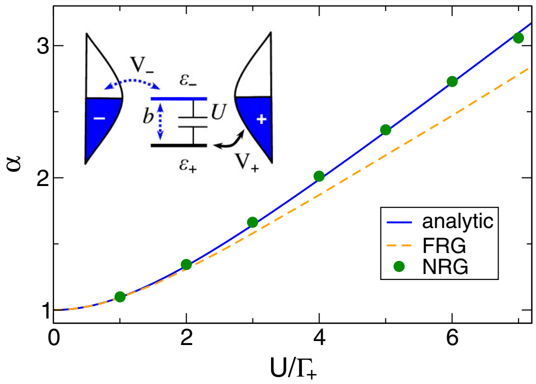

FIG. 1 (color online). The exponent α computed using the NRG, FRG, and Eqs. (8). NRG parameters: $\Gamma_+/D = 0.04$, $\Lambda = 1.7$, and 2800 states are retained. Inset: The model system. Two localized QD levels are coupled by tunneling to separate baths. Spinless electrons residing on the two levels experience a Coulomb repulsion U.

[9]. The energies $\epsilon_\pm$ are tuned using gate voltages. Depending on the specific realization, their tuning may inflict a similar change in b. We focus on realizations where $\epsilon_\pm$ can be tuned independently of b.

The bare energy scales that characterize tunneling in Eq. (1) are the level broadenings $\Gamma_\pm = \pi\rho V_\pm^2$ and the direct hopping amplitude b. The density of states (DOS) ρ is taken to be equal for both bands without loss of generality. Our interest is in the charging properties of the narrow level $d_-^\dagger$ as a function of ϵ_- in the limit where b and V_- are both small: $\Gamma_-, b \ll \Gamma_+$. Strictly at $b = V_- = 0$ ergodicity of the microcanonical ensemble is broken as a new conserved quantity arises: $\hat{n}_- \equiv d_-^\dagger d_-$ is either equal to 0 or 1. Comparing the total energies of the competing ground states with $\langle \hat{n}_- \rangle = 0$ and $\langle \hat{n}_- \rangle = 1$ as a function of ϵ_- one finds a critical value $\epsilon_- = \epsilon^*(\epsilon_+, U, V_+)$ at which the two become degenerate. For $\epsilon_+ = 0$, ϵ^* is pinned to zero by particle-hole symmetry if symmetric bands are assumed. In the limit $b, V_- \to 0$ the average occupation $\langle \hat{n}_- \rangle$ thus indicates a first-order transition (width $\Omega = 0$) as ϵ_- is swept across ϵ^*. It is the smoothening ($\Omega > 0$) of this transition at small but finite b, V_- for $U \geq 0$ that is addressed in this Letter.

Two regimes can be distinguished depending on ϵ_+. When $|\epsilon_+| \gg U, \Gamma_+$, the level $d_+^\dagger$ maintains an approximately fixed integer valence $\langle n_+ \rangle \in \{0, 1\}$, independent of ϵ_-. Hence, the charging of $d_-^\dagger$ is essentially single particle in nature with $\Omega = \Gamma_- + \Gamma_+ b^2/\epsilon_+^2$. The effect of interactions is contained in the simple Hartree renormalization, $\epsilon_- \to \epsilon_- + U(\langle n_+ \rangle - 1/2)$. Far more complex is the case of $|\epsilon_+| \ll \max\{U, \Gamma_+\}$, when the broad level is prone to strong valence fluctuations (for $\epsilon_- \to \epsilon^*$). Going from $U/\Gamma_+ \ll 1$ to $1 \ll U/\Gamma_+$ spans all physical regimes from weak to strong electronic correlations [16–18], which constitutes the main focus of our study. To this end we initially set $\epsilon_+ = 0$, which fixes $\epsilon^* = 0$. Using analytical and numerical tools we first obtain Ω in the case where either V_- or b is nonzero. The combined effect of V_- and b is next addressed by single-parameter scaling and FRG. Finally, we extend our analytical results to arbitrary ϵ_+.

Analytical approach.—To analytically determine the width Ω using minor approximations, we proceed in two steps. First, we derive a continuum-limit Hamiltonian where Γ_+ is incorporated in full. Second, an exact mapping of this Hamiltonian onto the anisotropic Kondo model is established. This allows usage of known results for the Kondo problem in order to extract Ω.

In the first step, we diagonalize the Hamiltonian $\mathcal{H}_+ = \sum_k \epsilon_k c_{k+}^\dagger c_{k+} + V_+ \sum_k \{c_{k+}^\dagger d_+ + d_+^\dagger c_{k+}\}$ using scattering theory. Expanding $d_+^\dagger$ in terms of the single-particle eigenmodes of $\mathcal{H}_+$ and converting to continuous constant-energy-shell operators [22], $\mathcal{H}$ takes the form of a generalized interacting resonant-level model with a single $d_-^\dagger$ level tunnel coupled to two bands: a narrow $\sigma = +$ band with a Lorentzian DOS of half-width Γ_+, and a flat $\sigma = -$ band with half-width $D \gg \Gamma_+$. In addition, the $d_-^\dagger$ level is capacitively coupled to the "+" band.

In the desired limit $b, \Gamma_- \ll \Gamma_+$, one can conveniently replace the Lorentzian DOS with a flat symmetric one of height $1/\pi\Gamma_+$ and half-width $D_+ = \pi\Gamma_+/2$ [22]. The elimination of all degrees of freedom in the energy interval $D_+ < |\epsilon| < D$ leads to renormalizations of the couplings of the order of $\Gamma_-/\Gamma_+ \ll 1$ or higher, which can be safely neglected. Converting at this point to left-moving fields, we obtain the continuum-limit Hamiltonian

$$\begin{aligned}\mathcal{H} = {}& i\hbar v_F \sum_{\sigma=\pm} \int_{-\infty}^{\infty} \psi_\sigma^\dagger(x) \partial_x \psi_\sigma(x) dx + \epsilon_- d_-^\dagger d_- \\ & + (b/2)\sqrt{a}\{\psi_+^\dagger(0) d_- + \text{H.c.}\} \\ & + Ua : \psi_+^\dagger(0)\psi_+(0) : \Delta\hat{n}_- \\ & + \sqrt{a\Gamma_+\Gamma_-}\{\psi_-^\dagger(0) d_- + \text{H.c.}\}, \end{aligned} \tag{2}$$

applicable at energies below Γ_+. Here, $a = \pi\hbar v_F/D_+$ is a new short-distance cutoff ("lattice spacing"), and $:\psi_+^\dagger \psi_+:$ stands for normal ordering with respect to the filled Fermi sea. The left-moving fields obey canonical anticommutation relations subject to the regularization $\delta(0) = 1/a$. The derivation of Eq. (2) is controlled by the small parameters $\Gamma_-/\Gamma_+ \ll 1$ and $b/\Gamma_+ \ll 1$, and hence is expected to become asymptotically exact as $\Gamma_-, b \to 0$.

If either $b = 0$ or $\Gamma_- = 0$, Eq. (2) can be treated using Abelian bosonization [23]. To this end, we introduce two bosonic fields $\Phi_\pm(x)$, one for each fermion field $\psi_\pm(x)$. With a proper choice of the phase-factor operators, the bosonized Hamiltonian reads

$$\begin{aligned} H = {}& \sum_{\sigma=\pm} \frac{\hbar v_F}{4\pi} \int_{-\infty}^{\infty} [\nabla\Phi_\sigma(x)]^2 dx + \epsilon_- d_-^\dagger d_- \\ & + \hbar v_F \frac{2\delta_U}{\pi} \nabla\Phi_+(0)\Delta\hat{n}_- + \frac{A}{\sqrt{2}}\{e^{i\Phi_\pm(0)} d_- + \text{H.c.}\}. \end{aligned} \tag{3}$$

The tunneling term in Eq. (3), proportional to A, depends on the case of interest; one takes $A = b/2$ and the upper sign ($A = \sqrt{\Gamma_+\Gamma_-}$, lower sign) for $\Gamma_- = 0$ ($b = 0$). The value of $\delta_U = \arctan(U/2\Gamma_+)$ is fixed by matching the $b = \Gamma_- = 0$ scattering phase shifts of the "+" band in the fermionic and the bosonic representations, for each sector with fixed integer occupancy of the "−" level.

Next, we manipulate Eq. (3) by (i) applying the canonical transformation $\mathcal{H}' = \hat{U}^\dagger \mathcal{H} \hat{U}$ with

$$\hat{U} = \exp[-i(2\delta_U/\pi)\Phi_+(0)\Delta\hat{n}_-], \qquad (4)$$

and (ii) converting to the "spin" and "charge" fields $\Phi_s(x)$ and $\Phi_c(x)$. The latter are defined as $\Phi_s(x) = \Phi_+(x)$ and $\Phi_c(x) = \Phi_-(x)$ for $\Gamma_- = 0$, and

$$\Phi_{s,c}(x) = [1 + (2\delta_U/\pi)^2]^{-1/2}\left[\Phi_\mp(x) \mp \frac{2\delta_U}{\pi}\Phi_\pm(x)\right] \qquad (5)$$

for $b = 0$ (the upper signs correspond to Φ_s). In this manner, the Hamiltonian acquires the unified form

$$\mathcal{H}' = \sum_{\mu=s,c} \frac{\hbar v_F}{4\pi} \int_{-\infty}^{\infty} [\nabla\Phi_\mu(x)]^2 dx + \epsilon_- d_-^\dagger d_- + 2^{-1/2} A\{e^{i\gamma\Phi_s(0)} d_- + d_-^\dagger e^{-i\gamma\Phi_s(0)}\}, \qquad (6)$$

where $\gamma = \sqrt{1 + (2\delta_U/\pi)^2}$ for $b = 0$ and $\gamma = 1 - 2\delta_U/\pi$ for $\Gamma_- = 0$.

The very same Hamiltonian with $0 < \gamma < \sqrt{2}$ also describes the anisotropic Kondo model with $0 < J_z$, where in standard notation $A = J_\perp/\sqrt{8}$ and $\gamma = \sqrt{2}[1 - (2/\pi) \times \arctan(\pi\rho J_z/4)]$ represent the transverse and longitudinal spin-exchange couplings, respectively, and $\epsilon_- = \mu_B g H$ corresponds to a local magnetic field. This representation of the Kondo model is obtained by [24] (i) bosonizing the Kondo Hamiltonian with two bosonic fields $\Phi_\uparrow(x)$ and $\Phi_\downarrow(x)$, (ii) converting to the spin and charge fields $\Phi_{s,c}(x) = [\Phi_\uparrow(x) \mp \Phi_\downarrow(x)]/\sqrt{2}$, (iii) employing $\mathcal{H}' = \hat{T}^\dagger \mathcal{H} \hat{T}$ with $\hat{T} = \exp[-i\sqrt{2}(2\delta_z/\pi)\Phi_s(0)\tau_z]$, τ_z being the z spin component and $\delta_z = \arctan(\pi\rho J_z/4)$, and (iv) representing the spin $\vec{\tau}$ in terms of the fermion $d_- = \tau^-$. This establishes a mapping between our problem with either $b = 0$ or $\Gamma_- = 0$ and the anisotropic Kondo model. In particular, charging of the $d_-^\dagger$ level is mapped onto the magnetization of the Kondo impurity, relating the width Ω to the Kondo temperature T_K.

We can now exploit known results for the Kondo problem. Specifically, RG equations perturbative in $J_\perp$ but nonperturbative in J_z [19] give $T_K \sim D_+(A/D_+)^{2/(2-\gamma^2)}$, which yields for our problem

$$\frac{\Omega}{\Gamma_+} \sim \begin{cases} (\Gamma_-/\Gamma_+)^\alpha & \text{if } b = 0, \\ (b/\Gamma_+)^{2\beta} & \text{if } \Gamma_- = 0, \end{cases} \qquad (7)$$

$$\alpha = \frac{1}{1 - (2\delta_U/\pi)^2}, \qquad \beta = \frac{1}{2 - [1 - (2\delta_U/\pi)]^2}. \qquad (8)$$

Thus, Ω is a power law of the relevant tunneling amplitude with an exponent that varies smoothly with U. In going from $U = 0$ to $U \gg \Gamma_+$, α grows monotonically from 1 to $\pi U/(8\Gamma_+)$ while β decreases from 1 to 1/2. The asymptote $\alpha = \pi U/(8\Gamma_+)$ coincides with the result of Ref. [17] [Eq. (29) with $\epsilon_0 = -U/2$], obtained using very different techniques. For $U = 0$, the noninteracting integer exponents are reproduced. Hence Eqs. (8) are precise both at small and large U. As shown next, these expressions remain highly accurate also at intermediate U, suggesting that they might actually be exact.

Numerical analysis.—To test Eqs. (8), we computed α and β numerically using the NRG [20] and FRG [21], each approach having its own distinct advantage. The NRG is extremely accurate in all parameter regimes of interest, while the FRG is approximative in U but offers a far more flexible framework for scanning parameters. The width $\Omega = 1/(\pi\chi_c)$ was obtained with either method from the inverse charge susceptibility $\chi_c = d\langle\hat{n}_-\rangle/d\epsilon_-$, evaluated at $\epsilon_- = 0$ and $T \to 0$. The exponents α and β were extracted from log-log fits (see the inset of Fig. 2). Our results, summarized in Figs. 1 and 2, reveal excellent agreement between Eqs. (8) and the NRG, to within numerical precision. The agreement extends to all interaction strengths from small to large U, confirming the accuracy of Eqs. (8) at all U. The FRG results for α coincide with those of the NRG up to $U/\Gamma_+ \approx 2$, above which they acquire a linear slope that is reduced by a factor of $8/\pi^2$ as compared to the NRG [17]. The exponent β is accurately reproduced up to larger values of U/Γ_+. In particular, the FRG data for α and β exactly reproduce the leading behaviors of Eqs. (8) at small U.

Combination of Γ_- and b.—The case where both Γ_- and b are nonzero lies beyond the scope of our bosonization treatment, but allows the formulation of a scaling law. To this end, consider the dimensionless quantity $\tilde{\Omega} = \Omega/D_+$, which depends on the three dimensionless parameters in Eq. (2): $\tilde{\Omega} = f(\tilde{V}, \tilde{b}, \delta_U)$, with $\tilde{V} = \sqrt{\Gamma_+\Gamma_-}/D_+$ and $\tilde{b} = b/D_+$. Given the exact RG trajectories, $\tilde{\Omega}$ evolves according to $\tilde{\Omega}' = \tilde{\Omega}/\xi = f(\tilde{V}', \tilde{b}', \delta_U', \{\lambda_i'\})$ upon reducing the bandwidth from D_+ to ξD_+ ($0 < \xi < 1$). Here, primes denote renormalized parameters and $\{\lambda_i'\}$ are the new couplings generated. At sufficiently weak tunneling the RG

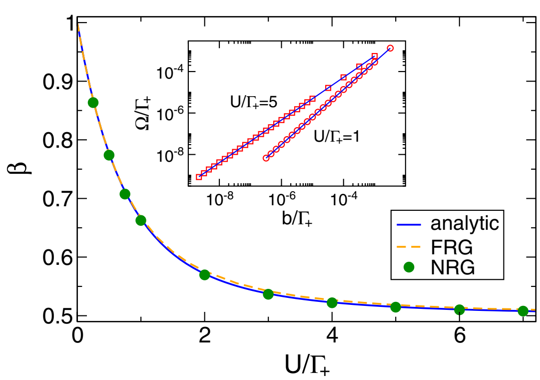

FIG. 2 (color online). The exponent β computed using the NRG, FRG, and Eqs. (8). NRG parameters: $\Gamma_+/D = 0.02$, $\Lambda = 1.6$, and 2000 states retained. Inset: Representative NRG data for Ω vs b, along with the log-log fits used to extract β.

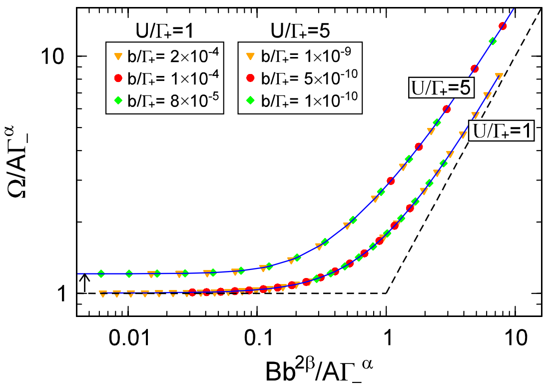

FIG. 3 (color online). A scaling plot of Ω for two (fixed) ratios U/Γ_+ and different combinations of Γ_- and b, obtained using the FRG. The coefficients A and B were extracted from the limiting cases where $b = 0$ and $\Gamma_- = 0$, respectively [25]. For clarity, the data for $U/\Gamma_+ = 5$ were multiplied by a constant as indicated by the arrow length. Dashed lines show the asymptotes $\mathcal{F} = 1$ and $\mathcal{F} = x$.

equations can be linearized with respect to the relevant couplings $\tilde{V}'$ and $\tilde{b}'$, resulting in their power-law growth with the exponents determined previously: $\tilde{V}' = \tilde{V}\xi^{-1/2\alpha}$ and $\tilde{b}' = \tilde{b}\xi^{-1/2\beta}$. Note that δ_U is left unchanged in this approximation, nor are there any new couplings generated. Consequently, $f(\tilde{V}, \tilde{b}, \delta_U) = \xi f(\tilde{V}\xi^{-1/2\alpha}, \tilde{b}\xi^{-1/2\beta}, \delta_U) = \tilde{\Omega}$ is a homogeneous function of ξ, taking the general form $f(\tilde{V}, \tilde{b}, \delta_U) = \tilde{V}^{2\alpha}\mathcal{G}(\tilde{b}^{2\beta}/\tilde{V}^{2\alpha}, \delta_U)$. Finally, defining the coefficients A and B from $\Omega|_{b=0} = A\Gamma_-^\alpha$ and $\Omega|_{\Gamma_-=0} = Bb^{2\beta}$, we arrive at the scaling form [25]

$$\Omega = A\Gamma_-^\alpha \mathcal{F}(Bb^{2\beta}/A\Gamma_-^\alpha; \delta_U), \tag{9}$$

with $\mathcal{F}(0; \delta_U) = 1$ and $\mathcal{F}(x \gg 1; \delta_U) = x$. In Fig. 3 we confirm the scaling form of Eq. (9) using FRG data.

Extension to arbitrary ϵ_+.—Our discussion has focused thus far on $\epsilon_+ = 0$. A nonzero ϵ_+ introduces the potential-scattering term $\mathcal{H}_{\rm ps} = \epsilon_+ a{:}\psi_+^\dagger(0)\psi_+(0){:}$ into Eq. (2). Consequently, δ_U in Eq. (3) is replaced with two distinct parameters $\delta_\pm = \arctan[(U \pm 2\epsilon_+)/2\Gamma_+]$, assigned to $\Delta\hat{n}_- = \pm 1/2$, respectively. An identical derivation, only with $2\delta_U\tilde{n}_- \to (\delta_+ + \delta_-)\Delta\hat{n}_- + (\delta_+ - \delta_-)/2$ in Eq. (4), leads then to the same Hamiltonian (6) with two modifications: (i) ϵ_-, and thus ϵ^*, acquires a shift proportional to $\delta_+^2 - \delta_-^2$, and (ii) δ_U is replaced with $(\delta_+ + \delta_-)/2$ in the expressions for γ. The end results for α and β are just Eqs. (8) with $\delta_U \to (\delta_+ + \delta_-)/2$, which properly reduce to the noninteracting limit $\alpha = \beta = 1$ when $|\epsilon_+| \gg U, \Gamma_+$. The effect of nonzero ϵ_+ is negligible for $|\epsilon_+| \ll \max\{U, \Gamma_+\}$. It becomes significant only as $|\epsilon_+|$ approaches $\max\{U, \Gamma_+\}$.

Summary.—We have resolved the fundamental question of the charging of a narrow QD level capacitively coupled to a broad one. The zero-tunneling fixed point is critical in the sense of being unstable. Finite tunneling is a relevant perturbation, driving the system to a strong-coupling Fermi-liquid fixed point. The inverse charge-fluctuation time Ω varies as a power of the bare tunneling amplitude, with a nonuniversal exponent that depends on the nature of tunneling, the strength of the capacitive coupling, and the width and position of the broad level. We have proven this scenario by devising a two-stage mapping of the original model onto the anisotropic Kondo problem, yielding accurate analytic expressions for the exponents. Our analytic predictions were confirmed by extensive numerical calculations within the frameworks of the NRG and FRG.

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