Dynamical repulsion-attraction transition of doublons

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Contents

1 Introduction

Transport investigation in strongly correlated materials out of equilibrium is a convenient way of controlling their properties and can lead to discover unexpected physics. One manifestation of strong correlations is the Mott insulator. Mott insulator is a clear example of strong correlations where doubly occupied sites play the role of carriers. This causes a big interest in the study of doublon dynamics in experimental and theoretical works due to development of the ultrafast time-resolved experimental techniques. There are exist ways to change the number of doublons in such materials are doping or pumping of the sample by laser pulse.

In work of [Hideo] described how the double occupancy changes with in the magnitude of the vector potential, which leads to a change in the sign of the Coulomb interaction.

In this paper, we want to discuss how the doublone-doublone interaction depends on the magnitude of the external electric field.

2 Model and method

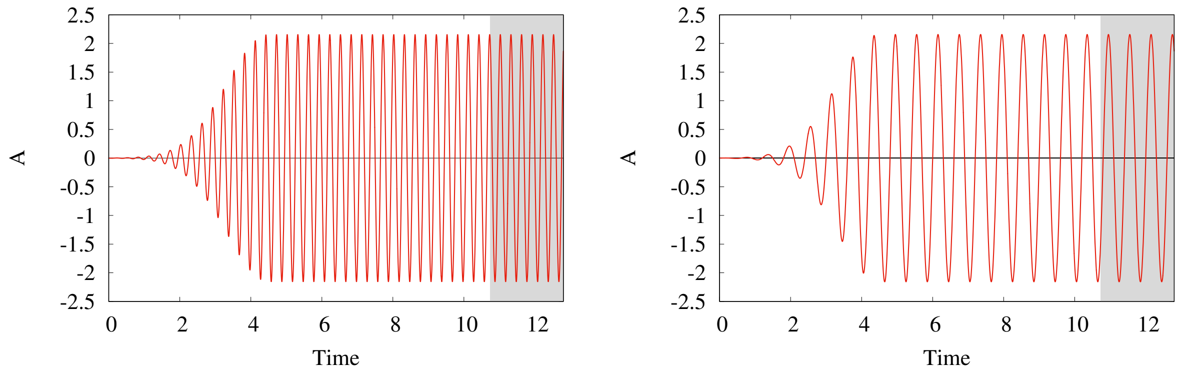
The Hamiltonian of the driven half-filled Hubbard model is

$$\begin{aligned} H(t) = \sum_{ij,\sigma} t_{ij} \exp\left(-i \int_{\mathbf{R}_j}^{\mathbf{R}_i} d\mathbf{r} \cdot \mathbf{A}(t)\right) c^\dagger_{i\sigma} c_{j\sigma} \\ + U \sum_i \left(n_{i\uparrow} - \frac{1}{2}\right)\left(n_{i\downarrow} - \frac{1}{2}\right), \end{aligned} \tag{1}$$

where t_{ij} are electron hopping amplitudes between sites i and j, $c^\dagger_{i\sigma}$ the creation operator for an electron of spin σ at site i, U the on-site interaction, $n = c^\dagger c$ the number operator. Time-dependent double occupancy defined as $d(t) = \langle n_\uparrow(t) n_\downarrow(t) \rangle$. To solve the model we use the nonequilibrium dynamical mean field theory (DMFT) [Aoki et al.(2014)Aoki, Tsuji, Eckstein, Kollar, Oka, and in combination with a weak coupling perturbative impurity solver (iterative perturbation theory

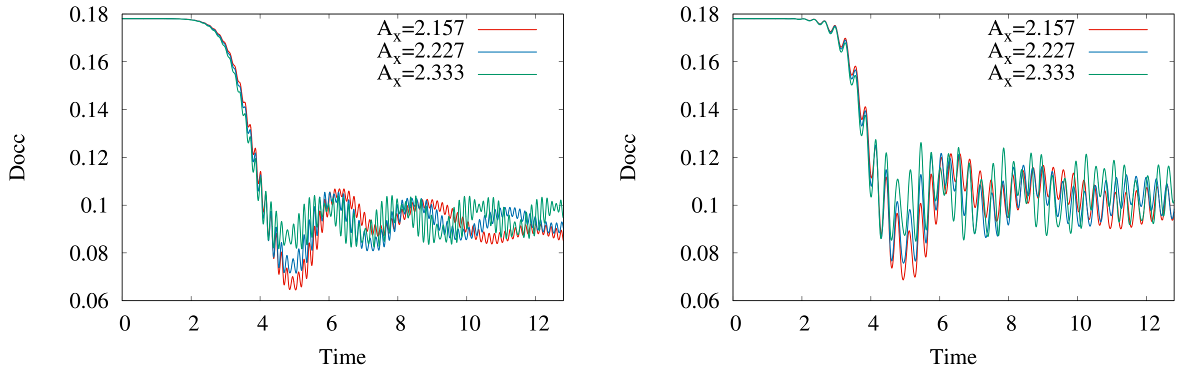
(IPT)) [Georges et al.(1996)Georges, Kotliar, Krauth, and Rozenberg, Eckstein and Werner(2011)]. We consider an 2D square lattice with dispersion law $\varepsilon(\mathbf{k}, t) = 2t \left[\cos(k_x + A_x(t)) + \cos(k_y + A_y(t))\right]$ and apply the electric field along the diagonal. In a gauge with pure vector potential $A(t)$, the electric field $E(t) = -\partial_t A(t)$ enters the calculation as a time-dependent shift of the noninteracting dispersion, $\epsilon_k \rightarrow \epsilon_{k-A(t)}$. We start at $t = 0$ in the equilibrium state at inverse temperature β=5 and switch on the vector potential as it shown in Fig. 1.

3 Shift of the Hubbard bands



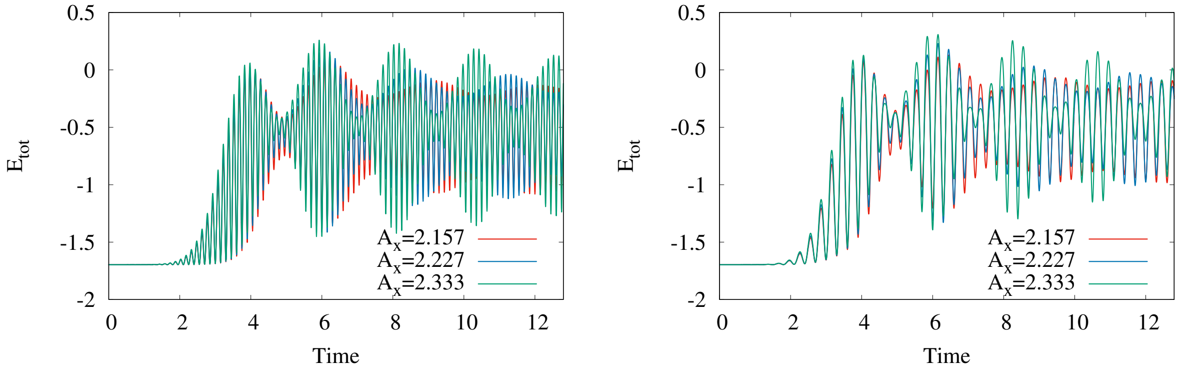
(a) (b)

Figure 1: Pulse (a)21, (b)10.



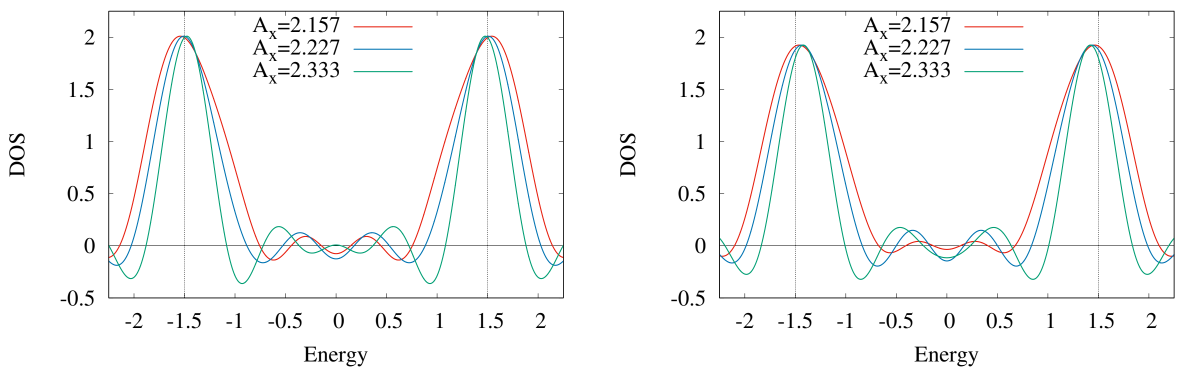
(a) (b)

Figure 2: docc



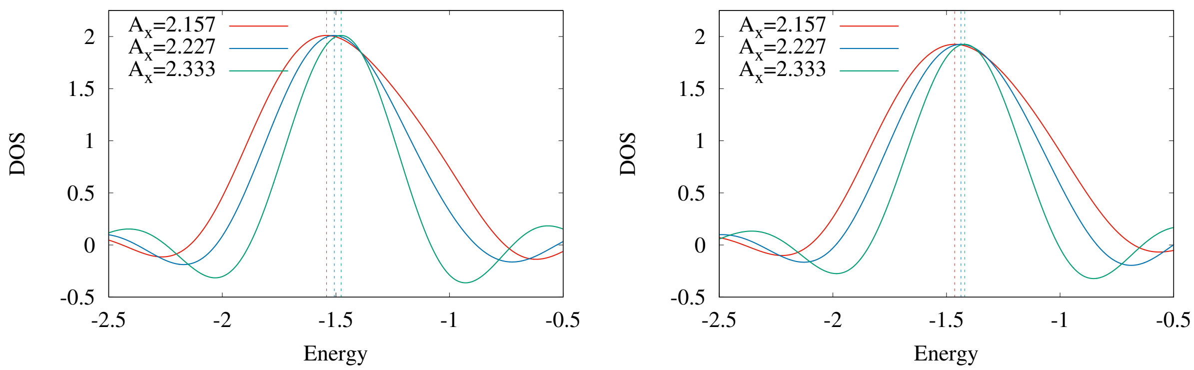
(a) (b)

Figure 3: Etot



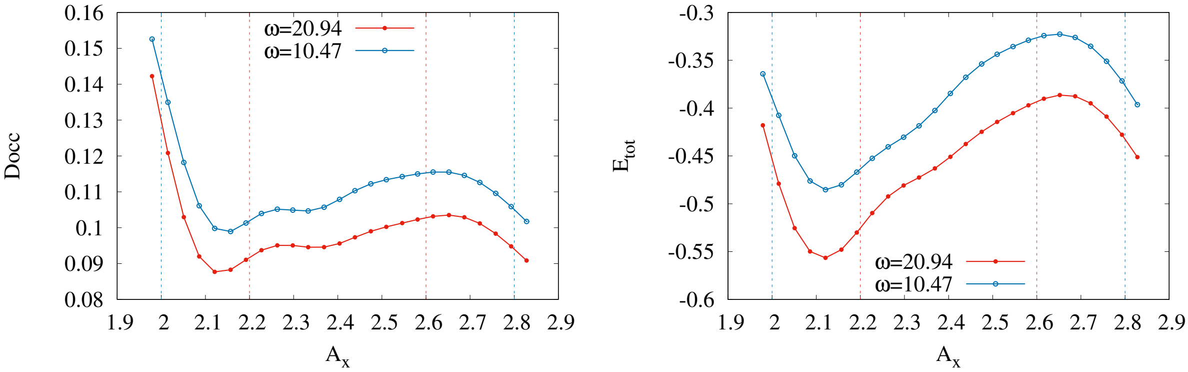
(a) (b)

Figure 4: DOS



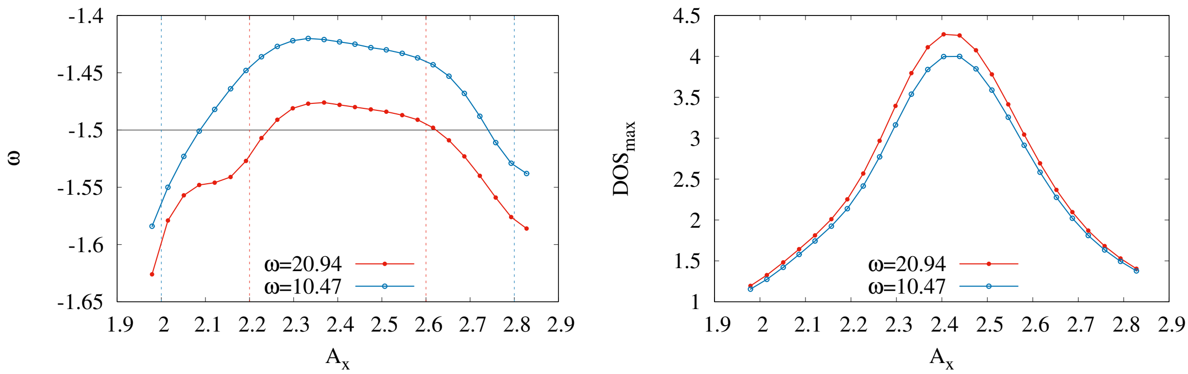
(a) (b)

Figure 5: DOS small



(a) (b)

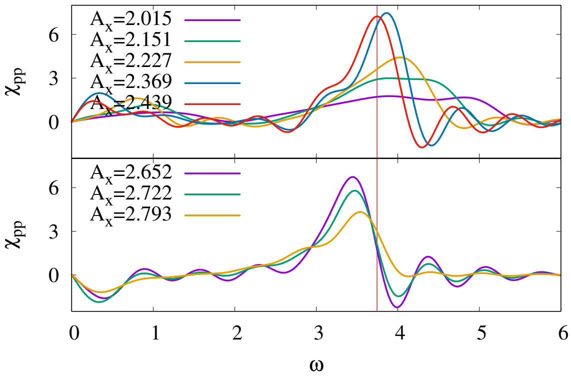
Figure 6: docc Etot



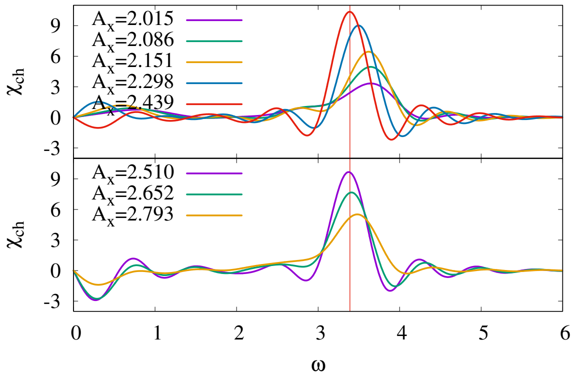
(a) (b)

Figure 7: DOS peak

4 Dispersion of doublons

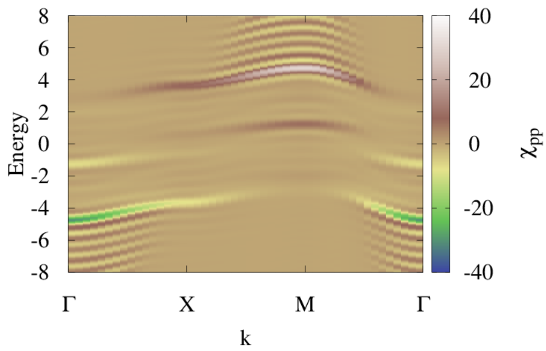


(a)

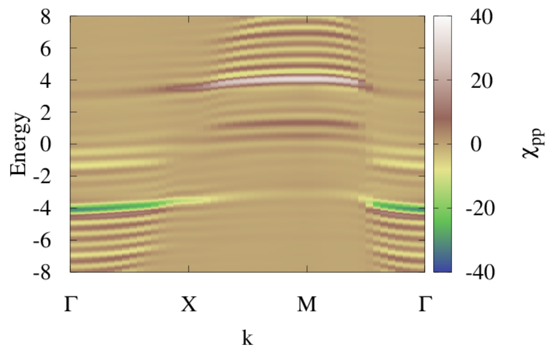


(b)

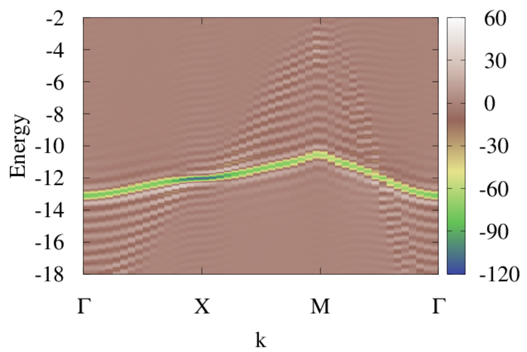
Figure 8: CHI loc pp ch



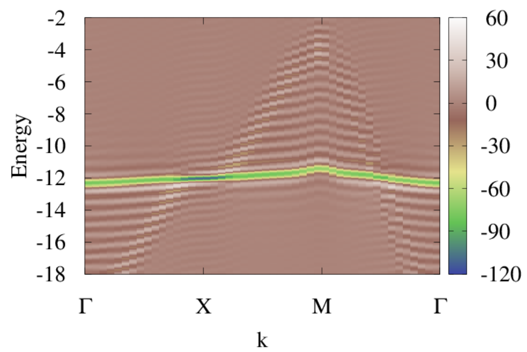
(a)



(b)



(c)



(d)

Figure 9: CHI k pp. A-dependence. (a) $A_x = 2.157$ $n = 0.5$, (b) $A_x = 2.333$ $n = 0.5$, (c) $A_x = 2.157$ $n = 1$, (d) $A_x = 2.333$ $n = 1$.

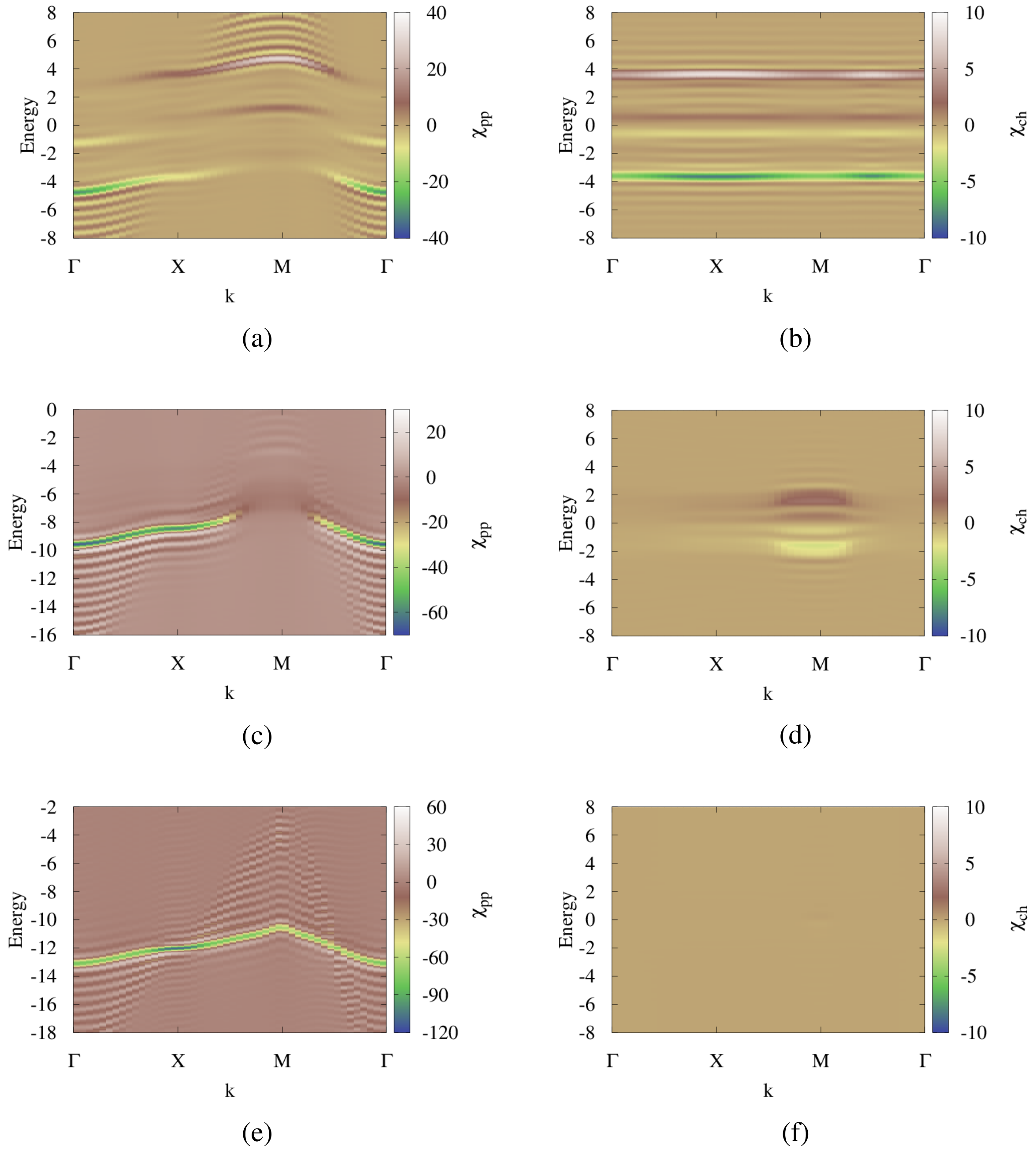


Figure 10: CHI k pp. μ-dependence, $A_x = 2.157$. (a) χ_{pp} $n = 0.5$, (b) χ_{ch} $n = 0.5$, (c) χ_{pp} $n = 0.875$, (d) χ_{ch} $n = 0.875$, (e) χ_{pp} $n = 1$, (f) χ_{ch} $n = 1$.

5 Summary

References

[Aoki et al.(2014)Aoki, Tsuji, Eckstein, Kollar, Oka, and Werner] H. Aoki, N. Tsuji, M. Eckstein, M. Kollar, T. Oka, and P. Werner. Nonequilibrium dynamical mean-field theory and its applications. *Rev. Mod. Phys.*, 86:779–837, Jun 2014. doi: 10.1103/RevModPhys.86.779. URL `https://link.aps.org/doi/10.1103/RevModPhys.86.779`.

[Eckstein and Werner(2011)] M. Eckstein and P. Werner. Damping of bloch oscillations in the hubbard model. *Phys. Rev. Lett.*, 107: 186406, Oct 2011. doi: 10.1103/PhysRevLett.107.186406. URL `https://link.aps.org/doi/10.1103/PhysRevLett.107.186406`.

[Georges et al.(1996)Georges, Kotliar, Krauth, and Rozenberg] A. Georges, G. Kotliar, W. Krauth, and M. J. Rozenberg. Dynamical mean-field theory of strongly correlated fermion systems and the limit of infinite dimensions. *Rev. Mod. Phys.*, 68:13–125, Jan 1996. doi: 10.1103/RevModPhys.68.13. URL `https://link.aps.org/doi/10.1103/RevModPhys.68.13`.