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Chebyshev expansion approach to the AC conductivity of the Anderson model

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Abstract. We propose an advanced Chebyshev expansion method for the numerical calculation of linear response functions at finite temperature. Its high stability and the small required resources allow for a comprehensive study of the optical conductivity $\sigma(\omega)$ of non-interacting electrons in a random potential (Anderson model) on large three-dimensional clusters. For low frequency the data follows the analytically expected power-law behaviour with an exponent that depends on disorder and has its minimum near the metal-insulator transition, where also the extrapolated DC conductivity continuously goes to zero. In view of the general applicability of the Chebyshev approach we briefly discuss its formulation for interacting quantum systems.

PACS. 78.20.Bh Theory, models, and numerical simulation – 72.15.Rn Localisation effects (Anderson or weak localisation) – 05.60.Gg Quantum transport

Rapid Note

The numerical calculation of linear response functions is one of the standard tasks in condensed matter theory and many other areas of physics. In practice, however, the number of degrees of freedom usually becomes enormously large and can easily reach $N \approx 10^6$ or more, e.g., for a quantum many body problem. A complete diagonalisation of such systems and a naive evaluation of linear response functions is prohibitive is such situations, since the required time would scale at least as N^3. The use and development of new numerical methods which are *linear* in the system size has therefore become an essential part of current research. In the present work we follow this line and propose an advanced Chebyshev expansion method for the calculation of dynamical correlation functions at finite temperature. It exceeds previous attempts, in particular, since it requires only a single simulation run for all temperatures and, if applied to non-interacting fermions, for all chemical potentials.

As a particularly interesting application, we study the optical (AC) conductivity $\sigma(\omega)$ of non-interacting electrons in a random potential, which has so far resisted a thorough numerical treatment. The basic model to describe this kind of problem and many of its features was proposed by Anderson almost fifty years ago [1], and since then attracted a considerable amount of analytical, numerical, and experimental work [2]. Starting from spinless fermions $c_i^{(\dagger)}$ which are allowed to hop between neighbouring sites of a crystal,

$$H = -t \sum_{\langle ij \rangle} \left(c_i^\dagger c_j + c_j^\dagger c_i \right) + \sum_i \epsilon_i c_i^\dagger c_i \,, \qquad (1)$$

disorder can be introduced in the form of a random, uniformly distributed local potential $\epsilon_i \in [-W/2, W/2]$ parameterised by the disorder strength W. Given this Hamiltonian the question arises, whether its one-particle eigenfunctions span the entire lattice, thus resembling the Bloch waves known from an ordered crystal ($W = 0$), or are localised in the vicinity of certain lattice sites. Naturally, this change in the spatial structure of the wave functions is reflected in the (DC) conductivity of the system, being insulating or metallic depending on the disorder strength W, the spatial dimension d, and the particle density (or chemical potential μ). Much of our current understanding of this disorder-induced metal-insulator transition is based on the one-parameter scaling theory of Abrahams et al. [3], which in $d \leq 2$ dimensions predicts insulating behaviour for any finite disorder $W > 0$ and a continuous metal-insulator transition at some $W_c(\mu) > 0$ for $d > 2$. The critical behaviour near the transition is usually described in terms of nonlinear σ-models [4] and is widely believed to follow power laws with a correlation/localisation length ξ diverging as $\xi \propto |W_c - W|^{-\nu}$, and the DC conductivity vanishing as $\sigma(0) \propto (W_c - W)^s$. Numerical work confirmed much of this general picture and over the last years focused on the precise determination of the critical line $W_c(\mu)$ and of the critical exponents, which so far could not be calculated analytically. For the above model the most reliable data ($W_c(0)/t = 16.54$ and $\nu = 1.57$, cf. Ref. [5]) is based on the transfer-matrix method [6], where in a quasi-one-dimensional geometry the correlation length ξ is obtained from the finite size scaling of the Lyapunov exponents. Unfortunately, approaches of this type cannot directly access the DC conductivity $\sigma(0)$ or its critical behaviour. Our knowledge of the exponent s is therefore mainly based on scaling arguments [7], namely, $s = (d-2)\nu$. However, the validity of the one-parameter

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scaling theory and of the corresponding critical behaviour has been repeatedly called into question [8,9], and instead the non-power-like critical behaviour known for the Bethe lattice has been proposed to hold also for hyper-cubic systems. The resolution of this certainly not completely settled issue may require the use of alternative numerical methods, which should preferably be based on true d dimensional systems and yield complementary critical quantities.

As noted before, here we want to focus on the numerical calculation of the optical conductivity $\sigma(\omega)$ of three-dimensional (cubic) clusters. This allows for a test of various analytical predictions for the finite frequency behaviour, and eventually we can draw conclusions about the zero-frequency response. In particular, for d dimensional systems Wegner [7] found $\sigma(\omega) \sim \omega^{(d-2)/d}$ to hold exactly at the metal-insulator transition, a prediction which is consistent also with the one-parameter scaling theory [10]. On the metallic side of the transition different studies [10–12] agree that for small enough frequency the conductivity should behave as $\Delta\sigma = \sigma(\omega) - \sigma(0) \sim \omega^{(d-2)/2}$, whereas on the insulating side we expect the well known $\sigma(\omega) \sim \omega^2$ behaviour independent of the spatial dimension [13]. As will become clear below, the numerical calculation of $\sigma(\omega)$ is a challenging task, which certainly is the reason that only the prediction for the critical point in $d = 3$, i.e., $\sigma(\omega) \sim \omega^{1/3}$, is confirmed so far [14,15]. Within linear response the real part of the optical conductivity is given by

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

where $|n\rangle$ and $|m\rangle$ denote eigenstates of the Hamiltonian with energies E_n and E_m, $\omega_{nm} = E_n - E_m$, $f(E) = 1/(\exp(\beta(E-\mu)) + 1)$ is the Fermi function, and $J_x = -\mathrm{i}t \sum_i (c_i^\dagger c_{i+x} - c_{i+x}^\dagger c_i)$ the x-component of the current operator. Even at zero temperature equation (2) involves a summation over matrix elements between *all* one-particle eigenstates of H, which can hardly be calculated for a reasonably large system. Consequently, until now, the number of numerical attempts to this problem is very small. Some authors relied on a full diagonalisation of the Hamiltonian and an explicit summation of the current matrix elements [14,16–18], but of course the system sizes manageable with this approach are very limited. Even the dramatically improved performance of present day computers allows only the study of clusters of about $L^3 = 20^3$ sites. More recently the so-called forced oscillator method [15] and the projection method [19] were applied to the problem, which increased the accessible system size to about 30^3 and 256^3 sites, respectively. However, the frequency and parameter ranges considered in these works were rather limited, and unfortunately the resolution as well as the statistical quality of the data seem to be insufficient for a detailed analysis of the low-frequency behaviour [19].

About a decade ago Silver and Röder [20] proposed the kernel polynomial method (KPM) for the calculation of the density of states of large Hamiltonian matrices, which, in addition, turned out to be a very robust and reliable tool for the calculation of temperature dependent static quantities and zero-temperature dynamical correlation functions of interacting systems (which in contrast to Eq. (2) require only a single summation over the matrix elements between the ground-state and excitations) [21]. In a nutshell, after appropriate rescaling of the Hamiltonian, $\tilde{H} = (H - b)/a$, and of the energy spectral quantities like the density of states, $\rho(E) = \sum_{n=0}^{N-1} \delta(E - E_n)/N$, are expanded in terms of Chebyshev polynomials $T_m(x) = \cos(m \operatorname{acos}(x))$. To alleviate the effects of a truncation of such a series the result is convoluted with a particular kernel (the Jackson kernel), and to a good approximation $\rho(E)$ then reads

$$\rho(E) \approx \frac{g_0\mu_0 + 2\sum_{m=1}^{M-1} g_m\mu_m\, T_m[(E-b)/a]}{\pi\sqrt{a^2 - (E-b)^2}}. \quad (3)$$

Here the g_m account for the kernel and the μ_m are the actual expansion coefficients, $\mu_m = \int \rho(x)\, T_m[(x - b)/a]\, dx = \mathrm{Tr}[T_m(\tilde{H})]/N$. It turns out that the numerical calculation of the coefficients μ_m does not require the full evaluation of the trace of the polynomial $T_m(\tilde{H})$. Instead, self-averaging properties, used also in Monte Carlo simulations, allow for an replacement of the trace by an average over a small number $R \ll N$ of random states $|r\rangle$. If, in addition, recursion relations for the Chebyshev polynomials are taken into account, for sparse Hamiltonians of dimension N the numerical effort for the calculation of all M coefficients μ_m is proportional to $RNM/2$, i.e., *linear* in N. Once the μ_m are known the reconstruction of the target function is facilitated by the close relation between Chebyshev expansion and Fourier transform, i.e., the availability of divide-and-conquer type algorithms (FFT).

So far we are aware of only one attempt [22] to generalise the kernel polynomial method to finite-temperature dynamical correlations (note that for non-interacting systems the numerical effort is equal for $T = 0$ and $T > 0$). In this recent letter Iitaka and Ebisuzaki [22] propose a Chebyshev expansion of the Boltzmann or Fermi weights (see Eq. (2)), which is used to generate a set of correspondingly weighted random vectors. These states are then subject to standard numerical time evolution and measurements of the targeted operator, and finally yield the considered correlation function. Although certainly being a useful approach, we argue that it is still unnecessarily complicated, mainly because each change in the temperature T or chemical potential μ requires a new simulation.

To avoid these complications we propose a slight increase in the level of abstraction, namely, the introduction of *two-dimensional* KPM. A closer inspection of equation (2) shows that $\sigma(\omega)$ is easily written as an integral over a matrix element density

$$j(x,y) = \frac{1}{L^d} \sum_{n,m} |\langle n|J_x|m\rangle|^2 \delta(x - E_n)\delta(y - E_m),$$

$$\sigma(\omega) = \frac{1}{\omega} \int_{-\infty}^{\infty} j(x, x+\omega)[f(x) - f(x+\omega)]\, dx. \quad (4)$$

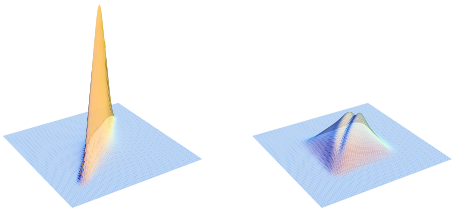

Fig. 1. The matrix element density $j(x,y)$ for the Anderson model at $W/t = 2$ and 12. Note the dip developing at $x = y$ which finally causes the vanishing DC conductivity.

The quantity $j(x,y)$, however, is of the same structure as the density of states, except for being a function of two variables. As was shown by Wang [23] some years ago, it can thus be expanded as a series of polynomials $T_l(x)T_m(y)$ and the expansion coefficients μ_{lm} are characterised by a similar trace, $\mu_{lm} = \mathrm{Tr}[T_l(\tilde{H})J_x T_m(\tilde{H})J_x]/L^d$. Again the trace can be replaced by an average over just a few random vectors $|r\rangle$, and the numerical effort for an expansion of order $l, m < M \ll N$ ranges between $2RNM$ and RNM^2, depending on whether memory is available for up to M vectors of dimension N or not. Probably overlooking the potential of the approach, so far only the zero temperature response was studied and, in particular, the back transformation of the expansion coefficients relied on pure truncated Chebyshev series [23]. The latter, however, suffer from unwanted high-frequency oscillations and the positivity of $j(x,y)$ is not ensured. We therefore generalised the Jackson kernel and the KPM to two dimensions. Combined with fast Fourier methods, which are available for arbitrary dimension, this leads to an easy and reliable method for the calculation of $j(x,y)$ and $\sigma(\omega)$.

Note the main advantage of this approach: Once we know the coefficients μ_{lm} and the resulting $j(x,y)$, we can immediately calculate $\sigma(\omega)$ for *all* temperatures and *all* chemical potentials, without repeating the most time consuming step of calculating μ_{lm} (and, for the present model, averaging over several realisations of disorder). In addition, as was shown in a number of works, standard KPM is numerically much more stable and allows much higher resolution than the popular Lanczos recursion approach [24]. We therefore believe that the new generalisation of KPM will also outperform the finite-temperature Lanczos methods proposed recently [25,26]. The generalisation of the approach to interacting systems is straightforward [27]. It merely requires a substitution of the Fermi function by the Boltzmann weight in equation (4), and a division of the result by the partition function, which is readily obtained from an expansion of the density of states.

Applying the approach to the Anderson model, we obtain the matrix element density $j(x,y)$ shown in Figure 1. Starting from a "shark fin" at weak disorder, with increasing W the density $j(x,y)$ spreads in the entire energy plane, simultaneously developing a sharp dip along $x = y$. A comparison with equation (4) reveals, that it is this dip which is responsible for the decreasing and finally vanishing DC conductivity. For $\mu = 0$ (band centre) and $T = 0$ the corresponding optical conductivity $\sigma(\omega)$ is given in Figure 2. Note, that the calculation is based on large finite clusters with up to $N = L^3 = 100^3$ sites and periodic boundary conditions, the data is averaged over up to $S = 440$ disordered samples, and the expansion order $M = 1024$ (or $M = 2048$ for the dashed sets in the inset). At weak disorder the conductivity is almost Drude like with only a small dip at low frequency. With increasing disorder this small-ω feature becomes more pronounced and finally leads to insulating behaviour at strong disorder. Beyond a sharpening maximum near $\omega \approx t$ the conductivity falls of almost with a power law and later exponentially.

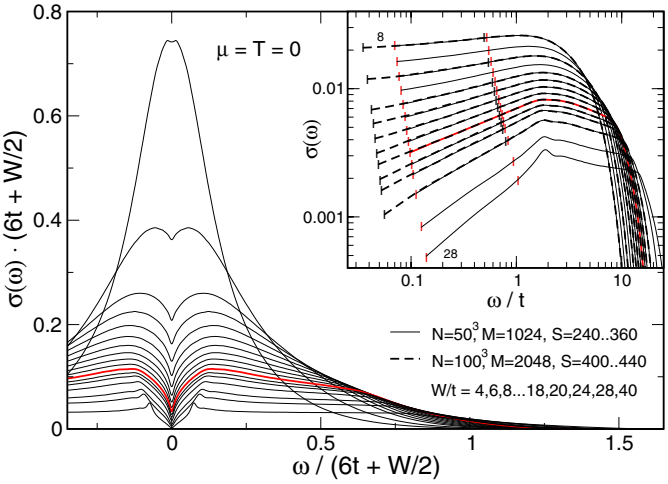

Fig. 2. Optical conductivity of the 3D Anderson model at $T = 0$ and $\mu = 0$ (band centre) for increasing disorder W. The thick red lines mark $W/t = 16$, which approximately corresponds to the critical disorder. Data denoted by solid lines is based on $N = 50^3$ site clusters, expansion order $M = 1024$, and $S = 240 \ldots 360$ disordered samples, dashed lines in the inset correspond to $N = 100^3$, $M = 2048$ and $S = 400 \ldots 440$.

The high precision of the data allows for a detailed comparison of the low frequency behaviour with the above mentioned analytical results. In the inset of Figure 2 we focus on the low frequency part and plot the conductivity data again on a double-logarithmic scale. Clearly, for disorder $W/t \geq 16$ the data follows a power law, whereas for $W/t < 16$ the slight upturn at low frequencies accounts for the finite DC conductivity. To substantiate these findings, in Figure 3 we show fits of the low-frequency data to $\sigma(\omega) = \sigma(0) + C\omega^\alpha$. Starting from the localised phase at large W the DC conductivity $\sigma(0)$ is zero and the exponent α decreases continuously with W, reaching $\alpha = 1/3$ near $W/t \approx 16$. Below that value $\sigma(0)$ increases continuously with decreasing disorder W, and the same seems to hold for α. Note that we slightly vary μ around zero to expand the data basis and estimate the error of the fits. Unfortunately, for $W/t < 16$ the three free parameters lead to a sizeable uncertainty in particular for the exponent α. Nevertheless, we can confirm the general trends, namely an increase of the exponent α from 1/3 at the critical point to eventually a value of 2 at very large disorder,

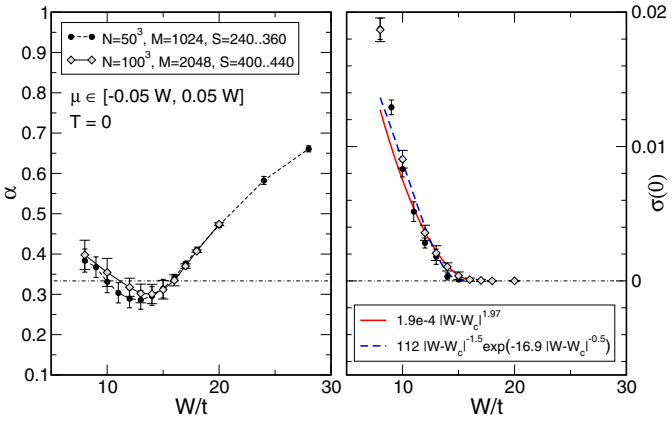

Fig. 3. Exponent α and DC conductivity $\sigma(0)$ obtained from fits of the low-frequency conductivity to $\sigma(\omega) = \sigma(0) + C\,\omega^{\alpha}$ (vertical bars in the inset of Figure 2 mark the underlying frequency range). Error bars are estimated by slightly varying μ in the range $-0.05W \ldots 0.05W$.

and an increase towards $\alpha = (d-2)/2 = 1/2$ for weak disorder. Although our data looks rather convincing, note one potential problem: The considered frequencies might still be too large for an observation of the correct scaling, since from analytical work [12] the $\sqrt{\omega}$ or ω^2 behaviour of $\sigma(\omega)$ is expected only for frequencies smaller than a cut-off of the order of $\omega_{\rm cr} \sim 1/(\rho(\mu)\xi^3)$, while for $\omega \gg \omega_{\rm cr}$ $\Delta\sigma \sim \omega^{1/3}$. On the other hand, also an increased resolution did not show any indication of such a cross-over, even though, particularly on the insulating side, the localisation length ξ rapidly decreases with W, reaching the order of 1 for the largest disorder values considered. We hope further studies can resolve this puzzling issue.

Keeping in mind the above subtleties, we can also try to address the critical behaviour expressed in $\sigma(0)$. As the comparison of data for 50^3 and 100^3 sites in Figure 2 illustrates, for the considered frequencies the AC conductivity does not suffer from noticeable finite-size effects. This is corroborated by estimates of the diffusion length L_ω (the distance electrons diffuse within a field cycle; cf. Ref. [10]), throughout yielding $L_\omega \ll L$. Therefore the fit parameter $\sigma(0)$ in Figure 3 should correspond to the thermodynamic limit of the DC conductivity, which for dimension $d = 3$ is widely believed to follow a $\sigma(0) \sim (W_c - W)^s$ law with $s = \nu \approx 1.57$. However, the curvature of $\sigma(0)$, derived from our data, seems to be larger, leading to s of the order of 2. On the other hand, we also obtained reasonable fits using the expression for the Bethe lattice [8], $\sigma(0) \sim (W_c - W)^{-3/2} \exp(-A(W_c - W)^{-1/2})$, which would contradict the behaviour generally assumed for the $d = 3$ Anderson model. Although resolving these interesting questions certainly requires an improvement of both the resolution and the statistical quality of the data, our results shed new light on the Anderson transition and illustrate the potential of the numerical approach.

In summary, we described a promising new technique for the numerical calculation of finite temperature dynamical correlation functions for both interacting and non-interacting quantum systems. By extending the Kernel Polynomial Method to functions of two variables, we avoid the disadvantages of thermal projection techniques, and obtain reliable results for all temperatures (and chemical potentials) from a single simulation run. Being a hybrid of the iterative schemes of numerical diagonalisation and of random sampling, the approach might also inspire new Monte-Carlo methods for correlation functions. Applying the method to the Anderson model we present comprehensive data for the AC conductivity, which substantially improves previous numerical studies with respect to accessible system size, considered frequency and parameter range, as well as statistical significance. In addition, we confirm analytical predictions for the low-frequency behaviour of the AC conductivity, but find indications that the critical behaviour of the DC conductivity might deviate from the commonly presumed form.

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27. More details to be published elsewhere

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