Resonant Thermalization of Periodically Driven Strongly Correlated Electrons

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We study the dynamics of the Fermi-Hubbard model driven by a time-periodic modulation of the interaction within nonequilibrium dynamical mean-field theory. For moderate interaction, we find clear evidence of thermalization to a genuine infinite-temperature state with no residual oscillations. Quite differently, in the strongly correlated regime, we find a quasistationary extremely long-lived state with oscillations synchronized with the drive (Floquet prethermalization). Remarkably, the nature of this state dramatically changes upon tuning the drive frequency. In particular, we show the existence of a critical frequency at which the system rapidly thermalizes despite the large interaction. We characterize this resonant thermalization and provide an analytical understanding in terms of a breakdown of the periodic Schrieffer-Wolff transformation.

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Recent advances in the ability to tailor and control light-matter interaction on an ultrafast timescale [1–4] have brought increasing interest in the manipulation of quantum phases of matter with periodic *driving* fields. Notable achievements are light-induced superconductivity [5,6], metal-to-insulator transition [7], and control of microscopic parameters such as the local interaction in organic Mott insulators [8] and the band gap in excitonic insulators [9]. Similar ideas are applied to ultracold atoms in optical lattices [10] where driving fields are used, for instance, to engineer topological states [11].

From a theoretical perspective, periodically driven, or *Floquet*, quantum systems are a long-standing subject of studies ranging from dynamical localization [12] and quantum dissipation [13] to quantum chaos [14] and, more recently, isolated quantum many-body systems [15]. Other topics of active research include drive-induced topological states [16,17] and artificial gauge fields [18], driven electron-phonon coupling [19–21], and integrable systems [22], correlated electrons [23–26], or topological systems [27,28] in the presence of dissipation.

In the absence of integrability and of many-body localization, isolated out-of-equilibrium quantum many-body systems are expected to show thermalization of local observables at long times [29]. Driven systems, which lack time translational invariance, are therefore brought to *thermalize* to a featureless infinite-temperature state consistent with maximum entropy and no energy conservation [30–33]. Yet, the transient dynamics may leave space to nontrivial extremely long-lived nonthermal states characterized by oscillations synchronized with the drive, a phenomenon known as Floquet prethermalization. This prethermal behavior can emerge in the high frequency limit [34–40] or be the consequence of a nearby integrable point in the system parameter space. In this case, as recently observed for weakly [41–43] and strongly [44,45] interacting systems, there are many quasi-integrals of motion that prevent thermalization except at very long times, similarly to what happens after a quantum quench [46]. However, many intriguing questions remain wide open especially concerning the intermediate coupling and frequency regimes, where the most remarkable phenomena are expected to occur.

In this Letter we consider the Fermi-Hubbard model as a paradigmatic example of strongly correlated electrons. The system is subject to a time-periodic modulation of the electron interaction, but it is otherwise isolated from any external reservoir. Starting from a thermal equilibrium state, we use nonequilibrium dynamical mean-field theory (DMFT) [47] to calculate the time evolution induced by the drive. First, we explicitly show that at moderate interaction the system thermalizes to the infinite-temperature state. Then, we turn to the regime of large interaction and find a long-lived prethermal state synchronized with the drive, except for a critical, resonant frequency where we find thermalization and a behavior reminiscent of a dynamical transition [48–50]. A periodic Schrieffer-Wolff transformation shows that the Floquet prethermalization is due to the quasiconservation of double occupancy at large interaction, with the resonant thermalization emerging in correspondence of a break down of such an expansion.

The system is governed by the following Hamiltonian:

$$H(t)=\sum_{i,j}\sum_{\sigma=\uparrow,\downarrow}V_{ij}c^{\dagger}_{i\sigma}c_{j\sigma}+U(t)\sum_{i}\left(n_{i\uparrow}-\frac{1}{2}\right)\left(n_{i\downarrow}-\frac{1}{2}\right), \tag{1}$$

where $U(t) = U_0 + \delta U \sin \Omega t$ is the periodically driven interaction and V_{ij} is the hopping, which is such that the bare density of states reads $\rho(\epsilon) = \sqrt{4V^2 - \epsilon^2}/(2\pi V^2)$ (Bethe lattice). We take V as unit of energy, frequency, and inverse of time ($\hbar = 1$). In these units the bare bandwidth is $W = 4$ and the critical point of the Mott transition in DMFT is at $U_c \simeq 4.8$ and at an inverse temperature $\beta_c \simeq 20$. We consider a thermal initial density matrix $\rho(0) = \exp[-\beta H(0)]$ with $\beta = 5$ and we fix the drive amplitude $\delta U = 2$ (cf. Supplemental Material [51], Sec. I). For all times the interaction remains repulsive and the system stays half-filled ($\langle n_\sigma \rangle = 0.5$) and particle-hole symmetric.

To calculate the time evolution induced by the drive we use nonequilibrium DMFT [47], which consists in mapping the lattice model described by Eq. (1) onto a quantum impurity problem with the following action:

$$\mathcal{S} = \mathcal{S}_{\rm loc} + \int_{\mathcal{C}} dt dt' \sum_{\sigma=\uparrow,\downarrow} c^\dagger_\sigma(t) \Delta_\sigma(t,t') c_\sigma(t'), \tag{2}$$

where $\mathcal{S}_{\rm loc}$ is the action associated with the local term in Eq. (1), $\mathcal{C}$ is the three branch Keldysh contour [52], and $\Delta_\sigma(t,t') = V^2 G_\sigma(t,t')$ is the hybridization between the impurity and a nonequilibrium bath, which is self-consistently determined from the impurity Green function $G_\sigma(t,t') = -i\langle T_{\mathcal{C}} c_\sigma(t) c^\dagger_\sigma(t')\rangle$. Within the DMFT mapping, the impurity Green function coincides with the local lattice Green function and from it we can calculate various quantities directly in the thermodynamic limit, such as the double occupancy $d(t) = \langle n_{i\uparrow}(t) n_{i\downarrow}(t)\rangle$ and the kinetic energy $K(t) = \sum_{ij\sigma} V_{ij} \langle c^\dagger_{i\sigma}(t) c_{j\sigma}(t)\rangle$. The computation of the impurity Green function is a challenging task and, despite recent progresses [53–55], an efficient and numerically exact approach is still lacking. Here we resort to the noncrossing approximation [56–63] which consists of a first order self-consistent hybridization expansion and which we implement through a Dyson equation for the impurity atomic-state propagator (cf. Supplemental Material [51], Sec. III). For moderate interaction, we benchmark the results with the next-order one-crossing approximation (cf. Supplemental Material [51], Sec. IV).

We start by discussing the results for moderate average interaction $U_0 = 4$ (Fig. 1). The double occupancy shows fast oscillations with frequency comparable to the one of the drive Ω superimposed to a slower but exponential relaxation. Quite interestingly, after the initial transient and despite the continuous driving, the oscillations get fully damped and the double occupancy reaches the value $d_{\rm th} = 0.25$ independently of the frequency. This is the value of a maximally disordered state and as such signals the thermalization to infinite temperature. With an exponential fit we can extract the thermalization time $\tau_{\rm th}$ which is minimum for $\Omega \simeq 4.8$ and diverges for large frequency.

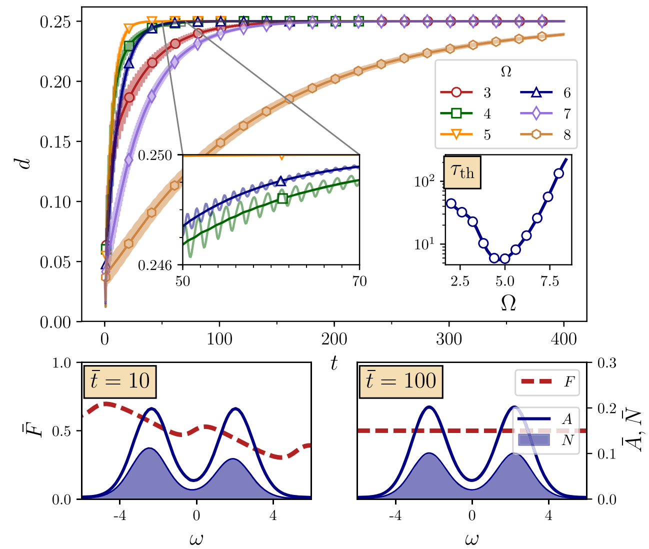

FIG. 1. Thermalization to infinite temperature ($U_0 = 4$). Top panel: Double occupancy $d(t)$ for various drive frequencies Ω shows oscillations (shade) on top of an exponential relaxation (solid line). Right inset: Thermalization time $\tau_{\rm th}(\Omega)$. Bottom panels: Averaged spectral function $\bar{A}(\omega, \bar{t})$, occupation function $\bar{N}(\omega, \bar{t})$, and distribution function $\bar{F}(\omega, \bar{t}) = \bar{N}(\omega, \bar{t})/\bar{A}(\omega, \bar{t})$ for $\Omega = 4$ show the evolution from the out-of-equilibrium state at $\bar{t} = 10$ to the infinite-temperature thermal state at $\bar{t} = 100$.

Thermalization is confirmed by the evolution of the Green function and, in particular, of the retarded component $G^R_\sigma(t,t') = -i\theta(t-t')\langle\{c_\sigma(t), c^\dagger_\sigma(t')\}\rangle$ and the lesser component $G^<_\sigma(t,t') = i\langle c^\dagger_\sigma(t') c_\sigma(t)\rangle$. In a thermal state these functions depend only on the difference $t - t' = \tau$ and their Fourier transform is related by the fluctuation-dissipation theorem. Out of equilibrium one can perform a Fourier transform with respect to τ at fixed $\bar{t} = (t+t')/2$ [64] and obtain the spectral function $A(\omega, \bar{t}) = -1/\pi \sum_\sigma {\rm Im} G^R_\sigma(\omega, \bar{t})$ and the occupation function $N(\omega, \bar{t}) = i/(2\pi) \sum_\sigma G^<_\sigma(\omega, \bar{t})$. As a consequence of the time-dependent interaction, these functions have oscillations in $\bar{t}$ with period $T = 2\pi/\Omega$ and are even negative for some ω. To extract meaningful information about the thermalization, which happens on times $\tau_{\rm th} \gg T$, we average $A(\omega, \bar{t})$ and $N(\omega, \bar{t})$ over a few periods and obtain positive $\bar{A}(\omega, \bar{t})$ and $\bar{N}(\omega, \bar{t})$ (cf. Supplemental Material [51], Sec. V). The distribution function $\bar{F}(\omega, \bar{t}) = \bar{N}(\omega, \bar{t})/\bar{A}(\omega, \bar{t})$ provides a simple indicator for thermalization since in the thermal state it equals the Fermi-Dirac distribution. In this case at early times we observe a nonthermal distribution with a pseudoperiodic structure in ω with period Ω. This feature is related to the so-called Floquet subbands characteristic of periodically driven systems [23]. Then, at later times we observe a remarkably flat distribution—clearly the only one to be at the same time thermal and pseudoperiodic. This establishes that the fluctuation-dissipation relation is satisfied with infinite temperature and therefore confirms thermalization.

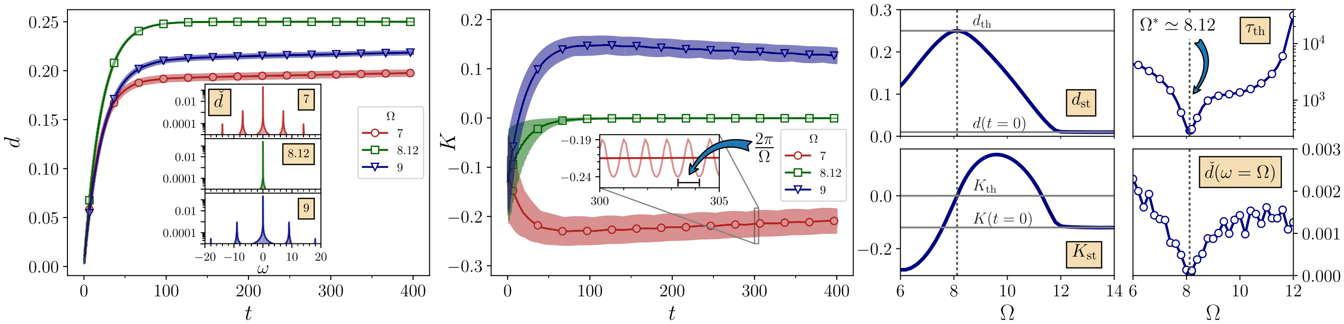

FIG. 2. Floquet prethermalization and resonant thermalization ($U_0 = 8$). Left panel: Double occupancy $d(t)$ for various drive frequencies Ω shows oscillations (shade) on top of an exponential relaxation (solid line). Central panel: same for kinetic energy. Inset of left panel: Fourier transform $\check{d}(\omega)$. Right panels: Top left: stationary value $d_{\mathrm{st}}(\Omega)$ with thermal value d_{th} and initial value $d(t=0)$ for reference. Bottom left: same for kinetic energy. Top right: estimated thermalization time $\tau_{\mathrm{th}}(\Omega)$. Bottom right: weight of the peak $\check{d}(\omega=\Omega)$. Dotted lines mark the resonant frequency $\Omega^* \simeq 8.12$. For $\Omega = 7, 9$ we see Floquet prethermalization with $d_{\mathrm{st}} \neq d_{\mathrm{th}}$, $K_{\mathrm{st}} \neq K_{\mathrm{th}}$ and $\check{d}$ peaked at $\omega = \pm\Omega, \pm 2\Omega$. For $\Omega = \Omega^*$ not only $d_{\mathrm{st}} = d_{\mathrm{th}}$ and $K_{\mathrm{st}} = K_{\mathrm{th}}$ but also the sharp minimum of $\tau_{\mathrm{th}}(\Omega)$ and the vanishing of $\check{d}(\omega=\Omega)$ signal the resonant thermalization.

We now turn to the strong coupling regime at large average interaction $U_0 = 8$ (Fig. 2). The transition from moderate interaction appears to be rather smooth (cf. Supplemental Material [51], Sec. I); however, for large interaction, in contrast with above, we find qualitative differences as a function of the drive frequency. As a first indication, while for short times also in this case local observables oscillate on top of an exponential relaxation, now the stationary value depends on frequency. As we detail in the following, this signals the existence of different dynamical regimes. In particular, we find thermalization and damping of the oscillations only for a critical frequency, which we estimate to be $\Omega^* \simeq 8.12$, while for the other frequencies we observe a long-lived prethermal state.

For frequency below Ω^* the double occupancy and the kinetic energy oscillate around an average which relaxes exponentially to a nonthermal plateau after the initial transient. While for moderate interaction these oscillations damp out, here they persist with constant amplitude. We calculate the Fourier transform $\check{d}(\omega) = \int_{\tau_{\mathrm{pth}}}^{t_{\max}} dt e^{i\omega t} d(t)$, where τ_{pth} is the prethermalization time when the plateau is attained and $t_{\max}$ is the maximum simulation time. The peaks of $\check{d}$ at multiples of Ω demonstrate the synchronization of the oscillations with the drive. This, together with the nonthermal value of the plateau, are the distinctive features of a Floquet prethermal state in which the system appears to be trapped for times longer than numerically accessible. Since the plateau has a slight linear positive slope, we can extrapolate it to intercept the thermal value $d_{\mathrm{th}} = 0.25$ and in this way estimate a thermalization time τ_{th} which turns out to be orders of magnitude larger than at moderate interaction.

For frequency above Ω^* we find a very similar prethermalization regime until, for $\Omega \simeq U_0 + W = 12$, we observe a sharp threshold behavior. This value corresponds to the maximum energy for single-particle excitations above which the system appears to be unable to absorb energy and local observables are almost constant and equal to their initial equilibrium values. Accordingly, the thermalization time grows exponentially with frequency, in agreement with rigorous bounds [35,39]. We remark also that, for a range of frequencies, the kinetic energy becomes positive, which is characteristic of a highly nonequilibrium state with population inversion. While a similar phenomenon is observed in other Floquet systems [24], here it cannot be ascribed to an effective change of sign of the interaction, since this would also cause the double occupancy to increase above 0.25.

The above picture radically changes for the critical frequency $\Omega^* \simeq 8.12$ where fast thermalization is found despite the large interaction. Here we observe an exponential relaxation of the double occupancy and of the kinetic energy to the thermal values, together with a full damping of oscillations. At this specific frequency the Floquet prethermal state is therefore melted away and the system is able to relax to the infinite-temperature thermal state. We name this phenomenon *resonant* thermalization since for Ω^* the periodic modulation of the interaction is resonant with the energy $\sim U_0$ of doublon excitations, i.e., excitations that change the double occupancy. This resonant condition allows the absorption of energy from the drive and the creation of doublons, which are otherwise suppressed by the large average interaction through a well-known bottleneck mechanism [65,66]. Remarkably, the behavior of the system around Ω^* is strongly reminiscent of a dynamical transition [48–50]. This is clearly seen in the estimated thermalization time $\tau_{\mathrm{th}}(\Omega)$ which has a sharp minimum for Ω^*, as well as from the peak at $\omega = \Omega$ of the Fourier transform $\check{d}(\omega)$. The weight of this peak goes to zero for Ω^* with singular behavior, indicating the breakdown of synchronization and the approach to the stationary thermal value.

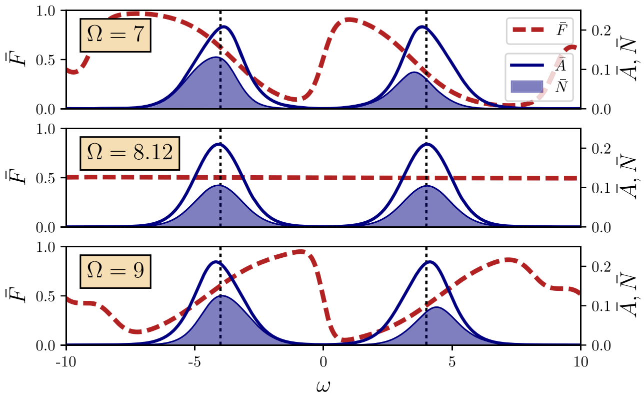

FIG. 3. Averaged spectral function $\bar{A}(\omega, \bar{t})$, occupation function $\bar{N}(\omega, \bar{t})$, and $\bar{F}(\omega, \bar{t}) = \bar{N}(\omega, \bar{t})/\bar{A}(\omega, \bar{t})$ for $U_0 = 8$ and $\bar{t} = 100$. Prethermalization for $\Omega = 7$, 9 and thermalization for $\Omega = \Omega^* \simeq 8.12$. For $\Omega = 9$ the population inversion is clear from the shift of $\bar{N}$ towards higher energy and the change of slop of $\bar{F}$ with respect to $\Omega = 7$. Dotted lines mark the approximate middle of the Hubbard bands.

The above results are corroborated by the evolution of the spectral, occupation, and distribution functions (Fig. 3). After the initial transient, these functions reach a stationary state independent of $\bar{t}$. This confirms that the plateau of the local observables corresponds to a true steady state of the system. For $\Omega \neq \Omega^*$ the distribution function $\bar{F}(\omega, \bar{t})$ is clearly nonthermal and pseudo-Ω periodic, as also found for the nonthermal transient at moderate interaction. On the opposite, for the critical frequency Ω^* we find a remarkably flat distribution which confirms the thermalization at infinite temperature. Interestingly, for $\Omega > \Omega^*$, corresponding to positive kinetic energy, we indeed find a population inversion, as it is clear from the shift towards high energy of $\bar{N}$ and the change of slope of $\bar{F}$ with respect to $\Omega < \Omega^*$.

To gain an analytical insight into the Floquet prethermalization and the resonant thermalization we use a Floquet Schrieffer-Wolff transformation [67–69]. This conveniently describes the strong coupling regime, where doublon excitations are suppressed because of the large average interaction, thus preventing the system from absorbing energy unless the frequency of the drive is resonant with the doublon energy. In practice, we introduce a time-periodic unitary $R(t) = \exp[S(t)]$ which eliminates perturbatively in V/U_0 the terms that do not conserve the double occupancy in the transformed Hamiltonian $\tilde{H} = e^S H e^{-S} - i\partial_t S$. This is obtained with an ansatz $S(t) = (V/U_0)[\alpha(t)K_+ - \alpha^*(t)K_-]$ where $\alpha(t)$ is a periodic function determined imposing the vanishing of the commutator $[\tilde{H}, \sum_i n_{i\uparrow} n_{i\downarrow}]$ up to terms of a given order in V/U_0, and where we decompose the kinetic energy in terms that do not change (K_0), increase (K_+), or decrease (K_-) the double occupancy (cf. Supplemental Material [51], Sec. VI). For generic drive frequency the transformation is well behaved and at first order in V/U_0 we find

$$d(t) = d(0) - 2(V/U_0)\mathrm{Re}\{\alpha(T)\mathrm{Tr}[\rho(0)K_+]\} + 2(V/U_0)\mathrm{Re}\{\alpha(t)e^{i\int_0^t U(t')dt'}\mathrm{Tr}[\rho(0)K_+(t)]\}, \quad (3)$$

where $K_+(t) \equiv e^{iVK_0 t}K_+ e^{-iVK_0 t}$. Equation (3) captures the Floquet prethermal state at long time multiples of $T = 2\pi/\Omega$ (stroboscopic evolution) when the double occupancy is synchronized with the drive and oscillates around a frequency-dependent nonthermal value. However, for the critical value $\Omega^* \simeq U_0$ and its submultiples, the function α develops a singularity and the transformation breaks down. This suggests that, at these frequencies, the Floquet prethermal state is unstable towards thermalization through nonperturbative processes in V/U_0, as captured by DMFT. Calculations at large interaction $U_0 = 14$ and drive amplitude $\delta U = 6$ clearly show the resonant thermalization for frequencies Ω^* and $\Omega^*/2$ (cf. Supplemental Material [51], Sec. II).

The results we have presented here have a potential impact on various experiments, ranging from ultracold atoms in driven optical lattices, where one should observe a sudden increase of the heating rate [70] at $\Omega = \Omega^*$, to photoexcited organic Mott insulators [8], where one should observe a sudden filling of the gap in the transient optical conductivity. We also envisage further theoretical study, in particular on the effect of nonlocal correlations in realistic lattices, which are likely to affect the lifetime of the prethermal plateau. Advances in the solution of the impurity problem would also be important, as they would permit further investigations of the transition between moderate and large interaction and the access to initial states at lower temperature.

In conclusion, to study periodically driven strongly correlated electrons, we have considered the Fermi-Hubbard model with time-periodic interaction. Within nonequilibrium DMFT we have calculated the evolution of local observables and of the local Green function, which provide evidence for thermalization or prethermalization. We have showed the existence of three dynamical regimes: (i) Thermalization to infinite temperature at moderate interaction, as expected for generic isolated quantum many-body systems; (ii) Floquet prethermalization at large interaction, characterized by oscillations of local observables around a nonthermal plateau and a stationary nonthermal distribution function; (iii) resonant thermalization at large interaction for an isolated critical frequency Ω^*, where local observables relax exponentially to the infinite-temperature thermal value, together with a damping of oscillations and a flat distribution function. We have then developed a periodic Schrieffer-Wolff transformation that captures the qualitative features of the Floquet prethermal state and whose breakdown for Ω^* indicates the nonperturbative nature of the resonant thermalization phenomenon.

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for details on the noncrossing and one-crossing approximations, the spectral analysis, and the Schrieffer-Wolff transformation.
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