I. INTRODUCTION

Electrons in materials are charged particles that repel each other through Coulomb interaction, but effective electron-electron attraction can be generated by coupling to lattice vibrations. The Hubbard model describes a lattice with on-site electron-electron interaction term $U$ which can be either positive (repulsion) or negative (attraction). The positive-$U$ Hubbard model is a minimal model for the cuprate family of superconducting materials and describes the competition between the delocalizing effects of electron hopping and localization effects of charge repulsion. The negative-$U$ Hubbard model is used as an effective description for certain systems with very strong electron-phonon coupling and for cold atoms in optical lattices. It has been used to study, for example, strong-coupling superconductors and the cross-over between the BEC and BCS superconducting regime.

There are very few works that directly address the differences between the repulsive and the attractive regime of the Hubbard model. While at the particle-hole symmetric point (i.e., at half filling, for one electron per lattice site), the two cases are trivially related by a partial particle-hole transformation that leads to $U \rightarrow -U$ and simply exchanges the spin and charge sectors, this is no longer the case at finite doping, since the doping corresponds to the magnetization under this mapping. Comparative studies of repulsive and attractive Hubbard models are very valuable for understanding more complex models such as the Hubbard-Holstein model, where for increasing electron-phonon (e-ph) coupling the effective electron-electron (e-e) interaction becomes attractive on low-energy scales, while remaining repulsive at higher energies. They are also of interest in the context of fermionic cold atoms trapped in optical lattices, where the strength and even the sign of the interaction can be continuously tuned by means of Feshbach resonances. In this work, we study the paramagnetic phase of the Hubbard model at moderate hole doping, $\langle n \rangle = 0.8$, for both signs of $U$ using the dynamical mean-field theory (DMFT). We focus on the experimentally most relevant properties: transport (resistivity and Seebeck coefficient, optical conductivity) and NMR ($1/T_1$ spin-lattice relaxation rate) characteristics as a function of temperature. The main new results of this work are the identification of the characteristic energy scales in the $U < 0$ model, observation of resilient quasiparticles for resistivity in excesses of the Mott-Ioffe-Regel value, and the non-monotonic temperature dependence of the spin-lattice relaxation rate.

This work is structured as follows. In Sec. II we introduce the model and discuss the partial particle-hole transformation. In Sec. III we describe the thermodynamic properties as a function of Hubbard coupling $U$ and temperature $T$. In Sec. IV we discuss the local and momentum-resolved spectral functions, the $U$-dependence of the quasiparticle renormalization factor $Z$, and the asymmetric structure of the self-energy $\Sigma$ and its temperature variation. In Sec. V we describe the transport properties and contrast the positive and negative $U$ and provide some details about the non-monotonous temperature dependences in the attractive Hubbard model. In Sec. VI we compare the spin-lattice relaxation rates. Section VII is devoted to the DMFT mapping in the attractive $U$ case, where the effective model is the particle-hole symmetric Anderson model.
impurity model at constant magnetization and we discuss to what degree the properties of the impurity model reflect in the fully self-consistent DMFT calculations. The final section concerns the experimental relevance of our calculations and presents some additional results for the optical conductivity that could aid in the interpretation of the measurements on zeolite materials.

II. MODEL AND METHOD

We study the Hubbard model

\[ H = \sum_{k\sigma} \epsilon_k c_k^{\dagger} c_{k\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}. \]  

(1)

Here \( \epsilon_k \) is the dispersion of electrons with wave-vector \( k \) and spin \( \sigma \), while \( U \) is the Hubbard coupling. Index \( i \) ranges over all lattice sites, while \( n_{i\sigma} = c_{i\sigma}^{\dagger} c_{i\sigma} \). We seek a non-ordered paramagnetic (homogeneous in space) solution of this model using the DMFT. In this approach, the bulk problem defined on the lattice maps onto a quantum impurity model (single impurity Anderson model) subject to a self-consistency condition for the hybridization functions. This technique takes into account all local quantum fluctuations exactly, while inter-site correlations are treated at the static mean-field level. This is a good approximation for problems where the most important effects are local in nature (Mott metal-insulator transition, etc.). Magnetic order, charge-density-wave, and superconducting DMFT solutions are also possible, but not allowed for in our calculations; even if the true ground state is ordered, our results are still valid above the ordering temperature. We work with the Bethe lattice that has non-interacting density of states \( \rho_0(\epsilon) = (2/\pi D) \sqrt{1 - (\epsilon/D)^2} \). As the impurity solver, we use the numerical renormalization group (NRG) with discretization parameter \( \Lambda = 2 \), twist averaging over \( N_z = 16 \) values, and keeping up to 12000 multiplets (or up to a truncation cutoff at energy \( 10\omega_N \), where \( \omega_N \) is the characteristic energy at the \( N \)-th NRG step). We remind the reader that the twist averaging in the NRG means that \( N_z \) separate NRG calculations are run for different choices of interleaved discretization grids (so-called \( z \) parameters) and the results are then averaged; this technique leads to a significant cancelation of the discretization artifacts of the method. Spectral broadening has been performed with parameter \( \alpha = 0.3 \). We use Broyden’s method to speed-up convergence of the DMFT iteration and to control the chemical potential in constant-occupancy calculation. The convergence criteria are very stringent (integrated absolute value of the difference of spectral functions less than \( 10^{-8} \)) in order to obtain reliable results for transport properties at low temperatures. In spite of these efforts, the residual oscillatory features in the self-energy remain problematic especially at low temperatures; for computing transport properties it is necessary to perform fitting with low-order polynomials around \( \omega = 0 \).

There is a relation between the repulsive and the attractive Hubbard model through the partial particle-hole (Lieb-Mattis) transformation defined as

\[ c_{i\uparrow}^{\dagger} \rightarrow d_{i\uparrow}^{\dagger}, \quad c_{i\downarrow}^{\dagger} \rightarrow (-1)^i d_{i\downarrow}^{\dagger}. \]  

(2)

For down spins, this is a mapping of the particle creation operators onto annihilation operators for the holes. The \((-1)^i\) factor indicates different prefactors for the two sublattices of a bipartite lattice. The transformation leaves the kinetic energy unchanged, but changes the sign of the quartic electron-electron coupling term, i.e., flips the sign of \( U \). Furthermore, it can be seen that the particle number operator for \( c \) particles maps onto the spin-\( z \) (magnetization) operator for \( d \) particles. While the spin-up Green’s function is invariant, the spin-down Green’s function is transformed. Since \( \langle (A; B) \rangle_z = -\langle (B; A) \rangle_{-z} \), the transformation is

\[ A_{i\downarrow}(\omega) \rightarrow A_{i\uparrow}(-\omega). \]  

(3)

This implies that the field-induced Zeeman splitting of the quasiparticle band in the \( U > 0 \) case corresponds to a uniform shift of the quasiparticle band through changes of the chemical potential.

Unless noted otherwise, the band filling is \( \langle n \rangle = 0.8 \), i.e., the hole doping level is \( \delta = 1 - \langle n \rangle = 0.2 \).

III. THERMODYNAMIC PROPERTIES

Figure 1: (Color online) Thermodynamic properties of the Hubbard model. (a) Double occupancy \( P_2 = \langle n_{\uparrow} n_{\downarrow} \rangle \). The inset shows the charge susceptibility, \( \chi_c = \partial \langle n \rangle / \partial \mu \). (b) Potential, kinetic and total energy per particle.

We first consider the static (thermodynamic) properties. In Fig. (a) we show the double occupancy \( P_2 = \langle n_{\uparrow} n_{\downarrow} \rangle \). The non-interacting result at \( U = 0 \), \( (n/2)^2 = 0.16 \), is rapidly reduced for repulsive \( U \) with maximum curvature in the range where the upper Hubbard band emerges (\( U \approx 2D \),...
see Fig. [4] and tends to zero as $1/U$. For attractive $U$, the double occupancy increases up to values around 0.4, at which point constant-occupancy DMFT calculations no longer converge due to a very high charge susceptibility (see the inset in Fig. [1]). It helps to perform calculations at a fixed chemical potential $\mu$ and determine the appropriate $\mu$ by bisection. The instability also manifests itself as a large spread of expectation values in the $z$-averaging method in the NRG calculations. For example, at $U/D = -2.85$, computed $\langle n \rangle$ values range from 0.741 to 0.861 for different discretization grids, thus the quantitative validity of the results becomes somewhat questionable (for comparison, generally the differences between $\langle n \rangle$ are of order $10^{-4}$). Such behavior is a well known precursor of phase transitions in NRG calculations. Remaining in the paramagnetic phase, for large $|U|$ one namely expects the formation of bipolarons. We denote the transition point by $U_0$. Below, we will determine its value to be

$$U_0/D = -2.89$$

(4)

for $\langle n \rangle = 0.8$ considered here. The charge susceptibility is large, but not divergent at $U = U_0$. This value is close in absolute value to that for the Mott metal-insulator-transition in the half-filled repulsive Hubbard model, $U_{c2}/D = 2.92$; the reason for this similarity will become clear in the following.

In Fig. [1b] we follow the kinetic and potential energies. The potential energy is given simply by $U\langle n_{\uparrow}n_{\downarrow}\rangle$, thus it does not bring any new information. $E_{\text{kin}}$ is minimal in the non-interacting case. It increases for both signs of $U$, because interactions always lead to increased particle localization which costs kinetic energy.

The entropy curves for attractive $U$ have a pronounced plateau at intermediate temperatures, see Fig. [2] for example, at $U/D = -2.25$ the low-temperature nearly linear region is followed by a plateau starting at $T = T_{\text{pl}} \approx 0.04D$, where the entropy is nearly pinned at $S \approx 0.89k_B$ up to $T \approx 0.15D$ at which point it starts to rise again. The temperature scale $T_{\text{pl}}$ is also visible in the chemical potential $\mu(T)$: for $T < T_{\text{pl}}$ the chemical potential is nearly constant, then it rapidly crosses over into a new decreasing regime that smoothly connects with the asymptotic linear behavior, see Fig. [3].

We note that under the $U \to -U$ mapping, the chemical potential corresponds to the magnetic field required to maintain the magnetization constant. In the following, we show that the plateau can be related to features seen in the double occupancy and spin-lattice relaxation curves, but not so well in the dc transport properties.

Figure 2: (Color online) Temperature dependence of entropy per lattice site for a set of $U$ values.

Figure 3: (Color online) Temperature dependence of the chemical potential (shifted by $-U/2$).

IV. ZERO-TEMPERATURE SPECTRAL FUNCTIONS

In the DMFT, the lattice (momentum-resolved) Green’s function is approximated using a self-energy function that depends only on the frequency but not on the momentum, so that

$$G_k(z) = \frac{1}{z + \mu - \epsilon_k - \Sigma(z)},$$

(5)

where $z$ is complex frequency (one may take $z = \omega + i\delta$ to obtain the retarded Green’s function). The local Green’s function is obtained as the $k$ average:

$$G_{\text{loc}}(z) = \frac{1}{N} \sum_k G_k(z) = \int \frac{\rho_0(\epsilon) d\epsilon}{z + \mu - \epsilon - \Sigma(z)}$$

(6)

where $N$ is the number of lattice sites and $G_0(z)$ is the non-interacting Green’s function of the chosen lattice. Momentum-resolved and local spectral functions are then defined as $A_k(\omega) = (-1/\pi)\text{Im}G_k(\omega + i\delta)$ and $A(\omega) = (-1/\pi)\text{Im}G_{\text{loc}}(\omega + i\delta)$.

In Fig. [4] we compare the local spectral functions $A(\omega)$ for both signs of $U$. For positive $U$, the results are well known: with increasing $U$, the upper and lower Hubbard bands emerge and there is a narrow quasiparticle (QP) band at the Fermi level. For very large $U$, the low-energy part of the spectrum no longer changes, while the upper Hubbard band shifts to higher energies. In the large-$U$ regime, the system is a doped Mott insulator, which is a Fermi liquid at low temperatures and a bad metal at high temperatures.

For negative $U$, the local spectral function also features Hubbard bands and a QP peak, but the evolution as a function
Figure 4: (Color online) Local spectral function $A(\omega)$ at zero temperature for (a) repulsive and (b) attractive case. (c) Quasiparticle renormalization factor $Z \equiv Z(T=0)$ as a function of $U$. $Z$ goes to zero at $U = U_0 \approx -2.89D$.

The temperature dependence of spectra for the attractive case is shown in Fig. 5, where we plot the momentum-resolved ($\epsilon$-dependent) spectral functions. We observe the gradual disappearance of the QP band (finished by $T \approx 0.15D$), while the high-energy Hubbard bands are not affected much in this temperature range.

We now compare the structure of the self-energy function in repulsive and attractive case. For weak interaction, they are qualitatively similar and can be reproduced using the perturbation theory: in $\text{Im}\Sigma(\omega)$ there are two broad peaks centered approximately at $\omega = \pm |U|$. For strong interactions, the case shown in Fig. 6(a), the differences become more pronounced. The $U/D = 4$ case has been thoroughly studied recently in $B \sim T_K$ regime in the language of the effective quantum impurity model with positive $U$. This is precisely the non-trivial cross-over regime between the well-understood $B = 0$ Kondo limit and the non-interacting $B \to \infty$ limit. The field was found to cause derenormalization of quasiparticles.

Figure 5: (Color online) Momentum-resolved spectral functions $A(\epsilon, \omega)$ for a range of temperatures for attractive interaction with $U/D = -2$.

of $U$ is quite different. This problem maps onto the half-filled repulsive Hubbard band in the presence of an external magnetic field of such intensity that the magnetization remains constant, see Fig. 3. With increasing $|U|$, the low-energy scale (Kondo temperature) is reduced exponentially, thus the QP band shrinks. The negative-$U$ model thus corresponds to the

\begin{equation}
Z(T) = \left(1 - \text{Re} \left[\frac{d\Sigma(\omega, T)}{d\omega}\right]_{\omega=0}\right)^{-1}
\end{equation}

at zero-temperature, $Z \equiv Z(T=0)$. It quantifies the renormalized mass $m^* = m/Z$ and the QP lifetime $\tau^* = Z \tau$. The system is a Fermi liquid for all $U > U_0$, where we have defined $U_0$ as the point where $Z$ goes to zero and the QP band disappears. For $U < U_0$ the system is a paramagnetic insulator, analogous to the Mott insulator in the repulsive Hubbard model at half-filling in magnetic field. (Note again that in our DMFT Ansatz we do not allow for any instability toward ordered phases, magnetic order for $U > 0$ or charge order and superconductivity for $U < 0$. The true ground state of the $U < 0$ model is superconducting.)
Ref.\cite{41}, where the strong particle-hole asymmetry in vicinity of the Fermi level has been pointed out. For strongly negative $U/D = -2.5$, we also find asymmetry in the low-energy part, but in this case the plateau in Im$\Sigma(\omega)$ is found on the hole side rather than on the particle side, and it is much less pronounced. The resonance structures remain rather sharp on both particle and hole sides; they tend toward small $\omega$ as $|U|$ increases, which reflects the structure of the spectral function with shrinking QP band (resonances in Im$\Sigma$ follow from the analytical structure of the Green’s functions and are expected between any two spectral peaks). For strongly attractive $U$, the asymmetry decreases for increasing $|U|$.

The temperature dependence of Im$\Sigma(\omega)$ in the attractive case reveals an interesting reversal of the asymmetry, see Fig. 6(b). This is another non-trivial effect of the constant-magnetization constraint; it indicates that the $T = 0$ self-energy does not permit an easy identification of the transport mechanisms at elevated temperatures.

\section{V. TRANSPORT PROPERTIES}

In the DMFT, the vertex corrections drop out and the optical conductivity is fully determined by the self-energy alone\cite{20,40,49}:

$$\sigma(\omega) = \frac{2\pi e^2}{\hbar} \int d\omega' F(\omega, \omega') \int d\omega' \Phi(\omega) A_e(\omega') A_e(\omega + \omega),$$

(8)

with $F(\omega, \omega') = [f(\omega') - f(\omega + \omega')]/\omega$, $f(\omega)$ is the Fermi function, $A_e(\omega) = -(1/\pi)\text{Im}[\omega + \mu - \epsilon - \Sigma(\omega)]^{-1}$, and $\Phi(\epsilon)$ is the transport function. For Bethe lattice, $\Phi(\epsilon) = \Phi(0)(1 - (\epsilon/D)^2)^{1/2}$. We find that the choice of the transport function has a strong effect on the results; it can even change the sign of the Seebeck coefficient.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig6.pdf}
\caption{(Color online) (a) Imaginary part of the self-energy at $T = 0$ for strongly repulsive and attractive interactions reveals particle-hole asymmetry at low energy scales in both cases. (b) Temperature dependence of Im$\Sigma(\omega)$ for the attractive Hubbard model at $U/D = -2.25$.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig7.pdf}
\caption{(Color online) Resistivity and Seebeck coefficient of the Hubbard model at constant temperature $T = 10^{-2}D$. The resistivity is expressed in units of the Mott-Ioffe-Regel value $\rho_0 = (e^2/\hbar)\Phi(0)/D$. The results for Seebeck coefficient for low-$|U|$, where the calculation is not reliable, have been omitted.}
\end{figure}

We consider first the dc resistivity $\rho = 1/\sigma(0)$ and the Seebeck coefficient (thermopower)\cite{50} at fixed low temperature as a function of the interaction strength $U$, see Fig. 7. The most notable feature is the rapid resistivity increase for large e-e attraction, $U \lesssim -2D$. This effect is much stronger than the growing resistivity for increasing e-e repulsion for $U > 0$. This can be explained by the strong decrease of the effective Kondo temperature, and the corresponding decrease of the QP lifetime $\tau^*$, see Fig. 6(b).

The thermopower (Seebeck coefficient) is defined as

$$S = \frac{k_B}{e_0 T} \frac{L_{12}}{L_{11}},$$

(9)

where the transport integrals in the infinite-$d$ limit are given as

$$L_{jk} = \int d\omega \left(-\frac{\partial f(\omega)}{\partial \omega}\right) \left[\sum_{\sigma} \int d\epsilon \Phi(\epsilon) A_{\sigma,\epsilon}(\omega)^2\right]^j \omega^{k-1}.$$  

(10)

The Seebeck coefficient for small $U$ is negative because of the asymmetry of the density of states around the Fermi level. For increasing interaction, it becomes more negative for repulsive $U$ and positive for a range of attractive $U$. This behavior can be explained by the previously discussed asymmetry in the self-energy. For $U$ approaching $U_0$, the Seebeck coefficient again turns negative.

In Fig. 8 we plot the temperature dependence of the transport properties. At low temperatures, we always find Fermi
liquid behavior \( \rho \propto T^2 \) below temperature \( T_{\text{FL}} \) for \( U > U_0 \).

In the repulsive case, \( T_{\text{FL}} \) is given by \( T_{\text{FL}} \approx 0.05 \delta D \) where \( \delta \) is doping with respect to half-filling, \( \delta = 1 - \langle n \rangle \) \(^{11}\). For large positive \( U \), the resistivity above \( T_{\text{FL}} \) increases linearly with negative intercept up to \( T^* \), where the slope changes and the resistivity is linear with positive intercept. \(^{11}\) In the attractive case, we find that the quadratic dependence typically extends to much higher temperatures; for \( U/D \gtrsim -2 \), it goes essentially up to the maximum resistivity at approximately \( T_{\text{max}} = ZD \). For even stronger e-e attraction, we find clearer separation between between the \( T_{\text{FL}} \) and \( T_{\text{max}} \) scales, see Fig. 9(b). We find that well-defined QP excitations survive almost up to the high temperature scale \( T_{\text{max}} \), similar to the resilient quasiparticles identified in the repulsive case which exist up to \( T_{\text{MIR}} \) where \( \rho \) reaches the MIR value. \(^{12}\) The surprising results is that in the attractive case at \( T_{\text{max}} \), the resistivity for large enough \( |U| \) surpasses the Mott-Ioffe-Regel limit, thus resilient quasiparticles exist even in this regime.

We now consider the thermopower, see Fig. 8(b). For positive \( U \), the sign change of \( S \) reveals a change of the dominant transport mechanism and finds its counterpart in the kink in \( \rho(T) \). For negative \( U \), the Seebeck coefficient remains negative for all temperatures, excepts for a small range of \( U \) where it is positive at small temperatures.

It is interesting to compare these findings for the attractive Hubbard model with the results for the transport properties of the repulsive \( U \) model at half-filling in the absence of the magnetic field (zero magnetization) reported, for example, in Ref. \(^{51}\). The common feature is the non-monotonic behavior of \( \rho(T) \) and the resistivity peak much in excess of the Mott-Ioffe-Regel limit at the point where the quasiparticles are no longer present. The difference is found in the behavior of the thermopower. In the attractive model, with the exception of \( U \) close to the transition point, it is monotonous at all temperatures and has no change of sign. In the repulsive model, however, it has a change of sign indicating the thermal destruction of the coherent Fermi liquid state, similar to what is also found in doped Mott insulator (i.e., positive \( U \) calculations at finite hole doping, as studied in this work and previously in Ref. \(^{41}\)). This difference in the thermopower can be traced back to the partial particle-hole mapping, Eq. (3), and its effect on the transport integrals. \( L_{jk} \) includes the factor

\[
A_{\epsilon,\uparrow}(\omega)^2 + A_{\epsilon,\downarrow}(\omega)^2,
\]

which maps to

\[
A_{\epsilon,\uparrow}(\omega)^2 + A_{\epsilon,\downarrow}(\omega)^2.
\]

This mostly affects \( L_{12} \) where the integrand is odd in \( \omega \) and thus sensitive to the asymmetry of spectral functions.

While in the repulsive case, the characteristic temperature scales \( T_{\text{FL}} \) and \( T_{\text{MIR}} \) are proportional to doping \( \delta = 1 - \langle n \rangle \), in the attractive case the amount of doping has little effect on the resistivity curves, see Fig. 10. \( T_{\text{max}} \) depends mostly only on \( U \), while the doping controls the peak value of resistivity, but even this dependence is found to be very weak. The results can be explained by the trends seen in the spectral function:
the QP band is not affected much by the amount of doping (there is a minor shift of its low-energy edge, while the high-energy edge is almost invariant), while there is a significant reorganization of spectral weight between the lower and upper Hubbard band (this reflects the changing magnetization in the language of the effective positive-\( U \) model at half-filling).

The optical conductivity at low temperatures shows the well-known characteristics of the Fermi liquid state: a pronounced Drude peak at \( \Omega = 0 \) due to transitions inside the QP band, peak(s) corresponding to transition between the QP band and the Hubbard bands near \( \Omega = U/2 \), and a more diffuse peak at \( \Omega = U \) due to the inter-Hubbard-band excitations.

The results for attractive interaction \( U/D = -2.25 \) are shown in Fig.\[11\]. At low temperatures the peaks are rather well defined and clearly separated. As the temperature increases, the Drude peak intensity decreases. For \( T \gtrsim T_{\text{FL}} \), the intensity of the peak at \( \Omega \approx U/2 \) also drops and shifts toward lower frequencies. In this temperature range of \( T \lesssim T_{\text{max}} \), the optical spectral weight is transferred mostly to the \( \Omega = U \) inter-Hubbard-band peak. As the temperature is increased further to \( T \gtrsim T_{\text{max}} \), there is a spectral redistribution in the opposite direction, from the \( \Omega = U \) region to low-frequency regions, which corresponds to the decreasing dc resistivity in the temperature interval from \( T_{\text{max}} \) to the plateau of nearly constant resistivity around \( T = 0.5D \).

For completeness, we also study the \( n \)-dependence of the optical conductivity at two characteristic temperature regimes \( (T/D = 10^{-2} \) is well in the Fermi liquid regime, \( T/D = 10^{-1} \) corresponds to the cross-over regime between the low-temperature and high-temperature asymptotics) for both signs of \( U \), see Fig.\[12\].

For positive \( U \), the results for the lower temperature \( T/D = 10^{-2} \) are easy to understand. With increasing doping (decreasing \( n \)), both Hubbard bands shift to higher energies, thus the corresponding optical peaks also move up. At the same time, the spectral weight of the QP band is increasing, while that of the Hubbard bands is decreasing. This is reflected in the decreasing weight of the peak at \( \Omega \approx U \) (upper Hubbard band, UHB), although that at \( \Omega \approx 0.5D \) (lower Hubbard band, LHB) is actually increasing due to the increasing density of initial QP states. At higher temperature \( T/D = 10^{-1} \), the QP-LHB transitions can no longer be resolved, but the general trend with increasing doping is similar as at \( T/D = 10^{-2} \).

The weak dependence of the optical conductivity on \( n \) for large negative \( U \) is expected, since in the effective model the changing magnetization leads to rather moderate weight redistribution: it mostly affects the total spectral weight in the atomic peaks, while their positions remain essentially the same. The results are also in agreement with the trends in the dc resistivity, shown in Fig.\[10\]. The most significant variation of the dc resistivity is found in the peak region from \( T \approx 0.1D \) to \( T \approx 0.2D \), and we also observe that in this temperature range the optical conductivity is affected on an extended frequency range from \( \Omega = 0 \) up to \( \Omega \approx 2D \) which includes the transitions inside the QP band and between the QP band and either Hubbard band: the main effect is that with increasing doping, the optical conductivity decreases almost uniformly, with no changes in peak positions. The behavior is different at the lower temperature of \( T = 0.01D \): the main effect there is a shift in the upper flank of the peak in \( \sigma(\Omega) \) at \( \Omega \approx U/2 \), which corresponds to transitions between the QP band and either Hubbard band, but little overall decrease in the optical conductivity.

VI. SPIN-LATTICE RELAXATION RATE

The spin susceptibility can be probed in nuclear magnetic resonance (NMR) experiments. The spin-lattice relaxation...
rate $1/T_1$ quantifies the decay of the nuclear magnetic moments and provides information about the fluctuations of the electronic magnetic moments:

$$\frac{1}{T_1} = 2k_BT \left( \frac{g_N\mu_B}{g_B} \right)^2 \sum_q |H_{hf}(q)|^2 \text{Im} \left[ \frac{\chi^+ - (q, \omega_N)}{\omega_N} \right],$$

where $\omega_N$ is the nuclear Larmor frequency which may be set to zero. If the hyperfine interaction $H_{hf}(q)$ is local (i.e., has very weak $q$ dependence), we are effectively probing the local magnetic susceptibility that is easily computed using the NRG. Furthermore, if there is no magnetic order, $\chi_{zz} = \frac{1}{2} \chi_{+-}$ due to isotropy in spin space. Thus, in the context of paramagnetic DMFT calculations, $1/T_1$ measures the slope of the imaginary part of $\chi_{\text{loc}}$ in the zero-frequency limit.

The temperature dependence of the relaxation rate is shown in Fig. 13(a). For large repulsive e-e interaction, it is monotonously decreasing with temperature: for $U/D = 4$ it drops by four orders of magnitude when going from $T = 0$ to $T \sim D$. For attractive $U$, the dependence is much more complex and non-monotonic. The case of $U/D = -2$ is typical for the strongly attractive regime. The pronounced minimum at $T \sim 0.1D$ corresponds to the maximum in $P_2(T) = \langle n_{\uparrow}n_{\downarrow} \rangle(T)$, see Fig. 13(b): higher double occupancy implies less developed local moments, i.e., increased itinerancy. (Note the opposite behavior for the repulsive case where $P_2$ starts by decreasing upon heating, i.e., increased localization, which can be explained by the higher entropy in the Mott insulating phase.) We also generally observe that the scale of temperature variations is significantly smaller in $U < 0$ case as compared to the $U > 0$ case.

The relaxation rate at $T = 0$ is plotted in Fig. 13(c). The general trend is expected: for the repulsive $U$ the system exhibits sizeable magnetic fluctuations which saturate in the large-$U$ limit, while for the attractive $U$ the spin fluctuations rapidly freeze out. In the interval $-2D < U < 2D$, $1/T_1$ depends exponentially on $U$, approximately as

$$\frac{1}{T_1} \propto \exp \left( \frac{dU}{D} \right), \quad \text{with} \quad d \approx 1.7.$$

For a more strongly attractive $U$, the reduction becomes even more pronounced. This is associated with the emergence of the sharp Kondo resonance in the charge sector.

VII. DISCUSSION

The non-monotonic temperature dependences in the attractive-$U$ Hubbard model have been explained through non-trivial properties of the positive-$U$ model in magnetic field at constant magnetization. In this section, we investigate to what extent this behavior is present already at the level of the quantum impurity model without the self-consistency loop. In other words, we consider the Anderson impurity model at the particle-hole symmetric point as a function of external magnetic field $B$ and temperature $T$, and study its properties along the constant magnetization contours. The magnetic field will be expressed in energy units (i.e., it includes the $g\mu_B$ prefactor, where $g$ is the $g$-factor and $\mu_B$ the Bohr magneton). We choose $U/D = 0.5$, $\delta = 0$ and a flat band with constant hybridization function $\Gamma/D = 0.05$. For this parameter set, the Kondo temperature according to Wilson’s
definition is $T_K/D = 10^{-3}$. We consider a temperature range up to $T = 0.05D = 50T_K$, where the Kondo peak is already strongly suppressed (but still visible as a small hump at the Fermi level), and magnetic fields up to $B = 0.02D = 20T_K$ where the spin polarization at low temperatures is 80% and there is strong Kondo peak splitting (although the peaks are still clearly present). The comments about the persistence of non-trivial low-frequency spectral features at $T$ and $B$ of several tens of $T_K$ are worth stressing again: the Kondo effect is a cross-over with logarithmic dependencies, thus it affects the system properties in a wide temperature and field range much above the $T_K$ scale. This has obvious implications for the physics of the Hubbard model considered within the DMFT approach, since a quasiparticle band must consequently be present on temperature scales much above $Z \sim T_K$, unless suppressed through the additional effect of the DMFT self-consistency constraint.

In Fig. 14(a) we plot the constant-magnetization contours in the $(T, B)$ plane. For low magnetization, the contours are almost linear: curvature is visible only at low temperatures and high fields. We note that the attractive Hubbard model at $(\mu) = 0.8$, the case we focused on in this work, corresponds to the $S_z = 0.1$ line which is nearly perfectly linear for $T > T_K$ and has some very weak curvature much below $T_K$. The impurity properties are best characterized by its thermodynamic properties, defined as the impurity contributions to the total quantities. In panels (b,c,d) we show the results for spin and charge susceptibility and the entropy in the $(T, B)$ plane, while panel (e) presents the spin susceptibility along a set of constant-magnetization contours. We observe that there are no sharp features in any of these results: the cross-overs are all smooth, with no visible kinks. This should be compared with the $\mu$ vs. $T$ curves for the attractive Hubbard model presented in Fig. 2 where a kink becomes noticeable for sufficiently negative $\mu$. Such kinks must thus be generated through the self-consistency loop and are a genuine lattice effect that is not present at the single-impurity level. The susceptibility curves in panel (e) indicate that the cross-over scale does not depend much on the magnetization. This property of the pure impurity model explains the results for the resistivity of the Hubbard model shown in Fig. 10 which indicate an analogous lack of dependence on the band filling.

In Fig. 15(a), we show the temperature and field dependence of the “conductivity” for a single spin species of the symmetric Anderson impurity model as a function of temperature and magnetic field. The quantity shown is actually

$$\chi(\omega) = \frac{1}{\beta} \int \frac{d\omega}{2\pi} \text{Im} \left\{ \chi(\omega) \right\} = 10^{-3},$$

i.e., the spin-resolved spectral function integrated with a thermal broadening kernel. A single spin is considered because under the partial particle-hole transformation, the original $U < 0$ spectral functions for both spins map to a single spin-resolved function of the $U > 0$ model (this is only true at the p-h symmetric point). The thermal kernel is the same as in the bulk expression for the dc conductivity [Eq. 7 in the $\Omega \rightarrow 0$ limit]. If the quantity $F(T, B)$ is evaluated along the constant-magnetization contours we obtain the results shown in Fig. 15(b): the conductivity is monotonically decreasing, thus this simple calculation does not explain the nonmonotonous transport properties of the bulk attractive-U Hubbard model.

One final remark is in order. Fig. 14 indicates that there is nothing special about the zero magnetization line at $B = 0$ and that the results along the zero magnetization contour do not differ drastically from those for finite magnetization lines. This simply shows that as the doping in the attractive $U$ Hubbard model is reduced toward zero, the results are smoothly connected with those for the repulsive $U$ Hubbard model at half-filling in the absence of the field, except for the effects of
the mapping of spectral functions, Eq. (3), on the transport properties, in particular the thermopower, as already commented above. This, together with the weak dependence on the doping $n$, also explains why the transition to the localized state at $U_0/D = -2.89$ for $n = 0.8$ is so close in absolute value to that for the Mott MIT at $U_c/D = 2.92$.

VIII. EXPERIMENTAL RELEVANCE

Zeolites are aluminosilicate materials with microporous structure consisting of cages or channels with large voids which can accommodate alkali cations. They show a variety of exotic electronic properties, including different magnetically ordered states and metal-insulator transitions. The $s$ electrons of alkali atoms are believed to be confined in the cages and the concentration of dopants strongly affects the electronic properties, since it changes not only the band filling, but also the electronic potential depth, thereby controlling the electron-electron repulsion. Furthermore, the cations can undergo large displacements, thus there is significant electron-phonon coupling leading to polaron effects. The appropriate model for such systems is thus some multi-orbital variant of the Hubbard-Holstein model which takes into account the large number of electron orbitals inside the cages, and their consecutive filling as the concentration of dopant atoms is increased. The minimal model, however, is the single-orbital Hubbard-Holstein model, which may be expected to describe at least qualitatively the electrons in the top-most electronic band near the Fermi level. A detailed study of this model is beyond the scope of the present work. Nevertheless, the Hubbard-Holstein model maps in the antiadiabatic limit onto the Hubbard model with effective interaction $U_{\text{eff}}$ that depends on the original e-e repulsion $U$ and on the value of the electron-phonon coupling $g$, thus some features of interest can be studied in this setting.

A question of direct experimental relevance is how the evolution of two key parameters, the band-occupancy $n$ and the e-e coupling $U$, is reflected in measurable quantities. The optical conductivity for a range of $n$ at constant $U$ was already shown (Fig. 12) and here we provide the results for a range of $U$ at constant $n$ in Fig. 16. The calculations are again performed at $T/D = 0.01$ and $T/D = 0.1$; the lower value is representative of low-temperature measurements, and the higher one of those near room temperature. As expected, the variation as a function of $U$ is much stronger than the dependence on $n$. It affects the optical conductivity on all frequency scales. At low $U$, the optical spectrum has a strong Drude peak with a “Drude foot” but it is otherwise featureless; well defined structure becomes observable only for $|U| \gtrsim D$. Note that in the true Hubbard-Holstein model we expect complex optical conductivity even for $U_{\text{eff}} = 0$, since the effective e-e coupling is itself a frequency dependent quantity.

The results of this work are also directly relevant for the experiments on fermionic cold atoms confined in optical lattice. The value and even the sign of the interparticle in-
Since fermions are difficult to cool down to very low temperatures (below $0.1E_F$, where $E_F$ is the Fermi energy), the ordered ground states (quantum magnetism) are not easy to reach. For this reason, our results for the paramagnetic regime above ordering temperatures are actually precisely in the parameter range accessible to experiments. Recently, experiments aiming to measure the transport properties have been successfully performed. Our results on the Hubbard model will become pertinent once similar experiments are performed on fermions on optical lattices. Such measurements should be able to detect the resistivity peak in excess of the MIR limit in the attractive $U$ case.

**IX. CONCLUSION**

We have compared the basic properties of the Hubbard model with either repulsive or attractive electron-electron interactions for the same generic value of the occupancy $\langle n \rangle = 0.8$. The negative-$U$ model can be understood in terms of the mapping via a partial particle-hole transformation to a positive-$U$ model at half-filling in external magnetic field such that the magnetization is fixed to some constant value. This constraint leads to some interesting features. The resistivity in the attractive model strongly increases as the system approaches the transition toward the negative-$U$ analogue of the Mott state, which is unstable toward bipolaron formation. Since the occupancy is fixed, there would be phase separation at finite temperatures, signaled in our calculations by the lack of convergence. The resistivity as a function of the temperature in the attractive model is non-monotonous: it has a maximum on the scale $T_{\text{max}} = ZD$ where the quasiparticles disappear. The NMR relaxation rate in the attractive model has a complex non-monotonic temperature dependence which reflects the non-monotonic behavior of the double occupancy.

**Acknowledgments**

R. Ž. and Ž. O. acknowledge the support of the Slovenian Research Agency (ARRS) under Program No. P1-0044.
Figure 16: (Color online) Optical conductivity for $n = 0.8$ for a range of repulsion parameters $U$. The finite width of the Drude peak for $U = 0$ is due to artificial broadening in the calculation. The absence of the Drude peak for $U/D = −2.5$ at $T/D = 0.1$ shows that the system is in the (bad) insulator regime.

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