Feshbach modulation spectroscopy of the Fermi-Hubbard model

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In the vicinity of a Feshbach resonance, a system of ultracold atoms in an optical lattice undergoes rich physical transformations which involve molecule formation and hopping of molecules on the lattice and thus goes beyond a single-band Hubbard model description. We explore theoretically the response of this system to a harmonic modulation of the magnetic field, and thus of the scattering length, *across* the Feshbach resonance. In the regime in which the single-band Hubbard model is still valid, we provide results for the doublon production as a function of the various parameters, such as frequency, amplitude, etc., that characterize the field modulation, as well as the lattice depth. The method may uncover a route towards the efficient creation of ultracold molecules and also provide an alternative to conventional lattice-depth-modulation spectroscopy.

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I. INTRODUCTION

The field of ultracold atoms in optical lattices has been opening up new possibilities which include a controlled experimental realization of the fermionic Hubbard model [1,2]. Further challenges and opportunities arise with the idea of creating and manipulating *molecules* in an optical lattice. Molecules in an optical lattice allow a much wider range of model Hamiltonians and physical phenomena to be emulated and studied than is possible with atoms. For example, spin models can be created by manipulating the internal structure of the molecule, and the interaction strength can be long ranged [3], e.g., by creating dipolar molecules. However, it is more difficult to cool molecules down to low temperatures via laser cooling due to their more complex level structure, which includes rotational and vibrational degrees of freedom (with some unique exceptions [4]). The cooling of individual atoms to a very low temperature followed by the formation of so-called preformed molecules in the optical lattice is thus a promising alternative [5–7]. In this paper, we explore theoretically the possibilities of achieving this by temporally modulating the magnetic field around a Feshbach resonance—we will refer to this as *Feshbach modulation*.

Near a Feshbach resonance, bound states of these preformed molecules occur. Depending on the value of the magnetic field, molecules form and hop from one lattice site to the other; these processes are governed by the complex Fermi resonance Hamiltonian (FRH) [8]. This Hamiltonian and the physical phenomena it supports are so complex that there has only been limited theory work performed on it, and a wide range of its rich behavior has not yet been explored thoroughly via experiment. Needless to say, it is crucial to understand the FRH physics in order to control and optimize the molecule-formation process, especially if one wants to find regimes where the formation might be more efficient than performing a simple field sweep across the Feshbach resonance. Experimentally, such an understanding of the FRH may be facilitated by Feshbach-modulation *spectroscopy*, which would be a study of the response of the system to a magnetic field which is periodically temporally modulated across a Feshbach resonance as a function of the frequency and the amplitude of the modulation.

The *theoretical* challenge, therefore, is to calculate the response of the FRH to such a time-varying magnetic field. The FRH is, however, rather difficult to treat theoretically. So in this work, we focus primarily on Feshbach-modulation spectroscopy in the off-resonance limit of the model, which is described by the simpler Fermi Hubbard model (FHM) (one could consider bosonic analogs as well, but for concreteness we discuss only the Fermi case here).

In case of the single-band Hubbard model, the so-called lattice modulation spectroscopy has proved to be useful for studying the nonequilibrium dynamics of the model, and for experimentally determining the value of the atom-atom interaction, given by U. In lattice-modulation spectroscopy, the intensity of the laser defining the optical lattice is varied harmonically. As a result, the optical lattice *depth* is modulated, which causes the hopping amplitude and the interaction strength to *both* change as a function of time, allowing the Mott gap to be measured directly in the experiment. Experimentally, this technique has been applied in a number of different situations, while numerous theoretical descriptions have also been given [2,9–26]. One of the motivations of this work exploring Feshbach-modulation spectroscopy is that the latter does not involve modulating *both* terms in the Hamiltonian. The reasons why this might be of interest is that it would both provide more precise control and allow the system to evolve in a more continuous fashion. For conventional lattice-modulation spectroscopy evolves the hopping to regimes where it becomes very small, essentially "turning off" the hopping of the particles, resulting in what is a more "kicked" driving of the system. If one can keep the hopping fixed in magnitude and modulate only the interaction, as one can by using Feshbach modulation, then this will correspond to a smoothly driven system, rather than a kicked one, which could have experimental advantages. Furthermore, lattice-modulation spectroscopy does not modify the sign of the interaction strength and is thus fundamentally limited when more general physics issues such as the molecule formation are to be studied.

The effects of a modulated magnetic field near a Feshbach resonance leading to a modulation of the scattering length have previously been investigated in a number of different contexts, both experimentally [27–30] and theoretically [31–36]. The

experimental efforts have been primarily focused on molecule formation in the simpler case when there is no optical lattice. In this regime, modulating the field at a frequency close to that corresponding to the binding energy for the molecules can both enhance their formation and also be used to measure their binding energy [28–30]. Theoretically, the effects were first explored for describing "Feshbach-resonance management" [31,32], which controlled "breathers" and solitons in trapped bosonic systems. Next, they were invoked to show how many-body effects and the periodic driving could push the tunneling to vanish [33], also in bosonic systems. More recently, they have been used to illustrate how one can obtain correlated hopping in bosonic systems when the amplitude of the magnetic-field oscillation is small and the frequency large compared to the interaction scales [34–36]. Relatively recent experiments on bosonic systems in an optical lattice [37] examined driven collective excitations. Here, we focus on the Fermi version of the Hubbard model and examine situations where the driving is pushed close enough to the Feshbach resonance that nonlinear effects become very important.

We thus consider the response of the system to a harmonic modulation of the magnetic field

$$B(t) = \bar{B} + \chi_{[0,t_{\rm mod}]}(t)\Delta B \sin \omega t \tag{1}$$

near the Feshbach resonance, where

$$\chi_I(t) = \begin{cases} 1 & \text{if} \quad t \in I \\ 0 & \text{otherwise} \end{cases} \tag{2}$$

is the characteristic function of the modulation interval. For the specific numerical calculations we have carried out, we consider a system of fermionic ^{40}K atoms subject to the ab Feshbach resonance [38] in an optical lattice with a laser wavelength of 1064 nm. We use strong-coupling-expansion techniques to calculate the doublon production as a function of the various parameters, $\bar{B}$, ΔB, and ω in Eq. (1), as well as the lattice depth, and analyze the results to uncover the factors that favor doublon formation and also permit the method to be of value as a spectroscopic tool.

The rest of this paper is organized as follows: In Sec. II, we present the model and the methods of calculation we use. In Sec. III, we present and discuss our results for the doublon production. Section IV contains our concluding discussion.

II. MODEL

As mentioned earlier, providing theoretical calculations for the full FRH in the presence of a time-dependent magnetic field (as described above) is currently beyond our reach. We treat instead the (Fermi) Hubbard model [39] which should be a reasonable approximation to the FRH in the early stages of the preformed molecule-formation process:

$$\mathcal{H}(t) = -J(t) \sum_{\langle i,j\rangle,\sigma} (c^\dagger_{i\sigma} c_{j\sigma} + \text{H.c.}) + U(t) \sum_i n_{i\uparrow} n_{i\downarrow} + \sum_{i\sigma} \epsilon_i n_{i\sigma}. \tag{3}$$

The time dependence of the lattice hopping and interaction reads $J(t) = J_0 = \text{const.}$ and $U(t) = g(t) \int |w(\vec{r}\,)|^4 d^3r$, where $w(\vec{r}\,)$ is the maximally localized Wannier function [40].

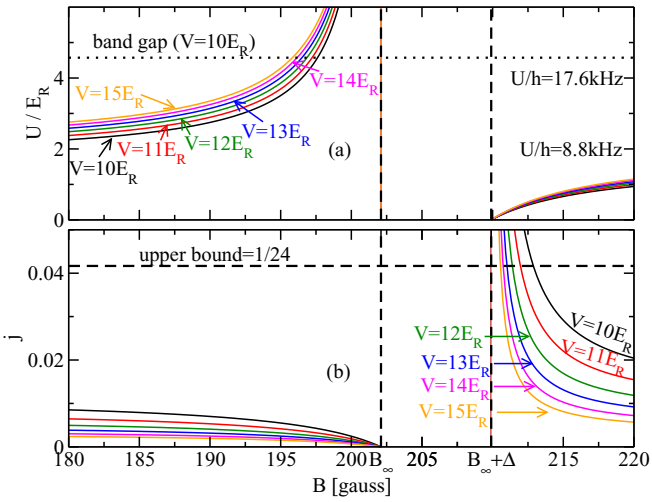

FIG. 1. (Color online) ab Feshbach resonances of the system ^{40}K for different lattice depths. The upper panel (a) shows the dependence of the interaction on the magnetic field and the lower panel (b) shows the resulting normalized hopping $j = J_0/U(B)$.

The time-dependent coupling constant $g(t) = 4\pi\hbar^2 a(t)/m$ is determined by the mass m of the ^{40}K atoms and the s-wave scattering length

$$a(t) = a_{bg}\left(1 - \frac{\Delta}{B(t) - B_\infty}\right), \tag{4}$$

where $a_{bg} = 174a_0$ is the background scattering, $B_\infty = 202.1G$ is the position of the Feshbach resonance, where the scattering length diverges, and $\Delta = 8.0G$ is its width.

For simplicity, we consider a translationally invariant lattice in three dimensions at half filling in the Mott-insulating phase and study the behavior of the double occupancy. With a higher double occupancy, molecule formation is more likely to occur in the later stages of the driving of the full FRH system. Computationally, we employ a strong-coupling approach which works well at finite temperatures larger than the hopping and has already successfully modelled conventional lattice-modulation spectroscopy [25,26,41]. In order to ensure the accuracy of the approach, we constrain the studied parameter range to a maximum value $j_{\max} := \max\{J_0/U(t)\}_{t\in\mathbb{R}} \approx 1/24$.

For each lattice depth, the Feshbach resonance has a different effect on the hopping relative to the interaction, i.e., on $j(t) := J_0/U(t)$, which we refer to as the *normalized hopping*. Also, the magnetic-field dependence of the hopping strength in units of the interaction, $j(B) := J_0/U(B)$, plays a key role in the Feshbach spectroscopy of the Hubbard model. Figure 1(b) shows this map for several lattice depths. Figure 1(a) shows the corresponding interaction strength. We limit our consideration to the interval $[0, j_{\max}]$ indicated by the horizontal dashed line in Fig. 1(b). In addition, we assume that the amplitude ΔB of the magnetic field is realistically smaller than 5 G for the necessary modulation frequency of a couple of kHz (which is near the magnitude of the average particle-particle interaction), since these numbers are experimentally reasonable. We also require the interaction to be significantly lower than the noninteracting band gap which is also displayed in Fig. 1(a) at lattice depth $V = 10E_R$. This,

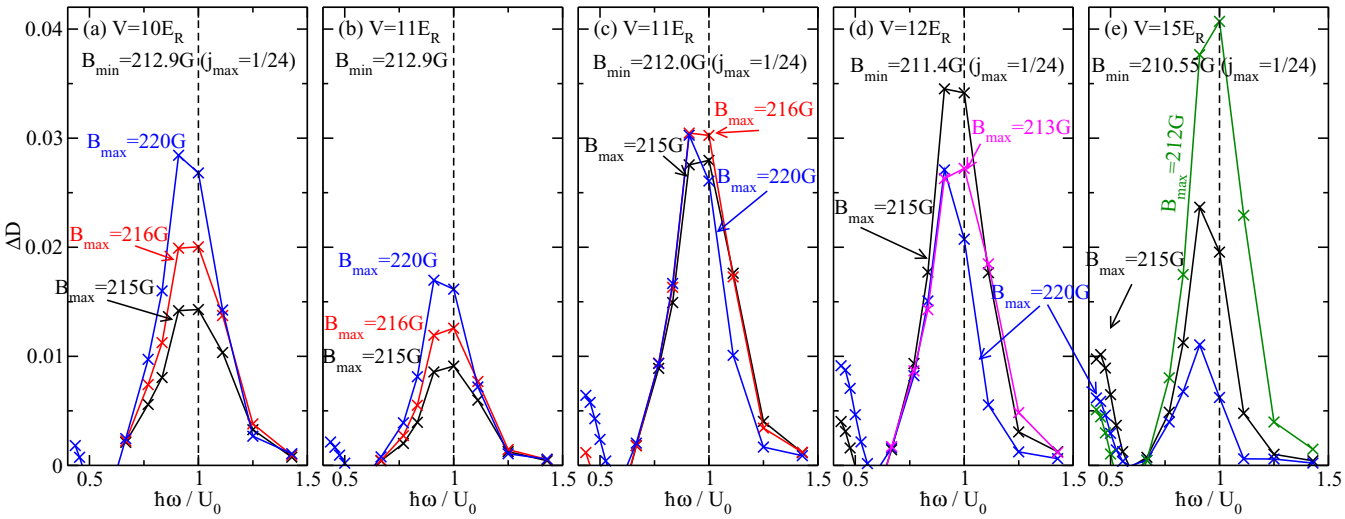

FIG. 2. (Color online) Doublon production at different values of $B_{\max}$. Each panel represents different values of V and $B_{\min}$. In panels (a), (c), (d), and (e), $B_{\min}$ is chosen such that $j_{\max} = 1/24$. The initial temperature is $k_B T = 0.1U_0$.

together with the requirement that the normalized hopping j, while small, should be large enough for the effects due to changes in it arising from changes in B to be measurable, constrains the considered parameter range to the right branches displayed in Fig. 1(b). Thus we consider magnetic-field values within the interval $(B_\infty + \Delta, 220G]$ and lattice depths equal to or larger than $10E_R$ (for smaller lattice depths, the band gap to the second band would be too small).

In experiments, the upper bound for the normalized hopping need not apply. However, in the vicinity of the resonance, the strong dependence of the normalized hopping on the field also results in a stronger dependence on the inhomogeneities of the magnetic field. It is therefore reasonable to keep the value of j below a certain threshold in experiments to reduce the effects of inhomogeneity.

In addition to the mean value of the magnetic field, other important parameters to be considered are the amplitude ΔB and the frequency ω of the field modulation. If the physical response of the system is sensitive to these values, this may help to determine unknown model properties (such as the lattice depth in the experiments) more precisely than is possible in lattice-modulation spectroscopy. In order to explore such possibilities, we investigate the frequency dependence of the doublon production rate for fixed windows of magnetic-field modulation.

The field modulation in Eq. (1) is parametrized by the magnetic-field amplitude ΔB, the average field value $\bar{B}$, the length of the modulation time interval t_{mod}, and the modulation frequency ω. ΔB and $\bar{B}$ can alteratively be expressed in terms of the minimum and maximum values of the field strength, $B_{\min} = \bar{B} - \Delta B$ and $B_{\max} = \bar{B} + \Delta B$. These values also determine the minimum and maximum values of the normalized hopping $j(B) = J_0/U(B)$. In order to translate $B_{\min}$ and $B_{\max}$ into $j_{\min}$ and $j_{\max}$, respectively, one uses Fig. 1(b).

III. RESULTS

We consider three field modulation intervals $[B_{\min}, B_{\max}]$ first, and compare the behavior for two lattice depths. Depending on the frequency, the field is modulated over a time interval $[0, t_{\max}]$, with

$$t_{\max}(\omega) = \left\lfloor \tilde{t}_{\max} \left(\frac{2\pi}{\omega} \right)^{-1} \right\rfloor \frac{2\pi}{\omega}, \tag{5}$$

and $\tilde{t}_{\max} U_0/\hbar = 29$, resulting in 2 to 6 field-modulation cycles for $\hbar\omega/U_0 = 0.5, \ldots, 1.5$, where $U_0 := U(\bar{B})$. Note that $\lfloor \cdots \rfloor$ denotes the floor operator which is equal to the closest integer to its argument which is not larger than its argument. As a physical observable, we study the excitation from the lower to the upper Hubbard band which is measured by the double occupancy per site:

$$D(t) = \langle n_\uparrow n_\downarrow \rangle(t), \tag{6}$$

and study the increase in this quantity, which we measure as

$$\Delta D := \frac{U_0}{h} \int_{\tilde{t}_{\max}+2-h/U_0}^{\tilde{t}_{\max}+2} dt\, D(t) - D(t_0). \tag{7}$$

That is, the end value has been averaged over one oscillation period of a resonantly excited Hubbard system and compared to the initial value $D(t_0)$.

Figures 2(a) and 2(b) shows the resulting frequency dependence of ΔD for three different values of $B_{\max}$, while we keep the minimum field value constant at $B_{\min} = 212.9G$. Figures 2(a) and 2(b) correspond to lattice depths $V = 10E_R$ and $V = 11E_R$, respectively. Since the normalized hopping $j_{\max}$ is smaller for a deeper lattice, fewer doublons are produced for $V = 11E_R$ than for $V = 10E_R$. However, the relative behavior of the curves as a function of $B_{\max}$ is qualitatively the same for the two lattice depths.

Hence we discuss the dependence of the resonance curves on $B_{\min}$ in more detail. Figure 2 shows several resonance curves for two slightly different values of $B_{\min}$ in Figs. 2(b) and 2(c), respectively. It shows that even the qualitative behavior of the Feshbach modulation can be quite sensitive to the details of the model. In Fig. 2(c), the shape and the strength of the different resonances are approximately the same. For the slightly larger value of $B_{\min}$ shown in Fig. 2(b), the resonance curves

change drastically as a function of $B_{\max}$. The reason for this qualitatively different behavior is that in the case of Fig. 2(c) a larger fraction of the steep portion of the normalized hopping j as a function of B (see Fig. 1) is sampled in the modulation procedure than in the case of Fig. 2(b). An effect which both the the cases of Figs. 2(b) and 2(c) have in common is that the maximum in doublon production is shifted towards smaller frequencies for larger values of $B_{\max}$. The reason for this may be the lower time-averaged value of the interaction strength for larger values of $B_{\max}$ in units of the respective values for $U_0 = U(\bar{B})$. For example, in the simplified case $B_{\min} = B_\infty + \Delta$, the time-averaged value of the interaction U_{tavg} can be approximately written as $U_{\text{tavg}}/U_0 = 1 - (U_{\text{bg}}/2U_0)b^2$, where U_{bg} is the interaction associated with the background scattering a_{bg} and $b = (B_{\max} - B_{\min})/2\Delta$. A similar relation can be derived for the more realistic $B_{\min} > B_\infty + \Delta$. However, since the width of the resonance is almost independent of $B_{\max}$ in both Figs. 2(b) and 2(c), this reasoning cannot be the whole story.

Furthermore, we can also compare the resonance curves for several lattice depths at a fixed maximum value $j_{\max}$ of the normalized hopping. This corresponds to adjusting $B_{\min}$ appropriately for each lattice depth such that the same value of $j_{\max}$ is obtained. In this case, we choose $j_{\max} = 1/24$, which is also the upper bound we introduced previously in order to ensure the convergence of the strong-coupling method. Figures 2(a), 2(c), 2(d), and 2(e) show data for different lattice depths at this constant maximum value of j. We again find that the dependence on $B_{\max}$ may depend very much on the lattice depth. While for the shallow lattice, $V = 10E_R$, increasing the modulation amplitude yields a stronger signal, we observe the *opposite* effect in a deeper lattice, $V = 15E_R$. This striking difference is due to the increasing nonlinearity of $j(B)$ as V increases. For a shallow lattice, $j(B)$ still exhibits a nearly linear behavior, so the peak strength is proportional to the amplitude. In a deep lattice, $j(B)$ is strongly nonlinear and the system is rather kicked than driven. An increased amplitude decreases the kick strength in a deep lattice, because j is close to $j_{\max}$ for shorter time spans during the modulation. As the lattice gets deeper, a second-order peak appears at $\hbar\omega = U_0/2$, which is approximately as strong as the first-order peak for strong modulation amplitudes. The lattice depths between $V = 10E_R$ and $V = 15E_R$ interpolate between these two behaviors. In the very deep lattice, for $V = 15E_R$, the strongest doublon production can be achieved with a rather small amplitude corresponding to $B_{\max} = 212G$, or $\Delta B \approx 0.73G$. Indeed, the doublon production in the Hubbard model is the precursor toward molecule formation in the FRH model. Unfortunately, our numerical techniques will not allow us to go farther with the calculation to examine those effects.

Finally, in order to compare different lattice depths, we fix the values of $B_{\min}$ and $B_{\max}$ in such a way that the normalized hopping oscillates between the same values $j_{\min} = 1/48$ and $j_{\max} = 1/24$. The resulting resonance curves at different lattice depths are shown in Fig. 3. In contrast to the scenarios discussed in Fig. 2, the curves are now essentially identical. This underlines the central role of the normalized hopping in interpreting both Feshbach- and lattice-depth-modulation spectroscopy. However, we also observe a tendency towards a stronger doublon production for deeper lattices. As can be seen in the left inset of Fig. 3, this is not related to the initial number

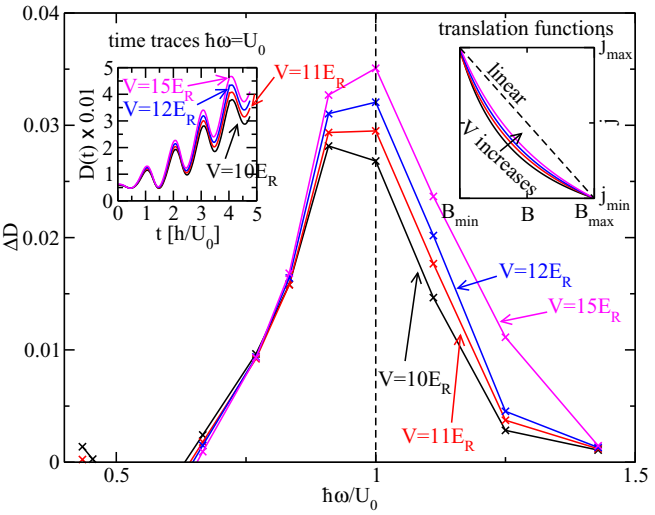

FIG. 3. (Color online) Magnetic modulation with the normalized hopping j oscillating within the interval $[j_{\min}, j_{\max}]$, with $j_{\max} = 1/24$ and $j_{\min} = j_{\max}/2$ for different lattice depths. The corresponding magnetic field intervals $I_B = [B_{\min}, B_{\max}]$ are $I_B(V = 10E_R) = [212.9G, 219.56G]$, $I_B(V = 11E_R) = [212.0G, 215.52G]$, $I_B(V = 12E_R) = [211.4G, 213.59G]$, $I_B(V = 15E_R) = [210.55G, 211.32G]$.

of doubly occupied sites, which is essentially identical for each lattice depth. Rather, the tendency is due to the shape of the translation function between magnetic field and renormalized hopping, as shown in the right inset of Fig. 3. As the lattice depth is increased, the convexity of the translation function is decreased and the latter approaches a linear behavior. This gives rise to an increase in the doublon production, and shows one of the advantages of being able to modulate the interaction independently of the hopping.

IV. CONCLUSIONS

In this work, we have explored Feshbach-modulation spectroscopy, where tuning and temporally modulating a magnetic field near a Feshbach resonance allows for the system to have a time-dependent interaction, with a constant hopping (the normalized hopping, of course is time dependent), as an alternative to conventional lattice-depth-modulation spectroscopy. This changes the behavior of the driving of the system from a more kicked drive in the conventional approach to a smoother evolution. We find that, in some cases, the signal can have strong resonant effects that require fine tuning of the magnetic field, and hence have the potential to produce higher-precision measurements. In addition, we find that the "two-photon" peak at a frequency equal to half the average interaction strength is often enhanced in these systems, making it easier to study nonlinear excitation effects. Finally, we conjecture that even more interesting behavior will occur when the Feshbach-modulation spectroscopy is pushed through the Feshbach resonance itself and allows for complete molecule formation. The many mutually coupled degrees of freedom in the FRH [8] promise a rich variety of physical effects which will be interesting to investigate both experimentally and theoretically. In particular, it will be interesting to explore the channels that lead to molecule formation spectroscopically.

We do not yet have the ability to model and calculate the behavior of such spectroscopy, but experiments could potentially investigate such effects in the near future.

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