Finite-temperature density-matrix renormalization group method for electron-phonon systems: Thermodynamics and Holstein-polaron spectral functions

David Jansen,1 Janez Bonča,2,3 and Fabian Heidrich-Meisner1

1Institut for Theoretical Physics, Georg-August-Universität Göttingen, D-37077 Göttingen, Germany
2J. Stefan Institute, 1000 Ljubljana, Slovenia
3Faculty of Mathematics and Physics, University of Ljubljana, 1000 Ljubljana, Slovenia

We investigate the thermodynamics and finite-temperature spectral functions of the Holstein polaron using a density-matrix renormalization group method. Our method combines purification and local basis optimization (LBO) as an efficient treatment of phonon modes. LBO is a scheme which relies on finding the optimal local basis by diagonalizing the local reduced density matrix. By transforming the state into this basis, one can truncate the local Hilbert space with a negligible loss of accuracy for a wide range of parameters. In this work, we focus on the crossover regime between large and small polarons of the Holstein model. Here, no analytical solution exists and we show that the thermal expectation values at low temperatures are independent of the phonon Hilbert space truncation provided the basis is chosen large enough. We then demonstrate that we can extract the electron spectral function and establish consistency with results from a finite-temperature Lanczos method. We additionally calculate the electron emission spectrum and the phonon spectral function and show that all the computations are significantly simplified by the local basis optimization. We observe that the electron emission spectrum shifts spectral weight to both lower frequencies and larger momenta as the temperature is increased. The phonon spectral function experiences a large broadening and the polaron peak at large momenta gets significantly flattened and merges almost completely into the free-phonon peak.

I. INTRODUCTION

Developments in experimental methods with ultra-fast dynamics (see, e.g., Refs. [1–5] and Refs. [6, 7] for a review) have reinforced the interest in the theoretical modeling of electron-phonon interactions. Despite the complexity of real materials, qualitative insights can be gained from model systems such as the Holstein model [8–43], hard-core boson-phonon models [44, 45], the t-J model augmented with phonons [46, 47] and spin-boson models [48–51]. It is believed that many experimental results can be interpreted by studying such toy Hamiltonians that contain important key features. A paradigmatic example is the Holstein-polaron model [8] which consists of one electron interacting with local bosons. Since the electron-boson interaction is the only mean of thermalization in the system (see, e.g., Ref. [52]), the model allows us to study this particular relaxation channel, which plays an important role in real materials, in a controlled way.

The Holstein polaron at zero temperature has been the subject of intense research [13, 17, 27, 53–57]. Recent developments in the field of thermalization in isolated quantum systems and quench dynamics have fueled the demand for additional research on the model at a finite temperature [52, 58–67]. In particular, the momentum dependence of the spectral function and the self-energy have recently been computed using a finite-temperature Lanczos method by Bonča et al. in Ref. [68], followed by a comparison between spectral properties of the Holstein polaron and an electron coupled to hard-core bosons [69].

In this paper, we introduce an alternative numerical approach. We demonstrate that a density-matrix renormalization group (DMRG) method [70–72] can efficiently reproduce the spectral function. We also compute the electron emission spectrum, which can be accessed in angle-resolved photoemission spectroscopy (ARPES) experiments [73–78], and the phonon spectral function. The method further allows us to compute thermodynamic observables for very large system sizes compared to other wave-function based methods.

We combine finite-temperature DMRG with purification [79–82], time-dependent DMRG (tDMRG) [72, 83–86] and local basis optimization (LBO) [87] to obtain an efficient scheme to both generate the finite-temperature matrix-product state (MPS) and to compute different Green’s functions. LBO, originally introduced by Zhang et al. in Ref. [87], has already been used for the real-time evolution [40, 43, 88, 89] and ground-state algorithms [43, 48, 90–96]. The DMRG method with purification requires an infinite-temperature state as its starting point which is approximate and strongly dependent on the truncation of the phonon Hilbert space. Our results, however, become independent of that truncation in the polaron-crossover regime at low temperatures, which is physically most relevant. This allows for the efficient computation of static and dynamic properties of the Holstein model at finite temperatures.

In particular, using finite-temperature states we compute the electron addition spectral function. This quantity has already been analyzed thoroughly at finite temperatures by Bonča et al. in Ref. [68] for a system with periodic boundary conditions. We show that we can resolve the same peaks as the finite-temperature Lanczos method and observe an excellent quantitative agreement. We additionally compute the electron emission spectrum and the phonon spectral function. The electron emission spectrum was computed in Ref. [58] for a two-site...
and two-electron system. Here, we focus on one electron and go up to twenty one sites. We further show that
the LBO scheme proposed in Ref. [88] becomes computationally beneficial at low temperatures and significantly
simplifies the computations of these spectral functions.

This paper is structured as follows. In Sec. II, we intro-
duce the Holstein-polaron model, the observables, and
the spectral functions. We proceed in Sec. III with a
description of the methods used. We introduce DMRG with
purification in Sec. III A, the time-evolution algorithm
in Sec. III B and the finite-temperature Lanczos method
in Sec. III C. In Sec. III D and Sec. III E, we show the
spectral functions for the single-site Holstein model. We
present the results for the thermodynamic expectation
values in Sec. IV and the results for the spectral func-
tions in Sec. V. In Sec. VI, we summarize the paper and
provide an outlook.

II. MODEL

A. The Holstein polaron

To study finite-temperature polaron properties we con-
consider the single-electron Holstein model [8]. The Hamil-
tonian is defined as

$$\hat{H} = \hat{H}_{\text{kin}} + \hat{H}_{\text{ph}} + \hat{H}_{e-ph}.$$  

(1)

The model has $L$ sites and we use open boundary condi-
tions, unless stated otherwise. We set $\hbar = 1$ throughout
this paper. The first term, the kinetic energy of the elec-
tron, then becomes

$$\hat{H}_{\text{kin}} = -t_0 \sum_{j=1}^{L-1} \left( \hat{c}^\dagger_j \hat{c}_{j+1} + \hat{c}^\dagger_{j+1} \hat{c}_j \right),$$  

(2)

with $\hat{c}^\dagger_j (\hat{c}_j)$ being the electron creation (anni-
hilation) operator on site $j$ and $t_0$ the hopping amplitu-
de. The second term is the phonon energy

$$\hat{H}_{\text{ph}} = \omega_0 \sum_{j=1}^{L} \hat{b}^\dagger_j \hat{b}_j,$$  

(3)

where $\hat{b}^\dagger (\hat{b}_j)$ is the creation (anni-
hilation) operator of an optical phonon on site $j$ with the
constant frequency $\omega_0$. The last term is the electron-phonon coupling

$$\hat{H}_{e-ph} = \gamma \sum_{j=1}^{L} \hat{n}_j \left( \hat{b}^\dagger_j + \hat{b}_j \right),$$  

(4)

with $\hat{n}_j = \hat{c}^\dagger_j \hat{c}_j$. We furthermore define the dimensionless
 coupling parameter

$$\lambda = \frac{\gamma^2}{2 t_0 \omega_0},$$  

(5)

which characterizes the crossover from a large ($\lambda < 1$) to
a small ($\lambda > 1$) polaron. In this work, we focus on the
intermediate regime and set $\lambda = 1$.

B. Thermodynamics

We first want to study the thermodynamics of the
model. The thermal expectation value of an observable $\hat{O}$
in the canonical ensemble at temperature $T$ is defined as

$$\langle \hat{O} \rangle_T = \text{Tr}[\hat{\rho}(T)\hat{O}],$$  

(6)

where $\hat{\rho}(T)$ is the thermal density matrix at temperature $T$.
In the canonical ensemble,

$$\hat{\rho}(T) = \frac{1}{Z} e^{-\beta \hat{H}},$$  

(7)

where we have set $k_B = 1$ such that $\beta = 1/T$ and $Z$ is
the partition function. We will focus on four observ-
ables: The total energy $E(T) = \langle \hat{H} \rangle_T$, the kinetic energy
$E_{\text{kin}}(T) = \langle \hat{H}_{\text{kin}} \rangle_T$, the coupling energy $E_{e-ph}(T) = \langle \hat{H}_{e-ph} \rangle_T$ and the phonon energy $E_{\text{ph}}(T) = \langle \hat{H}_{\text{ph}} \rangle_T$.

C. Spectral functions

We are also interested in dynamical quantities by in-
vestigating Green’s functions of operators acting on sites
$m$ and $n$. We define the greater Green’s function

$$G^>_T(m,n,t) = -i \langle \hat{c}_m(t) \hat{c}^\dagger_n(0) \rangle_{T,0},$$  

(8)

where the sub-indices $T,0$ indicate that the thermal ex-
pectation value is calculated in the zero-electron sector.
Since we use open boundary conditions, we construct the
Fourier transform into quasi-momentum space (see, e.g.,
Refs. [97, 98]) as

$$\hat{c}_k = \sqrt{\frac{2}{L+1}} \sum_{j=1}^{L} \sin(kj) \hat{c}_j,$$  

(9)

where $k = \pi m_k / (L + 1)$ and $1 \leq m_k \leq L$. The greater
Green’s function in $k$ and $\omega$ space then becomes

$$G_T^>(k,\omega) = -i \int_{-\infty}^{\infty} dt e^{i\omega t} \langle n | G_{T,0}(k,t) | 0 \rangle,$$  

(10)

where $\eta = 0^+$ is an artificial broadening. From the
greater Green’s function, we extract the electron spec-
tral function

$$A(k,\omega) = -\frac{1}{2\pi} \text{Im}[G_T^>(k,\omega)].$$  

(11)

Since we are in the zero-electron sector, Eq. (11) con-
tains all the information about the spectrum. Here, we
extend previous studies [58, 68] of the finite-temperature
Holstein polaron by also computing the lesser Green’s
function in the one-electron sector

$$G_T^<_{1}(m,n,t) = i \langle \hat{c}_{m}^\dagger(0) \hat{c}_n(t) \rangle_{T,1},$$  

(12)
which we use to obtain the electron emission spectrum

\[ A^+(k, \omega) = -\frac{1}{2\pi} \text{Im}[-G_T^{\omega}(k, \omega)]. \]  

We are further interested in the greater Green’s function in the phonon sector

\[ D_T^{\omega}(m, n, t) = -i \langle \hat{X}_m(t) \hat{X}_n(0) \rangle_{T,1}, \]  

where \( \hat{X}_n = \hat{b}_n + \hat{b}_n^\dagger \) is the phonon displacement. We use Eq. (14) to calculate the phonon spectral function

\[ B(k, \omega) = -\frac{1}{2\pi} \text{Im}[D_T^{\omega}(k, \omega)]. \]  

III. METHODS

In this section, we first describe our main numerical method, DMRG using purification and local basis optimization. We next briefly review the finite-temperature Lanczos method used in Ref. [68]. In order to guide the discussion of the numerical results, we compute the three spectral functions in the single-site limit.

A. Density-matrix renormalization group with purification

While the density-matrix renormalization group and matrix-product states were originally developed to find ground states [70–72], they have proven to be extremely useful tools for calculating spectral functions [99–104], carrying out the time evolution [72, 83–86], and finite-temperature calculations [79–81, 105–112] as well. There are several ways to utilize matrix-product states at finite temperatures. These include, among others, minimally entangled typical thermal state algorithms [113–115], purification algorithms [80–82] or a mixture of both [116, 117].

In this paper, we use the purification method [79] which doubles the system by adding an auxiliary space to the physical Hilbert space \( \mathcal{H}_P \rightarrow \mathcal{H}_P \otimes \mathcal{H}_A \). One can write down a state in this doubled Hilbert space \( |\psi\rangle \in \mathcal{H}_P \otimes \mathcal{H}_A \). If one now traces out the auxiliary space, one can simulate a mixed state in the physical Hilbert space with the density matrix

\[ \hat{\rho}_P = \text{Tr}_A[|\psi\rangle \langle \psi|]. \]  

Since we are working with a fixed number of electrons, we will use the notation where \( |\psi^0_\beta\rangle \) represents a state at temperature \( T \) with \( n \) electrons in the physical system. For example, the state \( |\psi^1_\beta=0\rangle \in \mathcal{H}_P \otimes \mathcal{H}_A \) can be expressed analytically. This state can then be used to simulate the density matrix from Eq. (7) for one electron at \( \beta = 0 \). The density matrix for \( \beta \neq 0 \) is generated by the evolution in imaginary time of \( |\psi^0_\beta\rangle \) as

\[ |\psi^n_\beta\rangle = e^{-\hat{H} \beta/2} |\psi^0_\beta\rangle. \]  

The thermal expectation value of an observable \( \hat{O} \) can then be calculated as

\[ \langle \hat{O} \rangle_{T,\beta} = \frac{\langle \psi^0_\beta | \hat{O} | \psi^0_\beta \rangle}{\langle \psi^0_\beta | \psi^0_\beta \rangle}. \]  

Since we use thermal states with both one and zero electrons we briefly illustrate how to generate both of them at \( \beta = 0 \). Since the Holstein model contains infinitely many local phonon degrees of freedom, we first introduce a local cutoff \( M \) which represents the maximal number of phonons on each site. We furthermore define a local basis state \( |\sigma_i\rangle = |n_i^e, n_i^{ph}\rangle \) with electron occupation \( n_i^e \in \{0, 1\} \) and phonon occupation \( n_i^{ph} \in \{0, \ldots, M\} \). This determines the local dimension \( d = 2(M + 1) \). We further write \( |\bar{\sigma}\rangle = |\sigma_1, \sigma_2, \ldots, \sigma_L\rangle \). The zero-electron state \( |\psi^0_{\beta=0}\rangle \) becomes

\[ |\psi^0_{\beta=0}\rangle = \sum_{\bar{\sigma}^P, \bar{\sigma}^A} A_1^{\bar{\sigma}^P, \bar{\sigma}^A} A_2^{\bar{\sigma}_2^P, \bar{\sigma}_2^A} \cdots A_L^{\bar{\sigma}_L^P, \bar{\sigma}_L^A} |\bar{\sigma}^P, \bar{\sigma}^A\rangle, \]  

where each \( A_i^{\bar{\sigma}_i^P, \bar{\sigma}_i^A} = \delta_{n_i^e, 0} \delta_{n_i^{ph}, 0} \delta_{n_i^{ph}, 0} \delta_{n_i^{ph}, 0} \delta_{n_i^{ph}, 0} \) is the local tensor corresponding to maximum entanglement between the physical site \( \sigma_i^P \) and the auxiliary site \( \sigma_i^A \). To generate the one-electron state \( |\psi^1_{\beta=0}\rangle \), we proceed in a similar fashion as in Ref. [118]. We first write down the maximum entangled one-electron tensor \( \tilde{A}_j^{\sigma_j^P, \sigma_j^A} = \delta_{n_j^e, 0} \delta_{n_j^{ph}, 0} \delta_{n_j^{ph}, 0} \delta_{n_j^{ph}, 0} \delta_{n_j^{ph}, 0} \). We then define our wave function as the superposition of terms which all have the one-electron tensor \( \tilde{A}_j^{\sigma_j^P, \sigma_j^A} \) at a different site \( j \). On the sites \( i \neq j \), we just place the zero-electron tensors \( A_i^{\bar{\sigma}_i^P, \bar{\sigma}_i^A} \) from Eq. (18). The total wave function becomes

\[ |\psi^1_{\beta=0}\rangle = \sum_{j=1}^L \sum_{\bar{\sigma}^P, \bar{\sigma}^A} A_1^{\bar{\sigma}_1^P, \bar{\sigma}_1^A} \cdots \tilde{A}_j^{\sigma_j^P, \sigma_j^A} \cdots A_L^{\bar{\sigma}_L^P, \bar{\sigma}_L^A} |\bar{\sigma}^P, \bar{\sigma}^A\rangle. \]  

After constructing \( |\psi^1_{\beta=0}\rangle \), one then generates the desired \( |\psi^n_{\beta}\rangle \) by imaginary-time evolution.

B. Time evolution with local basis optimization

Since we are interested in thermodynamics and spectral functions at finite temperatures, we need to carry out both imaginary and real-time evolution. This subsection explains the procedure and its application to electron-phonon systems. To calculate the time evolution we use tDMRG [83, 84] combined with local basis optimization (LBO) [87]. The idea of the local basis optimization is to find a numerically efficient representation of the phonon Hilbert space, thus reducing the computational cost. This has already been applied to the real-time evolution of pure states, e.g., by Brockt et al. [88] for the polaron problem, by Stolpp et al. [43] for a charge density wave, as well as in Refs. [40, 89]. In this paper, we
demonstrate that the local basis optimization is computationally beneficial for computing thermodynamics and real-time evolution at finite temperature for the Holstein polaron.

For the tDMRG method, we first write our Hamiltonian as a sum of terms \( \hat{H} \) which act on the two neighboring sites \( l \) and \( l + 1 \). For a time step \( dt \) \((-i\hat{H} dt\) for imaginary-time evolution) one can then carry out a second-order Trotter-Suzuki decomposition into even and odd terms
\[
e^{-i\hat{H} dt} = e^{-i\hat{H}_{\text{even}}/2}e^{-i\hat{H}_{\text{odd}} dt}e^{-i\hat{H}_{\text{even}}/2} + O(dt^3). \tag{20}
\]

One can further write each exponential as the product of local elements \( e^{-i\hat{H}_{\text{even}}/2} = \prod_{l_{\text{even}}} e^{-i\hat{H}_{l_{\text{even}}}/2} \). Since each physical site is connected to an auxiliary site, one must first apply a fermionic swap gate \([114, 119]\) to swap site \( \sigma^P \) and \( \sigma^\Lambda \). One then acts with the time evolution gate \( e^{-i\hat{H}_{l_{\text{odd}}}/2} \) followed by another gate which swaps \( \sigma^P \) and \( \sigma^\Lambda \) back.

To illustrate how the local basis optimization works, we assume that our MPS is already in an optimal local basis. Before we start the real-time evolution, we first obtain the desired state \( |\phi^P_n\rangle \) and that the local transformation matrices \( R^P_{\sigma^P} \) and \( R^\Lambda_{\sigma^\Lambda} \). Then we follow Ref. \([81]\) and compute the desired correlation functions
\[
C_{T,n}(m,l,t) = \langle \psi_\beta^m | \hat{A}_m(t/2) \hat{B}_l(-t/2) | \psi_\beta^m \rangle, \tag{25}
\]

where \( \hat{A}, \hat{B} \) are general operators and
\[
\hat{A}_m(t) = U(t/2) \hat{U}^A(t/2) \hat{A}_m U(t/2) \hat{U}^A(t/2) \hat{U}(t/2). \tag{26}
\]

In Eq. (26), \( \hat{U}^V(t/2) = e^{-i\hat{H}_{\text{tr}}t/2} \) acts on the part of the state in the physical Hilbert space and \( \hat{U}^A(t/2) = e^{i\hat{H}_{\text{tr}}t/2} \) correspondingly evolves the part of the state in the auxiliary space in the opposite direction. This is done to keep the entanglement entropy low during the real-time evolution \([107-111]\). Even though this procedure is not optimal \([112]\), it provides a natural extension of the local basis optimization to the auxiliary spaces and allows us to keep them in an optimal basis during the time evolution. We then obtain \( C_{T,n}(k,\omega) \) from \( C_{T,n}(m,l,t) \) by Fourier transformations in space and time.

We further use linear prediction \([81, 120, 121]\) to access larger times. Since we do the real-time evolution on states \( |\phi^P_n\rangle = \hat{A}_i |\psi^P_\beta\rangle \), which are not normalized, e.g. \( \langle \phi^P_n | \phi^P_m \rangle \neq 1 \), we do not renormalize the state after applying the time-evolution gate. Instead, we verify that the norm is of order \( O(1) \) for the temperatures considered here, such that the MPS truncation scheme remains valid. We further keep the change of norm below \( \leq 10^{-3} \) during the simulation time. For all imaginary-time evolutions, we use \( dt/\omega_0 = 0.1 \) and for the real-time evolution, we use \( dt/\omega_0 = 0.01 \). The real-time evolution is done up to a maximum time \( t_{\text{total}}/\omega_0 \). All DMRG calculations are carried out using \([122]\).

C. Finite-temperature Lanczos method

We now proceed by introducing alternative methods used as benchmarks. The thermodynamic quantities will be compared to exact diagonalization (ED) and the spectral function from Eq. (11) will be compared to the finite-temperature Lanczos method \([123, 124]\) (FTLM).

The finite-temperature Lanczos method data used here is obtained from Ref. \([68]\). The electron spectral function
is expressed as

\[ A(k, \omega) = Z^{-1} \sum_{r=1}^{R} \sum_{j=1}^{M} \sum_{n=1}^{N} e^{-\beta \epsilon_n} \langle \phi_n^0 | \phi_n^0 | \psi_j \rangle \times \langle \psi_j | e^{-\beta \epsilon_j} | \psi_j \rangle \delta(\omega - \epsilon_j + \epsilon_n^0) , \]

where \( Z \) is the partition function, \( |\phi_n^0 \rangle \) are random states in the zero-electron basis, and \( |\phi_n^0 \rangle \) are the zero-electron eigenstates and \( |\psi_j \rangle \) are the Lanczos vectors from the one-electron subspace with the corresponding energy \( \epsilon_j \). The variational Hilbert space [13, 17] is used to-gether with twisted boundary conditions [125–127] to limit finite-size effects.

D. Single-site spectral function and emission spectrum

In order to gain a better understanding of the emission spectrum at low temperatures, we derive an analytical expression for the single-site system. This is done for the spectral function in Ref. [128] and a detailed derivation is presented in Ref. [68]. This section is a simple extension of that work but is included for self consistency and to guide the discussion. The single-site Hamiltonian is

\[ \hat{H}_s = \gamma \hat{n} \hat{b}^\dagger \hat{b} + \omega_0 \hat{b}^\dagger \hat{b} \]  

The solution for the case of a single electron is given by the well-known coherent states

\[ |0_s \rangle = e^{-\tilde{g}^2} \sum_{m=0}^{\infty} \frac{(-\tilde{g})}{\sqrt{m!}} |m \rangle \]

where \( \tilde{g} = \gamma / \omega_0 \) and \( |m \rangle \) are bare phonon modes. The ground state \( |0_s \rangle \) has the energy \( E_{0,s} = -\omega_0 \tilde{g}^2 \). The excited states \( |m_s \rangle \) have an energy \( E_{m,s} = -\omega_0 \tilde{g}^2 + m \omega_0 \) and are given by

\[ |m_s \rangle = \frac{\{b^\dagger + \tilde{g}\}^m}{\sqrt{m!}} |0_s \rangle \]

The single-site spectral function is derived in Ref. [68], is

\[ A_s(\omega) = \frac{1}{Z} \sum_{n,m=0}^{\infty} e^{-\beta \omega_n} |\langle m_s | n \rangle|^2 \delta(\omega + E_n - E_{m,s}) \]

where \( |n \rangle \) are the bare phonon modes and \( E_n \) the corresponding energies. We show \( A_s(\omega) \) in Fig. 1(a) for \( \lambda = 1 \).

The electron emission spectrum is

\[ A_s^+(\omega) = \frac{1}{Z} \sum_{n,m=0}^{\infty} e^{-\beta E_{m,s}} |\langle n | m_s \rangle|^2 \delta(\omega + E_n - E_{m,s}) \]

The overlap between the coherent state and the normal mode is given by

\[ \langle n | m_s \rangle = e^{-\tilde{g}^2/2} \sum_{l=0}^{\min\{m,n\}} \frac{(-1)^n \tilde{g}^{n+m-2l}}{l!(m-l)!(n-l)!} \frac{\sqrt{m!}}{n!} \]

If we send \( T / \omega_0 \to 0 \), only the \( m = 0 \) term contributes in Eq. (32). This gives

\[ \langle n | 0_s \rangle = e^{-\tilde{g}^2/2} \frac{\sqrt{n!}}{n!} \]

The emission spectrum then takes the form

\[ A_s^+(\omega) = \sum_{n=0}^{\infty} e^{-\tilde{g}^2/2} \frac{1}{n!} \delta(\omega + n \omega_0 + \omega_0 \tilde{g}^2) \]

which has a polaron peak for \( n = 0 \) at \( \omega_{pol}/\omega_0 = -\omega_0 \tilde{g}^2 \). The spectrum further has peaks at negative \( \omega \), which are separated by \( \omega_0 \). It is also clear that at larger temperatures, peaks at \( \omega > -\omega_0 \tilde{g}^2 \) will appear.

In Fig 1(b), we show the single-site emission spectrum \( A_s^+(\omega) \). There, the peaks at \( \omega < \omega_0 \tilde{g}^2 \) are visible. One can also observe the peaks at \( \omega > \omega_0 \tilde{g}^2 \) appearing for larger temperatures.

E. Single-site phonon spectral function

The single-site phonon spectral function is

\[ B_s(\omega) = \frac{1}{Z} \sum_{n,m=0}^{\infty} e^{-\beta E_{m,s}} |\langle n_s | \hat{b} + \hat{b}^\dagger | m_s \rangle|^2 \times \delta(\omega + E_{m,s} - E_{n,s}) \]

We use that

\[ \hat{b} |0_s \rangle = -\tilde{g} |0_s \rangle \]

and

\[ \hat{b} |m_s \rangle = \sqrt{m} |(m-1)_s \rangle - \tilde{g} |m_s \rangle \]

to obtain

\[ \langle n_s | b + \hat{b} | m_s \rangle = \sqrt{n} \langle (n-1)_s | m_s \rangle + \sqrt{m} \langle n_s | (m-1)_s \rangle - 2 \tilde{g} \langle n_s | m_s \rangle \]

At \( T / \omega_0 = 0 \), the spectral function becomes

\[ B_s(\omega) = 4 \tilde{g}^2 \delta(\omega) + \delta(\omega - \omega_0) \]

\( B_s(\omega) \) is shown for different \( T / \omega_0 \) in Fig. 1(c). We observe two peaks separated by \( \omega_0 \) at the lowest temperatures as predicted in Eq. (40). This is the polaron peak and the free-phonon peak. When the temperature is increased, a smaller free-phonon peak starts to appear at \( -\omega_0 \).
IV. DMRG RESULTS FOR THERMODYNAMICS

In this section, we show the results for the thermodynamic quantities introduced in Sec. II B. Thermodynamics for electron-phonon models has already been studied with Monte Carlo methods, see, e.g., Refs. [129–132] for results for two-dimensional lattices. As explained in Sec. III A, the DMRG purification method starts at $T = \infty$. Finite temperatures are then obtained by imaginary-time evolution. For the Holstein-polaron model with a local phonon cutoff $M$, we have $\langle H \rangle_{T=\infty} / (\omega_0 L) = M/2$, such that depending on the phonon number truncation, the imaginary-time evolution will start at a different energy. Additionally, starting points with a finite $M$ are artificial since they do not represent the true $T = \infty$ limit of the system. For this reason, we first want to investigate whether there is a range of temperatures where we can produce states with expectation values that are independent of $M$ for the polaron in the crossover regime $\lambda = 1$. Since the results become $M$-dependent and unphysical for large $T/\omega_0$, we choose to focus on $0.1 \leq T/\omega_0 \leq 0.4$. Secondly, we want to investigate how the optimal local basis is affected by the imaginary-time evolution.

We first verify that the purification method reproduces values calculated with ED. In Fig. 2, we compare the results to ED for $L = 5$ and different $M$. We show the four observables defined in Sec. II B as a function of temperature $T/\omega_0$. One sees that the finite-temperature DMRG method (symbols) reproduces the ED (solid lines) for the corresponding $M$. The clear dependence of the observables on $M$ suggests that the local Hilbert space is not
chosen large enough to yield the correct low-temperature physics for these parameters. Most importantly, the DMRG method reproduces the ED results for the accessible system sizes. We proceed by comparing the expectation values for different system sizes $L$. The results are shown in Fig. 3. Notice that the ground-state energy is intensive in the single-electron problem. Therefore, $E/(\omega_0 L)$ should approach zero in the thermodynamic limit. This can be observed in Fig. 3(a). The figure also serves as a consistency check by showing that the imaginary-time evolution approaches the ground-state energy calculated with ground-state DMRG [70–72] (solid lines). Both the total energy $E$ and the phonon energy $E_{ph}$ are extensive at finite temperature, and therefore, we divide both of these expectation values by the system size $L$ to get a quantity that only depends on temperature for sufficiently large $L$. The observables $E_{kin}$ and $E_{e-ph}$ [Figs. 3(b) and (d)] are automatically intensive since there is only one electron in the system. Figure 3 therefore illustrates that the purification method gives access to thermodynamic quantities in systems with very large local Hilbert spaces.

We next demonstrate that the DMRG method can access values of $M$ large enough to obtain cutoff-independent results in the low-temperature regime. In Fig. 4, we show the same observables as in Fig. 2 with $L = 21$ and $M = 20, 30$ calculated with DMRG. We find that even though the two initial states start at two completely different energies $\langle \hat{H} \rangle_{T=0}/(\omega_0 L)$, they still converge to the same expectation value up to an accuracy of $O(10^{-5})$ below $T/\omega_0 \lesssim 0.5$. We thus conclude that we correctly reproduce results for the real phonon limit $M \to \infty$ below a certain temperature if $M$ is chosen large enough. Therefore, the method gives access to thermodynamics at temperatures for system sizes and phonon numbers unavailable to ED and regular Lanczos methods. For the rest of this paper, we choose $M = 20$.

To demonstrate that the imaginary-time evolution results are converged in the low-temperature limit, we vary $\rho_{bond}$ and $\rho_{LBO}$. As explained in Sec. III, the truncation of the bond dimension is controlled by $\rho_{bond}$ whereas $\rho_{LBO}$ controls the truncation of the optimal local basis of the MPS. In Figs. 5(a) and (c), we illustrate how $E_{kin}$ is affected by changes in $\rho_{bond}$ and $\rho_{LBO}$. The change is significant if one of the discarded weights is chosen too large. If $\rho_{bond}$ is too large, the expectation values lie above the converged value. In the other case, for $\rho_{LBO}$ too large, we start to get fluctuating expectation values. We do this test for all terms in the Hamiltonian in Eq. (1) and find that they are all converged for $\rho_{bond} = 10^{-7}$ and $\rho_{LBO} = 10^{-9}$ to an accuracy of $O(10^{-3})$. However, exactly how they behave for a too small cutoff is observable and system-size dependent. Since the expectation values already have converged for both $\rho_{bond}$ and $\rho_{LBO} = 10^{-7}$ [red triangles in Figs. 5(a) and (c)], the $10^{-9}$ markers (blue circles) are barely visible.

In Figs. 5(b) and (d), we analyze the maximum dimension $\max(d_{LBO})$ of the optimal basis of the physical Hilbert space. One clearly sees that this becomes equal to the bare phonon dimension $M + 1$ for large $T/\omega_0$. This
is expected since all the phonon modes become equally probable at $T/\omega_0 = \infty$. However, $\text{max}(d_{\text{LBO}})$ starts to decrease rapidly below a certain temperature and the rotation into the optimal basis becomes computationally beneficial for a given truncation error. This means that the eigenvalues of the reduced-density matrix first do not decay at all until a certain temperature is reached. After that, they start decreasing rapidly as a function of $T/\omega_0$. Figure 5(d) shows that this trend becomes more pronounced for larger $M$. Furthermore, it illustrates that as $M$ is increased, the rotation into the optimal basis becomes beneficial at higher $T/\omega_0$.

The accurate evaluation of thermal expectation values also serves as an important test for the spectral function calculations in Sec. V 2. In Appendix B, we show that the first temperature-dependent moments can be calculated by either integrating the spectral function or by computing thermal expectation values. We verify the accuracy of the spectral function by comparing both methods. For the rest of this work, we set $\rho_{\text{LBO}} = \rho_{\text{bond}} = 10^{-9}$ during the imaginary-time evolution.

V. SPECTRAL FUNCTIONS

1. Real-time evolution

We now proceed by calculating dynamical properties of our model. We first check that the real-time evolution converges with respect to $\rho_{\text{bond}}$ and $\rho_{\text{LBO}}$. This is illustrated in Fig. 6. There, we show the imaginary part of $G^r_{T,0}(m, n, t)$ from Eq. (8) with $m = n = 11$. From Figs. 6(a) and (b), it becomes apparent that as $\rho_{\text{bond}}$ is increased, the results are indiscernible on the scale of the figure. A similar behaviour is also seen with respect to $\rho_{\text{LBO}}$ [see Fig. 6(c)]. We can also report a large increase in the bond dimension as the temperature is increased (for details, see Appendix A). Since this limits the accessible times it will also limit the possible energy resolution after the Fourier transformation. As explained in Sec. III A, we additionally apply linear prediction. The spectral functions tend to oscillate around zero away from the peaks as a result of the finite time interval. By applying linear prediction, the oscillation amplitude goes from order $10^{-1}$ to $10^{-5}$ without changing the peak position or height in the spectrum. However, the exact decrease of the amplitude is spectral-function and temperature dependent. Due to the oscillations, we always show the absolute values of the spectral functions in the normalized log-scaled plots. The real-time evolution for all the following spectral functions is done with $\rho_{\text{bond}} = \rho_{\text{LBO}} = 10^{-8}$.

To test the accuracy of the method, we also derive the first temperature-dependent moment of the spectral functions and compare the thermal expectation values to our numerical data. The results in Appendix B show good agreement. We further want to emphasize that in the zero-electron sector, it is trivial to obtain the finite-temperature initial state for the real-time evolution since it only contains non-interacting local harmonic oscillators. For this reason, we compare results using both the trivially obtained thermal states and those obtained with the imaginary-time evolution algorithm to verify its correctness.

2. Electron spectral function and comparison to the FTLM

In Fig. 7, we show the electron spectral function $A(k, \omega)$ and compare it to results obtained with FTLM. We show the results for $T/\omega_0 = 0.1$ in Figs. 7(a) and (b) and $T/\omega_0 = 0.4$ in Figs. 7(c) and (d). Our method can resolve the same peak positions as the FTLM. One can identify the polaron peak at $\omega_{\text{pol}}/\omega_0 \approx -3.0$ and the peaks corresponding to the polaron with additional phonons separated by $n\omega_0$ in the incoherent part of the spectrum. We also observe a significant decrease of the quasi-particle weight for $k_{\text{min}}$ compared to $k_{\text{max}}$. This has already been reported in Ref. [68] and is consistent with other ground-state approaches [15, 18, 133–135].

In the inset, we show

$$I(k, \omega) = \int_{-\infty}^{\omega} d\omega' A(k, \omega').$$  (41)

There are only small differences between the FTLM and the DMRG data. The amplitude of the polaron peak exhibits small temperature-dependent differences between the two methods. For larger values of $k$, we also observe
some different weight distribution in the incoherent part of the spectrum. The results for \( I(k, \omega) \) still almost completely overlap. We want to emphasize that we show results for two different \( k \) values for the methods due to the difference in boundary conditions. For the DMRG method, we choose \( k_{\text{min}} = \pi/(L + 1) \), \( k_{\text{max}} = \pi L/(L + 1) \) and for the FTLM method, we select \( k_{\text{min}} = 0 \), \( k_{\text{max}} = \pi \). We conclude that despite these differences, the DMRG and FTLM method show a very good quantitative agreement.

Alternatively to computing the complete correlation function, one can calculate \( G^<_{T,0}(m, n, t) \) for a fixed \( n = L/2 \) and \( m \leq n \). This gives access to much larger system sizes, as illustrated in Fig. 8. There, we calculate the spectral function for \( L = 101 \). We first fix \( n = 51 \) and set \( G^<_{T,0}(n + m, n, t) = G^>_{T,0}(n - m, n, t) \). We then compute the Fourier transform into \( k \)-space as

\[
G^>_{T,0}(k, t) = \frac{1}{L} \sum_{m=1}^{L} e^{i(m-n)k} G^<_{T,0}(m, n, t).
\]

Here, we use periodic boundary-condition quasi-momenta with \( k = 2\pi m/L \) and \(-\frac{\pi}{4} \leq m \leq \frac{\pi}{4} \). This is often done (e.g., in Refs. [82, 136]) and the method works well here since the noninteracting harmonic oscillators are homogeneously distributed in the initial state and there is no electron in the system. In Fig. 8, we show comparison between data produced with periodic-boundary condition momenta (\( L = 101 \)) with results for open-boundary moment (\( L = 21 \)). Only small changes in the largest peaks (see Figs. 8(a) and (c)) can be seen even though the \( L = 101 \) data use \( k_{\text{min}} = 0 \), \( k_{\text{max}} = \pi \) while the \( L = 21 \) data use \( k_{\text{min}} = \pi/(L + 1) \), \( k_{\text{max}} = \pi L/(L + 1) \). This is, however, not the case for the other spectral functions studied in this work since the one-electron state has an inhomogeneous electron distribution. The previously described approach does, therefore, not fulfill the sum rules in those cases. Moreover, we mention that the calculations with the periodic boundary-condition Fourier transformation is more sensible to the choice of parameters for the linear prediction for our data.

In Fig. 9, we show \( A(k, \omega) \) as a function of \( \omega \) for all \( k \). Here, the spectral weight at \( \omega < \omega_{\text{pol}} \) [see Fig. 7(a)] becomes visible at larger \( T/\omega_0 \). This has been reported in Ref. [68] and corresponds to the electron absorbing a thermal phonon. One can also see that the polaron band structure is shifted downwards and renormalized compared to the free-fermion case which would have its ground-state energy at \( \omega/\omega_0 = -2 \) and a bandwidth of \( 4\omega_0 \). In all cases, we confirm that the sum rule \( \int_{-\infty}^{\infty} d\omega A(k, \omega) = 1 \) is fulfilled up to \( 10^{-3} \).

3. Electron emission spectrum

We next discuss \( A^+(k, \omega) \), defined in Eq. (13). Computationally, this function is the easiest to obtain with our method since the most demanding part of the calculation,
namely the real-time evolution, is done without an electron in the physical system. In Fig. 10, we show $A^\dagger(k, \omega)$ for two different temperatures. At low $T/\omega_0$, Fig. 10(b) unveils the presence of several peaks that are separated by $\omega_0$. The peaks can be understood by inspecting the single-site emission spectrum at low temperatures from Eq. (35). There, one clearly sees a peak at $-\gamma^2/\omega_0$. Furthermore, there are several peaks at negative $\omega$ separated with $\omega_0$. In Fig. 10(b), we have one main peak at the ground-state energy $\omega_{\text{pol}}/\omega_0 \approx -3$. This peak is also robust against an increase in temperature [see Fig. 10(c)]. The peaks at lower $\omega$, however, acquire more structure at elevated $T/\omega_0$. We also observe a peak at $\omega_{\text{pol}}/\omega_0 + 1$ which is completely suppressed at $T/\omega_0 = 0.1$. In Fig. 11, the complete function $A^\dagger(k, \omega)$ is plotted as a function of $k$ and $\omega$. At $T/\omega_0 = 0.4$ [Fig. 11(b)], we see two clear polaron bands starting at $\omega/\omega_0 = -3$ and $\omega/\omega_0 = -2$. Both have a bandwidth of $D \approx e^{-\gamma^2}4 \approx 0.54$, which is illustrated by the black dashed and solid lines. The peaks at lower frequencies also seem to shift towards higher frequencies and additional peaks appear to emerge at approximately $D$ away from the already existing ones at $\omega/\omega_0 < -3$.

In Fig. 10(a), we show the electron momentum distribution calculated for different system sizes. This quantity can be calculated directly as the thermal expectation value $\langle n_k \rangle_T$ or extracted from the lesser Green’s function

$$n_k = \int_{-\infty}^{\infty} d\omega A^\dagger(k, \omega). \quad (42)$$

As a consistency check, we show both. Figure 10(a) illustrates that some finite-size effects exist for small $L$, but as $L$ is increased, $n_k L$ converges. Note that with increasing $L$, the number of $k$-points also increases, however, $\sum_k n_k = 1$. This is, of course, different for the spectral function discussed in Sec. V 2, where

$$\int_{-\infty}^{\infty} d\omega A(k, \omega) = 1 \quad (43)$$

for all $k$ and $L$. We thus conclude that already at the low temperatures studied here, $n_k$ starts to flatten out and the difference in amplitude between the polaron peak and the other peaks decrease.
4. Phonon spectral function

We now move on to the phonon spectral function. Its ground-state properties have already been studied thoroughly (see, e.g., Refs. [27, 56]). In Ref. [56], Loos et al. used analytic and numerical methods to study this spectral function in a variety of parameter regimes. They found that the dominating features of the phonon spectral function are a free-phonon line and a renormalized band dispersion with additional structure appearing for intermediate electron-phonon coupling. Vidmar et al. [27] studied the low-energy spectrum and identified several bound and anti-bound states in different parameter regimes.

Here, we are interested in this function at finite temperature and in Fig. 12, we display $B(k, \omega)$ for $T/\omega_0 = 0.1$ and 0.4 for different $k$. At $T/\omega_0 = 0.1$, which is close to the ground state, we clearly recognize two distinct peaks, one at $\omega/\omega_0 = 1$ and another one that gets shifted with $k$. The peak at $\omega/\omega_0 = 1$ originates from the free phonon, whereas the other peak originates from the phonon being coupled to the electron. When temperature is increased, the phonon spectral function changes dramatically. For $k = L\pi/(L+1)$, the peaks get significantly broader and the polaron and the free-phonon peaks are almost completely merged. We also see structure appearing at $\omega/\omega_0 < 0$ which is suppressed at low temperatures, exactly as is the case for the single-site phonon spectral function in Sec. III.E.

In Fig. 13, we show the complete $B(k, \omega)$. Here, the polaron band structure with a width of $D \approx 4e^{-g^2}$ is visible. It also becomes clear that whereas we only observe the appearance of a free-phonon peak at negative frequencies in the single-site case, here, there is a complete reflected polaron band appearing for $T/\omega_0 = 0.4$ at $\omega/\omega_0 < 0$ [see Fig. 13(b)]. This is similar to what we find for the emission spectrum in Fig. 11.

VI. SUMMARY

We have generalized the DMRG method combined with purification and local basis optimization to efficiently compute static as well as dynamic properties of the Holstein polaron in the intermediate coupling regime at finite temperatures. We first showed that the method enabled us to generate thermal states at a finite temperature by performing imaginary-time evolution. We then computed the electron spectral function and showed that our results quantitatively agree with those obtained using the finite-temperature Lanczos method of Ref. [68]. We also analyzed the electron emission spectrum and found that the difference between the amplitude of the polaron peak and the other peaks decreased and that $n_k$ flattened out with increasing temperature. In addition, we observed an additional band appearing at larger $\omega$. Regarding the phonon spectral function, our work unveils that with increasing temperature, the spectrum broadens at larger momentum accompanied by the emergence of a mirrored image at $\omega < 0$.

We propose a number of future applications of the method introduced in this work. One direction would be to combine the local basis optimization with other time-evolution methods [137–141]. Another possible area of application is to calculate thermal expectation values combined with quench dynamics [40, 43, 50, 88, 89, 142–145] to test the predictions of the eigenstate thermalization hypothesis [52, 60–62, 64, 66, 67, 146]. The proposed method can also be generalized to investigate hetero-junctions containing vibrational degrees of free-
dom [132, 147–152] and to study the evolution of polaron states in manganites [153–156]. Further challenging continuations could involve the numerical study of time-dependent spectral functions (see, e.g., [77, 136]) relevant to time-dependent ARPES experiments [74, 75, 157, 158] or to compute the optical conductivity at finite temperatures (see, e.g., Refs. [29, 159, 160]).

ACKNOWLEDGMENT

We acknowledge useful discussions with A. Feiguin, E. Jeckelmann, C. Karrasch, S. Manmana, and C. Meyer. D.J. and F.H.-M. were funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) 217133147 via SFB 1073 (project B09). J.B. acknowledges the support by the program P1-0044 of the Slovenian Research Agency, support from the Centre for Integrated Nanotechnologies, a U.S. Department of Energy, Office of Basic Energy Sciences user facility, and funding from the Stewart Blusson Quantum Matter Institute.

Appendix A: Bond and LBO dimension in real-time evolution

In Fig. 14, we show the maximum bond dimension [Fig. 14(a) and Fig. 14(b)] and maximum local optimal basis dimension [Fig. 14(c)] as a function of time. The bond dimension is clearly dependent on the temperature and on the specific Green’s function. It increases a lot faster for the $G_{T,0}^{\gamma}(t, m, n)$ (red) and $D_{T,1}^{\gamma}(t, m, n)$ (blue). For these Greens’ functions, the real-time evolution is done with an electron in the physical system which causes the large increase in the bond dimension. One also sees that as temperature is increased, the computations become much more costly. This is especially true for the phonon Green’s function $D_{T,1}^{\gamma}(t, m, n)$. The drop at $t\omega_0 = 0$ comes from the fact that the imaginary-time evolution is carried out with $\rho_{LBO} = \rho_{bond} = 10^{-3}$, whereas the real-time evolution is done with $\rho_{LBO} = \rho_{bond} = 10^{-8}$. This leads to some states getting truncated away right at the beginning. This is not the case for the red curve that shows $G_{T,0}^{\gamma}(m, n, t)$. There, the insertion of the electron into the system directly leads to a much larger bond dimension. We also observe that the maximum dimension of the local optimal basis remains approximately constant during the real-time evolution for the Green’s functions in the one-electron sector. The dimension clearly increases for larger temperature [$T/\omega_0 = 0.1$ (symbols) and $T/\omega_0 = 0.4$ (solid lines)] but it is, in both cases, clearly beneficial. This does, of course, not imply that the modes in the optimal basis remain the same. When the Green’s function is calculated in the zero-electron sector, inserting the electron clearly leads to an increase in $\max(d_{LBO})$.

Appendix B: Moments

To validate that the method captures the correct finite-temperature behaviour we compute the first temperature-dependent moment for each spectral function. The moments are defined for the corresponding spectral function [here only shown for $A(k, \omega)$] as

$$M_{m,A}(k) = \int_{-\infty}^{\infty} \omega^m A(k, \omega) d\omega.$$  \hspace{1cm} (B1)

For $A(k, \omega)$, the first two moments (see Refs. [68, 134, 161]) become

$$M_{1,A}(k) = \epsilon(k), \hspace{1cm} (B2)$$

$$M_{2,A} = \epsilon^2(k) + \gamma^2(2n_{ph} + 1), \hspace{1cm} (B3)$$

where $n_{ph} = 1/\left(\exp(\omega_0/T) - 1\right)$, $\epsilon(k) = -2t_0 \cos(k)$ with the quasi momenta for open-boundary conditions used in this paper. For $A^+(k, \omega)$, the first moment is already temperature dependent

$$M_{1,A^+}(k) = \frac{2}{L+1} \sum_{i,j} \sin(ki) \sin(kj) \times \langle \hat{c}_i \hat{c}_j (\epsilon(k) + \gamma \hat{X}_i) \rangle_T.$$ \hspace{1cm} (B4)
and for $B(k, \omega)$ we obtain

\begin{align}
M_{1,B}(k) &= \omega_0, \\
M_{2,B}(k) &= \frac{2}{L+1} \sum_{i,j} \sin(ik) \sin(jk) \\
&\times \langle \omega_0(\hat{X}_i \hat{X}_j) + 2\gamma \hat{n}_i \hat{X}_j \rangle_T.
\end{align}

The results for the temperature-dependent moments are shown in Fig. 15. We see that they can be calculated quite accurately with our method. The mean differences for both temperatures are of the order $O(10^{-5})$ for all the first moments and $O(10^{-2})$ for the second moments. In contrast to the rest of the paper, we here use a Gaussian regularization for the spectral function. The moments show a dependence on the regularization parameter $\eta$. One must find a compromise between allowing for unphysical oscillations in the spectral function and the accuracy of the moments. We choose $\eta = 0.05/(6\pi)$. For the second moments, we further limit the integration to physical oscillations in the spectral function and the accuracy of the moments. We choose $\eta = 0.05/(6\pi)$. For the second moments, we further limit the integration to $\omega_{\min} \approx -10\omega_0 < \omega < \omega_{\max} \approx 10\omega_0$. We found that the results for the Gaussian regularization are much more robust against changes in $\omega_{\min}$ and $\omega_{\max}$ than the Lorenzian regularization.

[1] C. Gadermaier, A. S. Alexandrov, V. V. Kabanov, P. Kusar, T. Mertelj, X. Yao, C. Manzoni, D. Brida, G. Cerullo, and D. Mihailovic, Electron-phonon coupling in high-temperature cuprate superconductors determined from electron relaxation rates, Phys. Rev. Lett. 105, 257001 (2010).

[2] F. Novelli, G. De Filippis, V. Cataudella, M. Esposito, I. Vergara, F. Cilento, E. Sindici, A. Amaricci, C. Giannetti, D. Prabhakaran, S. Wall, A. Perucchi, S. Dal Conte, G. Cerullo, M. Capone, A. Mishchenko, M. Grüniger, N. Nagaosa, F. Parmigiani, and D. Fausti, Witnessing the formation and relaxation of dressed quasi-particles in a strongly correlated electron system, Nat. Commun. 5, 5112 (2014).

[3] S. Dal Conte, L. Vidmar, D. Golež, M. Mierzejewski, G. Goavi, S. Peli, F. Banfi, G. Ferrari, R. Comin, B. M. Ludbrook, L. Chauviere, N. D. Zhigadlo, H. Eisaki, M. Greven, S. Lupi, A. Damascelli, D. Brida, M. Capone, J. Bońca, G. Cerullo, and C. Giannetti, Snapshots of the retarded interaction of charge carriers with ultrafast fluctuations in cuprates, Nat. Phys. 11, 421 (2015).

[4] C. Giannetti, M. Capone, D. Fausti, M. Fabrizio, F. Parmigiani, and D. Mihailovic, Ultrafast optical spectroscopy of strongly correlated materials and high-temperature superconductors: a non-equilibrium approach, Adv. Phys. 65, 58 (2016).

[5] C. Hwang, W. Zhang, K. Kurashima, R. Kaindl, T. Adachi, Y. Koike, and A. Lanzara, Ultrafast dynamics of electron-phonon coupling in a metal, EPL 126, 57001 (2019).

[6] D. N. Basov, R. D. Averitt, D. van der Marel, M. Dressel, and K. Haule, Electrodynamos of correlated electron materials, Rev. Mod. Phys. 83, 471 (2011).

[7] J. Orenstein, Ultrafast spectroscopy of quantum materials, Phys. Today 65, 44 (2012).

[8] T. Holstein, Studies of polaron motion: Part I. The molecular-crystal model, Ann. Phys. (N. Y.) 8, 325 (1959).

[9] J. E. Hirsch and E. Fradkin, Phase diagram of one-dimensional electron-phonon systems. II. the molecular-crystal model, Phys. Rev. B 27, 4302 (1983).

[10] G. Wellein, H. Röder, and H. Fehske, Polarons and bipolarons in strongly interacting electron-phonon systems, Phys. Rev. B 53, 9666 (1996).

[11] G. Wellein and H. Fehske, Polaron band formation in the Holstein model, Phys. Rev. B 56, 4513 (1997).

[12] G. Wellein and H. Fehske, Self-trapping problem of electrons or excitons in one dimension, Phys. Rev. B 58, 6208 (1998).

[13] J. Bońca, S. A. Trugman, and I. Batistić, Holstein polaron, Phys. Rev. B 60, 1633 (1999).

[14] A. Weiße, H. Fehske, G. Wellein, and A. R. Bishop, Optimized phonon approach for the diagonalization

FIG. 15. Temperature dependent moments. The symbols are calculated by numerically integrating the moments as in Eq. (B1) and the solid lines correspond to the thermal expectation values thereof. For all data, we use a Gaussian regularization and $\eta = 0.05/(6\pi)$. (a) Second moment of the electron spectral function for the same parameters as in Fig. 9. (b) First moment of the electron emission spectrum for the same parameters as in Fig. 11. (c) Second moment of the phonon spectral function for the same parameters as in Fig. 13.
of electron-phonon problems, Phys. Rev. B 62, R747 (2000).
[15] H. Fehske, J. Loos, and G. Wellein, Lattice polaron formation: Effects of nonscreened electron-phonon interaction, Phys. Rev. B 61, 8016 (2000).
[16] A. Weiße, G. Wellein, and H. Fehske, Density-Matrix Algorithm for Phonon Hilbert Space Reduction in the Numerical Diagonalization of Quantum Many-Body Systems, in High Performance Computing in Science and Engineering ’01, pp. 131 (Springer Berlin Heidelberg, 2002).
[17] L.-C. Ku, S. A. Trugman, and J. Bonča, Dimensionality effects on the Holstein polaron, Phys. Rev. B 65, 174306 (2002).
[18] M. Hohenadler, M. Aichhorn, and W. von der Linden, Spectral function of electron-phonon models by cluster perturbation theory, Phys. Rev. B 68, 184304 (2003).
[19] M. Hohenadler, H. G. Evertz, and W. von der Linden, Quantum Monte Carlo and variational approaches to the Holstein model, Phys. Rev. B 69, 024301 (2004).
[20] H. Fehske, G. Wellein, G. Hager, A. Weiße, and A. R. Bishop, Quantum lattice dynamical effects on single-particle excitations in one-dimensional Mott and Peierls insulators, Phys. Rev. B 69, 165115 (2004).
[21] H. Fehske and S. A. Trugman, Numerical solution of the Holstein polaron problem, Polarons in Advanced Materials, volume 103 of Springer Series in Materials Science, 393–461 (Springer Netherlands, 2007).
[22] L.-C. Ku and S. A. Trugman, Quantum dynamics of polaron formation, Phys. Rev. B 75, 014307 (2007).
[23] H. Fehske, G. Hager, and E. Jeckelmann, Metallicity in the half-filled Holstein-Hubbard model, EPL 84, 57001 (2008).
[24] O. S. Barisic and S. Barisic, Phase diagram of the Holstein polaron in one dimension, Eur. Phys. J. B 64, 1 (2008).
[25] S. Ejima and H. Fehske, Luttinger parameters and momentum distribution function for the half-filled spinless fermion Holstein model: A DMRG approach, EPL 87, 27001 (2009).
[26] A. Alvermann, H. Fehske, and S. A. Trugman, Polarons and slow quantum phonons, Phys. Rev. B 81, 165113 (2010).
[27] L. Vidmar, J. Bonča, and S. A. Trugman, Emergence of states in the phonon spectral function of the Holstein polaron below and above the one-phonon continuum, Phys. Rev. B 82, 104304 (2010).
[28] L. Vidmar, J. Bonča, M. Mierzejewski, P. Prelovšek, and S. A. Trugman, Nonequilibrium dynamics of the Holstein polaron driven by an external electric field, Phys. Rev. B 83, 134301 (2011).
[29] G. L. Goodvin, A. S. Mishchenko, and M. Berciu, Optical conductivity of the Holstein polaron, Phys. Rev. Lett. 107, 076403 (2011).
[30] D. Golež, J. Bonča, and L. Vidmar, Dissociation of a Hubbard-Holstein bipolaron driven away from equilibrium by a constant electric field, Phys. Rev. B 85, 144304 (2012).
[31] G. De Filippis, V. Cataudella, A. S. Mishchenko, and N. Nagaosa, Optical conductivity of polarons: Double phonon cloud concept verified by diagrammatic Monte Carlo simulations, Phys. Rev. B 85, 094302 (2012).
[32] G. De Filippis, V. Cataudella, E. A. Nowadnick, T. P. Devereaux, A. S. Mishchenko, and N. Nagaosa, Quantum dynamics of the Hubbard-Holstein model in equilibrium and nonequilibrium: Application to pump-probe phenomena, Phys. Rev. Lett. 109, 176402 (2012).
[33] P. Werner and M. Eckstein, Phonon-enhanced relaxation and excitation in the Holstein-Hubbard model, Phys. Rev. B 88, 165108 (2013).
[34] S. Sayyad and M. Eckstein, Coexistence of excited polarons and metastable delocalized states in photoinduced metals, Phys. Rev. B 91, 104301 (2015).
[35] F. Dorfer, L. Vidmar, C. Brockt, E. Jeckelmann, and F. Heidrich-Meisner, Real-time decay of a highly excited charge carrier in the one-dimensional Holstein model, Phys. Rev. B 91, 104302 (2015).
[36] P. Werner and M. Eckstein, Field-induced polaron formation in the Holstein-Hubbard model, EPL 109, 37002 (2015).
[37] M. A. Sentef, A. F. Kemper, A. Georges, and C. Kolth, Theory of light-enhanced phonon-mediated superconductivity, Phys. Rev. B 93, 144506 (2016).
[38] Z. Huang, L. Wang, C. Wu, L. Chen, F. Grossmann, and Y. Zhao, Polaron dynamics with off-diagonal coupling: beyond the Ehrenfest approximation, Phys. Chem. Chem. Phys. 19, 1655 (2017).
[39] C. Dutreix and M. I. Katsnelson, Dynamical control of electron-phonon interactions with high-frequency light, Phys. Rev. B 95, 024306 (2017).
[40] C. Brockt and E. Jeckelmann, Scattering of an electronic wave packet by a one-dimensional electron-phonon-coupled structure, Phys. Rev. B 95, 064309 (2017).
[41] A. F. Kemper, M. A. Sentef, B. Moritz, T. P. Devereaux, and J. K. Freericks, Review of the theoretical description of time-resolved angle-resolved photoemission spectroscopy in electron-phonon mediated superconductors, Ann. Phys. (Berl.) 529, 1600235 (2017).
[42] H. Hashimoto and S. Ishihara, Photoinduced charge-order melting dynamics in a one-dimensional interacting Holstein model, Phys. Rev. B 96, 035154 (2017).
[43] J. Stolpp, J. Herbrych, F. Dorfner, E. Dagotto, and F. Heidrich-Meisner, Charge-density-wave melting in the one-dimensional Holstein model, Phys. Rev. B 101, 035134 (2020).
[44] A. Dey, M. Q. Lone, and S. Yarlagadda, Decohherence in models for hard-core bosons coupled to optical phonons, Phys. Rev. B 92, 094302 (2015).
[45] J. Kogoj, M. Mierzejewski, and J. Bonča, Nature of bosonic excitations revealed by high-energy charge carriers, Phys. Rev. Lett. 117, 227002 (2016).
[46] L. Vidmar, J. Bonča, S. Maekawa, and T. Tohyama, Bipolaron in the t-J model coupled to longitudinal and transverse quantum lattice vibrations, Phys. Rev. Lett. 103, 186401 (2009).
[47] L. Vidmar, J. Bonča, T. Tohyama, and S. Maekawa, Quantum dynamics of a driven correlated system coupled to phonons, Phys. Rev. Lett. 107, 246404 (2011).
[48] C. Guo, A. Weichselbaum, J. von Delft, and M. Voitja, Critical and strong-coupling phases in one- and two-bath spin-boson models, Phys. Rev. Lett. 108, 160401 (2012).
[49] B. Bruognolo, A. Weichselbaum, C. Guo, J. von Delft, I. Schneider, and M. Voitja, Two-bath spin-boson model: Phase diagram and critical properties, Phys. Rev. B 90, 245130 (2014).
[50] M. L. Wall, A. Safavi-Naini, and A. M. Rey, Simulating generic spin-boson models with matrix product states, Phys. Rev. A 94, 053637 (2016).

[51] S. A. Sato, A. Kelly, and A. Rubio, Coupled forward-backward trajectory approach for nonequilibrium electron-ion dynamics, Phys. Rev. B 97, 134308 (2018).

[52] D. Jansen, J. Stolpp, L. Vidmar, and F. Heidrich-Meisner, Eigenstate thermalization and quantum chaos in the Holstein polaron model, Phys. Rev. B 99, 155130 (2019).

[53] O. S. Barišić, Variational study of the Holstein polaron, Phys. Rev. B 65, 144301 (2002).

[54] O. S. Barišić, Calculation of excited polaron states in the Holstein model, Phys. Rev. B 69, 064302 (2004).

[55] O. S. Barišić, Holstein light quantum polarons on the one-dimensional lattice, Phys. Rev. B 73, 214304 (2006).

[56] J. Loos, M. Hohenadler, A. Alvermann, and H. Fehske, Phonon spectral function of the Holstein polaron, J. Phys. Condens. Matter 18, 7299 (2006).

[57] J. Loos, M. Hohenadler, and H. Fehske, Spectral functions of the spinless Holstein model, J. Phys. Condens. Matter 18, 2453 (2006).

[58] E. V. L. de Mello and J. Ranninger, Dynamical properties of small polarons, Phys. Rev. B 55, 14872 (1997).

[59] S. Paganelli and S. Ciuchi, Tunnelling system coupled to a harmonic oscillator: an analytical treatment, J. Phys. Condens. Matter 18, 7669 (2006).

[60] M. Rigol, V. Dunjko, and M. Olshanii, Thermalization and its mechanism for generic isolated quantum systems, Nature (London) 452, 854 (2008).

[61] M. Rigol and M. Srednicki, Alternatives to eigenstate thermalization, Phys. Rev. Lett. 108, 110601 (2012).

[62] S. Sorg, L. Vidmar, L. Pollet, and F. Heidrich-Meisner, Relaxation and thermalization in the one-dimensional Bose-Hubbard model: A case study for the interaction quantum quench from the atomic limit, Phys. Rev. A 90, 033606 (2014).

[63] A. S. Mishchenko, N. Nagao, G. De Filippis, A. de Candia, and V. Cataudella, Mobility of Holstein polaron at finite temperature: An unbiased approach, Phys. Rev. Lett. 114, 146401 (2015).

[64] L. D’Alessio, Y. Kafri, A. Polkovnikov, and M. Rigol, From quantum chaos and eigenstate thermalization to statistical mechanics and thermodynamics, Adv. Phys. 65, 239 (2016).

[65] L. Chen and Y. Zhao, Finite temperature dynamics of a Holstein polaron: The thermo-field dynamics approach, J. Chem. Phys. 147, 214102 (2017).

[66] J. M. Deutsch, Eigenstate thermalization hypothesis, Rep. Prog. Phys. 81, 082001 (2018).

[67] T. Mori, T. N. Ikeda, E. Kaminishi, and M. Ueda, Thermalization and prethermalization in isolated quantum systems: a theoretical overview, J. Phys. B 51, 112001 (2018).

[68] J. Bonča, S. A. Trugman, and M. Berciu, Spectral function of the Holstein polaron at finite temperature, Phys. Rev. B 100, 094307 (2019).

[69] J. Bonča, Spectral function of an electron coupled to hard-core bosons, Phys. Rev. B 102, 035135 (2020).

[70] S. R. White, Density matrix formulation for quantum renormalization groups, Phys. Rev. Lett. 69, 2863 (1992).

[71] U. Schollwöck, The density-matrix renormalization group, Rev. Mod. Phys. 77, 259 (2005).

[72] U. Schollwöck, The density-matrix renormalization group in the age of matrix product states, Ann. Phys. (N. Y.) 326, 96 (2011).

[73] W. Eberhardt and E. W. Plummer, Angle-resolved photoemission determination of the band structure and multielectron excitations in Ni, Phys. Rev. B 21, 3245 (1980).

[74] A. Damascelli, Z. Hussain, and Z.-X. Shen, Angle-resolved photoemission studies of the cuprate superconductors, Rev. Mod. Phys. 75, 473 (2003).

[75] A. Damascelli, Probing the electronic structure of complex systems by ARPES, Phys. Scr. T109, 61 (2004).

[76] C. Kirkegaard, T. K. Kim, and P. Hofmann, Self-energy determination and electron-phonon coupling on Bi(110), New J. Phys. 7, 99 (2005).

[77] J. K. Freericks, H. R. Krishnamurthy, and T. Pruschke, Theoretical description of time-resolved photoemission spectroscopy: Application to pump-probe experiments, Phys. Rev. Lett. 102, 136401 (2009).

[78] P. Hofmann, I. Y. Skydacheva, E. D. L. Rienks, and E. V. Chulkov, Electron-phonon coupling at surfaces and interfaces, New J. Phys. 11, 125005 (2009).

[79] F. Verstraete, J. J. García-Ripoll, and J. I. Cirac, Matrix product density operators: Simulation of finite-temperature and dissipative systems, Phys. Rev. Lett. 93, 207204 (2004).

[80] A. E. Feiguin and S. R. White, Finite-temperature density matrix renormalization using an enlarged Hilbert space, Phys. Rev. B 72, 220401 (2005).

[81] T. Barthel, U. Schollwöck, and S. R. White, Spectral functions in one-dimensional quantum systems at finite temperature using the density matrix renormalization group, Phys. Rev. B 79, 245101 (2009).

[82] A. E. Feiguin and G. A. Fiete, Spectral properties of a spin-incoherent Luttinger liquid, Phys. Rev. B 81, 075108 (2010).

[83] A. J. Daley, C. Kollath, U. Schollwöck, and G. Vidal, Time-dependent density-matrix renormalization-group using adaptive effective Hilbert spaces, J. Stat. Mech.: Theory Exp. 2004, P04005 (2004).

[84] S. R. White and A. E. Feiguin, Real-time evolution using the density matrix renormalization group, Phys. Rev. Lett. 93, 076401 (2004).

[85] G. Vidal, Efficient simulation of one-dimensional quantum many-body systems, Phys. Rev. Lett. 93, 040502 (2004).

[86] S. Pueckel, T. Khler, A. Swoboda, S. R. Manmana, U. Schollwöck, and C. Hubig, Time-evolution methods for matrix-product states, Ann. Phys. (N. Y.) 411, 167998 (2019).

[87] C. Zhang, E. Jeckelmann, and S. R. White, Density matrix approach to local Hilbert space reduction, Phys. Rev. Lett. 80, 2661 (1998).

[88] C. Brockt, F. Dorfner, L. Vidmar, F. Heidrich-Meisner, and E. Jeckelmann, Matrix-product-state method with a dynamical local basis optimization for bosonic systems out of equilibrium, Phys. Rev. B 92, 241106 (2015).

[89] F. A. Y. N. Schröder and A. W. Chin, Simulating open quantum dynamics with time-dependent variational matrix product states: Towards microscopic correlation of environment dynamics and reduced system evolution, Phys. Rev. B 93, 075105 (2016).
[90] R. J. Bursill, Density-matrix renormalization-group algorithm for quantum lattice systems with a large number of states per site, Phys. Rev. B 60, 1643 (1999).

[91] B. Friedman, Optimal phonon approach to the spin Peierls model with nonadiabatic spin-phonon coupling, Phys. Rev. B 61, 6701 (2000).

[92] W. Barford, R. J. Bursill, and M. Y. Lavrentiev, Breakdown of the adiabatic approximation in trans-polyacetylene, Phys. Rev. B 65, 075107 (2002).

[93] W. Barford and R. J. Bursill, Effect of quantum lattice fluctuations on the Peierls broken-symmetry ground state, Phys. Rev. B 73, 045106 (2006).

[94] H. Wong and Z.-D. Chen, Density-matrix renormalization group approach to the spin-boson model, Phys. Rev. B 77, 174305 (2008).

[95] O. R. Tozer and W. Barford, Localization of large polarons in the disordered Holstein model, Phys. Rev. B 89, 155434 (2014).

[96] F. Dorfner and F. Heidrich-Meisner, Properties of the single-site reduced density matrix in the Bose-Bose renormalization group model in the ground state and in quantum quenches, Phys. Rev. A 93, 063624 (2016).

[97] S. Ejima, H. Fehske, and F. Gebhard, Dynamic properties of the one-dimensional Bose-Hubbard model, EPL 93, 30002 (2011).

[98] T. Barthel, Precise evaluation of thermal response functions using the density matrix renormalization group schemes, New J. Phys. 15, 073010 (2013).

[99] C. Karrasch, J. H. Bardarson, and J. E. Moore, Reducing the numerical effort of finite-temperature density matrix renormalization group calculations, New J. Phys. 15, 083031 (2013).

[100] D. Kennes and C. Karrasch, Extending the range of real time density matrix renormalization group simulations, Comput. Phys. Commun. 200, 37 (2016).

[101] J. Hausschild, E. Levitani, J. H. Bardarson, E. Altman, M. P. Zaletel, and F. Pollmann, Finding purifications with minimal entanglement, Phys. Rev. B 98, 235163 (2018).

[102] S. R. White, Minimally entangled typical quantum states at finite temperature, Phys. Rev. Lett. 102, 190601 (2009).

[103] E. M. Stoudenmire and S. R. White, Minimally entangled typical thermal state algorithms, New J. Phys. 12, 055026 (2010).

[104] B. Bruogno, Z. Zhenyue, S. R. White, and E. M. Stoudenmire, Matrix product state techniques for two-dimensional systems at finite temperature, arXiv:1705.05578 (2017).

[105] C.-M. Chung and U. Schollwöck, Minimally entangled typical thermal states with auxiliary matrix-product-state bases, arXiv:1910.03320 (2019).

[106] J. Chen and E. M. Stoudenmire, Hybrid purification and sampling approach for thermal quantum systems, Phys. Rev. B 101, 195119 (2020).

[107] T. Barthel, Matrix product purifications for canonical ensembles and quantum number distributions, Phys. Rev. B 94, 115157 (2016).

[108] R. Orús, Advances on tensor network theory: symmetries, fermions, entanglement, and holography, Eur. Phys. J. B 87, 280 (2014).

[109] S. R. White and I. Affleck, Spectral function for two-dimensional systems at finite temperature, Phys. Rev. B 4494 (1997).

[110] T. Barthel, Matrix product states with auxiliary matrix-product-state bases, arXiv:1910.03329 (2019).

[111] A. Vaidyanathan, The Theory of Linear Prediction, Synthesis Lectures on Engineering Series (Morgan & Claypool, 2008).

[112] TTensor Library (version 3.1.0) http://itensor.org .

[113] J. Jakli and P. Prelovsek, Finite-temperature properties of doped antiferromagnets, Adv. Phys. 49, 1 (2000).

[114] P. Prelovšek and J. Bonča, Ground State and Finite Temperature Lanczos Methods, Strongly Correlated Systems: Numerical Methods, 1–30 (Springer Berlin Heidelberg, Berlin, Heidelberg, 2013).

[115] B. S. Shastry and B. Sutherland, Twisted boundary conditions and effective mass in Heisenberg-Ising and Hubbard rings, Phys. Rev. Lett. 65, 243 (1990).

[116] D. Poilblanc, Twisted boundary conditions in cluster calculations of the optical conductivity in two-dimensional lattice models, Phys. Rev. B 44, 9562 (1991).

[117] J. Bonča and P. Prelovšek, Thermodynamics of the planar Hubbard model, Phys. Rev. B 67, 085103 (2003).

[118] S. Ciuchi, F. de Pasquale, S. Fratini, and D. Feinberg, Dynamical mean-field theory of the small polaron, Phys. Rev. B 56, 4494 (1997).

[119] R. T. Scalettar, N. E. Bickers, and D. J. Scalapino, Competition of pairing and Peierls-charge-density-wave correlations in a two-dimensional electron-phonon
[130] Y. Wang, M. Claassen, C. D. Pemmaraju, C. Jia, B. Moritz, and T. P. Devereaux, Theoretical understanding of photon spectroscopies in correlated materials in and out of equilibrium, Nat. Rev. Mater. 3, 312 (2018).
[131] B. Lau, M. Berciu, and G. A. Sawatzky, Single-polaron properties of the one-dimensional breathing-mode Hamiltonian, Phys. Rev. B 76, 174305 (2007).
[132] G. L. Goodvin, M. Berciu, and G. A. Sawatzky, Green’s function of the Holstein polaron, Phys. Rev. B 74, 245104 (2006).
[133] M. Berciu and G. L. Goodvin, Systematic improvement of the momentum average approximation for the Green’s function of a Holstein polaron, Phys. Rev. B 76, 165109 (2007).
[134] S. Paeckel, B. Fauseweh, A. Ostekorn, T. Köhler, D. Manske, and S. R. Manmana, Detecting superconductivity out of equilibrium, Phys. Rev. B 101, 180507 (2020).
[135] J. Haegeman, J. I. Cirac, T. J. Osborne, I. Pižorn, H. Verschelde, and F. Verstraete, Time-dependent variational principle for quantum lattices, Phys. Rev. Lett. 107, 070601 (2011).
[136] J. Haegeman, C. Lubich, I. Oseledets, B. Vandereycken, and F. Verstraete, Unifying time evolution and optimization with matrix product states, Phys. Rev. B 94, 165116 (2016).
[137] M. Yang and S. R. White, Time dependent variational principle with ancillary Krylov subspace, arXiv:2005.061048 (2020).
[138] B. Kloss, D. R. Reichman, and R. Tempelaar, Multiset matrix product state calculations reveal mobile Franck-Condon excitations under strong Holstein-type coupling, Phys. Rev. Lett. 123, 126601 (2019).
[139] P. Secular, N. Gourianov, M. Lubasch, S. Dolgov, S. R. Clark, and D. Jaksch, Parallel time-dependent variational principle algorithm for matrix product states, Phys. Rev. B 101, 235123 (2020).
[140] Y. Murakami, P. Werner, N. Tsuji, and H. Aoki, Interaction quench in the Holstein model: Thermalization crossover from electron- to phonon-dominated relaxation, Phys. Rev. B 91, 045128 (2015).
[141] N. Das and N. Singh, Hot-electron relaxation in metals within the GtzeWflle memory function formalism, Int. J. Mod. Phys. B 30, 1650071 (2016).
[142] S. Ono, Thermalization in simple metals: Role of electron-phonon and phonon-phonon scattering, Phys. Rev. B 97, 054310 (2018).
[143] J. R. Mannouch, W. Barford, and S. Al-Assam, Ultrafast relaxation, decoherence, and localization of photoexcited states in π-conjugated polymers, J. Chem. Phys. 148, 034901 (2018).
[144] J. Kogoj, L. Vidmar, M. Mierzejewski, S. A. Trugman, and J. Bonča, Thermalization after photoexcitation from the perspective of optical spectroscopy, Phys. Rev. B 94, 014304 (2016).
[145] M. Galperin, M. A. Ratner, and A. Nitzan, Molecular transport junctions: vibrational effects, J. Phys. Condens. Matter 19, 103201 (2007).
[146] E. A. Osorio, T. Bjørnholm, J.-M. Lehn, M. Ruben, and H. S. J. van der Zant, Single-molecule transport in three-terminal devices, J. Phys. Condens. Matter 20, 374121 (2008).
[147] T. Koch, J. Loos, A. Alvermann, A. R. Bishop, and H. Fehske, Transport through a vibrating quantum dot: Polaronic effects, J. Phys. Conf. Ser. 220, 012014 (2010).
[148] N. A. Zimbovskaya and M. R. Pederson, Electron transport through molecular junctions, Phys. Rep. 509, 1 (2011).
[149] A. Khedri, T. A. Costi, and V. Meden, Nonequilibrium thermoelectric transport through vibrating molecular quantum dots, Phys. Rev. B 98, 195138 (2018).
[150] A. Dey and S. Yarlagadda, Temperature dependence of long coherence times of oxide charge qubits, Sci. Rep. 8, 3487 (2018).
[151] W. Westhäuser, S. Schramm, J. Hoffmann, and C. Jooss, Comparative study of magnetic and electric field induced insulator-metal-transitions in Pr1−xCaxMnO3 films, Eur. Phys. J. B 53, 323 (2006).
[152] Y. M. Sheu, S. A. Trugman, L. Yan, J. Qi, X. Q. Jia, A. J. Taylor, and R. P. Prasankumar, Polaronic transport induced by competing interfacial magnetic order in a La0.7Ca0.3MnO3/BiFeO3 heterostructure, Phys. Rev. X 4, 021001 (2014).
[153] D. Raiser, S. Mildner, B. Ifland, M. Sotoudeh, P. Bichl, S. Techert, and C. Jooss, Evolution of hot polaron states with a nanosecond lifetime in a manganite perovskite, Adv. Energy Mater. 7, 1602174 (2017).
[154] M. Sotoudeh, S. Rajpurohit, P. Bölch, D. Mierwaldt, J. Norpoth, V. Roddatis, S. Mildner, B. Kressdorf, B. Ifland, and C. Jooss, Electronic structure of Pr1−xCaxMnO3, Phys. Rev. B 95, 235150 (2017).
[155] M. Eckstein and M. Kollar, Measuring correlated electron dynamics with time-resolved photoemission spectroscopy, Phys. Rev. B 78, 245113 (2008).
[156] M. Lligges, I. Avigo, D. Golež, H. U. R. Strand, Y. Beyazit, K. Hanif, F. Diekmann, L. Stojchevska, M. Källåne, P. Zhou, K. Rossnagel, M. Eckstein, P. Werner, and U. Bovensiepen, Ultrafast double dynamics in photoexcited 1T-TaS2, Phys. Rev. Lett. 120, 166401 (2018).
[157] J. J. Mendoza-Arenas, D. F. Rojas-Gamboa, M. B. Pleonio, and J. Prior, Exciton transport enhancement across quantum Sn-Schrieffer-Heeger lattices with quartic nonlinearity, Phys. Rev. B 100, 104307 (2019).
[158] J. H. Fetherolf, D. Golež, and T. C. Berkelbach, A unifiedification of the Holstein polaron and dynamic disorder pictures of charge transport in organic crystals, Phys. Rev. X 10, 021062 (2020).
[159] P. E. Kornilovitch, Photoemission spectroscopy and sum rules in dilute electron-phonon systems, EPL 59, 735 (2002).