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Response to dynamical modulation of the optical lattice for fermions in the Hubbard model

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Fermionic atoms in a periodic optical lattice provide a realization of the single-band Hubbard model. Using quantum Monte Carlo simulations along with the maximum-entropy method, we evaluate the effect of a time-dependent perturbative modulation of the optical lattice amplitude on atomic correlations, revealed in the fraction of doubly occupied sites. We find that the effect of modulation depends strongly on the filling—the response of the double occupation is significantly different in the half-filled Mott insulator from that in the doped Fermi liquid region.

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A number of key properties of strongly correlated electron systems appear to be well described by simplified tight-binding Hamiltonians. For example, the square-lattice Hubbard model, with one particle per site, is known to possess the long-range antiferromagnetic order manifest in the parent compounds of high-temperature superconductors, whose CuO_2 sheets have square arrays of copper atoms with one hole per 3*d* shell. There are many analytic and numerical clues that suggest the doped Hubbard model might also possess the *d*-wave superconducting phase exhibited by the cuprates, as well as other nontrivial properties including stripes and pseudogap physics [1]. If this could be demonstrated rigorously, it would provide important insight into the mechanism of superconductivity in these materials.

Ultracold atomic systems offer an opportunity for closer connection between experiments and calculations for such model Hamiltonians. At present, experiments on fermionic atoms are exploring temperatures T which are of the order of the hopping integral J_0, probing correlations such as double occupancy D, and short-range spin order that develops at that temperature scale. In particular, the evolution of D with the ratio of interaction strength U to hopping J_0 has been shown to indicate the presence of a Mott metal-insulator transition [2,3]. The presence of a Mott gap in the excitation spectrum has also been inferred through peaks in D which arise through a dynamic modulation of the optical lattice depthsxs V [2].

The possibility that such a modulation might provide a useful probe was first suggested by Kollath *et al.* [4], based on earlier work with bosonic systems [5]. Using a time-dependent density-matrix renormalization-group method, it was shown that a peak existed in the induced double occupation at a frequency ω which matched the interaction strength U. The authors emphasized that the measurement was sensitive to near-neighbor spin correlations and the exchange gap, as well as the charge gap.

This "modulation spectroscopy" has been further explored theoretically by Huber and Rüegg [6] and Sensarma *et al.* [7]. In the former work, the frequency dependence of the shift in D was studied in the atomic and two-particle limits and within a slave boson mean-field theory. The latter work focused on observing local antiferromagnetic order at the superexchange scale. In both of these papers, the modulation was assumed to couple only to the kinetic energy.

In this paper, we extend previous work by studying the effect of the modulation of both the tunneling strength δJ and the on-site interaction strength δU due to variation of the optical lattice depth V, for the two-dimensional repulsive fermionic Hubbard Hamiltonian. The modulation by δU is shown to be quite significant in the parameter range of interest to current experiments. We find that the filling of the system plays a very important role in the response. Crucially, through the use of determinant quantum Monte Carlo simulations [8] and the maximum-entropy method [9,10], we provide results which treat the electron-electron correlations exactly.

In the low-energy limit, two species of repulsively interacting fermions confined to a periodic optical potential with wavelength λ and amplitude $V(t)$ can be described by the one-band Hubbard model [11],

$$\hat{H} = -J\hat{K} + U\hat{D} - \mu\hat{N}, \tag{1}$$

where the hopping or kinetic-energy operator is $\hat{K} = \sum_{\langle ij\rangle,\sigma}[\hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma} + \text{H.c.}]$, $\hat{D} = \sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$ is the double occupancy, and $\hat{N} = \sum_i \hat{n}_{i\uparrow} + \hat{n}_{i\downarrow}$ is the total number of particles, with $\hat{c}^{\dagger}_{i\sigma}$ $(\hat{c}_{i\sigma})$ the fermion creation (annihilation) operator, $\sigma = \uparrow,\downarrow$ the spin index, $\hat{n}_{i\sigma} = \hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma}$, and μ the chemical potential. The hopping (J) and interaction (U) can be expressed as [11] $J \approx (4/\sqrt{\pi})\, E_R\, v^{3/4} \exp(-2\sqrt{v})$ and $U \approx 4\sqrt{2\pi}\,(a_s/\lambda)\, E_R\, v^{3/4}$, where $v = V/E_R$ is the ratio of lattice depth to recoil energy, and a_s is the short-ranged *s*-wave scattering length.

It is clear from these expressions that a small time-dependent modulation of V changes both J and U. Writing $V(t) = V_0 + \delta V \sin(\omega t)$ and expanding J and U in the limit $\delta V \ll V_0$ yields $\hat{H} = \hat{H}_0 + \delta\hat{H}\sin(\omega t)$ with $\hat{H}_0$ given by Eq. (1) with J replaced by J_0 and U by U_0, and $\delta\hat{H} = -\delta J\hat{K} + \delta U\hat{D}$ with the time-dependent perturbations

$$\delta J = J_0\left(\frac{3}{4} - \sqrt{\frac{V_0}{E_R}}\right)\frac{\delta V}{V_0},$$
$$\delta U = \frac{3}{4}U_0\frac{\delta V}{V_0}. \tag{2}$$

For $\delta V > 0$, we have $\delta J < 0$ and $\delta U > 0$ so that an increase in the optical lattice amplitude suppresses hopping and increases the Hubbard repulsion. We emphasize that one cannot *a priori* neglect δJ or δU as they can be of the same order of magnitude if the experimental parameters of Ref. [2] are used.

Our aim is to understand how such a simultaneous modulation of the hopping and interaction parameters, as provided by fermions in a time-dependent optical lattice, probes fermion correlations in the Hubbard model. To this end, we study the time dependence of the average double occupancy $D(t) = \langle \hat{D} \rangle$. Within standard time-dependent perturbation theory, $D(t)$ satisfies, to linear order,

$$D(t) = D(t_0) - i \int_{t_0}^{t} dt' \, \langle [\hat{D}(t), \delta \hat{H}(t')] \rangle_0 \sin \omega t', \qquad (3)$$

where $\langle \hat{O} \rangle_0 = Z_0^{-1} \mathrm{Tr} e^{-\beta \hat{H}_0} \hat{O}$ and $\hat{O}(t) = e^{i \hat{H}_0 t} \hat{O} e^{-i \hat{H}_0 t}$. Equation (3) can be simplified by rewriting $\delta \hat{H}$ in terms of $\hat{H}_0$ as $\delta \hat{H} = (\delta J / J_0)(\hat{H}_0 + U_0[\alpha - 1]\hat{D})$, with $\alpha = (1 - \frac{4}{3}\sqrt{\frac{V_0}{E_R}})^{-1}$. When inserted into Eq. (3), the first term will give a vanishing contribution, leading to

$$D(t) = D(t_0) + \frac{U_0}{J_0}(\alpha - 1) \int_{t_0}^{\infty} dt' \, \delta J \, \chi_{\mathrm{DD}}(t - t') \sin \omega t', \qquad (4)$$

where $\chi_{\mathcal{O}\mathcal{O}}(t - t') = -i \langle [\hat{O}(t), \hat{O}(t')] \rangle_0 \theta(t - t')$. Formally setting $\alpha = 0$ amounts to neglecting the modulation of the interaction term. In contrast, experimentally, α typically varies within the range $-0.41 < \alpha < -0.28$. The simplification leading to Eq. (4) can be generalized to show that $\chi_{\mathrm{DD}}(t) = (J_0/U_0)^2 \chi_{\mathrm{KK}}(t)$, a fact that we shall use below in our analysis.

Numerically, we calculate the imaginary-time quantity $\chi_{\mathrm{DD}}(\tau)$ from determinant quantum Monte Carlo simulations [8] and analytically extrapolate to the corresponding imaginary part of the real-frequency quantity $\chi''_{\mathrm{DD}}(\omega)$ by inverting

$$\chi_{\mathrm{DD}}(i\nu_n) = -\frac{1}{\pi} \int_{-\infty}^{\infty} d\omega \, \frac{\chi''_{\mathrm{DD}}(\omega)}{i\nu_n - \omega} \qquad (5)$$

via the maximum-entropy method [9,10]. In Eq. (5) $i\nu_n = 2n\pi T$ is the bosonic Matsubara frequency, T is the temperature, and ω is the real frequency.

To illustrate the importance of incorporating the modulation of the interaction parameter U, in Fig. 1 we show the dependence with U_0/J_0 of the double-occupancy response function $\chi_{\mathrm{DD}}(i\nu_n = 0)$ (black curves, circles), for $n = \langle n_{i\uparrow} + n_{i\downarrow} \rangle = 1.0$ and $n = 1.4$, along with this quantity multiplied by $(1 - \alpha)$ (red curves, squares). Therefore, the black curves are the result from modulating δJ only, while the red curves also include the effect of modulating δU. The difference between the curves illustrates that δU should not be neglected. We observe from Fig. 1 that at half filling ($n = 1$), the double-occupancy response is largest in the intermediate interaction region and decreases with increasing U_0/J_0. This is in striking contrast to the behavior at $n = 1.4$, in which the double-occupancy response is small at weak coupling and saturates at large U_0/J_0. To confirm our numerical calculation, we analytically solved the case of a two-site Hubbard model and found qualitatively similar behavior. (See green curves in the insets of Fig. 1.)

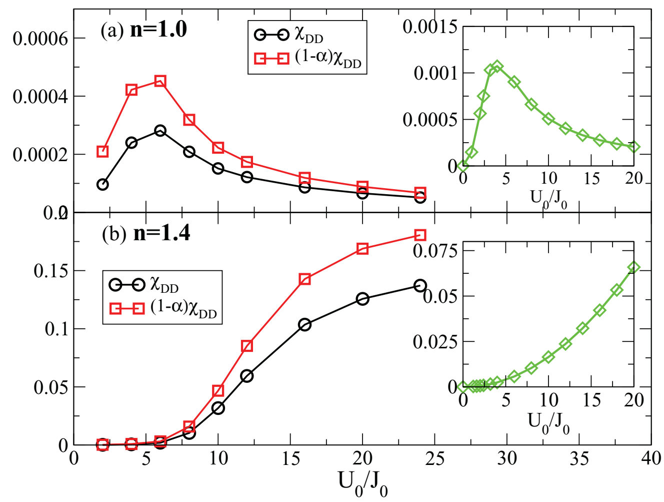

FIG. 1. (Color online) Data for (a) half filling, and (b) a filling of $n = 1.4$, for a two-dimensional 4×4 Hubbard lattice. Red curves (squares) show the quantity $(1 - \alpha)\chi_{\mathrm{DD}}$ that appears in the linear response of the double occupancy, evaluated at zero Matsubara frequency as a function of U_0/J_0. Neglecting the modulation of the Hubbard interaction amounts to setting $\alpha = 0$, yielding a smaller result (black curves, circles). For comparison, the green diamonds in the insets in both (a) and (b) are exact results for $(1 - \alpha)\chi_{\mathrm{DD}}$ for a two-site Hubbard model. α is determined by assuming $a_s/\lambda = 0.0119$, where $a_s = 240 a_0$ (a_0 is the Bohr radius) and $\lambda = 1064$ nm (following Ref. [2]); thus α can be found as a single-valued function of U_0/J_0.

We now turn to the full frequency-dependent dynamical susceptibility, which determines the response to the dynamical modulation, showing its evolution as a function of temperature (expressed in terms of $\beta J_0 = J_0/k_B T$) in Fig. 2. Figure 2(a) displays results at half filling, where Mott-insulating physics dominates. At this filling the low-frequency response is strongly suppressed for temperatures approaching zero (so that this quasipeak represents thermally excited states, not coherent excitations), with the predominant response occurring at frequencies close to U_0. This energy scale, corresponding to the Mott gap, is consistent with recent experimental results [2] which find a strong response in the double occupancy when $\omega \sim U_0$. The presence of the Mott gap also accounts for the much smaller values of χ'' in the top panels of Figs. 1 and 2. Figure 2(b) shows a filling $n = 1.4$, where an $\omega = 0$ peak remains robust for $T \to 0$. We attribute this peak to the presence of gapless excitations reflecting Fermi liquid behavior in this region. The peak at high ω represents coherent excitations at the band-gap scale which should be the distance between the lower and upper Hubbard bands.

In Fig. 3, we show the interaction dependence of $\chi''_{\mathrm{DD}}(\omega)$. Figure 3(a) displays the half-filled case where the peaks are centered at U_0. In Fig. 3(b), filling $n = 1.4$, we include the case of a larger lattice size (6×6) to show that finite-size effects are small. These results further verify the important role of filling in the response to dynamical modulation. Our findings can be qualitatively reproduced by neglecting vertex corrections in χ_{KK} and expressing the single-particle Green's function in the

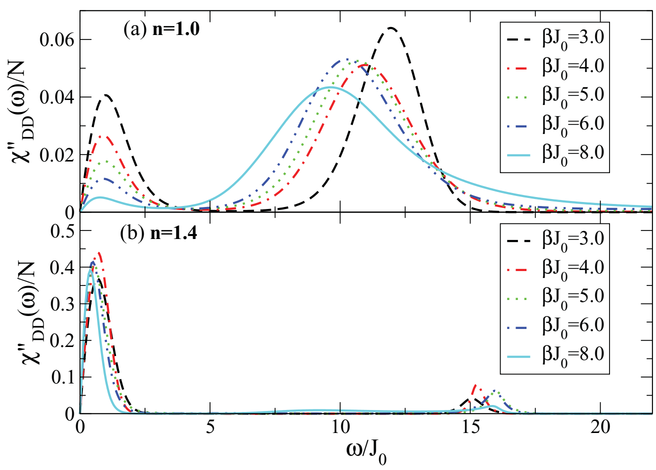

FIG. 2. (Color online) The imaginary component of the double-occupancy susceptibility $\chi''_{DD}(\omega)/N$ for $U_0/J_0 = 10.0$, a 4×4 square lattice, and various values of inverse temperature ($\beta = 1/T$). Results for (a) half filling, $n = 1.0$, and (b) a filling of $n = 1.4$, for $\beta J_0 = 3.0$ (dashed), 4.0 (dot-dashed), 5.0 (dotted), 6.0 (dot-dot-dashed), and 8.0 (solid). $N = 16$ is the system size.

Hubbard-I approximation. The latter corresponds to using an approximate self-energy of the form

$$\Sigma_\sigma(\omega) \sim \frac{U_0^2\, n_{\bar\sigma}(1 - n_{\bar\sigma})}{\omega + i\delta}. \tag{6}$$

We find that $\chi''_{KK}(\omega)$ [and hence $\chi''_{DD}(\omega)$] possesses poles at $\omega \sim 0, \pm[\sqrt{(\epsilon_{\mathbf{k}})^2 + 4U_0^2\, n_\sigma(1 - n_\sigma)}$), where $\epsilon_{\mathbf{k}}$ is the energy of a noninteracting quasiparticle with momentum $\mathbf{k}$. In the low-energy region, there are quasielastic peaks at approximately $\omega \sim 0$. Note that the peak vanishes at $\omega = 0$ because the imaginary part of the real-frequency susceptibility is an odd function $\chi''_{KK}(-\omega) = -\chi''_{KK}(\omega)$. In the high-energy region, the peaks are located at roughly $\omega \sim U_0 + \epsilon_{\mathbf{k}}^2/2U_0$. Therefore, at half filling, the peaks are at $\omega = U_0$ but they sit at higher frequencies away from half filling.

We now turn to the question of how the features in $\chi_{DD}(\omega)$ would be reflected in an experimental measurement of the double occupancy, by inserting our results for $\chi_{DD}(t)$ into Eq. (4). For this task, we need to obtain the real part of $\chi_{DD}(\omega)$ via the Kramers-Kronig relation; upon Fourier transforming we find the real-time dynamical response functions for the double occupancy to be strikingly different at half filling and away from half filling, as seen in Figs. 3(a) and 3(b). We see that filling $n = 1$ shows a response function that is tightly peaked at $t \to 0$, characterized by a single frequency scale $\omega \sim U_0$, while at $n = 1.4$ we see a broad behavior dominated by the two distinct frequencies associated with $\omega \sim 0$ and $\omega \sim U_0 + \epsilon_{\mathbf{k}}^2/2U_0$.

As in standard linear response theory, the real and imaginary parts of $\chi_{DD}(\omega)$ correspond to the in-phase and out-of-phase parts of the response, respectively. Thus, to linear order, an oscillatory driving of the optical lattice potential yields an oscillatory response at the same frequency, but with a phase lag characterized by the ratio of $\tan\phi(\omega) = \chi''_{DD}(\omega)/\chi'_{DD}(\omega)$.

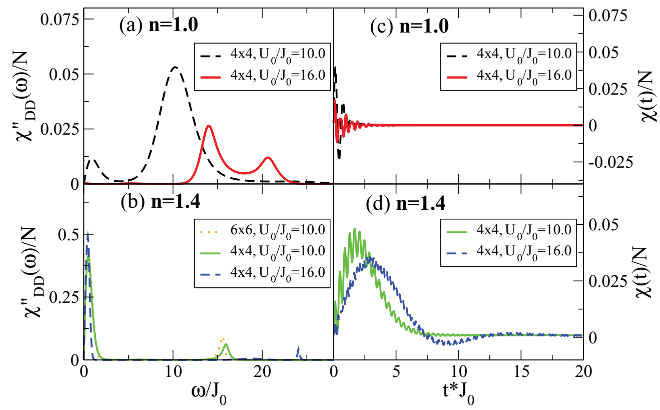

FIG. 3. (Color online) Left column: The imaginary part of the double-occupancy susceptibility $\chi''_{DD}(\omega)/N$ for $U_0/J_0 = 10$ and 16. (a) shows half-filling $n = 1.0$ results for a 4×4 lattice, $U_0/J_0 = 10.0$ (dashed black curve) and (solid red curve). (b) shows results for a filling $n = 1.4$ and for $U_0/J_0 = 10.0$, 6×6 square lattice (dotted orange curve), $U_0/J_0 = 10.0$, 4×4 lattice (solid green curve), and $U_0/J_0 = 16.0$, 4×4 lattice (dashed blue curve). Right column: The real-time double-occupancy response function $\chi_{DD}(t)$ for a 4×4 square lattice at half filling (c) for $U_0/J_0 = 10.0$ (dashed black curve) and 16.0 (solid red curve); and for $n = 1.4$ (d) with $U_0/J_0 = 10.0$ (solid green curve) and 16.0 (blue dashed curve). All results are at a temperature $T/J_0 = 2/3$.

This response has recently been observed directly [12]. We can then write the time-dependent double occupancy as

$$D(t) = D(0) + D(\omega)\sin[\omega t - \phi(\omega)], \tag{7}$$

where $D(\omega) = U_0/J_0(\alpha - 1)\delta J|\chi_{DD}(\omega)|$. We plot $D(\omega)$ and $\phi(\omega)$ in Fig. 4 for the case of $U_0/J_0 = 10$. We first note that, at low frequency $\omega \to 0$, Eq. (7) implies the time dependence of $D(t)$ to be precisely π out of phase with $\delta V(t)$. Therefore, an adiabatic increase of the optical lattice amplitude leads to a corresponding *suppression* of the double occupancy. At higher ω these plots show how the time-dependent linear response

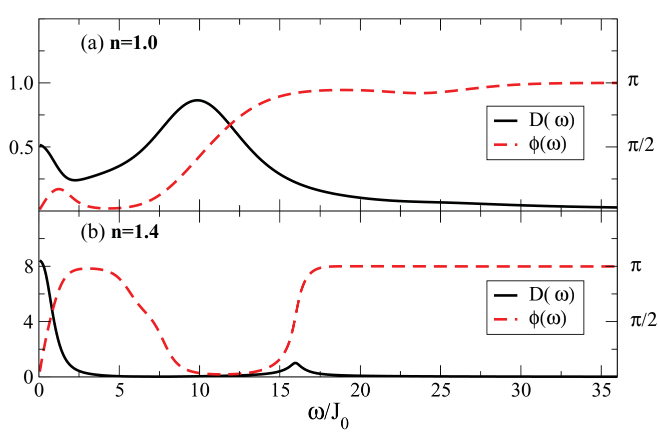

FIG. 4. (Color online) The frequency dependence of the double-occupancy linear response for a 4×4 lattice, interaction strength $U_0/J_0 = 10.0$, and temperature $T/J_0 = 2/3$. (a) shows half-filling results; (b) results for $n = 1.4$. Solid (black) curves shows the amplitude $D(\omega)$ while the dashed (red) curves display the phase shift $\phi(\omega)$ induced by the dynamical modulation.

of the double occupancy probes the underlying fermion correlations. As we expected, the half-filled case shows the strongest response when the driving frequency $\omega \sim U$, and with a phase that is shifted, by $\phi \approx \pi/2$, relative to the imposed modulation. At $\langle n \rangle = 1.4$, however, the predominant response is for $\omega = 0$, with phase shift $\phi \approx 0$.

In conclusion, we have investigated the dynamical properties of fermions in an optical lattice, realized by the Hubbard model subject to a periodic optical lattice modulation. We show that, even at the level of linear response, the dynamical double occupancy provides a sensitive probe of fermion correlations. Recent cold-atom experiments [12] studying the dynamical modulation of the optical lattice find a linear-in-time contribution to the double occupancy. Previous theoretical work has found such a contribution at quadratic order in the modulation parameter δV, with a coefficient proportional to the Fourier transform of the kinetic-energy correlation function [4]. Thus, we expect that our linear-response results apply at smaller $\delta V/V_0$, or after subtracting off this t-linear contribution to focus on the oscillatory component. Future extensions of our work will analyze the linear and quadratic-order contributions, as well as the effects of inhomogeneity due to a trapping potential.

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[1] D. J. Scalapino, in *Perspectives in Many-Particle Physics, Proceedings of the International School of Physics "E. Fermi" Course CXXI*, edited by R. A. Broglia, J. R. Schrieffer, and P. F. Bortignon (North-Holland, New York, 1994), and references cited therein.
[2] R. Jördens, N. Strohmaier, K. Günter, H. Moritz, and T. Esslinger, Nature (London) **455**, 204 (2008).
[3] U. Schneider, L. Hackermüller, S. Will, Th. Best, I. Bloch, T. A. Costi, R. W. Helmes, D. Rasch, and A. Rosch, Science **322**, 1529 (2008).
[4] C. Kollath, A. Iucci, I. P. McCulloch, and T. Giamarchi, Phys. Rev. A **74**, 041604(R) (2006).
[5] T. Stöferle, H. Moritz, C. Schori, M. Köhl, and T. Esslinger, Phys. Rev. Lett. **92**, 130403 (2004).
[6] S. D. Huber and A. Rüegg, Phys. Rev. Lett. **102**, 065301 (2009).
[7] R. Sensarma, D. Pekker, M. D. Lukin, and E. Demler, Phys. Rev. Lett. **103**, 035303 (2009).
[8] R. Blankenbecler, D. J. Scalapino, and R. L. Sugar, Phys. Rev. D **24**, 2278 (1981).
[9] J. E. Gubernatis, M. Jarrell, R. N. Silver, and D. S. Sivia, Phys. Rev. B **44**, 6011 (1991).
[10] M. Jarrell and J. E. Gubernatis, Phys. Rep. **269**, 133 (1996).
[11] I. Bloch, J. Dalibard, and W. Zwerger, Rev. Mod. Phys. **80**, 885 (2008).
[12] D. Greif, L. Tarruell, T. Uehlinger, R. Jördens, and T. Esslinger, Phys. Rev. Lett. **106**, 145302 (2011).