Dynamical Unbinding Transition in a Periodically Driven Mott Insulator

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We study the double occupancy in a fermionic Mott insulator at half-filling generated via a dynamical periodic modulation of the hopping amplitude. Tuning the modulation amplitude, we describe a crossover in the nature of double occupancy from a Fermi Golden Rule regime to damped Rabi oscillations. The decay time of excited states diverges at a critical modulation strength, signaling the transition to a dynamically bound non-equilibrium state of doublon-holon pairs. A setup using a fermionic quantum gas should allow to study the critical exponents.

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We study the response of interacting fermions on a lattice due to periodic modulation of the hopping amplitude (shaking), combining strongly correlated and non-equilibrium physics in a Mott insulator. Specifically, we analyze a half-filled Hubbard model (one particle per site) in the intermediate-temperature regime and determine the generation of double occupancy due to the shaking of a single bond; the remaining bonds assume the role of a reservoir. We map this problem onto a well-known impurity problem, a single impurity coupled to a band of delocalized states. The pumped bond plays the role of the impurity, the excited doublon-holon states which propagate through the lattice constitute the band states, and the strength Ω of the time-dependent drive represents the hybridization V; the strong interactions of the Mott state at half-filling is mapped onto an effective renormalized density of states of the reservoir.

Dynamical generation of double occupancy (DGDO) in a Mott insulator was studied previously for a uniform modulation of all bonds in a one-dimensional (1D) system using numerical methods and in a 3D system using perturbation theory in Ω. This has led to a description of DGDO in terms of Fermi’s Golden Rule (FGR) providing the rate by which the double occupancy is changed. On the other hand, it was noted that for intermediate modulation strength (Ω of the order of 1) dynamical generation of double occupancy due to the shaking of a single bond is a non-perturbative process requiring us to include the drive in a non-perturbative way. The transition from FGR to coherent Rabi oscillations should be observed.

Here, we focus on the intermediate to large Ω regime requiring us to include the drive in a non-perturbative way. We find that, besides the FGR regime and the regime of damped Rabi oscillations studied before, an additional regime of undamped Rabi oscillations appears at very strong drive: if Ω exceeds a critical strength Ωc, the dynamically generated doublon-holon pair has no time to separate but is coherently pumped back to the initial state with one particle per site. For very strong coupling, such a non-equilibrium state does not carry delocalized excitations and is therefore insulating. In quantum optics, this corresponds to a saturated atomic transition. Reducing the driving power below Ωc, the system undergoes a transition where the size of the bound doublon-holon pair diverges and the two excitations unbind. Thus, the transition from the undamped to damped Rabi oscillations is a unbinding transition. The reverse transition with increasing drive induces binding by pushing an isolated bound state out of a continuous spectrum. This situation resembles that of repulsively-bound atom pairs in an optical lattice as recently observed in cold atomic gases. The specific model presented here is motivated by a recent experiment using modulation spectroscopy as a probe in a system of cold Fermi atoms subject to an optical lattice.

We begin with a discussion of the d-dimensional model system, a single impurity (c) at energy εc coupled to a band with dispersion εk centered around ω = 0 with band width 2W = 4dV; in the Hamiltonian

\[ H_c = ε_c|c⟩⟨c| + \sum_k ε_k|k⟩⟨k| + V(|0⟩⟨0| + |c⟩⟨c|), \]

|c⟩ and |k⟩ are the impurity and (N) continuum states, and |0⟩ = ∑k |k⟩/√N is a localized (Wannier) state within the continuum which is coupled to the impurity through the hybridization V. As the Hamiltonian describes a single particle problem, the Green’s function of the localized state can be obtained explicitly,

\[ G_c(ω) = \langle c| (ω - H_c)^{-1} |c⟩ \]

with \[ G_c(ω) = \langle 0| (ω - H_b)^{-1} |0⟩ = N^{-1} \sum_k (ω - ε_k)^{-1} \]

the local Green’s function of the band; here, \[ H_b \] denotes the Hamiltonian of the band states. The coupling of the impurity to the continuum shifts its energy to \( \bar{ε} = ε_c + \frac{1}{N} \sum_k P \frac{V^2}{\bar{ε} - ε_k} \)

and renormalizes its weight \( Z \); if the energy of the new level \( \bar{ε} \) resides within the band continuum, it acquires a
finite width $\Gamma$. We concentrate on the situation where the (unrenormalized) energy $\varepsilon_c$ is within the band, $|\varepsilon_c| \leq W$.

For small hybridization $V \ll w$, the Green’s function is well approximated by replacing the band’s Green’s function by its value at $\omega = \varepsilon_c$ and we obtain a local spectral function

$$A(\omega) = -\frac{1}{\pi} \text{Im} G_c(\omega + i0^+) \approx \frac{V^2 \rho(\varepsilon_c)}{(\omega - \varepsilon_c^2 + \Gamma^2/4)},$$

where, the oscillator strength resides in a single level with energy $\varepsilon \approx \varepsilon_c$ broadened by the FGR result $\Gamma = 2\pi V^2 \rho(\varepsilon_c)$, where $\rho(\omega) = -\text{Im} G_B(\omega + i0^+)/\pi$ is the local density of states at the origin (we set $\hbar = 1$). Equation 4 leads to an exponential decay of $G_c(t) \propto \exp(-\Gamma t/2)$ in time.

Increasing the hybridization $V$ reveals corrections to the pure exponential behavior. A better approximation is obtained by retaining the $\omega$-dependence in $\rho(\omega)$ in the numerator of 4 but not in the denominator [13]. This generalized FGR result explains the rounding of $G_c(t) \approx 1 - \frac{V^2 t^2}{2}$ at short times and the algebraic saturation $G_c(t) \propto 1/t^{d+1}$ at large times; here, the exponent $\mu$ describes the behavior of the density of states near the band edge, cf. below. At strong coupling, $V \gg w$, the Green’s function can be approximated by $G_B(\omega) \approx \omega^{-1}$ and $A(\omega)$ exhibits two $\delta$-functions at $\omega = \pm V$, each with weight $Z = 1/2$; these are bound states which do not decay. The oscillations of the Green’s function $G_c(t > 0) = -i \cos(Vt)$ can be interpreted as Rabi oscillations between the states $|c|$ and $|0|$; dropping the second term $\propto w$ in 4 as compared to the last $\propto V$, leaves us with an effective two-level Hamiltonian, thus elucidating this result.

The crossover between these two regimes (the main target of this letter) depends on the shape of the local density of states $\rho(\omega)$. Coupling a level to an unstructured continuum, the damping, although vanishing as $V \to \infty$, remains finite for any finite $V$ [8]. Coupling the level to a finite-width continuum, the result depends on the shape of $\rho(\omega) \sim (W + \omega)^\mu$ near the (upper/lower) band edge [13]. In a non-interacting system with quadratic dispersion the power $\mu$ is $(d - 2)/2$. For $\varepsilon$ close (but outside) the band, the sum in [3] scales as $\sim V^2 (W - \varepsilon)^\mu$. In 1D, $\mu = -1/2$, the term diverges as $\varepsilon \to \pm W$ approaches the band and a solution exists for arbitrary small $W$, i.e., however small the hybridization, there exist two localized eigenstates, one above and one below the band. In 2D, $\mu = 0$ and the term scales as $\sim V^2 \log(W + \varepsilon)$ leading to the same conclusion with states exponentially close to the band. In 3D with $\mu = 1/2$, a finite hybridization $V > V_c$ is necessary to satisfy [8] with $\varepsilon$ outside the band. The critical hybridization $V_c$ marks an unbinding transition: for $V < V_c$ there is no bound state in the system and $G_c(t \to \infty) \to 0$, whereas for $V > V_c$ part of the spectral weight remains trapped in a bound state for arbitrarily long time and $G_c(t \to \infty)$ remains finite (but oscillatory).

Below, we are interested in the DGDO signal of interacting lattice fermions periodically driven across one bond. We map this problem onto the above impurity problem, with the interaction and many-body aspects manifesting themselves in (i) the bath’s density of states, which is replaced by a two-particle continuum characterized by an exponent $\mu_2 = 2\mu_1 + 1 = d - 1$ for a noninteracting particles and $\mu_{BR} = 2$ for strongly correlated particles; (ii) the initial state of the bond, which can be occupied by a singlet or a triplet; (iii) multiple excitations, which are created subsequently. We describe the system of interacting lattice fermions at half-filling by the Hubbard Hamiltonian

$$H_H = -w \sum_{\langle i,j \rangle, \sigma} (c^\dagger_{i \sigma} c_{j \sigma} + c^\dagger_{j \sigma} c_{i \sigma}) + U \sum_i n_{i \uparrow} n_{i \downarrow}$$

and account for the harmonic modulation (frequency $\nu$) of the hopping $w$ over the bond $t = 1, 2$ via

$$H_{\text{osc}}(t) = \Omega \cos(\nu t) \sum_{\sigma} (c^\dagger_{1 \sigma} c_{2 \sigma} + c^\dagger_{2 \sigma} c_{1 \sigma}).$$

Here, $c^\dagger_{1\sigma}$ are fermion operators creating particles with spin $\sigma$ in a Wannier state at site $i$ and the sum $\langle i,j \rangle$ runs over nearest neighbors for all $N$ lattice sites. The hopping amplitude is denoted by $w$ and $U$ is the on-site interaction. We restrict our analysis the strongly correlated intermediate-temperature ($T$) regime $w^2/U \ll w \sim k_B T \ll U$, such that the initial state is a Mott-like state with one particle per site. The oscillatory part, Eq. 6, generates double occupancy by coupling a spin-singlet on the bond $(1, 2)$ to a doublon-holon pair.

The DGDO signal is largest in the strongly correlated regime at half-filling $\frac{1}{2}$. In this case it is appropriate to truncate the full Hilbert space and keep only the two lowest-energy sectors $\alpha$ and $\beta$ of [5] at fixed particle number. The low-energy sector $\alpha$ (with width $w^2/U \ll k_B T$) is centered around the energy $E = 0$ and the eigenstates are well approximated by product states $\{|\{s\}_\alpha\}$ describing singly-occupied sites with spin configurations $\{s\}$. The next-higher energy sector $\beta$ (Hubbard bands) is centered around the energy $E = U$. The eigenstates in $\beta$ involve a (delocalized) empty site (holon) and a (delocalized) doubly occupied site (doublon) which form a two-particle continuum. We denote states of the doublon-holon continuum by $|i_\alpha, j_\beta; \{s\}'\rangle$ (where $i$ (j) denote empty (doubly occupied) sites) and $\{s\}'$ is the spin configuration of the remaining sites.

The time-dependent part $H_{\text{osc}}(t)$ couples the $\alpha$-sector to the $\beta$ states [7]. We find the average number of doublons $D(t) = P_{\alpha\beta}(t)$ from the probability $P_{\alpha\beta}(t)$ for a transition between the $\alpha$- and $\beta$-sectors; the latter can be obtained via $P_{\alpha\beta}(t) = 1 - P_{\alpha\beta}(t)$ from the persistence

$$P_{\alpha\beta}(t) = \frac{1}{N_\alpha} \sum_{\{s\}} \left| \langle \langle \{s\} | T e^{-i \int_0^t dt' H(t')} | \{s\}\rangle \rangle \right|^2,$$
i.e., the probability to stay in \( \alpha \); here \( N_\alpha = 2^N \) is the number of states in the \( \alpha \)-sector, \( N \) the number of lattice sites, and \( T \) denotes the time-ordering operator. In order to remove the time-dependence, we go to the interaction picture with respect to the reference Hamiltonian \( H_0 = -\nu \sum \langle s \rangle |\{ \{\} \rangle /|\{ \{\} \rangle| \). The new Hamiltonian then reads \( H'(t) = U(t)H(t) - H_0U(t) \) with \( U(t) = \exp(-iH_0t) \). As a consequence, all energies in the \( \alpha \)-sector are shifted by \( \nu \) with respect to the \( \beta \)-sector, such that the states overlap in energy for \( \nu \approx U \). Furthermore, we dispose of the time-dynamics in \( H_{\text{osc}} \) via a rotating wave approximation (dropping terms oscillating with frequency 2\( \nu \)) and obtain the new driving term (cf. Eq. (1))

\[
H'_{\text{osc}} = \Omega \sum_{\{ s \}' \rangle} \langle \{ s \}' | \alpha \beta \langle D; \{ s \}' | + \text{H.c.} \rangle + B \tag{8}
\]

with the relevant states in the \( \alpha-, \beta\)-sector

\[
\begin{align*}
|S; \{ s \}' \rangle_{\alpha} &= \{ 1, 2; \{ s \}' \rangle_{\alpha} - \{ 1, 2; \{ s \}' \rangle_{\alpha} / \sqrt{2}, \\
|D; \{ s \}' \rangle_{\beta} &= \{ 1, 2; \{ s \}' \rangle_{\beta} + \{ 1, 2; \{ s \}' \rangle_{\beta} / \sqrt{2}.
\end{align*}
\]

The operator \( B \) conserves the number of doubly occupied and empty sites and involves processes where empty/doubly occupied sites on the bond \( \langle 1, 2 \rangle \) interchange with singly occupied sites.

Assuming that the initial state is \( |S; \{ s \}' \rangle \alpha \) with \( \{ s \}' \) an arbitrary spin configuration, we are left with a single level coupled to a continuum via a hybridization energy \( \Omega \), i.e., the problem discussed above. The role of the local Green’s function \( G_c \) is played by \( G_{\alpha \alpha}(t) = -i\Theta(t) \alpha \langle S; \{ s \}' | T \exp[-i \int_0^t dt' H(t')] | S; \{ s \}' \rangle \alpha \), whose Fourier transform is given by (cf. Eq. (2))

\[
G_{\alpha \alpha}(\omega) = \int_0^\infty dt e^{i\omega t} G_{\alpha \alpha}(t) = \frac{1}{\omega - \delta - \Omega^2G(\omega)} \tag{9}
\]

with \( G(\omega) \) the Fourier transform of the (local) two-particle Green’s function of the \( \beta \)-sector

\[
G(t) = \frac{-i\Theta(t)}{N_\beta} \sum_{\{ s \}' \rangle} \beta \langle D; \{ s \}' | T e^{-iH_0t} | D; \{ s \}' \rangle \beta \tag{10}
\]

replacing the Green’s function \( G_b \) of the band. Here, \( N_\beta \) is the number of states in sector \( \beta \) and the detuning \( \delta = \nu - U \) replaces \( \epsilon \); below, we limit ourselves to the case \( \delta = 0 \) which describes the situation near \( \nu \approx U \).

Once \( G(\omega) \) is known, we can calculate the probability \( P_{\alpha \beta}(t) = 1 - P_{\alpha \alpha}(t) \) for a transition between the two sectors using Eq. (9) and

\[
P_{\alpha \alpha}(t) = \left[ 3 + |G_{\alpha \alpha}(t)|^2 \right] / 4; \tag{11}
\]

the two terms refer to triplet- (probability 3/4) and singlet- (\( |S; \{ s \}' \rangle \alpha \)) type initial states. In calculating the two-particle Green’s function Eq. (10), we make use of particle-hole symmetry and treat the doublon and the holon as independent particles, \( G(t) \approx ig(t)^2 \), except for the initial correlations between the doublon at 1 and the holon at 2. For the one-particle Green’s function \( g(t) \) we make use of the retraceable path approximation due to Brinkman and Rice (BR) \([14]\), with the additional prescription to exclude site 2 in the first hopping process as doublon-holon exchange is suppressed by \( w/U \). Every hop then is equivalent and the original BR result simplifies, generating the single particle Green’s function \( g(\omega) = 2w\omega_0^{-1} \left[ 1 - \sqrt{1 - (\omega_0/\omega)^2} \right] \), where \( \omega_0 = 2w\sqrt{2d - 1} \).

The two-particle Green’s function is the convolution \( G(\omega) = \int dz g(\omega - z)g(z) \) and we obtain

\[
G(\omega) = \frac{4x}{\omega_0} \left[ 1 + \frac{4}{3\pi} \left[ (x^2 - 1)K(x^{-1}) + (x^2 + 1)E(x^{-1}) \right] \right]
\]

with the corresponding two-particle density of states

\[
\rho(\omega) = \frac{16}{3\pi^2\omega_0} \left[ (x^2 + 1)E(\sqrt{1 - x^2}) - 2x^2K(\sqrt{1 - x^2}) \right]
\]

where \( x = \omega/2\omega_0 \) and \( K(x) \left| E(x) \right| \) is the complete elliptic integral of the first [second] kind \([13]\).

The weak to strong driving crossover is governed by the behavior of the density of states near the band edge. Expanding \( \rho(\omega) \) around the band edge at \( 2\omega_0 \), we find an exponent \( \mu_{\text{BR}} = 2 \) and hence the strongly correlated doublon-holon continuum features a transition from the FGR regime to Rabi oscillations at a critical drive \( \Omega_c > 0 \). We focus on the local spectral function \( A(\omega) \), cf. \([1]\), from which the propagator \( G_{\alpha \alpha}(t) = -i \int dz e^{-i\omega z} A(\omega) \) and the (directly measurable) number \( P_{\alpha \beta}(t) \) of doublons are easily derived, cf. Fig. 1. The limits of weak and strong driving lead to the similar results as described in Refs. \([6, 7]\) (see also the discussion below \([13]\)). Here, we concentrate on the regime near the transition
with $\Omega \approx \Omega_c$. This transition between different non-equilibrium states is dynamically triggered and marks the unbinding of the localized doublon-holon pairs. The critical modulation strength $\Omega_c$ is obtained by solving Eq. (3), $\bar{\omega} = \Omega_c^2 \text{Re} G(\bar{\xi})$ near the band edge $\bar{\xi} \to 2\omega_0$. For $\omega \geq 2\omega_0$, we find $\Omega_c = \omega_0/\sqrt{2-16/3\pi} \approx 1.82\omega_0$; approaching $\Omega_c$ from above, we find that $(\bar{\xi}-2\omega_0) \sim (\Omega-\Omega_c)^{\zeta}$ with the exponent $\zeta$ quantifying the level repulsion; here, $\zeta = 1$ and levels do not repel. At criticality $\Omega_c$, the oscillator strength in the two $\delta$-functions is $2Z_c = 3\pi/2 - 4 \approx 0.71$. For $\Omega < \Omega_c$, we trace the poles in the analytic continuation of Eq. (3) to the lower complex half-plane and determine the imaginary parts providing the inverse decay time of damped Rabi oscillations, $\tau^{-1} = -2\text{Im} \bar{\xi}$. Approaching $\Omega_c$ from below leads to a diverging decay time $\tau \sim |\Omega-\Omega_c|^{-\eta}$ with $\eta = 2$; an overview of these characteristics is presented in Fig. 2.

The above incoherent hopping in a random spin background above is basically independent of dimensionality (except for $\omega_0$); when hopping is in a polarized background, the coherent propagation of doublons/holons is given by the non-interacting band-dispersion and we expect a qualitatively different behavior in different dimensions, e.g., $\Omega_c = 0$ in 1D where $\mu_2 = 0$.

In restricting the many-body Hilbert space to the $\alpha$ and $\beta$-sectors, we have neglected excitations which involve two or more doublon-holon pairs. Such processes occur when the pair leaves the bond $\langle 1,2 \rangle$ within the time $1/\Omega$, which is the case for $w > \Omega$; the bond then is ready for a new excitation. When $\Omega \gg w$ (the Rabi oscillation regime), the doublon-holon pair remains localized around the sites 1,2 and thus blocks further excitations. In the opposite (FGR) limit ($\Omega \ll w$), the assumption of a single excitation is not valid and we need to include further excitations; within the FGR regime these are incoherent and independent. The probability that (at least) a single doublon-holon pair is created is given by $P_{\alpha\beta} = [1-|G_{\alpha\alpha}(t)|^2]/4 \equiv P_n$, cf. Eq. (11). Assuming independent processes, the probability $P_n(t)$ that $n$ (or more) doublon-holon pairs are created is given by $P_n(t) = P_{n-1}[1-|G_{\alpha\alpha}(t)|^2]/4$ and we find an average number of doublons

$$D(t) = \sum_n np_n = \sum_n P_n = 1 - |G_{\alpha\alpha}(t)|^2$$

where $p_n$ denote the probability that $n$ doublon-holon pairs are created. The previous relation $D(t) = P_{\alpha\beta}(t) = [1-|G_{\alpha\alpha}(t)|^2]/4$, Eq. (7), thus is only valid for $|G_{\alpha\alpha}(t)|^2 \approx 1$, i.e., at short times. Also, equation (12) describes the saturation at a value $D = 1/3$ for long times.

The system discussed in the present letter can be realized, e.g., in a setup with fermionic cold atoms subject to an optical lattice and interactions tuned by a Feshbach resonance. The dynamical driving of a single bond $\langle 1,2 \rangle$ can be achieved by an additional laser field modulating the potential well between the sites; note though, that we are interested in high-driving powers where $\Omega > w$. As it is impossible to achieve negative tunneling amplitudes, the bond $\langle 1,2 \rangle$ then needs to be driven around a static value $w_{12} \gg w$ of the hopping amplitude.

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