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Low-temperature Lanczos method for strongly correlated systems

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We present a modified finite-temperature Lanczos method for the evaluation of dynamical and static quantities of strongly correlated electron systems that complements the finite-temperature method introduced by Jaklič and Prelovšek for low temperatures. Together they allow accurate calculations at any temperature with moderate effort. As an example we calculate the static spin-correlation function and the regular part of the optical conductivity $\sigma^{reg}(\omega)$ of the one-dimensional Hubbard model at half filling and show in detail the connection between the ground-state and finite-temperature method. By using cluster perturbation theory, the finite-temperature spectral function is extended to the infinite system, clearly exhibiting the effects of spin-charge separation.

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The finite-temperature Lanczos method, introduced by Jaklič and Prelovšek,[1] has in recent years allowed the precise calculation of thermodynamic quantities of strongly correlated systems. It has been applied to the t-J model for the cuprates[2–8] and vanadates,[9,10] orbital t-J model,[11] Kondo lattice model,[12] Heisenberg model,[13] and static properties of the Hubbard model.[14,15] In principle, this method can be applied at all temperatures, but at low temperatures, the required number of random samples is very large. FTLM is restricted to small systems, and particularly at low temperatures, finite-size effects become important. They can be overcome, at least for properties derived from the single-particle Green's function, by using cluster perturbation theory (CPT),[16,17] which provides infinite system results with remarkable, accuracy.[18] However, CPT requires finite cluster Greens functions $G_{ab}(\omega)$ for all sites a,b, increasing the number of required Lanczos runs and matrix elements by a factor equal to the number of lattice sites. It therefore requires a sufficiently fast low-temperature method.

In this paper, we present a modified finite-temperature Lanczos method that allows us to calculate properties for large Hilbert spaces at low temperatures that are not accessible by the existing method. We show that a combination of our low-temperature Lanczos method (LTLM) with the FTLM allows an accurate calculation of thermodynamic properties at any temperature with moderate effort.

Let us first present the existing FTLM. For the case of a static expectation value of an operator $\mathcal{O}$

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \sum_{n}^{N} \langle n|\mathcal{O}e^{-\beta H}|n\rangle, \quad Z = \sum_{n}^{N} \langle n|e^{-\beta H}|n\rangle, \tag{1}$$

with $\beta = 1/T$ ($k_B = \hbar = 1$) and a sum over a complete orthonormal basis set $|n\rangle$, the FTLM approximation is

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \sum_{s} \frac{N_s}{R} \sum_{r}^{R} \sum_{m}^{M} e^{-\beta \varepsilon_m^{(r)}} \langle r|\Psi_m^{(r)}\rangle \langle \Psi_m^{(r)}|\mathcal{O}|r\rangle,$$

$$Z = \sum_{s} \frac{N_s}{R} \sum_{r}^{R} \sum_{m}^{M} |\langle r|\Psi_m^{(r)}\rangle|^2 e^{-\beta \varepsilon_m^{(r)}}, \tag{2}$$

with a sum over symmetry sectors s of dimension N_s and R random vectors $|r\rangle$ in each sector.[19] M is the number of Lanczos steps. For each random vector $|r\rangle$, a Lanczos procedure is performed, yielding M eigenenergies $\varepsilon_m^{(r)}$ and corresponding eigenvectors $|\Psi_m^{(r)}\rangle$. The trace in Eq. (1) requires N_s states, while very accurate results can be obtained via Eq. (2) even for a drastically reduced number of Lanczos steps $M \ll N_s$ and a partial random sampling of the Hilbert subspaces $R \ll N_s$.

For dynamical correlation functions $C(t) = \langle A(t)B \rangle$, FTLM calculates

$$C(t) = \frac{1}{Z} \sum_{s} \frac{N_s}{R} \sum_{r}^{R} \sum_{i,j}^{M} e^{-\beta \varepsilon_i^{(r)}} e^{-i(\tilde{\varepsilon}_j^{(r)} - \varepsilon_i^{(r)})t} \langle r|\Psi_i^{(r)}\rangle \times \langle \Psi_i^{(r)}|A|\tilde{\Psi}_j^{(r)}\rangle \langle \tilde{\Psi}_j^{(r)}|B|r\rangle. \tag{3}$$

Here, an initial vector

$$|\tilde{\Phi}_0^{(r)}\rangle = B|r\rangle / \sqrt{\langle r|B^\dagger B|r\rangle} \tag{4}$$

is used to generate additional eigenenergies $\tilde{\varepsilon}_j^{(r)}$ and eigenvectors $|\tilde{\Psi}_j^{(r)}\rangle$ from that part of the Hilbert space onto which the operator B projects. Hence, the term $\langle \tilde{\Psi}_j^{(r)}|B|r\rangle$ in Eq. (3) becomes sufficiently large.

Let us now consider the behavior of Eqs. (2) and (3) in the limit $T \to 0$. In this case, only the ground state $|\Psi_0\rangle$ contributes and we get

$$\langle \mathcal{O} \rangle = \sum_{r}^{R} \langle \Psi_0|\mathcal{O}|r\rangle \langle r|\Psi_0\rangle / \sum_{r}^{R} \langle \Psi_0|r\rangle \langle r|\Psi_0\rangle \tag{5}$$

and similarly for Eq. (3). Thus, the ground-state result will suffer from severe statistical fluctuations, although the exact (Lanczos) eigenvector $|\Psi_0\rangle$ is reached with every $|r\rangle$ and one random vector should be sufficient. Yet FTLM gets worse with decreasing temperature T.

The modifications we present in this paper are designed to overcome this limitation. Let us put forward a method for a static expectation value (1). We use a symmetric form

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \sum_{n}^{N} \langle n | e^{-(1/2)\beta H} \mathcal{O} e^{-(1/2)\beta H} | n \rangle. \tag{6}$$

As before, we approximate the trace by random sampling, but now we insert the approximate eigenbasis obtained by the Lanczos procedure twice, initially obtaining

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \sum_{s} \frac{N_s}{R} \sum_{r}^{R} \sum_{i,l}^{M} e^{-(1/2)\beta(\varepsilon_i^{(r)} + \varepsilon_l^{(r)})} \langle r | \Psi_l^{(r)} \rangle \times \langle \Psi_l^{(r)} | \mathcal{O} | \Psi_i^{(r)} \rangle \langle \Psi_i^{(r)} | r \rangle. \tag{7}$$

The partition function Z is calculated in the same way as in standard FTLM. The behavior in the limit $T \to 0$ is now different. If only the ground state $|\Psi_0\rangle$ contributes, Eq. (7) becomes

$$\langle \mathcal{O} \rangle = \sum_{r}^{R} \langle \Psi_0 | r \rangle \langle r | \Psi_0 \rangle \langle \Psi_0 | \mathcal{O} | \Psi_0 \rangle / \sum_{r}^{R} \langle \Psi_0 | r \rangle \langle r | \Psi_0 \rangle = \langle \Psi_0 | \mathcal{O} | \Psi_0 \rangle. \tag{8}$$

In agreement with ground-state Lanczos, one random vector suffices for the ground-state expectation value.

If we compute the numerators in Eq. (7) and Z separately, both suffer from pronounced statistical fluctuations, which however cancel exactly at $T=0$ as shown in Eq. (8). For finite T the fluctuations in numerator and denominator do not cancel exactly, but they are still strongly correlated. Separate error analysis for both terms would overestimate the statistical noise. These correlations are taken into account by employing a jackknife technique.[20]

For dynamical correlation functions, a straightforward variant of Eq. (3) suitable for low temperatures is

$$C(t) = \frac{1}{Z} \sum_{s} \frac{N_s}{R} \sum_{r}^{R} \sum_{ijl}^{M} e^{-(1/2)\beta(\varepsilon_i^{(r)} + \varepsilon_l^{(r)})} \times e^{-i[\tilde{\varepsilon}_j^{(r)} - (1/2)(\varepsilon_i^{(r)} + \varepsilon_l^{(r)})]t} \langle r | \Psi_l^r \rangle \langle \Psi_l^{(r)} | A | \tilde{\Psi}_j^{(r)} \rangle \times \langle \tilde{\Psi}_j^{(r)} | B | \Psi_i^{(r)} \rangle \langle \Psi_i^{(r)} | r \rangle. \tag{9}$$

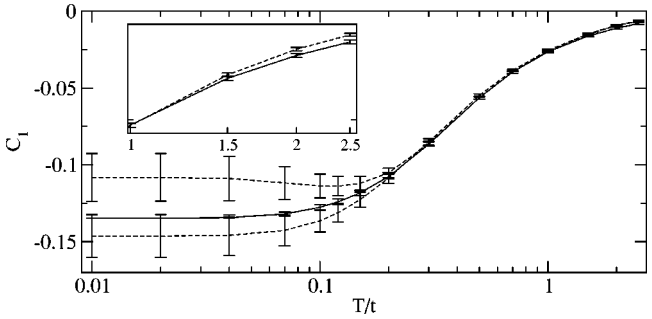

FIG. 1. Spin-correlation function $C_1 = \langle S_i^z S_{i+1}^z \rangle$ for the one-dimensional Hubbard model on a 12 site chain with periodic boundary conditions at $U=8t$ and $n=1$. Solid: LTLM with $\beta_c=1$, $\varepsilon_c=0.01$, $M=100$, and $R=25$. Dashed: Two independent runs of FTLM with $M=100$ and $R=25$. Inset: Deviation of C_1 in the high-temperature region beyond β_c. Here, $R=50$ in both cases.

In order to span the relevant subspace of the Hilbert space, we now choose initial vectors $|\tilde{\Phi}_0^{(r,i)}\rangle \propto B|\Psi_i^{(r)}\rangle$ for the second Lanczos run. With M such second Lanczos runs, the numerical effort would be much higher than for FTLM. For low temperatures, it can be reduced, since only the low-lying states contribute to the expectation values. We consider only states below a cutoff energy E_c, defined by

$$e^{-\beta_c(E_c - E_0)} < \varepsilon_c, \tag{10}$$

where ε_c defines the accuracy of the approximation and β_c is the minimal inverse temperature considered, and the calculation will be accurate for all $\beta > \beta_c$. We thus proceed as follows: For each random start vector $|r\rangle$, we perform an initial Lanczos run with M iterations. For each of the M_c states $|\psi_i^{(r)}\rangle$ with energies below E_c, we then calculate an initial vector $|\tilde{\Phi}_0^{(r,i)}\rangle \propto B|\Psi_i^{(r)}\rangle$ and perform a second run with M Lanczos iterations, obtaining an approximate eigenbasis $|\tilde{\Psi}_j^{(r,i)}\rangle$. Using these basis sets, the final form of LTLM is the same as Eqs. 7 and 9, with $\Sigma_{i,l}^{M}$ and $\tilde{\Psi}_j^{(r)}$ replaced by $\Sigma_{i,l}^{M_c}$ and $\tilde{\Psi}_j^{(r,i)}$, respectively.

Memory requirements of our method are the same as for standard FTLM, but the CPU time requirements differ significantly. CPU time is mainly determined by the number of matrix elements that have to be calculated. In the case of static expectation values, these are M for FTLM and M_c^2 for LTLM for each random vector. Therefore, both methods reach equivalent CPU time requirements per random vector when $M_c \approx \sqrt{M}$.

For dynamical correlation functions, the number of matrix elements to be calculated in the second Lanczos run is M^2 for FTLM and M_c^2 for LTLM. For LTLM, we have to perform M_c second Lanczos runs, but only one for FTLM. Thus, we have similar CPU time requirements per random vector for both methods when $M_c \approx M^{(2/3)}$. In the limit $T \to 0$, we have $M_c = 1$, and for $R=1$, LTLM is comparable to the ground-state Lanczos technique.

For both methods, CPU time is proportional to R, the number of random vectors. But, by design, far fewer random vectors are needed for the LTLM than for the FTLM at low temperatures for a given accuracy.

All considerations so far have been done without regarding reorthogonalization of Lanczos vectors. This procedure

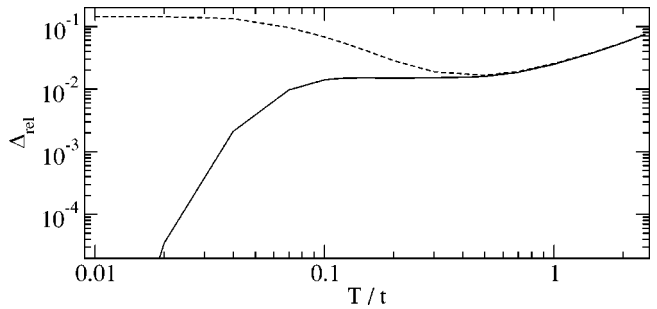

FIG. 2. Relative statistical errors $\Delta C_1 / C_1$ of LTLM (solid) and FTLM (dashed) with $R=25$ in both cases. Other parameters as in Fig. 1. The error of LTLM at $T=0.01t$ is $\Delta_{rel} = 10^{-8}$.

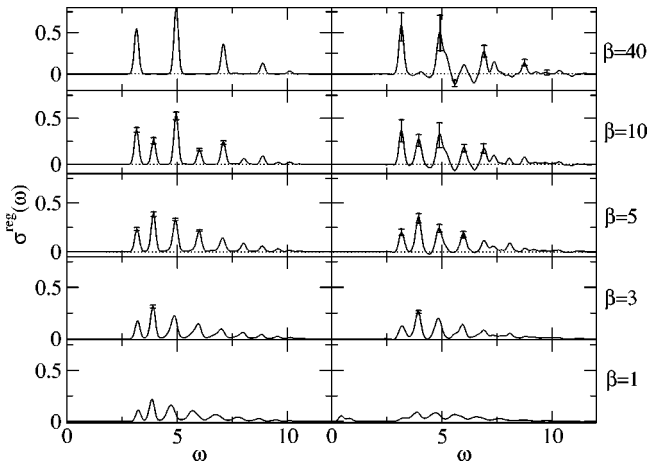

FIG. 3. Regular part of the optical conductivity of the one-dimensional Hubbard model on a 12 site chain with periodic boundary conditions at $U=6t$ and $n=1$. Left panel: LTLM calculations with $\beta_c=3$, $\varepsilon_c=0.01$, and $R=40$. Right panel: FTLM calculations with $R=50$. Number of Lanczos steps $M=100$ and additional broadening of $\sigma=0.1$. Dots mark the zero line. Only selected error bars are shown. For curves without error bars, the errors are smaller than the linewidth.

becomes important for $M \gtrsim 150$, where numerical roundoff errors become significant, and significantly increases CPU requirements.

Let us now demonstrate the method for the calculation of static and dynamical properties of the one-dimensional Hubbard model, with Hamiltonian

$$H=-t\sum_{i,\sigma}\,(c^{\dagger}_{i\sigma}c_{i+1,\sigma}+\text{H.c.})+U\sum_{i}\,n_{i\uparrow}n_{i\downarrow}\,. \qquad (11)$$

We specify energies in units of t. As an example, we calculate the static spin-correlation function $C_1=\langle S^z_i S^z_{i+1}\rangle$ on a 12 site chain with periodic boundary conditions at half filling ($n=1$). The number of basis states is $N=2\,704\,156$. Symmetry sectors are specified by momentum $\mathbf{k}$ and total spin S_z. The largest sector $S_z=\pm 1$ has 52 272 basis states. The sector $S_z=0$ is further reduced due to spin-up/(-down) symmetry. In Figs. 1 and 2, the convergence and statistical errors of LTLM and FTLM are compared at equal computational effort, with $R=25$ random samples per symmetry sector, each corresponding to sampling of $R/N_s \approx 0.05\%$ of the largest Hilbert subspace. At low temperatures, our method provides results that are orders of magnitude more precise than from standard FTLM, and which connect smoothly to the ground-state properties. We checked that for larger R, there is no systematic drift for either method, and the FTLM results converge towards those of LTLM. At intermediate temperatures, the statistical errors of LTLM increase and become similar to those of FTLM. Finally, considerably beyond the chosen cutoff temperature $1/\beta_c$, LTLM is no longer applicable and begins to show a systematic deviation.

Both FTLM and LTLM provide results for a range of temperatures from a single calculation. For FTLM, this range is limited towards low temperatures by statistical errors. For LTLM, it is limited by the chosen cutoff temperature $1/\beta_c$.

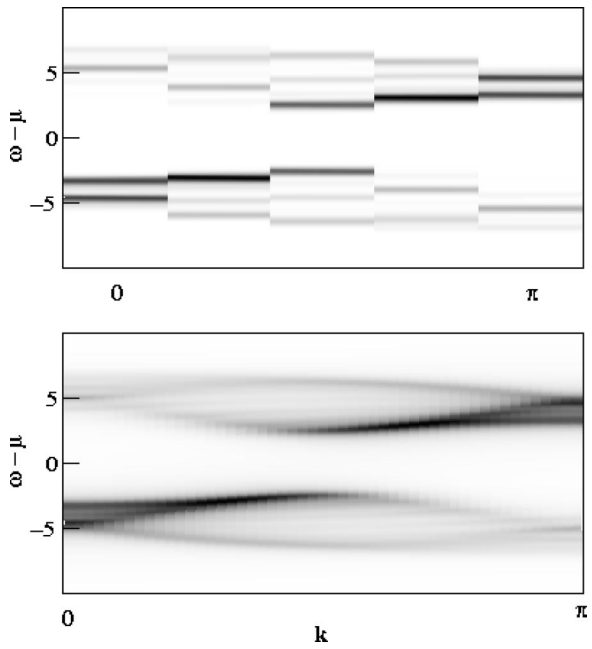

FIG. 4. Spectral function $A(\mathbf{k},\omega)$ obtained by LTLM for the one-dimensional Hubbard model at $U=8t$, $n=1$, and $\beta=10$. Parameters: $R=30$, $\beta_c=3$, and $\varepsilon_c=0.01$. Upper panel: 8 site chain with periodic boundary conditions. Lower panel: CPT result based on 8 site clusters.

Therefore, a combination of both methods provides precise results for all temperatures with moderate effort.

As an example of dynamical correlation functions we calculate the regular part of the optical conductivity, given by the current-current correlation function

$$\sigma^{reg}=\frac{1-e^{-\beta\omega}}{\omega}Re\int_0^{\infty}dt\,e^{i\omega t}\langle j(t)j\rangle, \qquad (12)$$

with the current operator $j=it\Sigma_{i,\sigma}(c^{\dagger}_{i\sigma}c_{i+1,\sigma}-\text{H.c.})$. In Fig. 3, we show results with approximately the same CPU time for both methods. Slightly above the ground-state, at $\beta=40$, LTLM approaches the exact ground-state result.[21,22] For intermediate temperatures $\beta=10$, 5, and 3, slight statistical fluctuations occur. With comparison to FTLM, we see that $\beta=1<\beta_c$ is indeed beyond the validity of this calculation. We also checked the accuracy of the results by using $M=200$ Lanczos steps instead of $M=100$, yielding the same LTLM spectra within statistical errors.

In contrast, FTLM suffers from strong statistical fluctuations at small temperatures. Error bars are very large and regions occur where $\sigma^{reg}(\omega)$ becomes negative, a clear indicator that we did not use enough random vectors for FTLM. As expected from our consideration of static expectation values, error bars of FTLM get smaller for higher temperatures. As for LTLM, we did calculations with $M=200$, yielding the, same curves within error bars but leading to a better convergence at the high-frequency side of the spectrum.

As mentioned in the beginning, at low temperature, finite-size effects become important. At least for properties derivable from the single-particle Green's function, these effects

can be overcome by using CPT.[16,17] In Fig. 4, we show the finite-temperature spectral function $A(\mathbf{k},\omega)$ obtained on a finite-size lattice with periodic boundary conditions, and the infinite lattice result obtained by CPT, which makes use of all the Green functions on the finite lattice as calculated by LTLM. In the latter, a smooth structure consisting of several branches can clearly be seen with spin-charge separation at $\mathbf{k}=0$ visible in the lower part of the spectrum.[16,23] On the finite-size cluster, however, this structure is not evident as it exhibits more discrete excitations. Further work on finite-temperature CPT is in progress.[18]

In conclusion, the method presented in this paper gives an accurate connection of the exact ground-state Lanczos method and the established FTLM. Using LTLM at low and FTLM at higher temperatures makes it possible to calculate static and dynamical properties of strongly correlated systems from $T=0$ up to $T=\infty$ with very good accuracy and rather small numerical effort.

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