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Lanczos method for the calculation of finite-temperature quantities in correlated systems

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A method, using the Lanczos diagonalization technique and random sampling, is introduced to evaluate finite-temperature static and dynamical quantities in small many-body quantum systems. As an example the method is applied to the calculation of the optical conductivity of a single charge-carrier hole in the system of strongly correlated electrons, as decribed by the t-J model.

In recent years, numerical methods have been extensively developed and applied to quantum many-body problems, in particular in connection with the challenging open theoretical questions of strongly correlated systems and electronic models of materials exhibiting superconductivity at high temperatures.[1]

Most frequently used numerical methods for these problems are the quantum Monte Carlo (QMC) method[2,3] and the exact diagonalization of small systems employing the Lanczos technique.[4] The QMC method enables the evaluation of static and some dynamical quantities at finite temperatures. For interacting fermions its application is however mainly restricted to a certain class of models which allow the decoupling of the interaction term, the prominent example being the Hubbard model.[2,3] QMC method is also plagued by the minus sign problem in the most challenging regimes of correlated systems. In contrast, the exact diagonalization of small correlated systems does not have any restrictions on the model and does not suffer numerical difficulties due to the fermionic sign. The deficiency of the method is in the relative smallness of system sizes, in spite of quite substantially increased system sizes in last five years, e.g., for the prototype two-dimensional (2D) t-J model[5–7] investigated later. So far the method has been essentially restricted to the evaluation of the $T = 0$ static and dynamical quantities,[1] i.e., properties of the ground state.

In this paper we introduce a method for the evaluation of finite-temperature properties, based on the Lanczos diagonalization technique for small systems. So far very few numerical calculations of quantities in small correlated systems have been performed at $T > 0$,[8] using the full or partial diagonalization within the basis set. Full diagonalization method allows only studies of rather small systems, since in general all eigenfunctions are needed simultaneously. In our method, presented below, we avoid the calculation of all eigenfunctions of the system. Instead, we introduce the procedure where the sampling over all states is reduced to a random partial sampling, while only approximate ground state and excited state wave functions, generated by the Lanczos technique, are used for the evalution of matrix elements. The size limitations of the method are effectively comparable to those encountered in the Lanczos-type diagonalization technique applied to the ground state calculations.

Let us present the method for the case of a statical expectation value of an operator A at general temperature T,

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

where $\beta = 1/T$ (we use $k_B = \hbar = 1$) and the sum runs over the chosen complete basis set of orthonormal wave functions $|n\rangle, n = 1, N$ spanning the Hamiltonian H. If we could perform the full diagonalization of the problem and find all eigenstates $|\Psi_l\rangle$ and corresponding energies E_l, we would express the result in a usual way,

$$\langle A\rangle = \sum_{l}^{N} e^{-\beta E_l}\langle l|A|l\rangle \Big/ \sum_{l}^{N} e^{-\beta E_l}. \tag{2}$$

We choose an alternative approach. With each basis function $|n\rangle$ we start a Lanczos procedure[4] $|\phi_0^n\rangle = |n\rangle$, generating an orthonormal set of functions $|\phi_m^n\rangle, m = 0, M$,

$$\begin{aligned} H|\phi_0^n\rangle &= a_{n0}|\phi_0^n\rangle + b_{n1}|\phi_1^n\rangle, \\ H|\phi_m^n\rangle &= b_{nm}|\phi_{m-1}^n\rangle + a_{nm}|\phi_m^n\rangle + b_{nm+1}|\phi_{m+1}^n\rangle, \\ & \qquad\qquad m = 1, M-1 \\ H|\phi_M^n\rangle &= b_{nM}|\phi_{M-1}^n\rangle + a_{nM}|\phi_M^n\rangle. \end{aligned} \tag{3}$$

For the chosen maximum number of Lanczos steps M we then diagonalize the tridiagonal matrix of coefficients a_{nm}, b_{nm} to find energies $\epsilon_{nm}, m = 0, M$ and the corresponding eigenfunctions $|\psi_m^n\rangle$. Within the restricted basis of the latter functions one can write the approximation for Eq. (2) as

$$\begin{aligned} \langle A\rangle &= Z^{-1}\sum_{n}^{N_0}\sum_{m}^{M}\langle n|\psi_m^n\rangle e^{-\beta\epsilon_{nm}}\langle\psi_m^n|A|n\rangle, \\ Z &= \sum_{n}^{N_0}\sum_{m}^{M}|\langle n|\psi_m^n\rangle|^2 e^{-\beta\epsilon_{nm}}. \end{aligned} \tag{4}$$

It is evident that the average evaluated via Eq. (4) is equivalent to Eq. (2) for the sampling over the full basis

set $N_0 = N$ and $M = N - 1$, i.e., for the Lanczos iteration, Eq. (3), pushed to exhaust the whole basis space.

Our basic claim is that very accurate results can be obtained via Eq. (4) even for a severly reduced number of Lanczos steps $M \ll N$ and for a partial random sampling of basis states $N_0 \ll N$, instead of the full sampling. Let us first investigate the method for the full sampling $N_0 = N$. The Lanczos procedure Eq. (3) represents an iterative action of the operator H on the initial function $|n\rangle$. Performing the (high temperature) expansion in β of the numerator and of the denominator of Eq. (4), it is easy to prove that both power series are correct up to the order M. On the other hand, $\langle A\rangle$ evaluated via Eq. (4) can yield very accurate results also for $T = 0$. It is a standard experience that the Lanczos procedure converges from an arbitrary initial function $|n\rangle$ (not orthogonal to the ground state) to the ground state energy E_0 and the corresponding wave function $|\Psi_0\rangle$ quite rapidly, typically in $M = M_0 \sim 50 \ll N$ steps. Hence for $M > M_0$ Eq. (4) yields a correct result at $T = 0$, i.e.,

$$\langle A\rangle = \sum_n^N \langle n|\Psi_0\rangle\langle\Psi_0|A|n\rangle \Big/ \sum_n^N |\langle n|\Psi_0\rangle|^2 = \langle\Psi_0|A|\Psi_0\rangle. \tag{5}$$

Hence, at full sampling our Lanczos-based method represents an optimum interpolation scheme between the high temperature $T \to \infty$ and the ground state $T = 0$ result. From Eq. (5) it follows that $M \sim M_0$ could be sufficient for the whole T regime.

We should also note the similarity of our method for the calculation of terms $\langle n|\exp(-\beta H)|n\rangle$ at chosen $|n\rangle$ to the usual Lanczos method for Green's (response) functions,[9] here extended to imaginary times $i\beta$. In analogy with the latter it would not be necessary[9,1] to involve wave functions in the calculation of, e.g., Z. On the other hand, nontrivial operators A in the nominator require the evaluation of off-diagonal terms, so the use of wave functions cannot be avoided.

The second important ingredient is the reduction of the sampling to the partial random one with $N_0 \ll N$. This step cannot be justified rigorously, but seems plausible in analogy with statistical Monte Carlo methods. The most severe test is expected to be the result at $T = 0$. For $M > M_0$ one can again use Eq. (5) where the sampling now runs only over random N_0 functions. In contrast to $T > 0$ only states $|n\rangle$ overlapping with the ground state $|\Psi_0\rangle$ contribute, hence statistical requirements are more severe. The exact result $\langle\Psi_0|A|\Psi_0\rangle$ can be approached only with $N_0 \sim N$, nevertheless we expect good convergence also for $N_0 \ll N$.

Even more interesting is the application of the method to the calculation of dynamical quantities. We choose as an example the optical conductivity, expressed within the linear response theory as

$$\sigma(\omega) = \frac{1 - e^{-\beta\omega}}{\omega} \int_{-\infty}^{\infty} dt\ e^{i\omega t} C(t),$$

$$C(t) = \langle j(t)j\rangle = Z^{-1} \sum_n \langle n|e^{(-\beta+it)H} j e^{-iHt} j|n\rangle. \tag{6}$$

In order to get the result at arbitrary β a double sum over all eigenstates $|\Psi_l\rangle, |\Psi_{l'}\rangle$ is required, i.e.,

$$C(t) = Z^{-1} \sum_{l,l'}^{N} e^{-\beta E_l} e^{i(E_l - E_{l'})t} |\langle\Psi_l|j|\Psi_{l'}\rangle|^2. \tag{7}$$

Instead, we use the approach described above for $\langle A\rangle$ generalized to dynamical $C(t)$,

$$C(t) = Z^{-1} \sum_n^{N_0} \sum_{m,k}^{M} \langle n|\psi_m^n\rangle e^{-\beta\epsilon_{nm}} e^{i(\epsilon_{nm} - \tilde{\epsilon}_{nk})t} \langle\psi_m^n|j|\tilde{\psi}_k^n\rangle\langle\tilde{\psi}_k^n|j|n\rangle. \tag{8}$$

Here, $|\tilde{\psi}_k^n\rangle$ and $\tilde{\epsilon}_{nk}$ are generated by the Lanczos procedure analogous to Eq. (3) via the orthonormal basis set $|\tilde{\phi}_k^n\rangle$, but with the initial condition

$$|\tilde{\phi}_0^n\rangle = j|n\rangle / \sqrt{\langle n|j^2|n\rangle}. \tag{9}$$

While for $N_0 = M = N$ expression (8) is equivalent to the exact one Eq. (7), arguments for using $N_0 \ll N$ and $M \ll N$ are analogous to those described above for the static case. For the full sampling $N_0 = N$ Eq. (8) yields correct series in $-\beta + it$ and it, respectively, up to the Mth order. Accordingly, $\sigma(\omega)$ has correct frequency moments $\langle\omega^p\rangle$, $p = 0, M$, for $\beta \to 0, T \to \infty$. At finite β the corresponding double series for the moments of $\sigma(\omega)$ are correct up to $\beta^{p+1}\langle\omega^{M-p}\rangle$, $p = 0, M$. Assuming that $M > M_0$ the method yields meaningful result also for $T = 0$, where Eq. (8) reduces in analogy to Eq. (5) to

$$C(t) = \sum_n^{N_0} \sum_k^{M} \langle\Psi_0|j|\tilde{\psi}_k^n\rangle\langle\tilde{\psi}_k^n|j|n\rangle\langle n|\Psi_0\rangle e^{i(E_0 - \tilde{\epsilon}_{nk})t}. \tag{10}$$

If M is large enough, the lowest states $|\tilde{\psi}_k^n\rangle$ and corresponding $\tilde{\epsilon}_{nk}$ become approximately independent of n. Hence the sum over n reduces to the unity operator and the result becomes again correct. It should be however stressed that generally more steps are needed to stabilize excited states, so that M should be considerably larger than M_0 to reproduce details of spectra at higher frequencies. Still frequency moments are expected to be reproduced up to the Mth order and in this sense the method yields after M steps the result similar to the one obtained by the Lanczos technique for dynamical response in the ground state.[9,10,7,1]

Before turning to the examples let us briefly mention the computational requirements of the method. Due to symmetries of the Hamiltonian the evaluation of $C(t)$ and $\sigma(\omega)$ can be separated into contributions of different symmetry sectors, leading to an essential reduction in storage requirements (as usually employed in the ground state calculations). Within each sector one chooses $|n\rangle$ which then serve as initial condition for two parallel Lanc-

zos procedures with M steps. In each of N_0 sampling steps we have to calculate M eigenfunctions $|\psi_m^n\rangle, |\tilde{\psi}_k^n\rangle$ and $M \times M$ matrix elements $\langle\psi_m^n|j|\tilde{\psi}_k^n\rangle$. The method requires $2N_0M$ Lanczos steps. Since in general a reorthogonalization of vectors is needed (see below), CPU time is determined by $\tau \propto N_0NM^2$. A similar estimate is obtained for the calculation of matrix elements. In contrast, a direct evaluation via the full diagonalization, Eq. (7), would need $\tau \propto N^3$.

Memory requirements are essentially determined by the number of basis states in the largest symmetry sector $N_1 \ll N$. Since CPU time limitations (in comparison with the ground state calculations) are quite severe for the method, it is important to use a vectorized Lanczos procedure, which on the other hand increases the memory requirements due to the precalculated Hamiltonian matrix.

Let us illustrate the method on the example of the optical conductivity $\sigma(\omega)$ in the t-J model, being the prototype model for strongly correlated electrons,[11]

$$H = -t\sum_{\langle ij\rangle s}(c_{js}^\dagger c_{is} + \text{H.c.}) + J\sum_{\langle ij\rangle}(\vec{S}_i \cdot \vec{S}_j - \tfrac{1}{4}n_i n_j), \tag{11}$$

where the double occupation of sites is forbidden. In particular, we investigate the dynamical response of a single charge-carrier hole $N_h = 1$, introduced into the reference undoped antiferromagnetic (AFM) spin state. This problem has been already investigated quite intensively using analytical techniques[12,13] as well as the exact diagonalization approach to small systems.[10,7] The latter studies were however so far restricted only to $T = 0$.

As a test we present results for $N_h = 1$ on the 4×4 square lattice. The total number of basis states for this problem is $N = 524\,288$. However, using sampling functions with definite symmetries, in our case the wave vector $\vec{q}$ and total spin S_z, $\sigma(\omega)$ is a sum of sector contributions, where the largest $S_z = \pm\frac{1}{2}$ contains $N_1 = 6435$ states. Within each sector we create N_0N_1/N random states $|n\rangle$, serving as initial conditions for the Lanczos iteration Eq. (3).

Let us first show the dependence of results on the number of Lanczos steps M. In Fig. 1 we present spectra $T\sigma(\omega)$ for $J = 0$ obtained for the sampling with $N_0 \sim 700$, i.e., $\delta = N_0/N \sim 0.005$ of states, at two different temperatures $T \gg t$ and $T = 0.5t$, and different $M = 60, 120, 180$. The main observation is that with increasing M spectra emerging from Eqs. (6) and (8) converge well to a smooth curve, as expected for higher T. Smaller M results in the appearance of regular oscillations, $\Delta\omega \sim \Delta E_m/M$, where ΔE_m seems to be related to the maximum energy span in the model. These oscillations do not contain any relevant information, so they could be eliminated, if necessary, by appropriate smoothing technique. Anyhow these oscillations become pronounced only at $T \gg t$, i.e., outside the most interesting regime. It should be mentioned that for the particular problem generally $M_0 \sim 50$ steps are needed to get good convergence for the ground state, hence one should choose preferably $M \gtrsim M_0$ steps. On the other hand, using $M \gg M_0$ requires a rather time-consuming additional reorthogonalization of Lanczos vectors, hence a compromise is needed when choosing M.

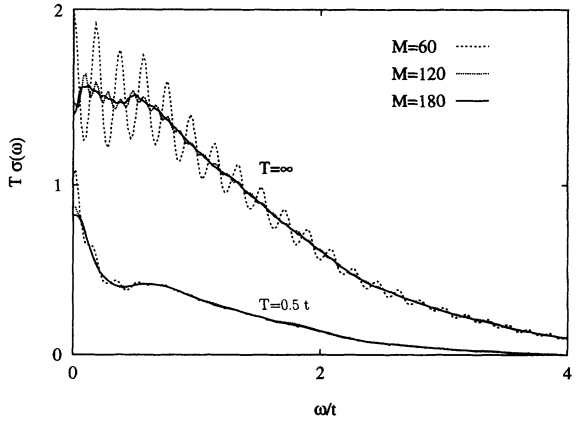

FIG. 1. Optical conductivity spectra $T\sigma(\omega)$ for a single hole in the t-$J = 0$ model on a 4×4 lattice at two different temperatures $T = \infty$ and $T = 0.5t$, as calculated using the random sampling over $N_0 = 720$ states and different number of Lanczos steps $M = 60, 120, 180$, respectively. Additional broadening of peaks with $\eta = 0.05$ is used.

The most stringent test for the random sampling are $T = 0$ spectra. Since at $J = 0$ the $T = 0$ spectra are trivial due to the ferromagnetic ground state, we present tests for $J = 0.3\,t$. In Fig. 2 we compare (a) the $T = 0$ result for $\sigma(\omega)$, obtained by the usual Lanczos method for the ground state $|\Psi_0\rangle$ (in fact due to the special sixfold degeneracy of the ground state of the 4×4 lattice we average over corresponding ground state spectra), and (b) the result obtained via Eqs. (6) and (10) with the random sampling over $\delta = 4 \times 10^{-5}$ and $\delta = 4 \times 10^{-4}$ of states, respectively. Since only the sampling over the degenerate ground states is contributing at $T = 0$, results in Fig. 2

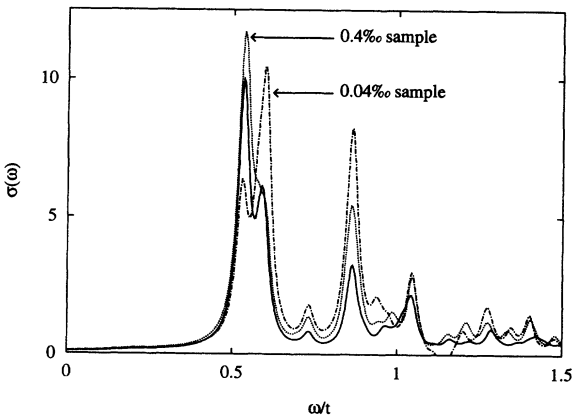

FIG. 2. $\sigma(\omega), T = 0$ spectra for a single hole in the t-J model with $J/t = 0.3$ on the 4×4 lattice. Full curve represents the exact $T = 0$ result (averaged over degenerate ground states), while dashed curves are obtained with $M = 120$ and with the random sampling over 4×10^{-4} and 4×10^{-5} of all states, respectively. Peaks are broadened additionally with $\eta = 0.02$.

correspond effectively to the sampling over 20 and 200 random states, respectively. It should be noted that in Fig. 2 we omit delta functions at the origin, the strength of which has to be determined indirectly. Presented results show that N_0 influences the intensities of peaks in the low-frequency part of spectra, and that convergence of those with N_0 is quite efficient. On the other hand, peak positions are mainly determined by M and are quite accurate at low frequencies for the presented examples. In the high-frequency regime details of the spectra are more dependent on M (as well as on N_0) and harder to reproduce exactly, as is also the case for the standard $T = 0$ Lanczos method.[7] Nevertheless, overall features, e.g., frequency moments, are expected to remain correct.

The method introduced in this paper is clearly feasible for the studies of finite-temperature statical and dynamical quantitites in correlated systems. More detailed results for the finite-temperature optical as well as the dc conductivity, obtained by this method, will be presented elsewhere. Since calculations presented here require quite modest computational effort, the method can be applied also to more demanding systems, e.g., t-J model either on larger lattices or with larger number of holes. In conclusion, we should also comment on the expected relation between $T > 0$ and $T = 0$ response functions obtained on small systems. There is a lot of evidence that several features of $T = 0$ spectra (in the low as well as in the high-frequency regime) are strongly system, i.e., size and shape, dependent and are therefore possibly not characteristic for the thermodynamic limit. The same could be true also for some static quantitites. $T > 0$ spectra are much smoother in general, even for small systems. Studying systems at $T > 0$, which are of interest by themselves, would therefore in addition allow an alternative limit $T \to 0$ to investigate challenging ground states of correlated systems.

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