Quantum critical entanglement in an Anderson model with a pseudogap

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Abstract

Quantum phase transitions are highly relevant to current research efforts in both superconductivity and quantum information. Numerical renormalization group (NRG) studies of quantum impurity models near a quantum critical point have given us a theoretical understanding of many low-temperature systems, successfully explaining the experimental properties of certain superconducting materials and quantum-dot systems. We study entanglement near the quantum critical point in an Anderson model with a pseudogap using the NRG, and successfully relate the entanglement entropy to established properties of the model.

I. INTRODUCTION AND BACKGROUND

Strongly-correlated electron systems have been the object of great interest over the past several decades for both their unusual properties and unique physics.[1] The strong interaction between electrons in these systems is responsible for a range of important phenomena, such as high-temperature superconductivity in cuprates, colossal magnetoresistance in manganites, and the Kondo effect.

This study concerns the Anderson model, one of the canonical quantum impurity models. These models were developed in an effort to understand the Kondo effect, in which coupling between a magnetic impurity and a metallic conduction band causes an anomalous increase in resistance at low temperatures. The Kondo effect is now well-understood, but these impurity models have since been revived in efforts to understand the physics of quantum dots, engineered nanostructures that are often called "artificial atoms" because they contain a small number of electrons and have atom-like electronic properties.[2] Like magnetic impurities, quantum dots possess a small number of degrees of freedom coupled to the bulk degrees of freedom of a macroscopic host, making modified quantum impurity models highly applicable to theoretical studies of their properties and behavior.

In recent years, there has been particular interest in quantum phase transitions in correlated systems such as cuprate superconductors, heavy-fermion materials, and quantum Hall systems.[1] A quantum phase transition is a transition at absolute zero between two different ground states as some nonthermal parameter (e.g., pressure, carrier concentration, applied magnetic field) is varied. Unlike conventional phase transitions such as the melting of ice, which are driven by thermal fluctuations, quantum phase transitions are governed by quantum mechanical fluctuations resulting from uncertainty at absolute zero. Quantum impurity systems provide a very useful arena in which to develop our understanding of quantum phase transitions. One case that has been particularly well-studied is pseudogap impurity models, which will be described in Section II. Studies of the Anderson and Kondo impurity models for pseudogap Fermi systems have established the existence of a quantum critical point (QCP) between a strong-coupling phase, in which the Kondo effect quenches the impurity degree of freedom, and a local-moment phase, in which the impurity behaves as a free spin degree of freedom.[3]

Like all quantum systems composed of multiple subsystems, quantum impurity systems

may be entangled. An entangled system is one whose state cannot be described by a product of the states of the subsystems. A system composed of two subsystems, 1 and 2, is therefore entangled if $|\Psi\rangle \neq |\psi_1\rangle_1 \, |\psi_2\rangle_2$. Consider, for example, a system of two spin-1/2 particles. The first particle has two available states: $|\uparrow\rangle_1$ and $|\downarrow\rangle_1$. Likewise, the second particle has two available states: $|\uparrow\rangle_2$ and $|\downarrow\rangle_2$. Consider the following overall state:

$$|\Psi\rangle = \frac{1}{\sqrt{2}} \, |\uparrow\rangle_1 \, |\downarrow\rangle_2 - \frac{1}{\sqrt{2}} \, |\downarrow\rangle_1 \, |\uparrow\rangle_2.$$

It is entangled — a measurement of one particle collapses the superposition of both (regardless of their spatial separation). If we measure one of the particles to have spin up, then the other particle must have spin down. If we measure one of the particles to have spin down, then the other particle must have spin up.

All proposed forms of quantum computation rely on entanglement between qubits.[4] In contrast to a conventional computer bit, which must be in one of two states, $|0\rangle$ or $|1\rangle$, a qubit in a quantum computer may be in an arbitrary superposition of the two, $|\Psi\rangle = a\,|0\rangle + b\,|1\rangle$, where a and b are complex coefficients that satisfy $|a|^2 + |b|^2 = 1$. Powerful algorithms, with a range of applications, have been developed to harness this property, though quantum information has yet to be fully realized. The tunability of quantum dots makes them viable candidates for implementation as qubits,[5] but we must first gain a theoretical understanding of how they become entangled in a macroscopic system. Quantum impurity models are ideally suited for this task.

Previous studies of quantum impurity models have demonstrated distinct peaks in entanglement entropy near a quantum critical point.[6] Here we examine the entanglement entropy near the quantum critical point in a pseudogap Anderson model, aiming to find and characterize similarly distinct behavior. There is also accumulating evidence that quantum criticality plays an important role in conventional superconductivity.[7] Recent experimental studies of the superconducting cuprates suggest that a QCP is hidden beneath the superconducting dome.[8] Though entanglement entropy is more directly relevant to quantum information, the potential for any additional understanding of QCPs to inform research in superconductivity further motivates this study.

II. METHODOLOGY

The Anderson impurity model consists of two electronic subsystems: the impurity level and the conduction band with which it interacts. The impurity level consists of a single orbital which, according to the Pauli exclusion principle, may either be empty, singly occupied by either an up-spin or down-spin electron, or doubly occupied with zero net spin. Its energy is $\epsilon_d < 0$, and there is a Coulomb repulsion energy U between two occupying electrons. An unoccupied impurity level therefore has zero energy, a half-filled impurity level has energy ϵ_d, and a full impurity level has energy $2\epsilon_d + U$. The model is particle-hole symmetric if $2\epsilon_d + U = 0$ in which case the empty and doubly occupied impurity configurations are degenerate.

The numerical renormalization group (NRG) is a proven method for solution of quantum impurity problems.[9] The continuum of energies in the conduction band is replaced by a discrete set of energies $\epsilon_{\pm n} = \pm\frac{1}{2}D(1+\Lambda^{-1})\Lambda^{-n}$ forming a sequence that focuses on the Fermi energy. Here $\Lambda > 1$ is a parameter introduced to create a separation of energy scales that allows the quantum impurity problem to be solved iteratively. The process begins at iteration 0 with the diagonalization of the Hamiltonian matrix corresponding to only the highest energy scale. At each subsequent iteration $N = 1, 2, \ldots$, the matrix is extended to include the next lowest energy scale. When the matrix becomes too large for feasible computation, the program retains only a fixed number of states having the lowest energy. The eigenstates retained at iteration N contain the information required for accurate calculation of physical properties in a range of temperatures around $T_N = \Lambda^{-N/2}D/k_B$. The resulting spectrum of eigenstates allows for the approximate calculation of various properties of the system, including the quantity of interest in this study, the entanglement entropy.

The Anderson model Hamiltonian is given by

$$H = \sum_{k,\sigma}[\epsilon_k c^\dagger_{k\sigma}c_{k\sigma} + V(d^\dagger_\sigma c_{k\sigma} + H.c.)] + \epsilon_d n_d + U n_{d\uparrow}n_{d\downarrow} \tag{1}$$

where $c_{k\sigma}$ annihilates a conduction-band electron of energy ϵ_k and spin-z component σ, d_σ annihilates an electron of energy ϵ_d in the impurity level, U is the Coulomb repulsion energy between two electrons in a full impurity level, V is the momentum-independent hybridization, $n_{d\sigma} = d^\dagger_\sigma d_\sigma$ measures the number of electrons with spin-z component σ in the impurity level, and $n_d = n_{d\uparrow} + n_{d\downarrow}$. We assume a simple power-law variation in the density

of states about the Fermi energy $\epsilon_F = 0$:

$$\rho(\epsilon) = \begin{cases} \rho_0 |\epsilon/D|^r, & |\epsilon| \le D \\ 0, & |\epsilon| > D \end{cases} \tag{2}$$

where $2D$ is the conduction bandwidth. The strength of the impurity-band interaction is characterized by the hybridization width $\Gamma = \pi\rho_0 V^2$, and its energy dependence by the exponent $r > 0$.

The properties of the pseudogap Anderson model are known[3] to be qualitatively different in three different ranges of the pseudogap exponent r: $0 < r \le r^* \simeq 0.375$, $r^* < r < \frac{1}{2}$, and $r \ge \frac{1}{2}$. In the latter two ranges the behavior is very sensitive to whether the model is particle-hole symmetric (achieved only for $U = -2\epsilon_d$) or asymmetric (any $U \ne -2\epsilon_d$). Accordingly, we have chosen to study the representative cases $r = 0.2$, 0.4, and 0.6, with $U = 0.2D$ and $\epsilon_d = -0.1D$ (symmetric) and $-0.05D$ (asymmetric).

In keeping U and ϵ_d constant, the multi-dimensional (in the parameter space) criticality was simplified to a one-dimensional criticality in Γ. For $\Gamma < \Gamma_c$, the system is in the local-moment phase with an impurity magnetic susceptibility χ satisfying $T\chi = \frac{1}{4}$ in the low-temperature limit, while for $\Gamma > \Gamma_c$, the system is in the strong-coupling phase with $T\chi = (T\chi)_{SC}$ in the low-temperature limit, where $(T\chi)_{SC} = r/8$ at particle-hole symmetry and $(T\chi)_{SC} = 0$ otherwise. The critical coupling Γ_c was then taken to be the point at which the susceptibility $T\chi$ plateaus at a value between $(T\chi)_{SC}$ and $\frac{1}{4}$ for the maximum number of iterations, or, equivalently, to the lowest temperature.

The entanglement entropy is given by

$$S_e = -\sum_i p_i \ln p_i \tag{3}$$

where p_i is the quantum-mechanical probability associated with each of the four impurity configurations i in the Anderson model. A small perturbation must be applied to offset any unentangled degeneracies. Since we focused on the low-temperature limit in which the Boltzman factor e^{-E_i/k_BT} corresponding to all positive-energy states is driven to zero, an infinitesimal perturbation suffices to eliminate the effect of any degeneracies on S_e. We apply a small, local, magnetic field h to offset the degeneracy between unentangled singly-occupied configurations while preserving degeneracies due to entangled Kondo resonances, which shield the impurity level from the field. We therefore compare the zero-field en-

TABLE I. Critical hybridization width Γ_c for symmetric and antisymmetric models with $U = 0.2$ and $r = 0.2$, 0.4, and 0.6. Although Γ_c was calculated to 20 decimal places using quadruple precision floating-point arithmetic, results here are reported only to the fourth decimal place.

r	$\epsilon_d = -0.1$	$\epsilon_d = -0.05$
0.2	0.0363	0.0276
0.4	0.1815	0.1111
0.6	n/a	0.2493

tanglement entropy $S_e(h = 0)$ with the limiting value of the entanglement entropy for an increasingly small local field $S_e(h \to 0) = \lim_{h\to 0} S_e(h)$.

All computation was performed using quadruple precision floating-point arithmetic. The NRG discretization was held constant at $\Lambda = 3$. After iteration N, all states of energy up to $15k_BT_N$ (where T_N is defined above) were retained to form the starting point for iteration $N + 1$.

III. RESULTS

The critical hybridization width for each of the studied combinations of r, U, and ϵ_d is listed in Table I. Exploratory calculations over a wide range of values $\Gamma > \Gamma_c$ confirm that in the strong-coupling phase the entanglement entropy is unaffected by a small magnetic field. This is to be expected because, in this phase, the impurity spin is screened by the conduction electrons (the Kondo effect). In contrast, calculations for $\Gamma < \Gamma_c$ reveal that the entanglement entropy is increasingly affected by a small field as Γ is shifted farther into the local-moment phase. This general trend is shown in Fig. 1.

In general, as Γ approaches Γ_c from below, $\lim_{h\to 0} S_e(h)$ converges at a progressively smaller field h. To minimize rounding errors in the NRG, we used no field value smaller than $h = 10^{-32}$, but this proved too large for complete convergence over a significant range of $\Gamma_c - \Gamma$ in the case of $r = 0.2$. For $\Gamma_c - \Gamma \leq 10^{-5}$ with $r = 0.2$, an extrapolation was necessary to obtain sufficiently precise results for $S_e(h \to 0)$ [relative to the magnitude of the desired quantity, $S_e(h = 0) - S_e(h \to 0)$]. In the $r = 0.2$ case S_e was therefore calculated for a range of field values: $h = 10^{-28}, 10^{-29}, 10^{-30}, 10^{-31}, 10^{-32}$. Extrapolations based on these results

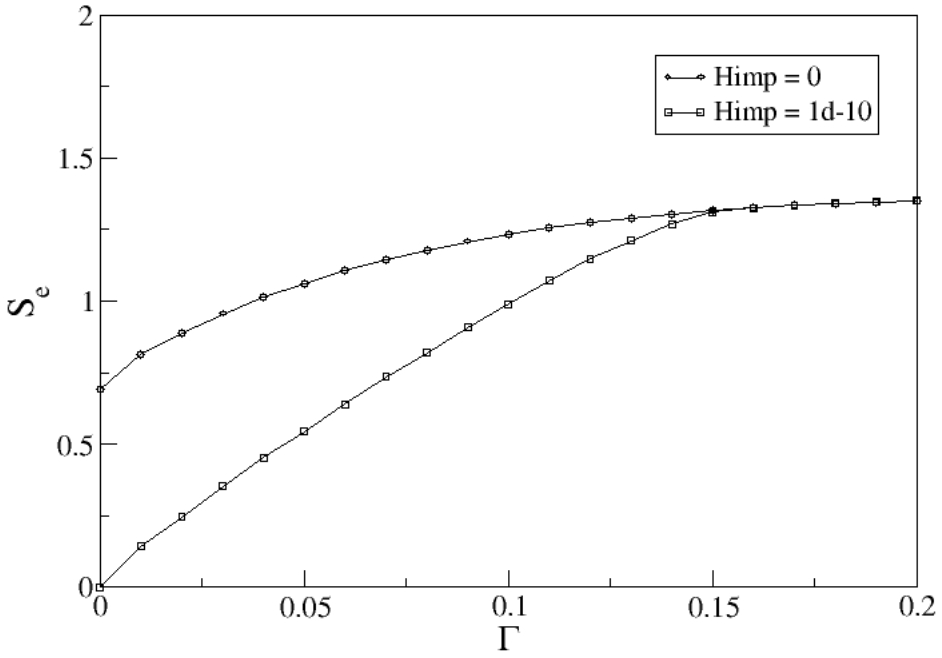


FIG. 1. Entanglement entropy S_e versus hybridization width Γ for the pseudogap Anderson model with $r = 0.4$ and $U = -2\epsilon_d = 0.2$. Data are shown for local magnetic fields $h = 0$ and $h = 10^{-10}$.

will be included in a future version of this paper. Collected results for $S_e(h = 0) - S_e(h \to 0)$ are graphed in Fig. 2, along with regression results for a power-law fit:

$$S_e(h = 0) - S_e(h \to 0) = A(\Gamma_c - \Gamma)^\eta. \tag{4}$$

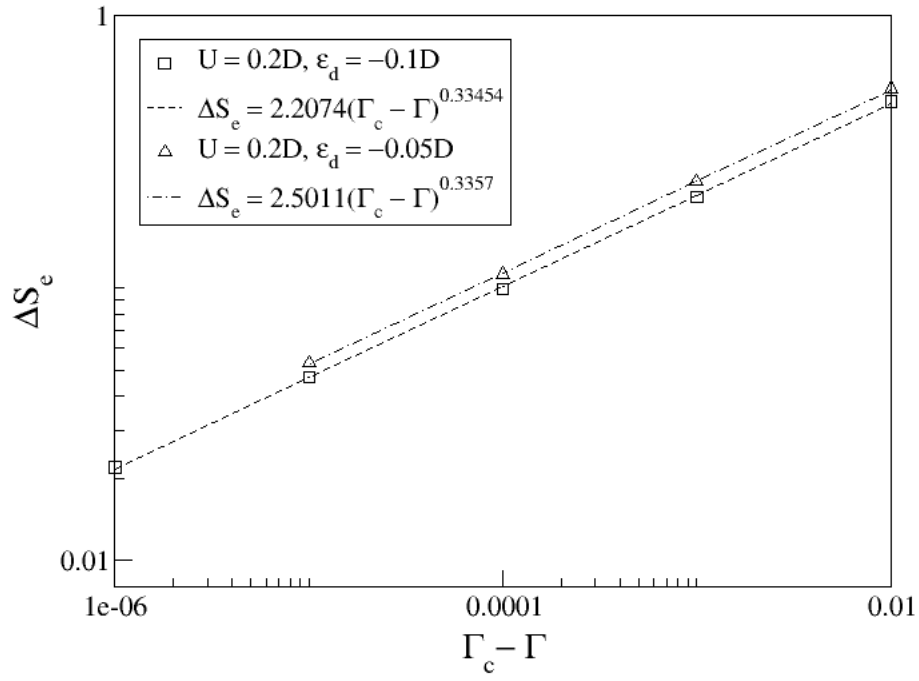
The trend in S_e indeed obeys this power law with smallest correlation coefficient $R = 0.9998868$.

IV. DISCUSSION AND CONCLUSION

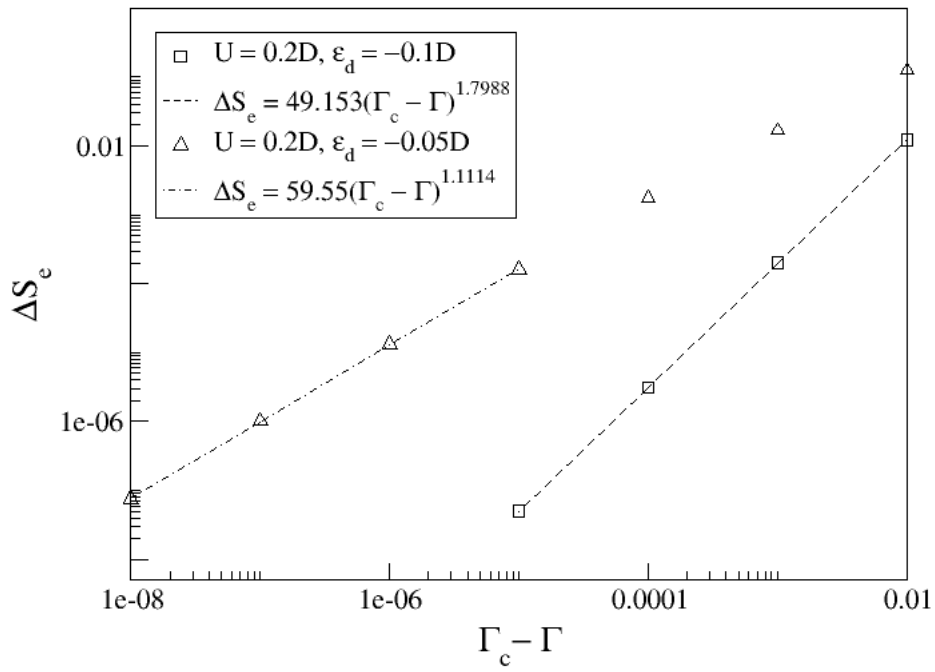
The power-law behavior we discovered may be explained in the context of the previous work of Ingersent and Si.[10] We relate $S_e(h = 0) - S_e(h \to 0)$ to the local magnetization m, beginning with the four probabilities p_i entering into Eq. (3). Since they must satisfy the condition $\sum_i p_i = 1$, only three are independent.

In zero field, $p_\uparrow = p_\downarrow$ so that $S_e(h = 0)$ depends on just two free quantities which we can

r = 0.2


1
0.01
1e-06
0.0001
0.01
ΔS_e
Γ_c − Γ
U = 0.2D, ε_d = −0.1D
ΔS_e = 2.2074(Γ_c − Γ)^0.33454
U = 0.2D, ε_d = −0.05D
ΔS_e = 2.5011(Γ_c − Γ)^0.3357

r = 0.4


0.01
1e-06
1e-08
1e-06
0.0001
0.01
ΔS_e
Γ_c − Γ
U = 0.2D, ε_d = −0.1D
ΔS_e = 49.153(Γ_c − Γ)^1.7988
U = 0.2D, ε_d = −0.05D
ΔS_e = 59.55(Γ_c − Γ)^1.1114

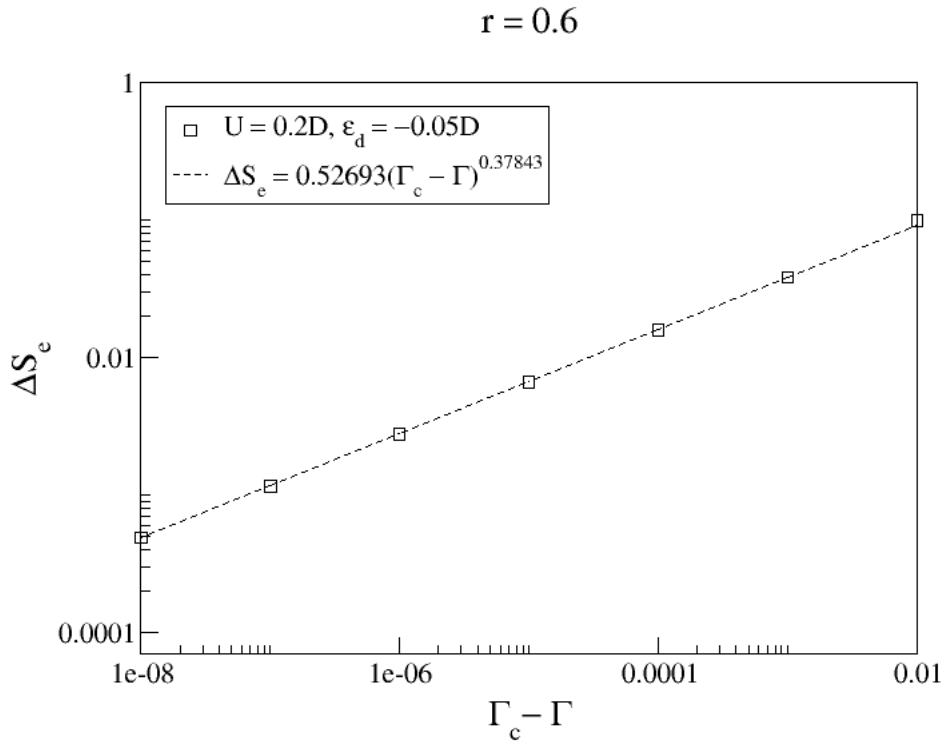


FIG. 2. The change in entanglement entropy $\Delta S_e = S_e(h=0) - S_e(h \to 0)$ caused by a vanishingly small magnetic field versus hybridization width $\Gamma_c - \Gamma$. The dashed line shows a power-law fit to the data points.

express in terms of the local-moment fraction $f = p_\uparrow + p_\downarrow$ and the charge $q = p_2 - p_0$. Here $p_\uparrow$ and $p_\downarrow$ are the probabilities of a singly-occupied impurity level with subscripts labeling the possible spin z directions, p_0 is the probability of an empty impurity level, and p_2 is the probability of a doubly-occupied impurity level. We may obtain the four probabilities from just the local-moment fraction and the charge: $p_\uparrow = p_\downarrow = \frac{1}{2}f$, $p_0 = \frac{1}{2}(1-f-q)$, and $p_2 = \frac{1}{2}(1-f+q)$. Then Eq. (3) gives:

$$S_e(0) = \ln 2 - f \ln f - \frac{1}{2}(1-f-q)\ln(1-f-q) - \frac{1}{2}(1-f+q)\ln(1-f+q) \qquad (5)$$

We may reasonably assume that a very small local magnetic field h does not affect the energy and hence the probability of the empty and doubly-occupied states. The local-moment fraction f and the charge q are therefore unchanged. However, in the local-moment phase, a field offsets the degeneracy between the two singly-occupied states, producing a

TABLE II. Entanglement-entropy exponents η obtained from fits to Eq. (4) compared to local-moment exponents β entering Eq. (7), calculated for for Coulomb repulsion energy $U = 0.2$ and different values of the impurity energy ϵ_d and the pseudogap exponent r.

r	ϵ_d	η	2β (Ref. 10)
0.2	-0.1	0.3345	0.3200
0.2	-0.05	0.3357	0.3200
0.4	-0.1	1.7988	1.8280
0.4	-0.05	1.0957	1.16
0.6	-0.05	0.37843	0.376

small nonzero magnetization $m = \frac{1}{2}(p_\uparrow - p_\downarrow) \ll \frac{1}{2}f$. We may then write the four probabilities in terms of f, q, and m: $p_\uparrow = \frac{1}{2}f + m$, $p_\downarrow = \frac{1}{2}f - m$, $p_0 = \frac{1}{2}(1 - f - q)$, and $p_2 = \frac{1}{2}(1 - f + q)$. Substituting into Eq. (3) and using $\ln(1 + x) = x - x^2/2 + \ldots$ (for $|x| \ll 1$) leads to the result

$$S_e(h) = S_e(0) - 2m^2/f \tag{6}$$

where $S_e(0)$ is given by Eq. (5).

It is known from Ingersent and Si[10] that

$$m \propto (\Gamma_c - \Gamma)^\beta. \tag{7}$$

By direct substitution into Eq. (6), we arrive at Eq. (4) with:

$$\eta = 2\beta. \tag{8}$$

Values for β calculated by Ingersent and Si are compared to our results for η in Table II. Though Eq. (8) is satisfied to only about two significant digits, we believe more accurate calculations in future work will provide confirmation of the relationship.

We have successfully established a power-law relationship between the entanglement entropy S_e and the hybridization width Γ, for several versions of the pseudogap Anderson model. In future work, we intend to consider additional values of the density-of-states exponent r across a finer spectrum in each region $r < r^*$, $r^* < r < \frac{1}{2}$, and $r > \frac{1}{2}$, and to study criticality in three parameters U, ϵ_d, and Γ. Integration of all these results into a single cohesive picture will provide a more complete understanding of entanglement at the quantum critical point in the Anderson model with a pseudogap.

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