Spectral Function of an Electron Coupled to Hard Core Bosons

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(Dated: July 20, 2020)

We have computed static and dynamic properties of an electron coupled to hard–core–boson (HCB) degrees of freedom in one spacial dimension. The polaron, an electron dressed with HCB excitations, remains light even in the strong coupling limit as its effective mass remains of the order of the free electron mass. This result is in a sharp contrast to the Holstein model where the electron effective mass increases exponentially with the electron–phonon coupling. HCB degrees of freedom mediate the attractive potential between two electrons that form a bound singlet bipolaron state at any non–zero coupling strength. In the low–frequency regime of the electron spectral function we observe a quasi–particle (QP) band that is separated from the continuum of states only in the central part of the Brillouin zone. The quasiparticle weight approaches zero as the QP band enters the continuum where it obtains a finite lifetime. At finite temperature an electron can annihilate thermally excited HCB’s. Such thermally activated processes lead to a buildup of the spectral weight below the QP band. While the investigated model bears a resemblance with the Holstein model, we point out many important differences that originate from the binary HCB excitation spectrum, which in turn mimics spin–$\frac{1}{2}$ degrees of freedom.

I. INTRODUCTION

We investigate static, dynamic and thermodynamic properties of an electron coupled to hard–core–boson (HCB) degrees of freedom. The model under the investigation resembles a well known Holstein model (HM)\textsuperscript{1} which has been a subject of extensive research\textsuperscript{2–10} starting from the HM, the HCB model (HCBM) is obtained by replacing each oscillator with its infinite degrees of freedom by a HCB representing a state that can be either occupied or un–occupied. Despite a significant reduction of inelastic degrees of freedom in comparison to the HM, the statistics of neighboring energy level spacings in HCBM remains well described by the Wigner-Dyson distribution\textsuperscript{11} characteristic of non–integrable ergodic quantum models. The reduction of HM to HCBM has further important consequences: HCBM possess a limited energy spectrum which further facilitates finite–temperature studies, reduction of inelastic degrees of freedom allows studies of larger–size systems approaching closer the thermodynamic limit.

An important motivation for the research presented in this manuscript originates from the research of high–temperature superconductivity where the quest for the origin of the attractive interaction between charge carriers is still active. Among the fundamental open questions is whether the attractive interaction is based on lattice degrees of freedom or is it due to the strong Coulomb interaction that generates the spin exchange coupling. Since the binary spectrum of a HCBs closely resembles a spin 1/2 degree of freedom, HCBM can be used to simulate properties of a spin–polaron\textsuperscript{22–24}, i.e. electron, interacting with spin degrees of freedom thus bridging the gap between research of lattice and spin models.

So far physical realization of systems with HCB’s is limited to ultracold atoms in optical lattices\textsuperscript{25–29}. Nevertheless, models where electrons are coupled to HCB’s may carry potential relevance to microscopic mechanisms of superconductivity. As we will show in this paper, the effective polaron mass remains small even in the limit of very strong electron-HCB coupling strength. We also demonstrate that HCB’s can mediate the necessary attractive potential for the formation of light bipolarons.

II. MODEL AND METHOD

We analyze a model with a single electron in a one–dimensional chain of size $L$ with periodic boundary conditions coupled to HCB degrees of freedom

\begin{equation}
H = -t_0 \sum_j (c_j^\dagger c_{j+1} + \text{H.c.}) - g \sum_j \hat{n}_j (b_j^\dagger + b_j) + \omega_0 \sum_j b_j^\dagger b_j,
\end{equation}

where $c_j$ and $b_j$ are electron and HCB creation operators at site $j$, respectively, and $\hat{n}_j = c_j^\dagger c_j$ represents the electron density operator. HCB’s are defined via the following commutation relation $[b_i, b_j^\dagger] = \delta_{i,j} (1 - 2b_i^\dagger b_i)$. Parameter $g$ measures the strength of coupling between the electron and HCB, $\omega_0$ denotes a dispersionless optical HCB frequency and $t_0$ nearest–neighbor hopping amplitude. From here on we set $t_0 = 1$.

In most calculations we have used full translationally invariant Hilbert space spanning $N_s = 2^L$ basis states. In case of zero-$T$ calculations we have implemented standard Lanczos\textsuperscript{30} technique. To determine static and dynamic properties of the model at finite-$T$ we have implemented the Finite Temperature Lanczos Method (FTLM) as described in Refs.\textsuperscript{31,32} where it has been shown that static thermodynamic properties of an operator $A$ can be evaluated via sampling over random states $|r\rangle$ defined in a subspace with one electron and
multiple HCB degrees of freedom, 
\[
\langle A \rangle_T = Z^{-1} \sum_{r=1}^{R} \sum_{j=1}^{M} e^{-\beta \epsilon_j} \langle r | \psi_j \rangle \langle \psi_j | A | r \rangle,
\]
where \(|\psi_j\rangle\) and \(\epsilon_j\) are Lanczos wave-functions and cor-
responding energies, respectively, in the sub-space with one ele-
tron, \(\beta = 1/T\), and \(Z\) is the partition function. Fur-
thermore, \(R\) represents the number of different random states, and
\(M\) is the number of Lanczos iterations.

The main goal of this work is to analyze the single-electron spectral
function, corresponding to electron addition, as obtained
via the corresponding retarded Green’s function
\[
A(\omega, k) = -\pi^{-1} \lim_{\eta \to 0^+} \mathcal{G}_R(\omega + i\eta, k),
\]
where at finite-\(T\) \(\mathcal{G}_R(\omega + i\eta, k)\) is obtained via the Gibbs en-
semble
\[
\mathcal{G}_R(\omega, k) = Z^{-1} \int_0^\infty dt \, e^{i\omega t} \sum_n \sum_{c} e^{-\beta \epsilon_n} \langle \phi_n^0 | c_k(t) c_{k}^\dagger(0) | \phi_n^0 \rangle,
\]
where \(\phi_n^0\) are multi HCB eigenstates of the Hamiltonian in Eq. (1) with no electron present in the system while \(c_j^\dagger\) are cor-
responding energies and \(c_k = 1/\sqrt{L} \sum_{j=1}^{L} \exp(ikj) c_j\). We
finally take advantage of the FTLM method \(22\) and replace the
trace over a complete set of states \(\langle \phi_n^0 |\) by the summa-
tion over random states \(\langle \phi^0 |\) = \(\sum_{n=1}^{N_0} \alpha_n \langle \phi_n^0 |\), where \(\alpha_n\) are
distributed randomly, and
\[
A(\omega, k) = Z^{-1} \sum_{r=1}^{R} \sum_{n=1}^{N_0} \sum_{j=1}^{M} e^{-\beta \epsilon_n} \langle \phi_n^0 | \langle \phi_n^0 | c_k \rangle | \psi_j \rangle
\]
\[
\langle \psi_j | c_{k}^\dagger | \psi_j \rangle \delta(\omega - \epsilon_j + \epsilon_n),
\]
where \(|\psi_j\rangle\) and \(\epsilon_j\) are Lanczos wave-functions and corre-
sponding energies, respectively, in the sub-space with one ele-
tron. Lanczos states are generated starting from states \(c_k^\dagger | \psi_j \rangle\). Furthermore, \(R \sim 100\) represents the number of dif-
ferent random states, \(N_0 = 2^k\) the size of the Hilbert space in
the zero-electron subspace and \(M\) is the number of Lanczos
iterations. We have used typically \(M = 50\) Lanczos itera-
tions to obtain static properties at finite-\(T\) and \(M = 500\) for
dynamic quantities combined with the Gram-Schmidt orthog-
onalization procedure to avoid spurious non-orthogonal states
that appear at large values of \(M\). The Lorentzian form of the delta
functions with the half width at half maximum (HWWM) \(\eta\) was used for graphi-
cal representations of \(A(\omega, k)\).

While our calculations were limited to rather small sys-
tem sizes \(L = 16\), we have expanded our calculations from
using only periodic boundary conditions towards the twisted
boundary conditions \(20\) that are equivalent to the intro-
duction of the magnetic flux penetrating the ring. In this ap-
proach the kinetic energy term in Eq. (1) is transformed to
\[
H_{\text{kin}} = -t_0 \sum_j (c_j^\dagger c_{j+1}^\dagger + H.c.), \quad \text{where } \theta \text{ represents a mag-
netic flux that penetrates the ring } \phi_m = \theta L/2\pi \text{ in units}
\]
of \(h/e_0\). Discrete \(k\)-points \(k_m = 2\pi n/L\) can thus be connected
by choosing \(\theta \in [0, 2\pi /L]\).

Further details concerning the construction of the transla-
tionally invariant basis states and comparison of the selected
ground state properties between a small basis set and a full
basis can be obtained in the Appendix A. We show in the
Appendix B that finite-size effects seem to be well under control
in all temperature regimes by comparing \(A(k, \omega)\) computed
on two different system sizes and different \(T\). In the Sub-
section E we also compute the lowest frequency moments of
\(A(k, \omega)\) and compare them with analytical results that are free
of finite–size effects, which in turn renders further insight into
the applicability of FTLM to the model under the investiga-
tion.

III. RESULTS

A. Zero-\(T\) properties

Figure 1: Ground-state properties computed using full basis on a
ring with \(L = 16\) taking into account the full translational symmetry:
a) the kinetic energy \(E_{\text{kin}} = \langle \psi_k | H \psi_k \rangle - 2t_0 \sum_j c_j c_{j+1}^\dagger H.c. | \psi_k \rangle\) vs. \(g\) at
different \(\omega_0\), b) the total number of HCBs \(N_0 = \langle \psi_k | \sum_j b_j^\dagger b_j | \psi_k \rangle\) and
c) the effective mass \(m_{\text{eff}} = \langle \partial^2 E(k) / \partial k^2 \rangle_{k=0}^{-1}\) compared to the
free electron mass \(m^0 = 1/2t_0\) where \(E(k) = \langle \psi_k | H | \psi_k \rangle\),
where \(|\psi_k\rangle\) is the ground state polaron wave function with
momentum \(k\). Thin lines represent the inverse of the quasiparticle weight
defined as \(Z_{\omega_0}(k) = \langle |\psi_k | c_k^\dagger | 0 \rangle^2 \rangle\) at \(k = 0\) where \(|0\rangle\) is the state
with no electron and no HCB excitations. In d) through f) we show
\(k\)-dependent properties at fixed coupling \(g\) of the total energy \(E(k)\)
in d), \(N_0(k)\) in e) and in f) the quasiparticle weight \(Z_{\omega_0}(k)\). Hor-
izontal lines in d) indicated values of \(\omega_0\).

In Figs. 1(a) through (c) we show some characteristic
ground state properties of the model at \(k = 0\). With increas-
ing the electron-boson coupling \(g\) the kinetic energy \(E_{\text{kin}}\) in-
creases but shows a tendency towards saturation at larger \(g\),
as seen in Fig. 1(a). \(E_{\text{kin}}\) also increases with increasing \(\omega_0\) at
fixed \(g\) which stands in contrast to a decrease of the total num-
ber of HCB’s \(N_0\) with increasing \(\omega_0\), seen in Fig. 1(b). Further
elaborating on results at fixed $g$: at smaller $\omega_0$ the electron is dressed up with a larger number of HCB excitations than at larger values of $\omega_0$, nevertheless, its kinetic energy is less affected by the presence by the HCB cloud at smaller $\omega_0$. It is furthermore instructive to compare the slow increase of $N_b$ with increasing $g$ to the increase of the number of phonons in the strong coupling limit in the HM where $N_{ph} = (g/\omega_0)^2$. This profound difference between the two models is trivially explained since the maximal on–site occupancy of HCB’s is limited to 1. In Fig. 1(c) we display the effective polaron mass $m_{eff}$. In the small–$g$ limit the perturbation theory can be applied and results in the following polaron dispersion relation:

$$E(k) = \epsilon(k) + \frac{1}{L} \sum_q \frac{g^2}{\epsilon(k) - \epsilon(k + q) - \omega_0},$$

(6)

where $\epsilon(k) = -t_0 \cos(k)$ is the free electron dispersion relation. In this limit $m_{eff}/m_0 - 1 \propto g^2$ just as in the HM, while at larger $g$ it displays a slow sub–logarithmic increase with $g$. Here, the difference with the HM is even more pronounced since it is well known that in the strong coupling limit of the HM $m_{eff}/m_0 = \exp[(g/\omega_0)^2]$. In the case of the HM $m_{eff}$ can be determined from $Z_{qp}(k = 0)^{-1} = m_{eff}/m_0$, as shown in Ref. In Fig. 1(c) we show along $m_{eff}/m_0$ also $Z_{qp}^{-1}$. The agreement between both quantities is good for large $\omega_0$ at any $g$, but starts to deviate strongly at small $\omega_0$.

In Figs. 1(d) through (f) we show $k$–dependent properties of the electron coupled to HCB’s at fixed $g = 2$ and various $\omega_0$. We start with the discussion of the dispersion relation representing the polaron energy $E(k) = \langle \psi_k | H | \psi_k \rangle$, where $| \psi_k \rangle$ is the ground state wave function with momentum $k$, shifted by $E(k = 0)$ which facilitates a quantitative comparison between results corresponding to different values of $\omega_0$, as shown in Fig. 1(d). Common to all cases is a quadratic increase at small $k$ followed by an abrupt flattening of the band at a value of $k_0$ corresponding to $E(k_0) - E(0) = \omega_0$. It seems as if the polaron band, also known as the quasi–particle (QP) band intercepts the continuum of states that starts at the energy $\omega_0$ above $E(0)$. This is in a sharp contrast to the Holstein polaron case where the QP band remains separated from the continuum in the whole Brillouin zone. A similar $k$–dependence is observed in the mean HCB number $N_b(k)$, Fig. 1(e). The QP weight $Z_{qp}(k)$ provides information about the electronic character of the polaronic state. In Figs. 1(f) we observe a disappearance of $Z_{qp}$ at $k_0$ where the QP band enters the continuum. This result suggests that the ground state $| \psi_k \rangle$ for $k = k_0$ contains nearly free electron contribution of a state $c_k^\dagger | 0 \rangle$. Instead, $| \psi_k \rangle$ is composed of a polaron in the state $k = 0$ that contains a significant amount of the free–electron wavefunction $c_k^\dagger | 0 \rangle$, and an extra HCB excitation in the state $k$. This is further consistent with results presented in Fig. 2 where we show the electron kinetic energy $E_{kin}(k) = \langle \psi_k | H_{kin} | \psi_k \rangle$. Naively, one would expect $E_{kin}(k)$ to resemble a renormalized free–electron dispersion relation. In contrast, $E_{kin}(k)$ shows a non–monotonic behavior whereby at larger $k > k_0$ it again reaches its value at zero momentum, i.e. $E_{kin}(k = 0) < E_{kin}(k > k_0)$, consistent with the above hypothesis.

Before switching to the description of finite–$T$ properties of the HCBM we show that the electron–HCB interaction leads to a formation of bound pairs of polarons or bipolarons. To test this assumption we investigate a system with two electrons coupled with HCB’s in the presence of a Coulomb on–site interaction $U$

$$H = -t_0 \sum_{j,\sigma \in [\uparrow, \downarrow]} (c_{j,\sigma}^\dagger c_{j+1,\sigma} + H.c.) - g \sum_j n_j (b_j^\dagger + b_j) + U \sum_j n_j \bar{n}_j + \omega_0 \sum_j b_j^\dagger b_j, \quad (7)$$

where $n_j = n_{j+1} + n_{j}$ and $\bar{n}_j = c_{j,\uparrow}^\dagger c_{j,\downarrow}$. We have computed the binding energy of a bipolaron defined as $\Delta = E_2 - E_1$ where $E_2$ is the ground state energy of two electrons with opposite spin orientation and $E_1$ is the ground state energy of a system with one electron. In Fig. 3 we present $\Delta$ vs. $g$ for different values of the HCB frequency $\omega_0$. Results show that at $U = 0$ the bipolaron remains bound irrespective of the coupling strength as well as $\omega_0$ while at finite $U = 1$ there exists a critical value of $g_c$. This result is consistent with $\Delta$ computed in the atomic limit, i.e. at $t_0 = 0$ where we obtain the following expression for the binding energy:

$$\Delta = \sqrt{4g^2 + \omega_0^2} - \frac{1}{2} \sqrt{16g^2 + \omega_0^2} - \omega_0/2 + U, \quad (8)$$

which leads to a $\Delta < 0$ for $U = 0$ at arbitrary $|g| > 0$.

To get further insight into the shape of the bipolaron we also present in Fig. 3 the density–density correlation function

$$\gamma(j) = \frac{\sum_{\bar{n}_j = 0} \langle \psi_0 | n_j n_{j+1} | \psi_0 \rangle}{\sum_{\bar{n}_j = 0} \langle \psi_0 | n_j n_{j+1} | \psi_0 \rangle}, \quad (9)$$

defined so as $\sum_j \gamma(j) = 1$. The $\Delta < 0$ regime is reflected in an exponentially decaying form of $\gamma(j)$. At finite–$U$ the bound state is formed from two electrons positioned predominantly on neighboring sites. This results bears a similarity to a $S1$ bipolaron in the Holstein–Hubbard model [23, 36].

**B. Finite–$T$ properties**

In Figs. 4 we present selected thermodynamic properties of the model. The total energy of the system increases with $T$ as well as with $\omega_0$, see Fig. 4(a). This is in part due to the
the electron–HCB coupling part of the Hamiltonian in Eq. \(1:\)

\[
E_g = -\langle g \sum_j \bar{n}_j (b_j + b_j)^\dagger \rangle \tau
\]

and in d) the number of HCB per site \(n_b = N_b / L\) along with the HCB thermal distribution functions \(n_b^0 = \frac{1}{\exp[j\omega_0\pi\tau]}\), shown using thin black lines.

Figure 3: \(\Delta\) vs. \(g\) for different values of \(\omega_0\) as shown in the legends for \(U = 0\) and 1 in (a) and (b), respectively. In (c) and (d) we present \(\gamma(j)\) at fixed \(g = 2\) while the other parameters of the model are the same as in (a) and (b). All results were computed on a system with 13 sites using periodic boundary conditions.

Figure 4: Finite-\(T\) properties of selected expectation values computed on a system with \(L = 16\) presented on a semi–log plot. In a) we present the energy of the system \(E(T) = \langle H \rangle \tau\) per site \(L\) where the expectation value is taken using FTLM method, as described in Eq (2) similarly, in b) we present \(E_{\text{kin}}(T)\), in c) we display the electron–HCB coupling part of the Hamiltonian in Eq. (1) \(E_g = -\langle g \sum_j \bar{n}_j (b_j + b_j)^\dagger \rangle \tau\) and in d) the number of HCB per site \(n_b = N_b / L\) along with the HCB thermal distribution functions \(n_b^0 = \frac{1}{\exp[j\omega_0\pi\tau]}\), shown using thin black lines.

In Fig. 5 we present the single particle density matrix \(\bar{n}_k\) vs. \(T\) computed using \(\omega_0 = 1\), \(g = 2\) and \(L = 16\).

The HCB occupancy per site \(n_b\) closely follows the Fermi–Dirac–like distribution, characteristic for HCBs \(n_b^0 \sim 1/[\exp(j\omega_0) + 1]\), as shown in Fig. 4(d) by thin black lines. In the high-\(T\) limit, i.e. for \(T >> \omega_0\), numerical results clearly approach \(n_b \rightarrow 1/2\).

In Figs. 6 we present density plots representing \(A(\omega, k)\) in the entire Brillouin zone (BZ) at fixed coupling \(g = 2\) and two different sets of \(\omega_0 = 1\) and 0.2. For a more quantitative analysis we also display with dashed lines the corresponding ground–state polaron energy \(E(k) = \langle \psi_k | H | \psi_k \rangle\), where \(|\psi_k\rangle\) is the ground state polaron wave function with momentum \(k\). We focus first on \(\omega_0 = 1\) and small \(T/\omega_0 = 0.05\) where we clearly observe in the low–\(\omega\) regime the QP band only in a limited part of the Brillouin zone, \(k \in [-0.6\pi, 0.6\pi]\). The spectral weight of the QP band is given by \(Z_{\text{qp}}(k)\). Outside this interval the QP band enters the continuum of states and \(Z_{\text{qp}}\) approaches zero, also consistent with Figs. (1)(d) and (f).

In the Appendix we show that only a partial separation of the QP band from the continuum is a consequence of the HCB commutation relation. In a model where the Hilbert space of HCBM is expanded to contain up to two phonon degrees of freedom per site, the QP band remains visible throughout the entire BZ and approaches the lower edge of the continuum near the edge of the BZ.

This behavior is in a sharp contrast to the HM case where the QP band extends through the whole BZ and is entirely located below the continuum. Within the incoherent part
of the spectra we observe a rather well defined band of high-energy excitations with its maximal intensity around the edges of the BZ. The separation between the QP band and these high-energy excitation can be estimated from the energies computed in the atomic limit of the model, \( t_0 = 0 \)

\[
\epsilon_{\pm}^{0} = \frac{1}{2}(\omega_0 \pm \sqrt{\omega_0^2 + 4g^2})
\]

that gives the energy gap \( \Delta_{\text{exp}} = \sqrt{\omega_0^2 + 4g^2} = 4.1 \), which further determines an estimate of the separation between the two bands. With increasing \( T \) additional spectral weight develops below the QP band predominantly around the center of the BZ, as seen in Figs. (b) and (c). This buildup of the spectra below the QP band appears because at elevated \( T \) an electron can annihilate a thermally excited HCB.

Remnants of the QP band remain clearly distinguishable even at \( T = \omega_0 \), the same holds also for the well pronounced peaks around the edges of the BZ in the high-frequency regime. In contrast to the HM case, the extra spectral weight that develops below the QP band extends only \( \omega_0 \) below the bottom of the QP band consistent with the fact that only a single HCB is allowed per site.

In spectral functions at small \( \omega_0 = 0.2 \), shown in Figs. (d) through (f), the QP band is barely visible even at small \( T/\omega_0 = 0.05 \), it merges with the continuum around \( k \sim 0.35\pi \). This is also consistent with the behavior of \( Z_{qp} \), shown in Fig. (f), that at \( k \sim 0.35\pi \) approaches zero. In contrast to the \( \omega_0 = 1 \) case where the QP band is well separated from the incoherent continuum, at \( \omega_0 = 0.2 \) we find rather large spectral weight just above the QP band. Towards the edge of the BZ the incoherent part of the spectrum consists of a series of separated and split bands.

In Fig. (f) we show comparison between \( A(\omega, k) \) as obtained from the HCBM and the standard HM using identical model parameters. Most notable distinction is observed already at small \( T/\omega_0 = 0.1 \), as shown in Figs. (a) and (d). While in the HCBM a single well defined QP band in the vicinity of the center of the BZ is observed, in the HM there are multiple well defined bands separated by \( \omega_0 \) above the QP band extending throughout the entire BZ. Spacing between multiple bands observed in the case of HM model can be explained by inspecting the energy spectra in the atomic limit of the model given by \( \epsilon_{\pm}^{0} = -g^2/\omega_0 + n\omega_0 \). In addition we find larger effective mass in the HM that is reflected in a less dispersive QP band in comparison to the HCB case. A quantitative analysis yields a mass ratio \( m_{\text{eff}}^{\text{HM}} / m_{\text{eff}}^{\text{HCB}} \sim 1.6 \).

Shifting now the comparison to finite-\( T \) results we observe additional spectral weight that emerges with increasing \( T \) below the respective QP bands in both cases. Nevertheless, in the HCBM the latter is limited to the energy interval \( |E(k), E(k) - \omega_0| \) and remains restricted to the center of the BZ, while in the HM case it appears as replicas of the nearly flat QP bands located at energies \( E(k) - n\omega_0 \) and with decreasing intensity as \( n \in \mathbb{N} \) increases.

### D. Self-energies

In order to study the life–time of the QP peaks at elevated \( T \), we have computed the corresponding self–energies. In Fig. (g) we show a direct comparison between a family of \( A(\omega, k) \) obtained in the interval \( k \in [0, \pi] \) and the imaginary parts of matching self–energies \( \Sigma' (\omega, k) \) for two different values of \( \omega_0 = 1 \) and 0.2 at low–\( T/\omega_0 = 0.05 \) as well as for high–\( T/\omega_0 = 1 \). Results of \( \Sigma' (\omega, k) \) were obtained from the relation \( \mathcal{G}^{R}(\omega, k) = 1/(\omega - \epsilon(k) - \Sigma(\omega, k)) \) where \( \epsilon(k) \) is the free electron energy \( \epsilon(k) = -2\hbar_0 \cos(k) \). From comparison of Figs. (g) and (c) we notice that \( \Sigma' (\omega, k) \sim 0 \) in the frequency regime that corresponds to the well defined QP band in Fig. (a). In Fig. (g) this regime however does not extend though the entire BZ since \( \Sigma' (\omega, k) \) becomes finite already around \( k_0 = 3\pi/4 \) and at the value of \( \omega \) corresponding to the lowest peak in \( A(\omega, k_0) \). This behavior shows that a well defined quasiparticle with an infinitely long lifetime exists only.
in a limited region of the BZ. In Fig. 8(g), corresponding to \( \omega_0 = 0.2 \), the regime of \( \Sigma''(\omega, k) \sim 0 \) is even more limited to the vicinity of the QP peak at \( k = 0 \). In both cases \( \Sigma''(\omega, k) \) displays rather pronounced \( k \)-dependence which is in contrast to the HM case. At elevated \( T \) \( \Sigma''(\omega, k) \) deviates significantly from zero already at frequencies, corresponding to the positions of QP peaks as seen in Figs. 8(d) and (h). This result demonstrates the importance of incoherent processes that originate from thermal collisions.

### E. Frequency moments

We have computed the lowest frequency moments of the spectral function. As already shown in Refs. [19,20], frequency moments of the single polaron spectral function can be obtained analytically using the following relation

\[
M_n(k) = \int_{-\infty}^{\infty} \omega^n A(\omega, k) d\omega = \langle \langle [c_k, H], [H], \ldots, [H]c_k^\dagger \rangle_T \rangle_T,
\]

where \( \langle \ldots \rangle_T \) represents the thermal average over zero-electron states and the number of commutators corresponds to the order of the frequency moment. Taking into account the HCB commutation relation \([b_i, b_j^\dagger] = \delta_{ij}(1 - 2b_i^\dagger b_i)\) analytical expressions may be obtained for arbitrary moments even at finite-\( T \). Here we list just a few:

\[
\begin{align*}
M_0(k) &= 1, \\
M_1(k) &= \epsilon(k), \\
M_2(k) &= \epsilon^2(k) + g^2, \\
M_3(k) &= \epsilon^3(k) + 2g^2\epsilon(k) + g^2\omega_0(1 - 2n_0^0),
\end{align*}
\]

where \( \epsilon(k) = -2t_0 \cos(k) \) and \( n_0^0 = 1/\langle \exp(\omega_0/T) + 1 \rangle \). Note that \( M_0(k) \) through \( M_2(k) \) do not depend on \( T \).

In Figs. 9 we plot \( M_n(k) \); \( n \in \{1, 2, 3\} \) extracted from \( A(\omega, k) \) for a set of temperatures \( T \in \{0.2, 0.4, \ldots 2.0\} \). Ex-
Figure 9: $M_1(k)$, $M_2(k)$ and $M_3(k)$ at $\omega_0 = 1$ and $g = 2$. In all plots we present with open symbols frequency moments obtained from numerical results of $A(\omega, k)$ computed on $L = 16$ sites system with twisted boundary conditions, just as in Fig. 6, but for 10 different values of $T \in \{0.2, 0.4, \ldots, 2.0\}$. Results for the lowest $T = 0.2$ and 0.4 are represented with blue and green circles, respectively, while the rest of results for $T \geq 0.6$ are shown in red. Blue lines represent analytic results from Eq. [12]. In (c) we observe a slight downward shift of numerical data with increasing $T$, which is nearly perfectly captured by a set of thin lines representing $M_3(k)$, Eq. [12].

IV. SUMMARY

We have computed typical ground state as well as finite-$T$ static and dynamic properties of an electron coupled to inelastic HCB degrees of freedom. While the model resembles a widely investigated HM, the limitation of infinite phonon degrees of freedom to HCB’s brings about important differences. A polaron, dressed with HCB excitations remains light, its effective mass remains of the order of the free electron mass even in the limit of strong coupling. Still, the model remains within a class of non-integrable models that exhibit ergodic properties at elevated temperatures.

In the electron spectral function we observe a dispersive QP peak forming a QP band with its maximal spectral weight centered around the center of the BZ. The peak remains separated from the continuum of states only in the central part of the BZ. With increasing momentum the weight of the QP band approaches zero as the peak enters the continuum while the imaginary part of the self-energy starts deviating from zero, which in turn signals the appearance of a finite lifetime. This result is in contrast to the HM where the QP band remains separated from the continuum throughout the whole BZ. With increasing $T$ additional features in the spectral function emerge in a form of an additional spectral weight below the QP band already at temperatures below $\omega_0$. These features appear due to processes where an electron annihilates one or more thermally excited HCB’s.

As mentioned in the introduction, models where electrons are coupled to HCB’s may carry potential relevance to microscopic mechanisms of superconductivity where the attraction between electrons is mediated by HCB degrees of freedom. Such mechanisms have been comprehensively investigated in connection to bipolaron formation mediated by lattice vibrations. One of the shortcomings of these theories are exponentially large effective polaron and bipolaron masses in the strong electron phonon coupling regime. We have also shown that in a system of two electrons with total spin $S = 0$ and in the absence of the on-site Coulomb interaction a bound bipolaron exists at any finite HCB–electron coupling strength $g$. In the case of finite Coulomb interaction there exists a threshold value of $g_c$. Since the effective polaron mass remains small even in the limit of very strong electron-HCB coupling regime, HCB–mediated electron electron interaction leads to formation of light bipolarons.

Acknowledgments

I acknowledge 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. I also acknowledge the hospitality of dr. M. Stout and loving support of my wife J. Bonča Vidmar.

Appendix A:

To gain further physical intuition into the ground–state properties of the HCBM as well as into the numerical approach used in this work, we have diagonalised the model in...
a restricted translationally invariant basis that spans only 14 states, obtained by acting with the off-diagonal part of Hamiltonian in Eq. [1]. i.e.

\begin{equation}
H_{\text{eff}} = H_{\text{0}} + H_g = -t_0 \sum_j (c_j^\dagger c_{j+1} + \text{H.c.}) - g \sum_j \hat{n}_j (b_j^\dagger + b_j). \tag{A1}
\end{equation}

\(N_h\) times on a state with a single electron in a translationally invariant state \(k\) with zero HCB degrees of freedom to obtain a limited basis set

\[ \{ |\phi_{k,i}^{(N_h)}\rangle \} = H_{\text{eff}}^{N_h} c_k^\dagger |0\rangle. \tag{A2} \]

Translationally invariant basis states are represented by HCB position coordinates \(i\) as \([i_1, i_2, \ldots, i_{N_{\text{HCB}}}]\) where \(N_{\text{HCB}}\) denotes the number of HCB's of a particular parent state. Due to the translational invariance, the electron position is kept fixed and does not need to be indexed. For the case of \(N_h = 4\) we obtain 14 states: \(|0\rangle_k = c_k^\dagger |\rangle_{0,k} |\pm 1\rangle_k, |0, \pm 1\rangle_k, |\pm 2\rangle_k, |\pm 3\rangle_k, |0, \pm 2\rangle_k, |1, 2\rangle_k, |1, -2\rangle_k\). We next list just a few non–zero matrix elements:

\[ \begin{align*}
    k \langle 0 | H | 0 \rangle_k &= -2t_0 \cos(k); \\
    k \langle 0 | H | 0 \rangle_k &= k \langle \pm 1 | H | \pm 1 \rangle_k = \omega_0 \ldots \\
    k \langle 0 | H | 0 \rangle_k &= k \langle \pm 1 | H | 0 \rangle_k = -g; \\
    k \langle 0 | H | 0 \rangle_k &= k \langle \pm 1 | H | \pm 2 \rangle_k = -t_0 e^{\mp ik} \\
    k \langle 0 | H | 0 \rangle_k &= k \langle \pm 1 | H | 0 \rangle_k = 2\omega_0.
\end{align*} \tag{A3} \]

In Fig. [A1] we show a comparison between results obtained using a full translationally invariant basis (FB) on a \(L = 16\) sites system with \(N_{\text{HCB}} = 2^L\) states with those obtained using only 14 limited basis states (LBS) as listed above. Note also that results presented in the main body of the paper have been obtained using the full translationally invariant basis. The only exemption from this rule are results of the HM presented in Fig.[7] where LBS states have been used combined with the standard Lanczos technique[23] and described in details in Refs.[30]. Using LBS we expectedly obtain considerably higher energies in comparison to the FB while it is also evident that differences between results decrease with increasing \(\omega_0\) at fixed coupling \(g\). This consistently holds true for all quantities, shown in Fig. [A1]. It is rather surprising that the comparison of \(m_{\text{eff}}/m_0\) for the largest \(\omega_0 = 1\) shows nearly identical results obtained using substantially different numbers of basis states. Some of the main characteristics of ground–state properties may be discerned even from considerably reduced LBS, such as a decrease of \(Z_{\text{qp}}(k)\) with increasing \(k\) and a slow increase of \(m_{\text{eff}}/m_0\) with \(g\). Nevertheless, much larger systems with complete basis states are needed to obtain some of the most interesting properties of the polaron, such as the disappearance of the \(Z_{\text{qp}}(k)\) with increasing \(k\), and crossing of the QP band with the continuum of states that is reflected in the flattening of \(E(k)\) at \(k_0\), given by the solution of \(E(k_0) = E(0) + \omega_0\). In addition, using FB as opposed to LBS is necessary to investigate finite–\(T\) properties of the model where multiple HCB excitations are needed to properly describe thermally activated processes.

![Figure A1: Ground-state properties computed using full basis on a ring with \(L = 16\) with \(N_{\text{HCB}} = 2^L\) parent states (thick lines) taking into account the full translational symmetry in comparison with calculations using only \(N_{\text{HCB}} = 14\) parent states (thin lines): a) and b): \(k\)–dependent energy \(E(k) – E(0)\) and \(Z_{\text{qp}}(k)\), respectively, at fixed coupling \(g\); c) the effective mass \(m_{\text{eff}}/m_0 = 2t_0(\pi E(k)/\partial k^2|_{k=0})^{-1}\) vs. \(g\).]

**Appendix B: Finite-size analysis**

We investigate the extent of finite–\(T\) effects on the spectral function. In Fig. [B1] we present results obtained on two different systems with \(L = 12\) and 16 sites. In both cases \(A(\omega, k)\) were computed on discrete \(k\)–points according to periodic as well as twisted boundary conditions, equivalent to \(k_{n,m} = 2\pi n/L + m\theta\) with \(n \in [-L/2, L/2]\) and \(\theta = 2\pi/(M L)\); \(m \in [0, M\theta - 1]\). For \(L = 12\) and 16 systems we have chosen \(M = 4\) and 3, respectively. As a result, for each system size \(A(\omega, k)\) were computed using \(M \theta = L + 1\) nonequivalent \(k\)-points. Despite substantially different system sizes results are qualitatively identical at any \(T\).

Last, we follow the evolution of \(A(\omega, k)\) with increasing number of allowed bosonic excitations per site starting from the HCBM in Fig. [B2(a)], over a truncated HM (THM) where we allow up to 2 phonon quanta per site, to the HM in Fig. [B2(c)] where we have expanded the Hilbert space up to maximal 22 phonon excitations per site. The emphasis of this analysis is on the evolution of the QP band. While in the HCBM the QP band enters the continuum at finite \(k_0\), already in the HMR it flattens out and shows a tendency to disperse below the continuum almost towards the edge of the BZ, as seen in Fig. [B2(b)]. Note that in the case of the HM \(g = 2\) represents the strong coupling limit, \(\lambda = 2\), where we observe a nearly flat QP band with a substantially reduced QP weight, followed by a series of nearly flat bands, separated by \(\omega_0\) as predicted by the strong coupling theory.
Figure B1: $A(\omega, k)$ for $\omega_0 = 1$, $g = 2$ for two different system sizes $L = 12$ shown in (a) through (c) and $L = 16$ shown in (d), through (f) and three different values of $T/\omega_0$ as specified in figures. In all cases $A(\omega, k)$ was computed in 25 equally spaced non-equivalent $k$-points in the interval $k \in [0, \pi]$ with increments of $\Delta k = \pi/24$. Note, in all figures from (a) to (f) the same color coding was used to enable direct comparison between different cases.

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Figure B2: \(A(\omega, k)\) for \(\omega_0 = 1, g = 2\) for a) the HCBM, b) the truncated HM (THM) with up to 2 phonon quanta per site, and c) the HM with up to 22 phonon quanta per site.