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Renyi entropy of the interacting Fermi liquid

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Entanglement properties, including the Renyi α entropies and scaling laws, are becoming increasingly important in condensed-matter physics because they can be used to determine physical properties and the "fingerprint" of quantum phases. In this work we use variational quantum Monte Carlo to compute the Renyi α entropies, their scaling laws, and the relationship between different α entropies for one of the most important phases in condensed matter, the interacting Fermi liquid. We also investigate the relationship between the scaling laws and the discontinuity in the momentum distribution at the Fermi surface. Contrary to recent theoretical predictions, we find that interactions increase the prefactor for the α-entropy scaling laws for all particle interaction strengths and forms. We also show that a theory of these scaling laws for the interacting systems may be developed by extending the free theory to incorporate properties of the momentum distribution.

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The Renyi α entropies, which provide a measure of entanglement between two spatial regions of a system, have been used to identify exotic phases, emergent Fermi surfaces, and to locate quantum phase transitions.[1–5] Their scaling laws provide information about whether the system is gapped or critical, the number of degrees of freedom in the low-energy theory, and several other fundamental physical properties of the system.[6–8] The relationships between different-order Renyi α entropies provide the most complete characterization of a quantum phase and are equivalent to the full spectrum of the density matrix, the entanglement spectrum.[9]

In two and three dimensions, quantum Monte Carlo techniques have recently been proven useful for computing α entropies for interacting systems.[10,11] Much of this work so far has been focused on exotic phases and critical bosonic systems, leaving many important phases, including the interacting Fermi liquid, to be explored.[3,10,12,13] The Fermi liquid is one of the most ubiquitous models in condensed-matter physics and is thought to represent the ground state of most "normal" fermionic Hamiltonians.

In addition to being of fundamental importance, the Fermi liquid is also interesting due to the area law violation of its α-entropy scaling laws.[14,15] In two dimensions (2D), the Widom conjecture predicts a leading-order $L \log L$ scaling for noninteracting systems with a Fermi surface and has been verified numerically.[16] This conjecture was proposed to describe the limiting behavior of certain operators that are identical to those that determine the entanglement scaling laws for noninteracting systems.[14] Furthermore, the conjecture predicts that the prefactor of the leading scaling term only depends on the shape of the Fermi surface and the shape of the real-space surface of the region. Recent theoretical studies of the interacting Fermi liquid in 2D have predicted that the leading Renyi α-entropy scaling laws are identical to the free case.[17,18]

Although many low-energy properties of the interacting Fermi liquid are well described by Fermi liquid theory, we find that the Renyi entropies are not. The prefactor of the leading scaling behavior of the Renyi entropies for the interacting Fermi liquid is larger than that predicted by the Widom conjecture. This result is shown to hold for short- and long-range interparticle potentials, and all interaction strengths and Renyi entropies computed in this work. We compute the quasiparticle renormalization factor Z to quantify interaction strength in the system and show that the prefactor of the leading Renyi entropy scaling law increases as interaction strength increases.

The Renyi α entropies are defined as

$$S_\alpha(\rho_A) = \frac{1}{1-\alpha} \log\left[\mathrm{Tr}\left(\rho_A^\alpha\right)\right], \tag{1}$$

where ρ_A is the spatially reduced density matrix of a system partitioned into two regions, A and B.

Unbiased estimates of these entropies for trial wave functions can be calculated in variational quantum Monte Carlo (VMC). The VMC method is used for computing observables from many-body wave functions and does not have a fermion sign problem. It has been used to calculate accurate energies and Fermi liquid parameters for the electron gas, helium-3, and several related Fermi liquid systems.[19–21] We use it to compute the α entropies via the swap operator,[10]

$$\mathrm{Tr}(\rho_A^\alpha) = \langle \Psi_1 \otimes \cdots \otimes \Psi_\alpha | \, \widehat{\mathrm{SWAP}}_\alpha | \Psi_1 \otimes \cdots \otimes \Psi_\alpha \rangle, \tag{2}$$

for an integer valued $\alpha > 1$. This operator works by cyclically swapping coordinates between α statistically independent copies of the system, each sampling Ψ^2.

In practice, the expectation value of the swap operator $\mathrm{Tr}(\rho_A^\alpha)$ decays rapidly as region A increases in size. To compute Renyi α entropies for large regions we factorize the swap operator into two parts: sign and magnitude.[3] These two pieces are computed separately and then summed to obtain the full value. This factorization is not an approximation and does not change the values we compute for S_α.

Computational details. In this work the swap operator for S_2 was used without factorization for circular regions A up to $\langle N \rangle = 16$ for a simulation cell of 137 electrons and with the sign factorization technique for $\langle N \rangle = 16$, 25, and 36 in 261 electron systems. We computed S_2 for regions of $\langle N \rangle = 1$–16 for the 137 particle simulation cell using the unfactorized estimator for the modified Pöschl-Teller potential (MPT). When factorization is unnecessary we are able to increase our computational efficiency by computing the swap operator for several region sizes at the same time. To increase

TABLE I. Coulomb potential: r_s is the Wigner-Seitz radius of the electron gas, $r_s = 0$ is the noninteracting system, $\Delta S_2/L = l + m \log L$, and Z is the quasiparticle renormalization factor. Corr$= (E_{VMC} - E_{HF})/(E_{DMC} - E_{HF})$ is the ratio of correlation energy the wave function recovers and provides a metric for wave-function quality.

r_s	m	l	Z	Corr
1	0.005(1)	0.001(1)	0.755(1)	0.991
5	0.035(1)	0.001(3)	0.450(1)	0.990
10	0.053(2)	0.027(3)	0.295(1)	0.988
20	0.073(2)	0.065(4)	0.134(1)	0.985

the efficiency of the sign factorization technique we moved pairs of particles, one in each system, together. Approximately 10^6 CPU hours were spent on the smaller systems and the same on the larger. For the higher-order α entropies we were restricted to $\langle N \rangle = 16$ or fewer electrons for the 261 electron system. All quantum Monte Carlo calculations are performed in QMCPACK.[22] By integrating out regions that are a small fraction of the system size, we minimize interactions of region A and its periodic neighbors. For small subregions we see oscillations, small relative to S_2, that decay as the subregion length increases for both the interacting and noninteracting cases.[23] Fits are performed on $\Delta S_2/L$ to minimize the effect of oscillations on the fitted parameters.

Wave functions. The ground-state wave function for the noninteracting Fermi gas (FG) Hamiltonian is $\Psi_{FG}(R) = \langle R|(\prod_{k<k_f} c_k^\dagger|0\rangle)$. To this we add a Jastrow correlation factor and optimize to obtain the trial wave function for the spin-polarized homogeneous electron gas (HEG), $\Psi_{HEG}(R) = \mathcal{J}(R)\Psi_{FG}(R)$, with $\mathcal{J}(R) = \exp(\sum_{i<j} U(r_{ij}))$ and U some function with optimizable parameters.[21] For the modified MPT, as with the HEG, we use an optimized trial wave function of the Slater-Jastrow form, $\Psi_{MPT}(R) = \mathcal{J}(R)\Psi_{FG}(R)$.

The Slater-Jastrow trial wave function for the interacting Hamiltonians adds additional correlation between particle pairs. We parametrize the Jastrow by a flexible B-spline function with fixed cusp conditions depending on the potential and optimize them using a variant of the linear method.[24] For the HEG wave function we eliminate the divergence in the electron-electron energy as $r_{ij} \to 0$ by including a cusp in the Jastrow.[21] For the MPT wave function, $\Psi_{MPT}(R)$, there is no singularity in the potential and therefore no cusp in the Jastrow.

The degree to which the trial wave function represents the ground-state Fermi liquid in VMC depends on its overlap with the exact ground-state wave function. We estimate the quality of our trial wave function by looking at the amount of correlation energy the wave function recovers in VMC relative to fixed-node-diffusion quantum Monte Carlo, $E_{\text{corr}} = E_{DMC} - E_{HF}$.[21] For exact wave functions this is 100%. We recover more than 98% of this correlation energy for all densities and potentials, shown in Tables I and II. Further tests of the wave-function quality were performed at $r_s = 5$, with a wave function of the Slater-Jastrow backflow form,[19] yielding no significant changes from the results presented here.

TABLE II. Modified Pöschl-Teller potential. V_0 is the strength of the potential for the modified Pöschl-Teller potential, and all other labels are as in Table I.

V_0	m	l	Z	Corr
10	0.032(1)	0.007(2)	0.504(6)	0.984
20	0.062(1)	0.028(1)	0.316(5)	0.981

The noninteracting reference entropies are computed using the correlation function technique using the same number of electrons as the corresponding VMC calculation and are converged with respect to real-space grid.[25]

Results. With these techniques, we first consider the Renyi α entropies of the spin-polarized homogeneous electron gas. Starting from the noninteracting Fermi-gas Hamiltonian in hartree units, $H_{FG} = \frac{-1}{2}\sum_i \nabla_i^2$, the HEG Hamiltonian is obtained by adding the Coulomb potential, $V_C = \sum_{i<j} r_{ij}^{-1} + C(r_s)$, with $r_{ij} = |r_i - r_j|$ the distance between electrons i and j, and a constant $C(r_s)$ due to a uniform positive background charge.

In Fig. 1 we plot S_2^{HEG}, the scaling laws for the HEG at different Wigner-Seitz radii $r_s = (\pi\nu)^{-1/2}$ with ν the number density. For all our scaling-law plots, we rescale all lengths, $L \to L/(\sqrt{\pi} r_s) = \sqrt{\pi \langle N_A \rangle}$, with N_A the average number of particles in the region, so that $S_\alpha(L)$ for the noninteracting Fermi liquid has no r_s dependence. Under this rescaling, all interacting S_α will collapse to the noninteracting S_α^{FG} if interactions are irrelevant. The noninteracting data is then fit by the leading scaling form predicted by the Widom conjecture, $S(L) = m_0(L/l_0)\log(L/l_0)$, and we find $m_0 = 0.032(2)$ and $l_0 = 0.113(5)$.[14,23]

We define $\Delta S_\alpha = S_\alpha^{HEG} - S_\alpha^{FG}$ as the difference between the interacting and noninteracting Renyi α entropies for the

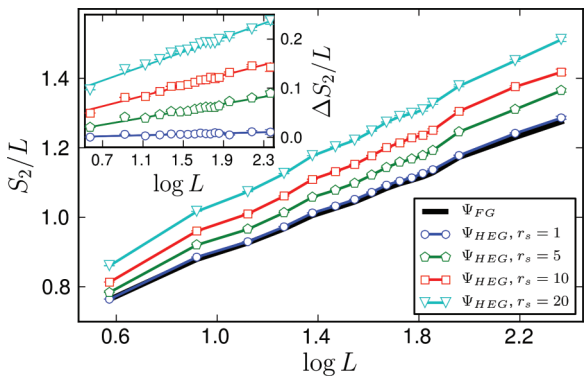

FIG. 1. (Color online) Scaling form for the spin-polarized electron gas. (Main plot) S_2/L for the spin-polarized interacting electron gas at $r_s = 1,5,10,20$ and the noninteracting Fermi liquid. L is scaled so that without interactions all lines lie on top of Ψ_{FG} results. The high-density $r_s = 1$ data falls on top of the noninteracting liquid while the lower-density, more strongly correlated liquids have larger Renyi 2 entropies. The Ψ_{FG} reference is the exact noninteracting S_2 computed using the same number of particles as the interacting system for each L. (Inset) $\Delta S_2/L = (S_2^{HEG} - S_2^{FG})/L$ plotted against $\log L$. The 2 entropy for the interacting case scales the same as the noninteracting case with a larger prefactor. The lines are from a fit to $\Delta S_2/L = l + m \log L$ shown in Table I.

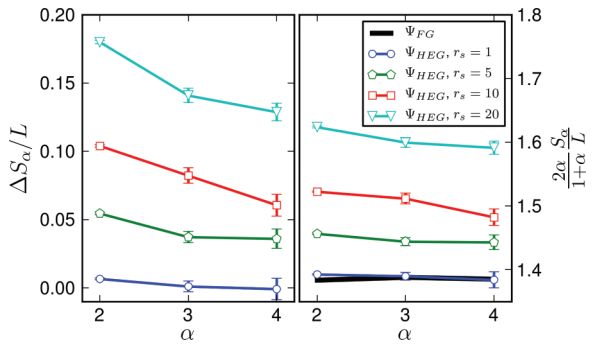

FIG. 2. (Color online) Relationship between α entropies for the spin-polarized electron gas. (Left) $\Delta S_\alpha / L = (S_\alpha^{HEG} - S_\alpha^{FG})/L$ for $\alpha = 2,3,4$ for region A size $\log L \approx 1.5$, $\langle N_A \rangle = 6.25$. S_α increases as correlations increase and decreases as α increases. (Right) $\frac{2\alpha}{1+\alpha} \frac{S_\alpha}{L}$ for $\alpha = 2,3,4$. Besides some small L oscillations, this scaling makes the noninteracting Renyi α entropies linear in α. Interactions modify this relationship: the rescaled α entropies decrease as α gets larger.

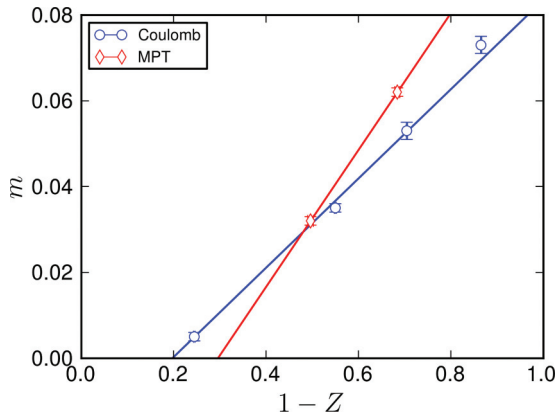

FIG. 3. (Color online) Relationship between particle interaction strength and modification of leading scaling law for S_2. Slope difference, m: $\Delta S_2 / L = (S_2^{HEG} - S_2^{FG})/L = l + m \log L$, as a function of $1 - Z$ for the Coulomb and modified Pöschl-Teller potential at all correlation strengths considered. Lines are guides to the eye from linear fits. For all interaction forms and strengths the prefactor of the leading scaling law is increased. Beyond some minimal $Z \approx 0.8$ the relationship for m and $1 - Z$ is linear within error bars for the Coulomb potential.

HEG and plot them as the inset of Fig. 1. We find $\Delta S_2 / L$ is well fit to the two-parameter form $l + m \log L$ presented in Table I. These plots demonstrate the extent to which the scaling laws are changed from the noninteracting case. As the Wigner-Seitz radius is increased, so too is the prefactor of the leading scaling term m. This increase in the Renyi α-entropy scaling laws is a violation of the Widom conjecture and shows that the interacting system is more entangled than its noninteracting counterpart.

Changes from the noninteracting theory are also seen for the higher-order Renyi α entropies. In the left graph of Fig. 2, $\Delta S_\alpha / L$ is plotted for the higher-order α entropy for a region of size $\langle N \rangle = 6.25$. The simple relationship between noninteracting S_α does not hold when Coulomb interactions are included, as shown on the right graph of Fig. 2. Upon rescaling, $\frac{S_\alpha}{L} \to \frac{2\alpha}{1+\alpha} \frac{S_\alpha}{L}$, the noninteracting Renyi α entropy is constant as a function of α. The difference between the interacting and noninteracting S_α decreases as α gets larger. As α increases the Renyi entropy is more strongly dominated by the largest eigenvalues in the density matrix spectrum. Because the interacting and noninteracting entropies converge as α gets larger, it indicates that the largest values in the spectrum of the density matrix may be universal.

To determine if these scaling-law changes are due to the long-range nature of the Coulomb interparticle potential, we also compute the scaling laws for a Hamiltonian with a short-range potential, the modified Pöschl-Teller potential. The MPT, $V_{MPT} = V_0 \sum_{i<j} \cosh^{-2}(r_{ij})$, is a well-tested short-range potential for the Fermi gas that has been used to model cold atom systems.[26,27] The parameter V_0 can be tuned to increase the correlation of the system and the effective range is set to the Wigner-Seitz radius, $r_s = 1$.[26]

The fitting parameters of $\Delta S_2 / L$ for the MPT at all V_0 computed are listed in Table II. Despite the short range of this interparticle potential, we still find modifications to the noninteracting scaling laws for S_2. Because the Widom conjecture depends on having a discontinuity in occupation of the momentum states at the Fermi surface, it is interesting to consider properties of the momentum distribution for these interacting systems. We do so by computing the quasiparticle renormalization factor Z.[28] Z provides a metric for particle correlation strength and is equal to the magnitude of the break in the momentum distribution at the Fermi surface. As shown in Fig. 3, the scaling laws for the MPT systems show qualitative agreement with the HEG with the same Z. As interparticle correlations are strengthened Z decreases, and the prefactor for the leading scaling behavior of the Renyi α entropies increases. For the HEG this results in a linear relationship for Z between 0.2 and 0.8. This result suggests a modification of the scaling-law prefactor based on the Widom conjecture due to the momentum distribution of the interacting system.

We consider the possibility that the scaling laws we observed are due to subleading terms that have not decayed for our largest calculations. For the data sets we have generated there is no evidence that, within our error bars, the leading-order scaling term is actually a decaying subleading term. Furthermore, there is no theoretical support for a subleading term which scales as the leading term for small systems but decays as the system size L gets large.

Conclusions. These fundamentally nonperturbative Renyi α-entropy results for interacting Fermi liquid show an increase in the leading scaling-law prefactor beyond the one predicted by the Widom conjecture. These results hold for all wave-function forms, correlation strengths, and interparticle potentials considered in this work. This does not rule out a universal scaling-law theory. However, it may be more complicated than the noninteracting theory to account for the modifications to the leading scaling term. Development of such a theory is likely to benefit from investigation of momentum distribution properties, such as Z, on the Renyi α entropies. Further entanglement studies of scaling laws and Fermi liquid parameters for interacting systems, such as paramagnetic electron gases, Wigner crystals, and realistic Coulombic systems, are essential for determining the exact relationship between them. We expect further studies will help

resolve this issue and contribute to how we understand the role of entanglement in condensed-matter physics.

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[1] T. J. Osborne and M. A. Nielsen, Phys. Rev. A **66**, 032110 (2002).
[2] Y. Chen, P. Zanardi, Z. D. Wang, and F. C. Zhang, New J. Phys. **8**, 97 (2006).
[3] Y. Zhang, T. Grover, and A. Vishwanath, Phys. Rev. Lett. **107**, 067202 (2011).
[4] A. Kitaev and J. Preskill, Phys. Rev. Lett. **96**, 110404 (2006).
[5] G. Vidal, J. I. Latorre, E. Rico, and A. Kitaev, Phys. Rev. Lett. **90**, 227902 (2003).
[6] L. Amico, R. Fazio, A. Osterloh, and V. Vedral, Rev. Mod. Phys. **80**, 517 (2008).
[7] J. Eisert, M. Cramer, and M. B. Plenio, Rev. Mod. Phys. **82**, 277 (2010).
[8] E. Fradkin and J. E. Moore, Phys. Rev. Lett. **97**, 050404 (2006).
[9] H. Li and F. D. M. Haldane, Phys. Rev. Lett. **101**, 010504 (2008).
[10] M. B. Hastings, I. González, A. B. Kallin, and R. G. Melko, Phys. Rev. Lett. **104**, 157201 (2010).
[11] N. M. Tubman and J. McMinis, arXiv:1204.4731.
[12] A. B. Kallin, M. B. Hastings, R. G. Melko, and R. R. P. Singh, Phys. Rev. B **84**, 165134 (2011).
[13] H. Ju, A. B. Kallin, P. Fendley, M. B. Hastings, and R. G. Melko, Phys. Rev. B **85**, 165121 (2012).
[14] D. Gioev and I. Klich, Phys. Rev. Lett. **96**, 100503 (2006).
[15] M. M. Wolf, Phys. Rev. Lett. **96**, 010404 (2006).
[16] W. Li, L. Ding, R. Yu, T. Roscilde, and S. Haas, Phys. Rev. B **74**, 073103 (2006).
[17] W. Ding, A. Seidel, and K. Yang, Phys. Rev. X **2**, 011012 (2012).
[18] B. Swingle, Phys. Rev. Lett. **105**, 050502 (2010).
[19] Y. Kwon, D. M. Ceperley, and R. M. Martin, Phys. Rev. B **48**, 12037 (1993).
[20] Y. Kwon, D. M. Ceperley, and R. M. Martin, Phys. Rev. B **50**, 1684 (1994).
[21] W. M. C. Foulkes, L. Mitas, R. J. Needs, and G. Rajagopal, Rev. Mod. Phys. **73**, 33 (2001).
[22] J. Kim, K. Esler, J. McMinis, M. Morales, B. Clark, J. Gergely, S. Chiesa, K. Delaney, J. Vincent, and D. Ceperley, "QMCPACKsimulation suite", http://qmcpack.cmscc.org.
[23] P. Calabrese, M. Mintchev, and E. Vicari, Europhys. Lett. **97**, 20009 (2012).
[24] C. J. Umrigar, J. Toulouse, C. Filippi, S. Sorella, and R. G. Hennig, Phys. Rev. Lett. **98**, 110201 (2007).
[25] I. Peschel, J. Phys. A: Math. Gen. **36**, L205 (2003).
[26] J. Carlson, S.-Y. Chang, V. R. Pandharipande, and K. E. Schmidt, Phys. Rev. Lett. **91**, 050401 (2003).
[27] A. J. Morris, P. Lopez Rios, and R. J. Needs, Phys. Rev. A **81**, 033619 (2010).
[28] M. Holzmann, B. Bernu, V. Olevano, R. M. Martin, and D. M. Ceperley, Phys. Rev. B **79**, 041308 (2009).