Dynamics of Thermalization in Small Hubbard-Model Systems

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We study numerically the thermalization and temporal evolution of a two-site subsystem of a fermionic Hubbard model prepared far from equilibrium at a definite energy. Even for very small systems near quantum degeneracy, the subsystem can reach a steady state resembling equilibrium. This occurs for a nonperturbative coupling between the subsystem and the rest of the lattice where relaxation to equilibrium is Gaussian in time, in sharp contrast to perturbative results. We find similar results for random couplings, suggesting such behavior is generic for small systems.

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Understanding the origin of statistical mechanics from a purely quantum-mechanical description is an interesting area of active research [1–9]. Of particular interest is the situation of an isolated quantum system partitioned into a subsystem and a bath. We ask the question: how do observables on the subsystem thermalize when the total system is in a pure state? Seminal works [1,2] have demonstrated the concept of "canonical typicality" that most random pure states of well-defined energy for the total system lead to thermalized reduced density matrices (RDMs) for the small subsystem. Numerical works have demonstrated thermalization in spin or boson systems for various observables of the subsystem [3–5] (and of the entire closed system [6,10]). Recent theoretical work [11] has investigated whether thermalization of small subsystems, initially far from equilibrium, is generic.

In this Letter, we investigate the temporal relaxation towards a steady state, focusing on the regime where the steady state appears thermalized. We consider a small Hubbard ring of fermions away from half-filling, with two adjacent sites as a subsystem and the other sites as a bath. We prepare the system in a product state of subsystem and bath pure states in a narrow energy window. Even for such a small system, we find a steady-state RDM close to a thermal state, down to quantum degenerate temperatures. Moreover, we find that the RDM diagonal elements approach a steady state as an exponential decay for weak subsystem-bath coupling. This becomes a Gaussian decay at a nonperturbative coupling, with a decay rate that departs significantly from the Fermi golden rule. We note that this is distinct from the Gaussian behavior in driven systems that remain out of equilibrium [12], and in decoherence dynamics [13] of off-diagonal RDM elements in systems that cannot thermalize.

The Model.—Taking motivation from cold atoms in optical lattices [14,15] where local addressing is possible, we study a local cluster in a generic (nonintegrable) interacting system with a quasicontinuous spectrum. We will examine how a local subsystem (S) thermalizes with the rest of the system as a bath (B) via unitary evolution of the whole system under the Hamiltonian $H = H_S + H_B + \lambda V$ where H_S (H_B), with eigenstates $|s\rangle_S$ ($|b\rangle_B$) of energy ε_s (ϵ_b), acts solely on the subsystem (bath). λV is the coupling between the subsystem and the bath. For $\lambda = 0$, the eigenstates are products of subsystem and bath eigenstates, denoted $|sb\rangle$, with energies $E_{sb} = \varepsilon_s + \epsilon_b$. The homogeneous case corresponds to $\lambda = 1$. Specifically, we choose a two-site subsystem in an L-site Hubbard ring of fermions:

$$\begin{aligned} H_S &= -\sum_{\sigma=\uparrow,\downarrow} J_\sigma (c^\dagger_{1\sigma} c_{2\sigma} + \text{H.c.}) + U(n_{1\uparrow}n_{1\downarrow} + n_{2\uparrow}n_{2\downarrow}), \\ H_B &= -\sum_{i=3}^{L-1} \sum_{\sigma=\uparrow,\downarrow} J_\sigma (c^\dagger_{i\sigma} c_{i+1,\sigma} + \text{H.c.}) + U\sum_{i=3}^{L} n_{i\uparrow}n_{i\downarrow}, \\ V &= -\sum_{\sigma=\uparrow,\downarrow} J_\sigma [(c^\dagger_{2\sigma} c_{3\sigma} + c^\dagger_{1\sigma} c_{L\sigma}) + \text{H.c.}], \end{aligned} \tag{1}$$

where $n_{i\sigma} = c^\dagger_{i\sigma} c_{i\sigma}$ is the number operator on site i with spin σ. The lattice is a ring with the subsystem sites at $i =$ 1, 2 and bath sites at $i = 3$ to L. The hopping integrals are $J_\sigma = J[1 + \xi \text{sgn}(\sigma)]$, with a nonzero $\xi = 0.05$ to remove level degeneracies due to spin rotation symmetry. We set the on-site repulsion $U = J$ to give us a metallic system with interacting bath modes while avoiding the formation of strong features in the many-body density of states at $U \gg J$ arising from Hubbard interactions. We will let J be the unit of energy. This Hamiltonian preserves the total particle number N and spin component S^z, but not the total spin S^2. In this work, we fill the $L = 9$ lattice with 8 fermions of total spin $S^z = 0$. The two-site subsystem has 16 eigenstates and the bath has 8281 eigenstates, while the composite system has a total of 15 876 states with average level spacing $\Delta \simeq 10^{-3}$. This is small enough to allow exact diagonalization, but large enough to provide a smooth density of states.

Consider a system prepared in a pure state of the form

$$|\Psi(t=0), E_0\rangle = \sum_{b_i=b_l}^{b_u} \frac{1}{\sqrt{B}} |s_i b_i\rangle, \tag{2}$$

where $|s_i\rangle_S$ is the initial subsystem state, e.g., $|\uparrow,\uparrow\rangle_S$ with parallel spins on the two sites. $|\Psi(t=0)\rangle$ contains a linear combination of B bath eigenstates $|b_i\rangle_B$ within an energy shell of width δ_B, chosen such that $\langle\Psi|H|\Psi\rangle = E_0$. The width δ_B ($=0.5$ in this work) is small on the scale for variations in the density of states. The system evolves in time: $|\Psi(t)\rangle = e^{-iHt}|\Psi(0)\rangle$. The subsystem is described completely by the RDM which traces over the bath states $|b\rangle_B$: $\rho(t) = \mathrm{Tr}_B|\Psi(t)\rangle\langle\Psi(t)|$. This is evaluated using the eigenstates of H from exact diagonalization.

Equilibrium states.—Before discussing relaxation dynamics during thermalization, we identify first the parameter regime where ρ does relax to thermal equilibrium. We say that a subsystem thermalizes if its RDM $\rho(t)$ approaches the thermal RDM ω after some time t (shorter than Δ^{-1}). The thermal RDM, ω, is diagonal with elements $\omega_{ss} = {}_S\langle s|\omega|s\rangle_S \propto N_B(E_0 - \varepsilon_s, N - n_s, S^z - s_s^z)$, where $|s\rangle_S$ is a subsystem eigenstate $|s\rangle_S$ with energy ε_s, n_s particles and spin s_s^z and $N_B(E, n_b, s_b^z)$ is the number of bath states with energies in $[E, E+\delta E]$ with n_b particles and spin s_b^z. We have to specify energy, number, and spin because they are globally conserved by the Hamiltonian H. We can define an effective temperature $T = [\partial \log N_B/\partial E|_{E_0}]^{-1}$ provided that the system is in a state with energy uncertainty $\delta E \gg \Delta$, the level spacing. (In the thermodynamic limit, ω takes the form of a Gibbs canonical distribution [10]—if particles are not exchanged with the bath, $\omega_{ss} \propto e^{-\varepsilon_s/T}$.)

We now present our results for a system starting from the initial states (2). We avoid the regime of very small subsystem-bath coupling λ where the subsystem RDM, ρ, is strongly dependent on the initial state even at long times due to finite-size effects. Nevertheless, we find that even such a small system can reach a steady state for couplings λ larger than a surprisingly small crossover value $\lambda_{\mathrm{th}} \ll 1$. The RDM becomes virtually diagonal—even the sum over the fluctuating off-diagonal elements, $[\sum_{s\neq s'} r_{ss'}^2]^{1/2}$, is 10^{-1} to 10^{-3} smaller than each diagonal element. Figure 1 shows the steady-state values of the diagonal elements of the RDM, $r = \lim_{\tau\to\infty}\int_0^\tau \rho(t)dt/\tau$ as a function of the composite energy E_0 for a coupling of $\lambda = 0.5$. For a variety of initial states, $\rho(t)$ is only weakly dependent on the details of the initial state at long times for $-3 \lesssim E_0 \lesssim 6$, approaching the thermal form ω expected from the canonical ensemble.

Next, we establish the range of the coupling λ over which the system forgets its initial state and thermalizes. We expect the system to retain memory of the initial state at weak coupling ($\lambda \ll 1$). Moreover, for $\lambda \gg 1$, the eigenspectrum becomes significantly altered by the coupling, splitting into several bands and we see oscillations. This is a feature of the projection of the initial state on the strongly coupled link. Therefore, we expect that the loss of memory of the initial state and thermalization are possible only in a range of intermediate couplings. To quantify this, we calculated the root-mean-square variation in diagonal RDM elements due to using different initial subsystem states: $\Delta r = \frac{1}{2}\sum_s[\langle r_{ss}^2\rangle - \langle r_{ss}\rangle^2]^{1/2}$, with $\langle\ldots\rangle$ averaging over all 16 initial states in the subsystem Fock basis (i.e., eigenstates at $J=0$). A small Δr indicates memory loss. We have also measured the closeness to the thermal state ω using $\sigma_\omega = \frac{1}{2}\sum_s\langle|r_{ss} - \omega_{ss}|\rangle$. We see from Fig. 2 that memory loss and thermalization occur in the intermediate range $\lambda_{\mathrm{th}} \lesssim \lambda \lesssim 3$ with crossover value $\lambda_{\mathrm{th}} \simeq 0.1$ at $E_0 = -2$ and 1.77.

We also find that the relative probabilities of different states in the $n_s = 2$, $s_s^z = 0$ sector fit a Boltzmann form: $\log r_{ss} = -\varepsilon_s/T_{\mathrm{eff}} + \mathrm{const}$. For states near the center of

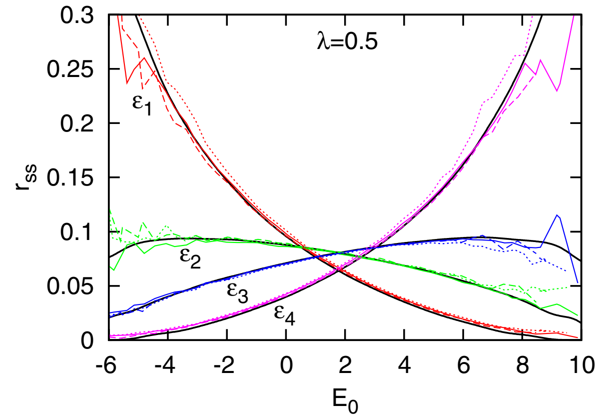

FIG. 1 (color online). Time average of diagonal RDM elements, r_{ss}, for the $n_s = 2$, $s_s^z = 0$ sector as a function of composite energy E_0, for initial subsystem states $|\uparrow\downarrow,\uparrow\rangle_S$ (solid line), $|\uparrow,\uparrow\rangle_S$ (dashed), and $|\uparrow,\downarrow\rangle_S$ (dotted). The four elements are labeled by their energies, ascending from ε_1 to ε_4. Thick lines: the corresponding elements for the thermal state ω, found by counting bath states with spin $S^z - s_s^z$ and $N - n_s$ particles within a Gaussian energy window of width $\delta E = 0.5$, centered on energy $E_0 - \varepsilon_s$.

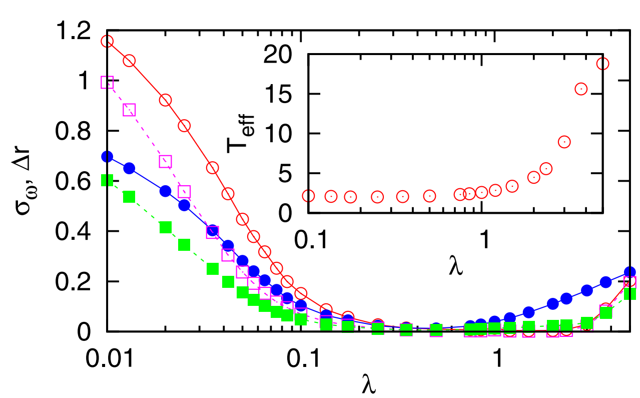

FIG. 2 (color online). Dependence on the initial state Δr (solid) and distance from the thermal state σ_ω (hollow) as a function of coupling λ, at composite energies $E_0 = -2$ (circle) and 1.77 (square). Inset: effective temperature T_{eff} for $E_0 = -2$.

the eigenspectrum ($E_0 \simeq 1.77$), the effective temperature $T_{\rm eff}$ is infinite. At $E_0 = -2$, we find $T_{\rm eff} \simeq 2$ up to $\lambda \sim 2$ (Fig. 2, inset). We estimate the chemical potential to be $2J \simeq 2$ so that, unlike in previous work, we see thermalization at temperatures down to quantum degeneracy.

We note that these thermalized systems are surprisingly small. Popescu *et al.* [2] give an estimate of the number d_R of composite-system eigenstates spanned by the initial state sufficient for thermalization—if the probability that $\sigma_\omega > Y = 0.1$ is at least as small as $X = 0.01$, then $d_R > (9\pi^3/2Y^2)\ln(2/X) \simeq 70\,000$. This is almost 2 orders of magnitude larger than the number of states ($\gtrsim \delta_B/\Delta$) spanned by our initial state which is as low as 950. Moreover, we find thermalization at $U = J$ for smaller systems than at $U \ll J$. We believe strong inelastic scattering in the interacting bath enables efficient thermalization at $U = J$ when system size is larger than the inelastic scattering length ($\propto J^2/U^2$ for small U/J).

Time evolution.—Having established the coupling range for thermalization for model (1), we will now discuss our main results for the temporal relaxation towards the steady state. Figure 3 shows examples of the time evolution of the diagonal RDM element $\rho_{ss}(t)$ with $s = s_i$ for two coupling strengths. This should decay from unity. The system is again prepared in the product state (2) with $|s_i\rangle_S = |\uparrow,\uparrow\rangle_S$. These results are computed for energy $E_0 = -2$. We do not expect our results to depend strongly on E_0 unless the system is close to a strongly correlated ground state.

We find qualitatively different relaxation behavior for perturbative and nonperturbative couplings (Fig. 3). Whereas the RDM relaxes towards the steady state exponentially in time at weak coupling ($\lambda < \lambda_{\rm exp}$), the relaxation follows a Gaussian form at larger coupling ($\lambda > \lambda_{\rm Gauss}$). Interestingly, this Gaussian regime covers the coupling range where the system thermalizes.

We can understand our results at short times or weak coupling. At short times, we can approximate $|\Psi(t)\rangle \simeq (1 - iHt)|\Psi(0)\rangle$. It can be shown (and our numerics agree) that the element $\rho_{s_is_i}(t) \simeq 1 - \Gamma_1^2 t^2$ for $t < t_1 = 1/\max(E_{sb} - E_0)$, with $\Gamma_1 = \lambda[\sum_{s\neq s_i,b}|\langle sb|V|\Psi(0)\rangle|^2]^{1/2}$. The maximum energy difference between states coupled by hopping (V) is of the order of the single-particle bandwidth $4J$ and so $t_1 \simeq 1/4$.

At weak coupling, we can go beyond t_1 by treating the coupling λV as a perturbation to the uncoupled Hamiltonian $H_S + H_B$. It is readily shown that, to leading order in λ, the RDM element corresponding to a subsystem state $s \neq s_i$ is approximated by $\tilde\rho(t)$:

$$\tilde\rho_{\,ss}(t) = \frac{4\lambda^2}{B}\sum_b \left|\sum_{b_i=b_l}^{b_u} \frac{\sin[(E_{sb} - E_{s_ib_i})\frac{t}{2}]}{E_{sb} - E_{s_ib_i}}\langle sb|V|s_ib_i\rangle\right|^2 \quad (3)$$

after the composite system is prepared in the state (2). The element $\tilde\rho_{s_is_i}$ is most readily found by using $\mathrm{Tr}(\tilde\rho) = 1$ to give $\tilde\rho_{s_is_i}(t) = 1 - \sum_{s\neq s_i}\tilde\rho_{ss}(t)$. This perturbation theory is valid until time t_2 when $\rho_{s_is_i}$ has dropped significantly below unity. For times between t_1 and t_2, Eq. (3) follows the Fermi golden rule (FGR): $\rho_{s_is_i}(t)$ decreases linearly in time with $d\rho_{s_is_i}/dt \propto -\lambda^2$. Beyond the FGR regime, we expect to see exponential decay (see, e.g., approximate Markovian schemes of the Lindblad type [16]) as is found in our data (Fig. 3, left) for $\lambda \lesssim \lambda_{\rm exp} = 0.1$. In our case, the initial state is not a bath eigenstate. This gives small fluctuations on top of a simple linear-t decay, due to interference between terms in the inner sum in (3).

We check in Fig. 4 that the FGR prediction agrees quantitatively with $d\rho_{s_is_i}/dt|_{t=0}$ for $E_0 = -2$ and 1.77, found from the parameters obtained for the exponential fit to $\rho_{s_is_i}$ for $t > t_1$: $\rho_{s_is_i}(t) \sim Ae^{-(t-t_0)/\tau} + (1 - A)$. The FGR rate $\gamma_{\rm FGR}$ is found by averaging (3) over a time t between t_1 and t_2: $-\gamma_{\rm FGR}t = \int_0^t[\tilde\rho_{s_is_i}(t') - 1]dt'/t$. This procedure is needed for a nonzero level spacing Δ. We point out that the exponential fit fails at very weak coupling ($\lambda \sim 10^{-2}$) when the system barely relaxes.

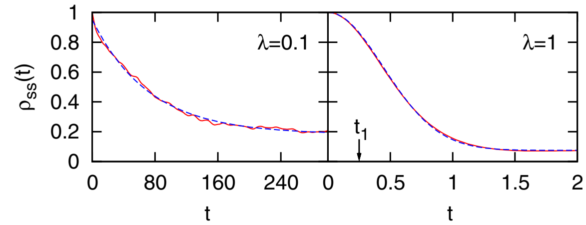

FIG. 3 (color online). The RDM element ρ_{ss} as a function of time t with $s = |\uparrow,\uparrow\rangle$ for the initial state (2) at total energy $E_0 = -2$ ($T_{\rm eff} \simeq 2$) with $s_i = s$. Left: coupling $\lambda = 0.1$ with exponential fit (dashed). Right: $\lambda = 1$ with Gaussian fit (dashed).

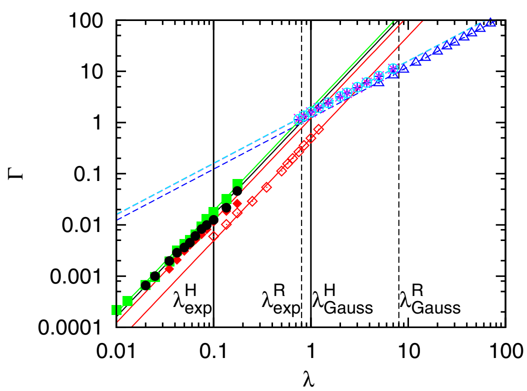

FIG. 4 (color online). Rates of decay of $\rho_{s_is_i}$ for the subsystem state $s_i = |\uparrow,\uparrow\rangle$ with initial state (2) at $E_0 = -2$ (● or +) and 1.77 (■ or ×) and random model at $E_0 = -2$ (○ or △). Weak coupling or exponential decay: $-d\rho_{s_is_i}/dt|_{t=0}$ at short times found from exponential fits (●,■,○) agree with Fermi golden rule prediction, $\gamma_{\rm FGR}$ (solid lines, gradient 2). Moderate coupling or Gaussian decay: fit to Gaussian with rate Γ (×, +, △) agrees with Γ_1 (dashed lines, gradient 1). Vertical lines mark estimates of the crossover values $\lambda_{\rm exp}$ and $\lambda_{\rm Gauss}$ [λ^H (λ^R) for Hubbard (random) models]. Data in the crossover region are rates obtained from attempted fits to either form.

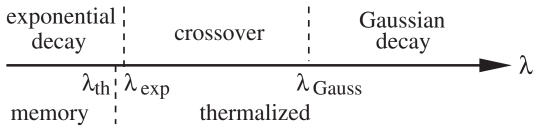

FIG. 5. Schematic behavior of the reduced density matrix $\rho(t)$ as a function of subsystem-bath coupling λ. Top: relaxation to steady state. Bottom: steady state of $\rho(t)$. Memory of initial state also occurs at large λ in the Hubbard case.

We now consider larger couplings where $\lambda \sim O(1)$. Instead of exponential relaxation, we find a good fit (Fig. 3, right) to a Gaussian decay: $\rho_{s_i s_i}(t) \sim Ce^{-\Gamma^2 t^2} + (1 - C)$. This is seen for couplings $\lambda \gtrsim \lambda_{\text{Gauss}} = 1$. The decay rate Γ now increases linearly with λ and is as large as the bandwidth scale $1/t_1 \simeq 4$. It appears insensitive to energy E_0. Interestingly, we see in Fig. 4 that, in the regime where $\Gamma t_1 \sim 1$, the decay rate Γ is well approximated by Γ_1 from the short-time expansion, which suggests $\Gamma = \Gamma_1/C^{1/2}$. (In our data, $0.97 < C^{1/2} < 1$.) In other words, perturbation theory gives the early-time precursor to the full Gaussian form. This suggests the interpretation that the time interval of validity of the Fermi golden rule ($t_1 < t < t_2$) narrows and vanishes as λ increases to λ_{Gauss}. For coupling range $\lambda_{\text{exp}} < \lambda < \lambda_{\text{Gauss}}$, the behavior is less clear-cut—the decay starts as a Gaussian but becomes exponential at later times. The amplitude of this exponential tail decreases with increasing λ, becoming negligible as λ reaches λ_{Gauss}.

Random couplings.—To verify that the two regimes of relaxation are not specific to our model Hamiltonian, we proceeded to study an alternative model where the subsystem-bath coupling V is replaced by a random Hermitian matrix W which still respects the conservation of the global particle number N and spin S^z. Each nonzero matrix element of W is Gaussian distributed, with the variance chosen such that $\text{Tr}(W^2) = \text{Tr}(V^2)$. Thus, we can compare $H = H_S + H_B + \lambda V$ with $H = H_S + H_B + \lambda W$ with similar decay rates. In this model, we expect $1/t_1$ to be of the order of the full bandwidth ~ 20 for $N = 8$, $S^z = 0$. We find exponential relaxation at weak coupling, $\lambda \lesssim \lambda_{\text{exp}} = 0.8$, and we recover Gaussian relaxation with a linear-λ decay rate for $\lambda \gtrsim \lambda_{\text{Gauss}} = 8$ (Fig. 4, hollow symbols). The crossover values λ_{exp} and λ_{Gauss} occur at nominally higher couplings than for the Hubbard ring (1). They become closer to the Hubbard-ring values if we mimic the structure of V by restricting the states coupled by W: $\langle s'b'|W|sb\rangle \neq 0$ only if $|E_{s'b'} - E_{sb}| < 4J$, the single-particle bandwidth.

We summarize our results in Fig. 5. We have shown that a two-site subsystem of the Hubbard model relaxes to steady states resembling canonical thermal states, even for systems with a handful of sites and at quantum degenerate energies. This occurs at a nonperturbative coupling between the subsystem and bath, corresponding to nearly homogeneous systems. In this regime, the reduced density matrix $\rho(t)$ displays Gaussian relaxation to the thermal state, with a decay rate Γ linear in the coupling λ. This contrasts sharply with the perturbative regime where $\rho(t)$ exhibits an exponential relaxation with a λ^2 decay rate. We believe that the Gaussian relaxation to thermalization is a generic feature of closed nanoscale systems, as is supported by our results for random Hamiltonians.

Finally, we note that it can be shown that $\Gamma_1 t_1 \sim \lambda J t_1 \sim \lambda$ irrespective of system size. The subsystem thermalizes on the time scale of a few hops between the subsystem and the bath, by inelastic collisions of the fermions within this time scale. This should be insensitive to system size for systems larger than the inelastic scattering length. Therefore, we speculate that the observed Gaussian relaxation should remain for large systems.

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