Chebyshev expansion method for finite-T dynamical correlations – Optical response of the Anderson model –

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Abstract

The numerical calculation of dynamical correlation functions, like optical conductivities, spin structure factors and other (linear) response functions, is one of the typical problems in condensed matter physics. At zero temperature Chebyshev expansion and the Kernel Polynomial Method (KPM) [1] proved to be a valuable tool for this kind of problem, for both interacting and non-interacting quantum systems. We present a non-trivial extension of these methods to finite temperature [2]. To demonstrate the power of the approach we calculate the optical conductivity of non-interacting electrons in a random potential (Anderson model).

Kernel Polynomial Method

KPM was proposed a decade ago for the calculation of the density of states of large Hamiltonian matrices [1],

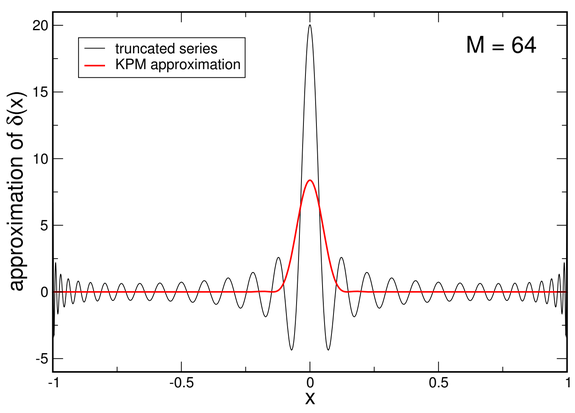
$$\rho(E) = \frac{1}{N}\sum_{n=0}^{N-1} \delta(E-E_n)\,. \tag{1}$$

The function of interest is expanded in terms of the functions $\phi_m(x) = \frac{T_m(x)}{\pi\sqrt{1-x^2}}$, derived from the Chebyshev polynomials $T_m(x) = \cos(m\,\mathrm{acos}(x))$.

To alleviate the effects of a truncation of such a series the result is convoluted with the Jackson kernel,

$$K_M(x,y) = g_0\phi_0(x)\phi_0(y) + 2\sum_{m=1}^{M-1} g_m\phi_m(x)\phi_m(y)\,, \tag{2}$$

$$g_m = \frac{(M-m+1)\cos\frac{\pi m}{M+1} + \sin\frac{\pi m}{M+1}\cot\frac{\pi}{M+1}}{M+1}. \tag{3}$$



Expansion of $\delta(x)$: Plain truncated series versus KPM.

The KPM approximation of $\rho(E)$ then reads

$$\rho(E) \approx \frac{g_0\mu_0 + 2\sum_{m=1}^{M-1} g_m\mu_m\, T_m[(E-b)/a]}{\pi\sqrt{a^2-(E-b)^2}}, \tag{4}$$

with expansion coefficients μ_m given by the trace

$$\mu_m = a\int_{-1}^{1} \rho(ax+b)\,T_m(x)\,dx = \frac{1}{N}\mathrm{Tr}\left[T_m\left(\frac{H-b}{a}\right)\right]. \tag{5}$$

Main advantages of KPM:

- Full evaluation of the trace not required, the average over a small number of random vectors $|r\rangle$ is sufficient.
- Recursion relations for T_m allow for an iterative calculation of the μ_m based on matrix-vector multiplications.
- For sparse Hamiltonian matrices the numerical effort is linear in the dimension N.

Dynamical correlation functions

KPM is easily applied [1] to zero-temperature dynamical correlation functions of interacting systems, e.g.,

$$\sigma(\omega) = \frac{1}{\omega N}\sum_{n>0} |\langle n|J|0\rangle|^2\;\delta(\omega-E_n+E_0)\,. \tag{6}$$

Finite temperature correlations are far more complex due to the double summation over matrix elements between all eigenstates and the thermal weighting,

$$\sigma(\omega) = \sum_{n,m}\frac{|\langle n|J|m\rangle|^2}{\omega ZN}\,(e^{-\beta E_n} - e^{-\beta E_m})\;\delta(\omega-\omega_{mn})\,. \tag{7}$$

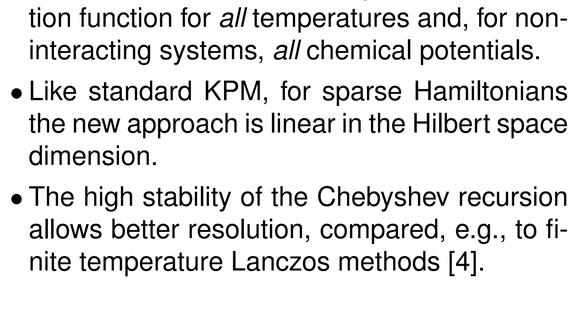
Previous attempts [3] are based on a Chebyshev / KPM expansion of the thermal weighting factors and explicit numerical time evolution ⇒ slow and complicated, since every change in temperature requires a new simulation.

New approach [2]: Rewrite $\sigma(\omega)$ as

$$\sigma(\omega) = \frac{1}{\omega ZN}\int_{-\infty}^{\infty} j(y+\omega,y)\left(e^{-\beta y} - e^{-\beta(y+\omega)}\right)dy \tag{8}$$

with a matrix element density

$$j(x,y) = \sum_{n,m} |\langle n|J|m\rangle|^2\;\delta(x-E_n)\;\delta(y-E_m) \tag{9}$$



Matrix element density for the Anderson model at $W = 2$ and 12.

Introducing *two-dimensional* KPM we can easily expand $j(x,y)$, a function of two variables, in terms of

$$\phi_{lm}(x,y) = \frac{T_l(x)T_m(y)}{\pi^2\sqrt{(1-x^2)(1-y^2)}}, \tag{10}$$

and the expansion coefficients μ_{lm} are again characterised by a trace,

$$\mu_{lm} = \mathrm{Tr}\left(T_l(\tilde{H})J_xT_m(\tilde{H})J_x\right). \tag{11}$$

Advantages of the new approach:

- Knowing μ_{lm} and $j(x,y)$ from a single simulation, we can calculate the dynamical correlation function for *all* temperatures and, for non-interacting systems, *all* chemical potentials.
- Like standard KPM, for sparse Hamiltonians the new approach is linear in the Hilbert space dimension.
- The high stability of the Chebyshev recursion allows better resolution, compared, e.g., to finite temperature Lanczos methods [4].

AC conductivity of the Anderson model

As a particularly interesting example we consider the optical conductivity of the Anderson model [5],

$$H = -t\sum_{\langle ij\rangle}\left(c_i^\dagger c_j + c_j^\dagger c_i\right) + \sum_i \varepsilon_i c_i^\dagger c_i\,, \tag{12}$$

which describes the motion of electrons in a disordered crystal, characterised by a random on-site potential $\varepsilon_i \in [-W/2, W/2]$. For spatial dimension $d > 2$ the system is known to undergo a continuous metal-insulator transition, caused by the onset of localisation of the single-particle eigenfunctions of H.

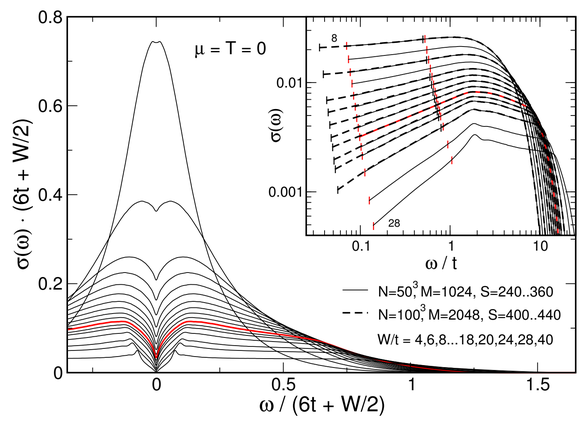
For this model of non-interacting fermions the optical conductivity reads

$$\sigma(\omega) = \sum_{n,m}\frac{|\langle n|J_x|m\rangle|^2}{\omega L^d}(f(E_m)-f(E_n))\,\delta(\omega-\omega_{nm})\,, \tag{13}$$

where $\omega_{nm} = E_n - E_m$, $f(E) = [e^{\beta(E-\mu)}+1]^{-1}$ is the Fermi function and

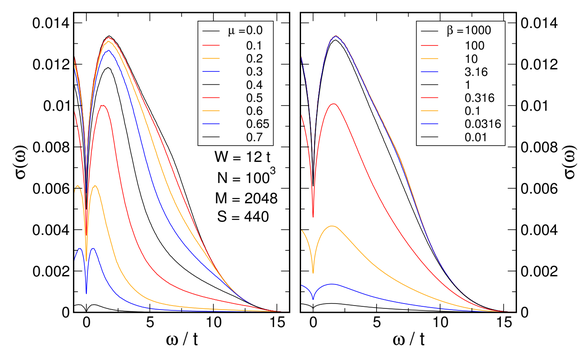
$$J_x = -\mathrm{i}t\sum_i\left(c_i^\dagger c_{i+x} - c_{i+x}^\dagger c_i\right) \tag{14}$$

the x-component of the current operator. Note, that for finite band-filling, $\mu > 0$, the complexity of the numerical problem is the same for $T = 0$ and $T > 0$. In both cases the calculation of matrix elements between all eigenstates is required.



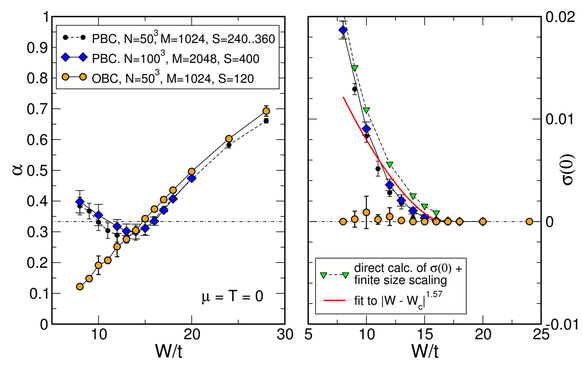
Optical conductivity of the 3D Anderson model (PBC) at $T = \mu = 0$.

Previous studies of $\sigma(\omega)$ were mostly based on a complete diagonalisation of H and an explicit calculation of the matrix elements. Naturally, the accessible system sizes were very limited ($N = L^3 \le 20^3$). The new approach yields high-resolution $\sigma(\omega)$ data for systems with 10^6 sites or more.



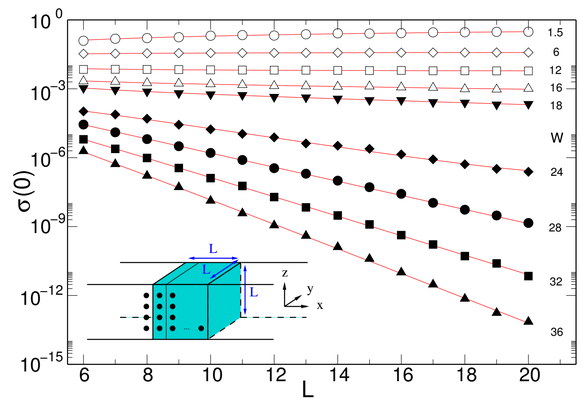
Dependence of $\sigma(\omega)$ on $\beta = 1/T$ and μ.

Based on these results we can check analytical predictions for the low-frequency behaviour of $\sigma(\omega)$. For a $d > 2$ dimensional system one-parameter scaling theory and renormalisation group arguments [6] yield $\Delta\sigma = \sigma(\omega) - \sigma(0) \sim \omega^{(d-2)/2}$ for the metallic phase, $\sigma(\omega) \sim \omega^{(d-2)/d}$ exactly at the transition, and $\sigma(\omega) \sim \omega^2$ on the insulating side [7].



Fits of the low-frequency data to $\sigma(\omega) = \sigma(0) + C\omega^\alpha$.

Fits of our numerical data confirm these predictions, i.e., for $W \ge W_c$ we find an exponent that increases from $\alpha = 1/3$, and $\sigma(0) = 0$. In the metallic phase, for PBC α increases towards $1/2$ and $\sigma(0)$ becomes finite. Within OBC no current can flow and the response is that of an insulator, $\sigma(0) = 0$ and further decreasing α.



Finite size scaling of directly calculated σ_{dc}.

To check the consistency of the fit parameter $\sigma(0)$ we considered a Landauer Büttiker type setup and calculated σ_{dc} directly using a numerical Greens function approach [8]. Finite size scaling with the ansatz $\sigma_{dc} \propto Le^{-L/\lambda}/(a+L)$ yields good agreement with $\sigma(0)$.

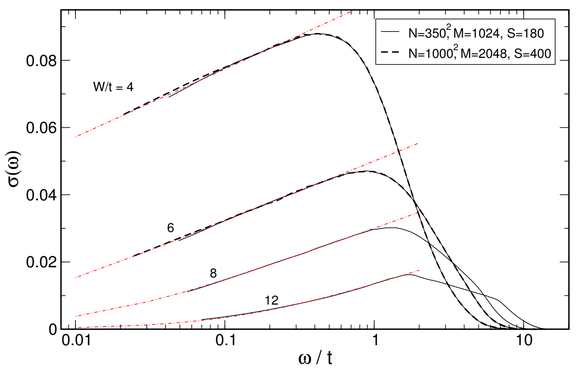
Note that fitting the power law $\sigma_{dc} \equiv \sigma(0) \propto |W - W_c|^s$ leads to a critical exponent larger than the expected $s = (d-2)\nu \approx 1.57$, a puzzle we hope to understand in future studies.

Weak localisation and beyond

The new approach allows also the study of large two-dimensional systems, which are expected to be insulating for any non-zero disorder. In contrast to $d > 2$, from the diffusion approximation [9] we now expect a logarithmic low-frequency behaviour of $\sigma(\omega)$. The data illustrates, however, that for increased disorder higher order corrections [10],

$$\sigma(\omega) \propto \ln(1+\omega/\omega_0)\,, \tag{15}$$

need to be taken into account.



Optical conductivity of the 2D Anderson model (PBC) at $T = \mu = 0$ and fits to Eq. (15).

Conclusions

Based on the Kernel Polynomial Method we propose a promising new approach for the numerical calculation of finite-temperature dynamical correlation functions. Its application to the Anderson model yields the optical conductivity of large finite clusters and confirms analytical predictions for the low-frequency behaviour.

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