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<tr>
<td>Citation</td>
<td>Ghosh, S., Miniatura, C., Cherroret, N., &amp; Delande, D. (2017). Coherent forward scattering as a signature of Anderson metal-insulator transitions. Physical Review A, 95(4), 041602-</td>
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<tr>
<td>Date</td>
<td>2017</td>
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<tr>
<td>URL</td>
<td><a href="http://hdl.handle.net/10220/43524">http://hdl.handle.net/10220/43524</a></td>
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Coherent forward scattering as a signature of Anderson metal-insulator transitions

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(Received 28 July 2016; revised manuscript received 7 February 2017; published 14 April 2017)

We show that the coherent forward scattering (CFS) interference peak amplitude sharply jumps from zero to a finite value upon crossing a metal-insulator transition. Extensive numerical simulations reveal that the CFS peak contrast obeys the one-parameter scaling hypothesis and gives access to the critical exponents of the transition. We also discover that the critical CFS peak directly controls the spectral compressibility at the transition where eigenfunctions are multifractal, and we demonstrate the universality of this property with respect to various types of disorder.

DOI: 10.1103/PhysRevA.95.041602

About 60 years ago, Anderson established that interference can completely suppress diffusion [1]. Later, it was even predicted that three-dimensional (3D) systems exhibit a genuine disorder-driven metal-insulator transition (MIT) [2,3]. Since then, various classes of MITs, with different critical properties, have been identified [4,5]. Generically, a MIT features a mobility edge separating a metallic phase, where waves are extended and propagate diffusively, from an insulating phase where waves are localized. Recently observed in spinless time-reversal invariant systems [6–10], Anderson MITs still remain challenging and elusive in more exotic configurations where time reversal or spin rotation is broken, or when interactions are present [11,12]. Furthermore, transport properties near the critical point, affected by the multifractal character of the eigenstates [13], have been little studied in actual experiments [14].

Related to Anderson localization (AL), coherent forward scattering (CFS) is a robust interference effect which triggers a macroscopic peak in the forward direction of the momentum distribution \( n(k,t) \) obtained after an initial plane wave \( | \vec{k}_0 \rangle \) has evolved through a bulk disordered system [15–17]. While CFS resembles the well-known coherent backscattering (CBS) effect, which is due to the pair interference of time-reversed scattering sequences and yields a peak in the backward direction [18], the two effects turn out to be fundamentally different. Indeed, the CBS peak relies on time-reversal symmetry (TRS) [19] and exists on both sides of the MIT, with no discontinuous behavior as the mobility edge is crossed [20]. In marked contrast, CFS requires Anderson localization to show up (it is absent in the metallic phase) and is present whether or not TRS is broken [21,22]. While the experimental observation of CBS in momentum space has been recently achieved with cold atoms [23], observations of CFS are lacking. On the theoretical side, CFS has been studied in one dimension and two dimensions [15,17,21], but not in three dimensions where an Anderson MIT takes place. In this Rapid Communication, we numerically demonstrate that the CFS contrast constitutes a reliable and measurable order parameter for MITs: (i) It jumps abruptly from zero in the metallic phase to a finite value in the insulating phase, (ii) obeys the one-parameter scaling hypothesis and gives access to the critical exponents of the transition, and (iii) directly controls the spectral compressibility at the transition, where eigenfunctions are multifractal. Using large-scale numerical investigations, we prove that the latter property is universal and we validate the conjecture that links the critical spectral compressibility to the fractal information dimension of the Anderson MIT in the orthogonal Gaussian ensemble (GOE).

In the left panel of Fig. 1, we show a density plot of the momentum distribution \( n(k,t) \) resulting from the numerical propagation over long times of an initial plane wave \( | \vec{k}_0 \rangle \) in a 3D random potential, in the insulating (top), critical (middle), and metallic phases (bottom). While the CBS peak at \( k = -k_0 \) is present in the three phases, the CFS peak at \( k = k_0 \) only exists in the critical and insulating regimes. These results have been obtained with the 3D tight-binding Anderson Hamiltonian \( \hat{H} = -J \sum_{ij} c_i^\dagger c_j + \sum_i V_i c_i^\dagger c_i \), with nearest-neighbor hopping only (strength \( J \)) and periodic boundary conditions. Lattice sites \( i \) and \( j \) run over a simple 3D cubic lattice comprising \( M^3 = 120^3 \) sites with spacing \( a \). The system is virtually infinite as its size is larger than the longest distance traveled during the simulations. The random on-site potential energies \( V_i \) are taken from the distribution \( P(V_i) = 1/W \) within \([-W/2, W/2]\), and correlations between sites \( i \) and \( j \) are described by the correlation function \( C_{ij} = \overline{V_i V_j} = \overline{V_i^2} \delta_{ij} \). We select a given energy \( E \) by applying the filtering operator \( F_\sigma(E) = \exp[-(E - \hat{H})^2/2\sigma^2] \) onto the initial plane-wave state \( | \vec{k}_0 \rangle \). Following the most accurate known numerical results [24], we choose \( E = J \) and vary the disorder strength around the critical point \( W_c(E) \approx 16.53J \) of the Anderson MIT. The width of the filter is \( \sigma = 0.5J \), so that \( W_c \) is almost independent of \( E \) in the selected range. We then evolve this filtered state with \( U(t) = \exp(-i \hat{H}t/\hbar) \). Our numerical scheme uses an expansion of the filtering and evolution operators in terms of Chebyshev polynomials of \( \hat{H} \); see Ref. [17] for
details. This procedure is repeated for 6000 different disorder configurations to compute the disorder-average momentum distribution \( n(k,t) \).

Let us now discuss the time dynamics of CBS and CFS across the MIT. The evolution of the CBS peak is simple: Whatever \( W \), this peak becomes sizable after a few mean free times \( \tau \) [20] and its amplitude shows no discontinuity as the mobility edge is crossed. To analyze the dynamics of CFS, we use the CBS and CFS contrasts \( C_F \) and \( C_B \) (defined as the peak height above the background of the momentum distribution at \( \pm k_0 \) over the background) [17]. As shown below, the CFS contrast \( C_F \) is a smoking gun of Anderson localization, as it vanishes at long times in the localized regime and grows to a large value—of the order of unity—in the localized regime. The CBS contrast behaves very differently, as it is not singular at the Anderson transition: It is almost exactly unity in the diffusive regime and slowly decreases far in the localized regime. We thus chose to compute the normalized contrast \( \Lambda(W,t) = C_F/C_B \). This definition proves less sensitive to statistical fluctuations of the background than \( C_F \) and \( C_B \) themselves. The same conclusion and similar quantitative results, although a bit more noisy, are obtained if one uses \( C_F \) only as the critical quantity. In a system where time-reversal symmetry is broken [22], the CFS peak is still present, but the CBS peak disappears. In such a situation, one has to directly use \( C_F \) to characterize the transition.

The time evolution of \( \Lambda \) in the three phases is shown in the right panel of Fig. 1. In the metallic phase \( W < W_c \), a small CFS peak appears after a few \( \tau \) and rapidly dies off, \( \Lambda(t \to \infty) \to 0 \). In the insulating phase \( W > W_c \), the CFS peak steadily grows on the much longer Heisenberg time scale (see below) and eventually saturates to the CBS peak value, \( \Lambda(t \to \infty) \to 1 \). At the critical point, the peak very quickly saturates at \( \Lambda(W_c) = \Lambda_c \approx 0.34 \). In other words, localization triggers a macroscopic CFS peak, which is discontinuous across the MIT, a behavior markedly different from the one of CBS.

Figure 2(a) shows \( \Lambda \) as a function of \( W \) for increasing times. The observed step is steeper as time increases, as expected for the behavior of a critical quantity across a phase transition where time plays the role of the system size. At long times, \( \Lambda \) is 0 in the metallic regime and jumps to 1 in the insulating regime, irrespective of the exact value of \( W \) chosen in each regime. Noticeably, all curves cross at the critical point of the MIT, \( W_c/J \approx 16.5 \), where \( \Lambda_c \approx 0.34 \). This important result reveals that exactly at the critical point, \( \Lambda \) is time independent. As will be seen below, this value is universal and related to the multifractal properties of eigenstates at criticality.

In the metallic phase, perturbative techniques explain the long-time dynamics of CFS by a sum of two interference contributions, one featuring a concatenation of two maximally crossed diagram series and the other being its time-reversed counterpart [15,17,21]. We find

\[
W < W_c : \quad \Lambda(t) \sim \frac{1}{2\pi \hbar D \sqrt{D_t}}.
\]

where \( \rho \) is the disorder-averaged density of states per unit volume (DOS) and \( D \) the diffusion coefficient. Figure 3(a) confirms that \( \Lambda(t) \) behaves indeed as \( 1/\sqrt{t} \) in the metallic phase. In the insulating phase, we expand the initial state \(|k_0\rangle\)
Critical value $\Lambda_c \approx 0.34$ reflects entirely the behavior of the CFS contrast.

The behavior of $\Lambda$ at long—but not infinite—times can also be computed from Eq. (2). Indeed, within RMT, the $\varphi_n(k)$ and the $\epsilon_n$ are statistically uncorrelated variables and the average of each term in the expansion of the square in Eq. (2) breaks into the product of averages over the $\varphi_n(k)$ and the $\epsilon_n$. The latter is proportional to the Fourier transform of the DOS-DOS correlator $K(\omega) = \rho(E + \hbar \omega/2)\rho(E - \hbar \omega/2)/\rho^2 - 1$, i.e., to the spectral form factor $K(t)$, leading to $\Lambda(t) = 2\pi \hbar \rho M^2 K(t)**(16,17).** Following the correlated volume approach [25], we obtain $K(t)$ by estimating the 3D hybridization of localized states with energies lying within a mean level spacing $\Delta = 2\pi \hbar / \tau_H$. This gives $K(\omega) \sim \delta(h \rho M^2 \omega) + (\delta_{\text{loc}}/M)^3 \ln^3(|\omega|\tau_H/4\pi)$ for $|\omega| \tau_H \ll 1$. After a Fourier transform, we obtain

$$W > W_c: \quad \Lambda(W,t) \approx 1 - \alpha \frac{\ln^2(\eta t/\tau_H)}{(t/\tau_H)^4}$$

The phenomenological constants $\alpha$ and $\eta$ respectively account for subdominant corrections in the distribution of localized states and for a possible numerical prefactor in the definition of $\tau_H$. The time scale $\tau_H = 2\pi \hbar \rho M^2$ is the Heisenberg time, i.e., the inverse of the mean level spacing $\Delta$ within a localization volume. It is the typical time beyond which off-diagonal terms in Eq. (2) average to zero. Note that the previous reasoning is invalid in the metallic phase since eigenstates are delocalized over an infinite volume: No minimum energy scale can show up in the expansion Eq. (2) and off-diagonal terms never average to zero.

As shown by Eq. (4), $\Lambda$ depends on $W$ and $t$ only through the parameter $t/\tau_H$. This property is confirmed numerically in Fig. 3(b), where all numerical points obtained for different $W$ collapse onto a single curve. This one-parameter scaling law can be extended to the whole range of disorder strengths if one introduces a “system size” $L = [t/(2\pi \hbar \rho)]^{1/3}$ and defines a correlation length $\xi \propto \delta_{\text{loc}}$ in the insulating phase and $\xi \propto (2\pi \hbar \rho D)^{-1/3}$ in the metallic one [17]. Then, both Eqs. (1) and (4) depend on $L/\xi$ only, suggesting that $\Lambda$ is a natural one-parameter scaling observable to study an Anderson MIT. Following the historic scaling theory of AL [3], the scaling function $\beta = d(\ln \Lambda)/d(\ln L)$ should depend on $L$ only. This is confirmed in Fig. 4, where points obtained by numerically computing $\Lambda$ at various times and disorder strengths all fall on the same curve. As time increases, the system goes metallic when $\beta(\Lambda) < 0$ and insulating when $\beta(\Lambda) > 0$. The critical phase is signaled by the fixed point $\beta(\Lambda_c) = 0$. In the vicinity of the MIT, the correlation length diverges as $\xi \propto |W - W_c|^{-v}$, where $v$ is the critical exponent. To accurately determine the critical parameters $W_c$ and $v$, we use a finite-time scaling analysis which consists of writing $\Lambda = F(\chi^{1/\nu})$ with $|\chi| \propto \xi^{-1/\nu}$ (scaling hypothesis) and fitting the numerical data with a double Taylor expansion

$$\Lambda = \sum_{m=0}^\infty F_m W^{m/\nu}$$

and

$$\chi = \sum_{m=0}^\infty b_m (W - W_c)^m,$$

where $F_m$, $b_m$, $W_c$, and $v$ are the fit parameters [20]. With our 1095 data points, we obtain a good fit for $n_R = m_R = 2$, achieving a chi square per degree of freedom $\approx 1.6$. The uncertainties of $W_c$ and $v$ are obtained by dividing the whole configuration sample into several independent subsets and estimating $W_c$ and $v$ for each subset. This approach gives $W_c/J = 16.53 \pm 0.03$
Assuming that the relation to the form factor still holds at the critical point, we infer $\Lambda_c = \lim_{t \to 0} 2 \pi \hbar M^2 K(t) = \kappa(W_c) \equiv \kappa_c$, a positive quantity quantifying the statistical fluctuations of the energy spectrum known as the spectral compressibility [27]. In the metallic phase, the spectrum is rigid—approximately described by GOE random matrices—and fluctuations are small, $\kappa \to 0$. In the insulating phase, fluctuations are large and $\kappa = 1$. At the mobility edge, $\kappa_c$ takes on an intermediate value depending only on the universality class of the MIT and carrying information on the multifractal character of the critical eigenstates [28]. It has been conjectured that $\kappa_c = 1 - D_1/3$, where the “information dimension” $D_1$ gives the amount of entropy of the critical eigenstates [29]. For the Anderson model, $D_1 = 1.95 \pm 0.005$ [30], which leads to the prediction $\kappa_c = \kappa_c = 0.347$, in excellent agreement with the numerically measured value $\Lambda_c = 0.342 \pm 0.01$. The alternate conjecture [31] $2 \kappa_c = 1 - D_2/3$ predicts $\kappa_c \approx 0.29$, deviating significantly from our numerical results. This demonstrates that the CFS peak at criticality is a direct universal experimental probe of $D_1$, independent of the disorder distribution and spatial correlation.

In conclusion, we have shown that CFS constitutes an experimentally measurable order parameter for Anderson MITs. The peak contrast obeys a one-parameter scaling law, gives direct access to properties which are in general extremely difficult to assess, such as the critical exponents, and exhibits a universal value at criticality related to the multifractal properties of eigenstates. Unlike CBS, which is absent when TRS is broken, CFS is robust, universal, and does not require any specific symmetry. It could thus be used to characterize different types of MITs beyond the conventional GOE class.

S.G. acknowledges the support of the PHC Merlion Programme of the French Embassy in Singapore. This work was granted access to the HPC resources of TGCC under the allocation No. 2015-057083 and No. 2016-057644 made by GENCI (Grand Equipement National de Calcul Intensif) and to the HPC resources of MesosPSL financed by the Region Ile de France and the project Equip@Mesos (Reference No. ANR-10-EQPX-29-01) of the program Investissements d’Avenir supervised by the Agence Nationale pour la Recherche. This research is supported by the National Research Foundation, Prime Minister’s Office, Singapore and the Ministry of Education, Singapore under the Research Centres of Excellence programme.