

Numerical investigation of polaron effects in strongly correlated electron-phonon systems

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Abstract

A parallelized exact diagonalization method is adopted to be used in combination with cluster perturbation theory, allowing to obtain accurate results for the single-particle spectral properties of strongly correlated electron-phonon models. On modern supercomputers and compute clusters, the code developed here represents a versatile tool to address open problems in condensed matter physics, as illustrated for the Holstein polaron problem.

Introduction The interaction between electrons and lattice fluctuations (phonons) is known to play an important role in many materials, giving rise to fascinating phenomena such as, e. g., superconductivity. The complexity even of simplified theoretical models motivates the application of unbiased numerical methods to advance our understanding of the underlying physics.

The ongoing development of high-performance computers allows to enter the most interesting and realistic parameter regions by developing parallel codes which can be run on modern supercomputers. In this project, a parallel exact diagonalization (ED) code is modified to be used in combination with cluster perturbation theory (CPT) [1], an approach which has received a lot of attention recently due to its reliability and broad applicability. Most importantly, the resulting method can be used to study problems of significantly higher difficulty by exploiting parallel systems, and achieves better accuracy than previous implementations. The calculated single-particle spectra may be compared to photoemission experiments.

Method The most time-consuming part of the CPT calculations is the diagonalization of a many-body problem defined on decoupled clusters of typically $N = 4 - 16$ lattice sites, at the heart of which lies an iterative algorithm (e. g., Lanczos) based on sparse matrix-vector multiplication (MVM) with matrix dimensions of up to 10^{10} —increasing exponentially with N . While short-range

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correlations are thus described exactly within each cluster, the electronic hopping between neighbouring clusters can be taken into account analytically in a strong-coupling approximation [1].

While single-processor machines are usually sufficient in applications of CPT to Hubbard models—with electronic degrees of freedom only—the fully quantum-mechanical treatment of the electron-lattice interaction gives rise to significantly enhanced memory requirements (order $10^3 - 10^6$). The number of possible phonon configurations is à priori infinite, even for $N < \infty$, but can be restricted to a finite, sufficiently large number in actual calculations [2]. Progress has been made in this project by incorporating an analytical separation of the symmetric zero-momentum phonon mode, thereby decreasing the matrix dimension for the same parameters and accuracy [3]. Furthermore, we obtain a noticeably higher accuracy and reliability by employing a kernel polynomial method based on an expansion of the spectrum in Chebyshev polynomials instead of the widely used spectral decoding method, which usually faces problems due to numerical instability and a nonuniform energy resolution [2].

Resources used The parallelization of the ED code is done at the sparse MVM step using MPI for portability reasons. To reduce the required memory—being the limiting factor in most computations—the nonzero entries of the sparse matrix are not stored but recomputed in each MVM step. In that case the iterative solver (Lanczos) used requires storage of three vectors of the matrix dimension only. We can further minimize the space for temporary communication buffers by mapping an inherent parallel structure of the physical model² onto our parallelization approach, i. e. we parallelize the code by distributing the electronic basis states through the MPI processes. This approach minimizes total memory consumption but introduces load imbalances and requires an high speed network such as *Myrinet* or *Infiniband*.

For the project under consideration, we so far focused on small system sizes ($N \leq 10$) in order to carefully test the correctness of the results by comparing them to exact (ED) methods. The maximum matrix dimension was about 10^9 requiring roughly 30 GBytes of main memory. These computations were done on the *AMD Opteron cluster* with *Myrinet2000* interconnect at HLRS using a maximum of 16 nodes (32 CPUs).

Results To illustrate the capabilities of the code developed, we present results for the inverse photoemission spectrum $A(k, \omega)$.³ This problem has been studied using CPT before [4], but these calculations were restricted to phonon frequencies larger than the electronic hopping integral, i. e., $\omega_0 > t$. Please note that the largest matrix dimension in [4] was 1.9×10^5 .

In contrast, most polaronic materials are characterized by $\omega_0 \ll t$, and here we consider a value $\omega_0/t = 0.4$, also at intermediate coupling, as well as a slightly larger cluster with $N = 10$, since finite-size effects become more

²The total Hilbert space is a direct product of electronic and phononic basis states.

³Here, $A(k, \omega)$ gives the probability for an electron added to the system to end up in a state with momentum k and energy ω (see [4] for details).

important for small ω_0 . Converged results in this case require a significantly larger matrix dimension 5.3×10^7 . Employing the abovementioned separation of the symmetric phonon mode this can be reduced by more than a factor of two without any loss of accuracy. Moreover, the benefit of this modification increases noticeably with increasing electron density and electron-phonon interaction. The present calculation can easily be done in less than 40 hours on one dual-processor AMD Opteron node using about 1 GByte of memory, and the results shown in Fig.1 reveal a narrow, low-energy polaron band which flattens at large momenta k , and an incoherent part which closely follows the free-electron dispersion [4].

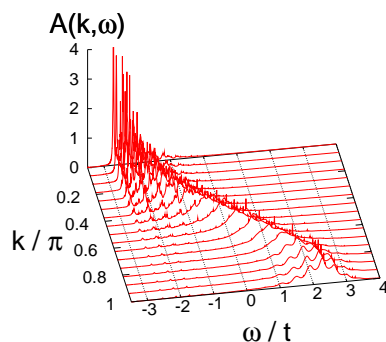


Figure 1: Single-particle spectral function of the one-dimensional Holstein polaron in the adiabatic intermediate electron-phonon coupling regime. Here $N = 10$, $\omega_0/t = 0.4$ and $\lambda = 1$ (see also [4]).

Outlook The method developed here can be applied to any model with local interactions only, with or without lattice degrees of freedom. Consequently, it allows future studies of a variety of interesting problems of significantly higher complexity than the example presented here. Among others, we will investigate the effect of carrier density on the spectra of the Holstein and the Holstein-Hubbard model. Finally, this project has stimulated current work on an extension of CPT to calculate the phonon Green function.

Acknowledgements The work has been performed under the Project HPC-EUROPA (RII3-CT-2003-506079), with the support of the European Community - Research Infrastructure Action under the FP6 “Structuring the European Research Area” Programme. We would like to acknowledge support from the HLR Stuttgart.

References

- [1] Sénéchal et al., Phys. Rev. Lett. **84**, 522 (2000), Sénéchal et al., Phys. Rev. B **66**, 075129 (2002).
- [2] Bäuml et al., Phys. Rev. B **58**, 3663 (1998).
- [3] Sykora et al., Phys. Rev. B **71**, 045112 (2005).
- [4] Hohenadler et al., Phys. Rev. B **68**, 184304 (2003).