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Equation of State and Thermometry of the 2D SU(N) Fermi-Hubbard Model

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(Received 30 May 2023; accepted 9 January 2024; published 21 February 2024)

We characterize the equation of state (EoS) of the SU($N > 2$) Fermi-Hubbard Model (FHM) in a two-dimensional single-layer square optical lattice. We probe the density and the site occupation probabilities as functions of interaction strength and temperature for $N = 3$, 4, and 6. Our measurements are used as a benchmark for state-of-the-art numerical methods including determinantal quantum Monte Carlo and numerical linked cluster expansion. By probing the density fluctuations, we compare temperatures determined in a model-independent way by fitting measurements to numerically calculated EoS results, making this a particularly interesting new step in the exploration and characterization of the SU(N) FHM.

DOI: 10.1103/PhysRevLett.132.083401

The interest in the square lattice SU(2) Fermi-Hubbard Model (FHM) has been historically driven by its suitability to describing cuprate superconductors, owing to their layered character and exceptionally simple band structure near the Fermi surface. For other more complex and multiorbital materials, however, descriptions with $N > 2$ spin components have long been used, which, in addition to being of fundamental interest, provide an elegant approximation of degenerate orbitals using a higher symmetry group. Larger N systems, in particular in 2D geometries, are relevant for describing the physics of transition-metal oxides [1–3], orbitally selective Mott transitions [4–7], graphene's SU(4) spin valley symmetry [8], twisted-bilayer graphene [9–12], the Kondo effect [13,14], heavy fermion behavior [15], and achieving robust itinerant ferromagnetism [16,17]. The SU(N) FHM is a special case of the $N > 2$ models that enjoys a higher symmetry group that stabilizes quantum fluctuations [18], making it a fertile ground for theory, and constituting a baseline to more complex multiorbital models. The determination of the $N > 2$ equation of state (EoS) of the SU(N) FHM is an important milestone in the attempt of understanding its properties. However, the exponential scaling of the Hilbert space with N and the increased severity of the fermion sign problem [19] make its numerical simulation more challenging than the $N = 2$ case [20–23].

Ultracold atoms in an optical lattice have provided valuable quantum simulations of the SU(2) FHM [24]. They complement and can sometimes outperform classical simulations [25,26]. More recently, the SU($N > 2$) FHM has been successfully explored with ultracold alkaline-earthlike atoms such as ^{173}Yb or ^{87}Sr in optical lattices, which naturally feature a full SU(N) symmetry in the atomic ground state [27–35]. A substantial effort has been placed in probing the thermodynamics and the short-range correlations of the model for different spin degeneracies and lattice geometries, and experiments have gone well beyond the regime that can be calculated with theory [36–42]. However, the SU(N) generalization remains much less explored and understood compared to the SU(2) case [43]. This is particularly true in two dimensions, where the thermodynamics of the SU(2) FHM at intermediate temperatures have been studied extensively [44–60].

In this Letter, we probe the equation of state of the two-dimensional SU(N) FHM in a square lattice at intermediate temperatures in both the metallic and the Mott regime and compare our results with numerical calculations. In particular, we determine the in-lattice temperature and entropy by fitting experimental data using numerical methods such as determinantal quantum Monte Carlo (DQMC) [61,62] and numerical linked cluster expansion (NLCE) [63,64]. We additionally determine the entropies in the 2D bulk

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before loading and after unloading from the lattice potential, and separately characterize the system inside the lattice with a thermometry relying on the fluctuation-dissipation theorem (FDT) based on the measurement of density fluctuations, without requiring modeling by theory.

The SU(N) FHM Hamiltonian is given by

$$\hat{H} = -t \sum_{\langle i,j\rangle,\sigma} \left(\hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + \mathrm{H.c.} \right) + \frac{U}{2} \sum_{i,\sigma\neq\tau} \hat{n}_{i\sigma} \hat{n}_{i\tau} - \sum_{i,\sigma} \mu_i \hat{n}_{i\sigma}, \quad (1)$$

where $\hat{c}^{\dagger}_{i\sigma}$ and $\hat{c}_{i\sigma}$ represent the fermionic creation and annihilation operators at site i with spin $\sigma \in \{1 \ldots N\}$, $\hat{n}_{i\sigma} = \hat{c}^{\dagger}_{i\sigma} \hat{c}_{i\sigma}$ is the number operator, $\langle i, j\rangle$ denotes next-neighbor lattice sites, t is the hopping amplitude, U is the on-site interaction strength, and μ denotes the chemical potential, which absorbs the contribution of the trap confinement in the local density approximation [65].

In this Letter, we directly probe the local density, components of the site-occupation distribution, and the density fluctuations within the detection resolution of a few lattice sites. By differentiating the density with respect to the local chemical potential, we evaluate the isothermal compressibility $\kappa = \partial n/\partial\mu|_T$. Crucially, we implement a 2D single-layer SU(N) ensemble that we probe with perpendicular absorption imaging with a resolution of a few lattice sites. This avoids integrating over inhomogeneous stacks of 2D systems [66,67] and allows us to directly access the density profile without complex reconstruction techniques required in 3D [37] and access density fluctuations as an additional thermodynamic *in situ* observable.

In our experiment, we load a degenerate Fermi gas of ^{173}Yb with tunable $N \leq 6$ equally populated components [see Fig. 1(a)] and an entropy per particle $s/k_{\mathrm{B}} \gtrsim 1.0$ into the single, horizontal layer of a vertical lattice. In this layer, we adiabatically ramp up a 2D square lattice potential with a wavelength of $\lambda = 759$ nm and a spacing of $d = \lambda/2$ [see Fig. 1(b)]. By modifying the lattice depth, we can tune the strength of the interactions. We measure the density distribution using *in situ*, saturated absorption imaging with a spatial resolution of approximately $2\ \mu\mathrm{m} \approx 5d$ [68].

The measured 2D density $n(x, y)$ of an SU(6) ensemble is shown in Fig. 1(c) for different interaction strengths and the same initial state preparation in the 2D bulk (the potential without in-plane lattices). Because of the harmonic confinement generated by the Gaussian profile of the lattice beams, the chemical potential varies across the trap, sampling different regions of the EoS. For increasing interactions, and in particular when the on-site interaction is larger than the square lattice bandwidth ($U/t \gtrsim 8$), we observe the emergence of plateaus at integer density which we associate with an incompressible regime, a signature of a Mott insulating state [78].

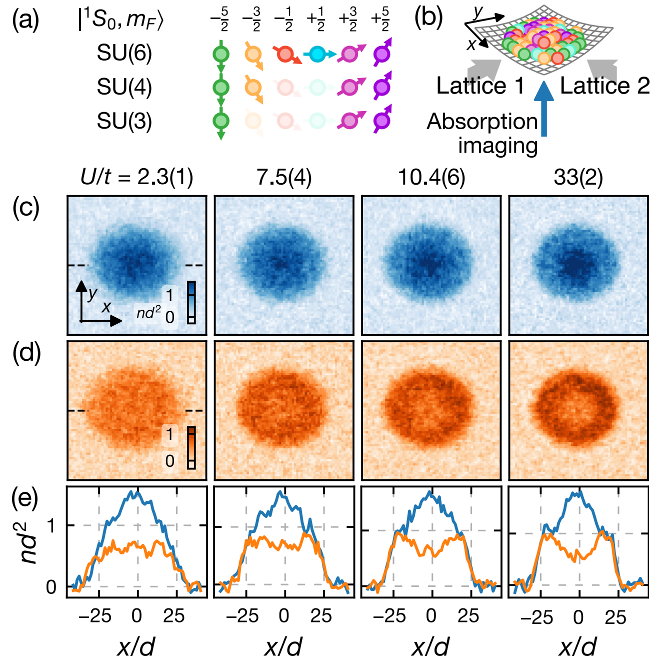

FIG. 1. Probing the 2D SU(N) Fermi-Hubbard model with ultracold atoms. (a) The $^1S_0$ ground state of ^{173}Yb naturally features an SU(6) symmetry, which can be freely tuned to $N \leq 6$ by preparing a suitable combination of the nuclear spin states $m_F = -5/2, -3/2, \ldots, +5/2$ (colored circles and arrows). (b) Schematic of the experimental setup showing a gas in a single layer 2D square lattice with harmonic confinement detected with absorption imaging along gravity. The square lattice is created by superimposing two orthogonal retro-reflected in-plane lattices. (c) Spatial distribution of the density $n(x, y)$ for $N = 6$. Each cloud shown in the horizontal frame has been prepared with the same initial entropy in the bulk and loaded into the lattice to a different U/t value. (d) Singly occupied sites after parity projection. Each horizontal frame corresponds to the same state shown in the same column of (c). (e) Density profiles for the data shown in (c) and (d) along the corresponding dashed lines in the left frames. Each image was produced using the averaging of eight shots after center of mass alignment [68].

As a distinctive probe of number squeezing effects in and close to the Mott regime [79–81], we determine the occupation number distribution by measuring the parity-projected density. After tuning U/t, we freeze the motion of the atoms by rapidly increasing the lattice depth and applying a photoassociation beam [36], which converts on-site pairs into excited-state molecules that are subsequently lost. The process removes > 99% of the on-site pairs and ≈5% of the remaining atoms [68]. Figure 1(d) shows the distribution of the singly occupied sites corresponding to the same states of Fig. 1(c). The increase in depletion in the center with increasing interaction strength is a consequence of number squeezing to a high atom pair fraction.

To access different spin degeneracies, we prepare $N < 6$ ensembles by removing spin components using optical pumping [68]. In Figs. 2(a)–2(d), we show the EoS as a

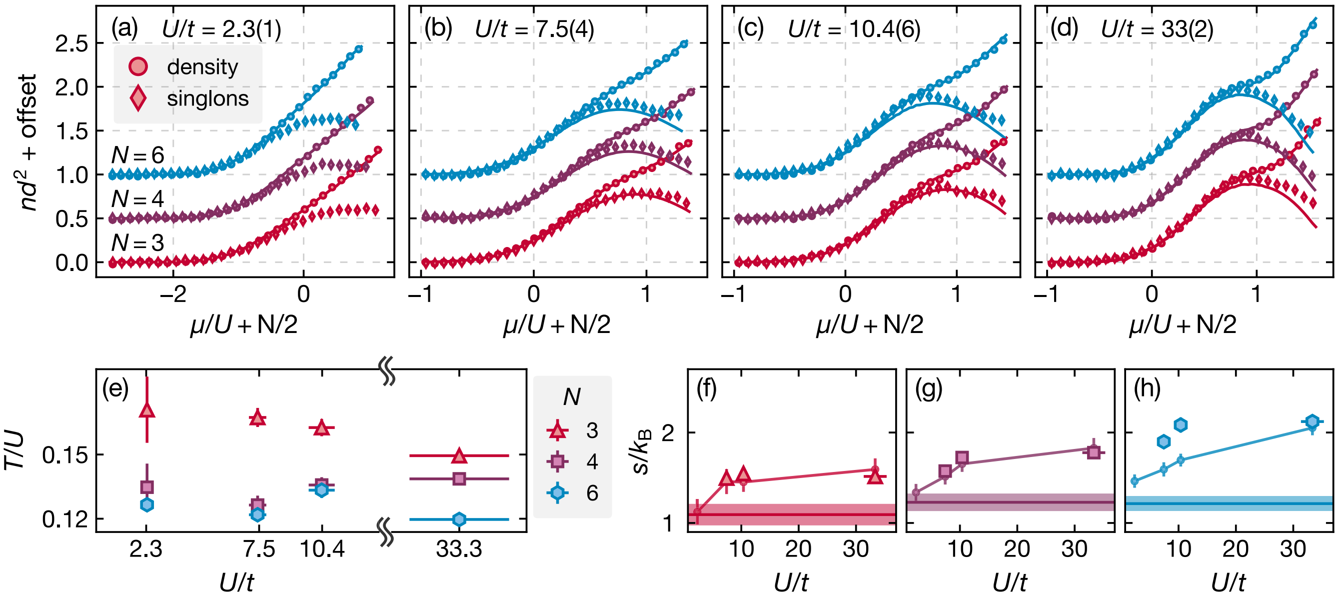

FIG. 2. Equation of state for the SU(N) Fermi-Hubbard model with $N = 6$ (blue), $N = 4$ (purple), and $N = 3$ (red). (a)–(d) Density (circles) and singly occupied sites (diamonds) as a function of the chemical potential. Data for $N = 4$ and $N = 6$ have been offset by $0.5nd^2$ and $1.0nd^2$ along the vertical axis, respectively. Continuous lines associated to the density curves correspond to the fit of the EoS calculations to the total density as described in the text. The theory used for the fit is DQMC for $U/t = 2.3(1)$ and NLCE for the other values of U/t. The results from this fit model are also used to calculate the expected pair and single-site distribution measurement. The chemical potential is defined with respect to the reference half filling [$nd^2(\mu = 0) = N/2$]. For each U/t, we fit the average of 15 frames with similar atom number after center-of-mass alignment [68]. Error bars are the standard error of the mean (s.e.m.). (e) Temperature according to the fit of the EoS shown in (a)–(d). (f)–(h) Entropy per particle. Horizontal line: entropy in the 2D bulk before loading into the lattice; triangles, squares, hexagons: entropy in the lattice according to the fit of the EoS; small circles: entropy in the 2D bulk after a round-trip experiment. The entropy in the bulk takes into account the effect of the interactions and the 3D anisotropic density of states [68]. Error bars correspond to the s.e.m. of the fit results.

function of the local chemical potential μ/U for $N \in \{6, 4, 3\}$. The chemical potential at a given location is calculated from the potential of the trap $\mu(x, y) = \mu_0 - \frac{1}{2}(\kappa_x x^2 + \kappa_y y^2)$. The exact shape of the potential is determined by fitting the density, where the trap frequencies are left as free parameters. We use a combined fit of the densities for $N = 3$, 4, and 6 for each separate U/t, but verify that separate fits for each N return values compatible with those of the combined fit. The fit of the EoS is performed in two dimensions, leaving as free parameters the temperatures $T(U/t, N)$ and the chemical potential $\mu_0(U/t, N)$ at the center of the trap. The theoretical density is convolved with the reconstructed point spread function (PSF) [68] to take into account the imaging imperfections.

For the EoS of Fig. 2, each spin mixture has been prepared with the same initial entropy per particle $s/k_B = 1.2(1)$ in the 2D bulk before ramping up the lattice. We fit and benchmark NLCE and DQMC [68] which are commonly used state-of-the-art methods for finite-temperature SU(2) Hubbard models in the regime we are considering but have only recently been extended and applied to the SU(N) experimental regime, which requires calculations away from $nd^2 = 1$ [23,41]. This is, to our knowledge, the first application of SU(N) NLCE to noninteger filling, and to the calculation of the occupancy distributions. Moreover, compared to previous works, the calculation has been extended to higher orders [68] to ensure a better convergence at low temperatures. For $U/t = 7.5(4)$ and 10.4(6) we fit both DQMC and NLCE, observing an excellent agreement between the theory and the experiment when fitting the temperature and the chemical potential at the center of the trap to the same data set with different numerical methods [68]. For $U/t = 33(2)$, we use NLCE and a high-temperature series expansion (HTSE-2), observing also in this case an excellent agreement [68]. For $U/t = 2.3(1)$, the temperature lies below the range of convergence of NLCE and we resort to DQMC alone. In Figs. 2(a)–2(d), for the cases in which we fit more than one model, we only plot the NLCE results, because the lines would overlap.

In addition to the total density, in Figs. 2(a)–2(d) we also characterize the distribution of on-site occupation numbers by removing doublons using the pair removal process described above. Experimental measurements (diamonds) are compared with the NLCE prediction (lines) based on the fit of the density, without additional free fit parameters, and agree well with the experimental data whenever available. As opposed to the $N = 2$ case, where only double occupancies are allowed, higher occupancies occur for $N > 2$. Although the numbers of these occupancies are small for the results considered at the temperatures and chemical potentials presented here, the photoassociation technique can be used to probe triple occupancies and their dynamics [82].

The harmonic confinement of the trap returned by the density fit can be compared to the confinement obtained from an independent measurement of the oscillatory motion of the atoms in the combined dipole potentials [68]. We find a discrepancy between about 13% for $U/t = 7.5(4)$ and 40% for $U/t = 33(2)$, which is not fully explained by tolerances or the trap loading model. A possible contribution could be a lack of adiabaticity during the loading into the lattice [83–85]. However, neither varying the speed of the lattice ramps up to a factor of four (up to 1 s length) nor variations of the atom number lead to significant changes in the fit results. This would require the nonadiabatic effects to produce minimal changes in density and parity profiles [68].

In Fig. 2(e) we plot the temperatures obtained by the fits of the EoS. We observe a smaller temperature for larger N, a behavior expected due to the Pomeranchuk effect [30,86], but somewhat weaker than the ideal theoretical predictions [21,86] with the temperatures for $N = 4$ and 6 differing from each other by up to 20%. We interpret this as a consequence of the heating not depending on N during the loading process, resulting in different entropies in the lattice. This is supported by the results presented in Figs. 2(f)–2(h). We find that, despite the initial entropy in the 2D bulk before loading into the lattice being independent of N, the entropy returned by the fit of the EoS is larger for larger N, which explains the weakening of the Pomeranchuk effect. For $U/t = 2.34$ entropy results are not yet converged at those such low temperatures and therefore are not presented. We also determine the entropy per particle in the 2D bulk after a round-trip experiment, which adds an inverted ramp back to the 2D bulk system. In this case, we obtain entropies comparable to those reported by the fit in the lattice for $N = 3$ and $N = 4$ but smaller for $N = 6$, similar to previous observations [37] and potentially indicating nonadiabatic effects in the preparation or return ramp.

Complementary to the measurement of the EoS, the new possibility to directly access the density in the 2D SU(N)-system allows us to probe the density fluctuations. For an integration area of size $A \gg d^2$, the variance of the detected atom number is related to the isothermal compressibility κ and the temperature T through the fluctuation-dissipation theorem [87]:

$$\mathrm{var}\left(\int_A n \; dA\right) = k_B T \kappa A = k_B T A \frac{\partial n}{\partial \mu}\bigg|_T. \qquad (2)$$

By measuring the density fluctuations, we can access the temperature with spatial resolution, without applying an

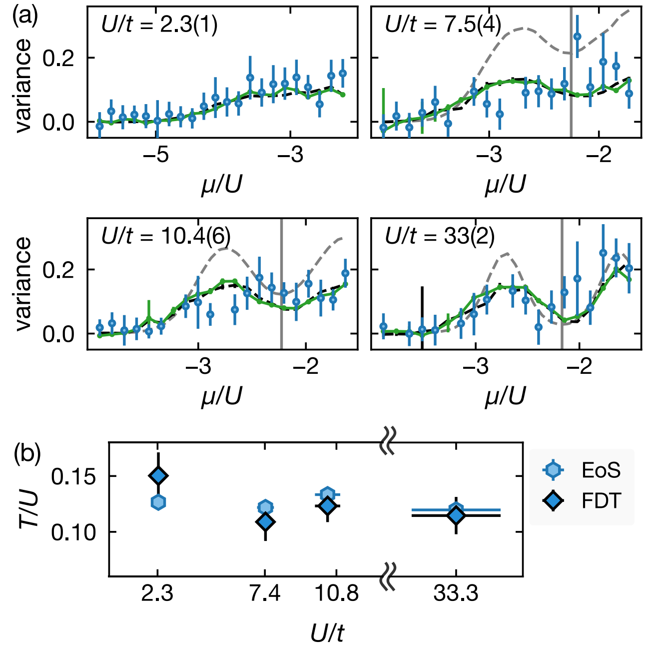

FIG. 3. (a) Measured density fluctuations (blue) for $N = 6$ as a function of the chemical potential for different interaction strengths. The data points have been obtained from the variance of 15 frames [same as Figs. 2(a)–2(d)] computed on spatially binned probe areas of size $\approx 5.1 \times 5.1 d^2$ (4×4 square camera pixels). The photon shot noise has been subtracted and a PSF correction has been taken into account [68]. The green line corresponds to the numerically differentiated compressibility κ times the temperature T_{EoS} obtained from the EoS fit of the averaged data, while the black dashed line corresponds to the theory-derived compressibility times T_{EoS}. The vertical line indicates $\mu(nd^2 = 1)$. The gray dashed line corresponds to the on-site density fluctuations $\delta\hat{n}_0^2 = \langle\hat{n}^2\rangle - \langle\hat{n}\rangle^2$ calculated with NLCE for T_{EoS}. (b) Comparison of the temperatures T_{FDT} (dark blue diamonds) and T_{EoS} (light blue hexagons). Error bars are the s.e.m.

EoS model to the dataset [60]. In Fig. 3(a) we show such density fluctuations mapped to the chemical potential for different U/t values and $N = 6$. Similar measurements for $N = 3$ and $N = 4$ are presented in the Supplemental Material [68]. For strong interactions, we observe a reduction of the fluctuations in the proximity of $nd^2 = 1$, where we expect an incompressible Mott-insulating regime. These measurements determine the temperature independently of the EoS fits, although the calibration values for the density and the trap configuration in this particular case were partially obtained from EoS-fitted datasets. Notably, the fluctuation amplitude is determined by area integration as described in Eq. (2), and therefore agrees with the thermodynamic fluctuations from the FDT as opposed to the expected on-site fluctuations $\delta\hat{n}_0^2 = \langle\hat{n}^2\rangle - \langle\hat{n}\rangle^2$ (gray dashed line). This discrepancy illustrates the role of nonvanishing short-range density correlations.

The FDT holds locally for each density. In thermal equilibrium, the ratio between the fluctuations and the compressibility is constant. We use the FDT to check this assumption and extract the temperature of the system. For this purpose, we determine the isothermal compressibility $\kappa(\mu)$ directly from the density profile data with three-point differentiation and fit the temperature T_{FDT} as the proportionality factor between the fluctuations and the compressibility. In Fig. 3(b) we compare T_{FDT} (diamonds) with the temperature T_{EoS} (hexagons) returned by the fit of the EoS. We observe a good agreement for all interactions. Moreover, we see that the residuals of the FDT analysis typically show similar temperatures at the center and at the edge of the cloud, indicating that there are no strong deviations from thermal equilibrium [68].

In conclusion, we report the measurement of the equation of state of the 2D SU(N) FHM across the Mott crossover for temperatures comparable with or below the hopping energy and we compare the experiment with state-of-the-art numerical models. Moreover, with direct access to a single 2D plane system, we can independently determine temperatures in the experiment with spatial resolution using density fluctuation analysis, which allows one to e.g. cross-check thermal equilibrium. This measurement characterizes the EoS also in regimes hard to reach by current numerical methods. When compared to the experimental data, we find the theoretical calculations describe well the properties of the SU(N) gas for the applicable range of temperatures. The temperature measurements also indicate that thermal equilibration is not inhibited even in the case of deep lattices in a temperature range where the onset of spin correlations between sites is expected.

The implementation of the directly accessible 2D ensemble, together with the accompanying theoretical description, paves the way toward more direct quantum simulation of the typically 2D models of interest in naturally occurring systems with SU($N > 2$) representations such as transition metal oxides and orbitally selective Mott transitions. An intriguing example is the case of cerium volume collapse, where there is a long-standing debate whether the single orbital Hubbard model ($N = 2$) or the double-orbital Hubbard model ($N = 4$) [88–91] is the correct description. While in the condensed matter examples the SU(N) symmetry is typically only approximately realized; cold atom representations provide an essentially exact realization of SU(N), allowing one to implement fully SU(N)-symmetric and previously purely theoretical models. It should even be possible to smoothly connect both regimes in a continuous way by controlled symmetry breaking using e.g. optical state manipulation or state-dependent potentials [32,39,92], but more generally alkaline-earthlike quantum simulations of SU(N) FHM can provide insight into the validity of the SU(N) approximation in more realistic models.

We thank Alexander Impertro for his contributions in the early phase of the experiment. We thank Hao-Tian Wei for useful conversations and the exact diagonalization code used in the NLCE. N. D. O. acknowledges funding from the International Max Planck Research School for Quantum Science and Technology. E. I. G. P. is supported by Grant No. DE-SC-0022311, funded by the U.S. Department of Energy, Office of Science, and acknowledges support from the Robert A. Welch Foundation (C-1872) and the National Science Foundation (PHY-1848304). K. H. acknowledges support from the Robert A. Welch Foundation (C-1872) and the National Science Foundation (PHY-1848304), and the W. F. Keck Foundation (Grant No. 995764). Computing resources were supported in part by the Big-Data Private-Cloud Research Cyberinfrastructure MRI award funded by NSF under Grant No. CNS-1338099 and by Rice University's Center for Research Computing (CRC). K. H.'s contribution benefited from discussions at the Aspen Center for Physics, supported by the National Science Foundation Grant No. PHY1066293, and the KITP, which was supported in part by the National Science Foundation under Grant No. NSF PHY1748958. R. T. S. is supported by Grant No. DE-SC0014671 funded by the U.S. Department of Energy, Office of Science.

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