Anderson transition in three-dimensional disordered systems with symplectic symmetry

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The Anderson transition in a 3D system with symplectic symmetry is investigated numerically. From a one-parameter scaling analysis the critical exponent $\nu$ of the localization length is extracted and estimated to be $\nu = 1.3\pm0.2$. The level statistics at the critical point are also analyzed and shown to be scale independent. The form of the energy level spacing distribution $P(s)$ at the critical point is found to be different from that for the orthogonal ensemble suggesting that the breaking of spin rotation symmetry is relevant at the critical point.

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Since the original work by Anderson [1] there has been considerable interest in the metal-insulator transition in disordered electron systems [3-6]. Critical phenomena at the Anderson transition are conventionally classified according to the universality class into which the system falls: orthogonal, unitary or symplectic [3-6]. The Anderson transition has been studied intensively numerically, analytically and experimentally. Nevertheless, in spite of this effort, we believe it is fair to say that some aspects of the Anderson transition remain puzzling. For example, the critical exponent $\nu$ of the localization length has been estimated for three-dimensional (3D) systems with orthogonal $\mathbb{O}$ and unitary symmetry $\mathbb{U}$ by means of finite-size scaling. The estimated numerical values of the critical exponent for these two universality classes have turned out to be rather close to each other. At present it is unclear whether or not this is an accidental coincidence. An obvious question immediately presents itself; does this coincidence also occur for the symplectic symmetry class? And if so does this coincidence also hold for other characteristics of the critical point?

Systems belonging to the symplectic universality class exhibit the Anderson transition even in two-dimensions (2D) $\mathbb{S}$, while systems belonging to the unitary and orthogonal classes do not, in general, exhibit any Anderson transition in 2D. Thus we also have the opportunity, when studying symplectic systems, to see how the critical behavior at the Anderson transition depends on the dimensionality of the system.

The statistical properties of energy levels $\mathbb{P}$ in the vicinity of the Anderson transition, and at the critical point in particular, have attracted considerable attention recently [3-6,21-23]. On the metallic side of the transition it has been demonstrated that the energy level statistics can be described by random matrix theory $\mathbb{P}$: for example, the spacing $s$ between successive energy levels is well described by a distribution function $P(s)$ which is quite close to the Wigner surmise. In contrast, on the insulating side of the transition, energy levels are uncorrelated and the spacing distribution is Poissonian. At the critical point, where the metal-insulator transition takes place, it has been claimed [6,7] that the energy level statistics are also universal but different from those predicted by random matrix theory. These so called critical statistics are believed to be universal in the sense that they depend neither on the system-size nor on the details of the model Hamiltonian. It is expected that these critical statistics should be determined only by the symmetry of the system and that they should be reflected in the critical behavior at the Anderson transition $\mathbb{P}$.

The existence of universal critical statistics has been demonstrated numerically for a 3D orthogonal system and for several 2D systems $\mathbb{P}$ [21-23]. For 2D symplectic systems, it has been observed that the level spacing distribution at the critical point $(P_c(s))$ exhibits a power-law behavior as $P_c(s) \sim s^4$ for $s \ll 1$ [21,22]. For 2D unitary systems it has been found that the spacing distribution behaves as $P_c(s) \sim s^2$ for $s \ll 1$ [22]. These behaviors of the level correlations for small $s$ are consistent with random matrix theory. However, it has also been reported [24] that in 3D $P_c(s)$ is unaffected by the presence of an Aharonov-Bohm flux (AB flux), even though the AB flux should break time reversal symmetry. If, as is claimed in [24], $P_c(s)$ is insensitive to the breaking of time reversal symmetry it immedi-
ately prompts the question; is $P_c(s)$ also insensitive to the breaking of spin rotation symmetry?

In this letter, we consider a 3D system with symplectic symmetry. In particular, we estimate the critical exponent $\nu$ for the localization length and examine the spacing distribution $P_c(s)$ of the energy levels in the critical regime.

The model we adopt here is described by the Hamiltonian

$$H = \sum_{<i,j>, \sigma, \sigma'} V_{i, \sigma} C_{i, \sigma}^\dagger C_{j, \sigma'} + \sum_{i, \sigma} \xi_i C_{i, \sigma}^\dagger C_{i, \sigma}$$

with

$$V_{i, \sigma} = V[\exp(-i\theta \sigma_k)]_{\sigma, \sigma'}, \quad k = \hat{x}, \hat{y}, \hat{z},$$

where $C_{i, \sigma}^\dagger$ denotes a creation (annihilation) operator of an electron at the site $i$ with spin $\sigma$, and $\{\sigma_x, \sigma_y, \sigma_z\}$ denote the Pauli matrices. The lattice sites $i$ are supposed to lie on a simple cubic lattice. The strength of the hopping amplitude is denoted by $V$. The site-diagonal potentials $\{\xi_i\}$ are assumed to be distributed independently, and their distribution is taken to be uniform in the range $[-W/2, W/2]$. The parameter $\theta$ characterizes the strength of the spin-orbit coupling. For $\theta = 0$ orthogonal symmetry is recovered. Here, two cases of strong spin-orbit coupling, $\theta = \pi/6$ and $\theta = \pi/4$, are studied. The length is scaled by the lattice spacing and $\hat{x}(\hat{y}, \hat{z})$ denotes the unit vector in the $x$- ($y$, $z$)-direction. We note that this model is a 3D generalization of the Ando model [10] proposed for a 2D symplectic system. It is easy to verify that the Hamiltonian is invariant under time reversal. In the following, we confine ourselves to the case of the band center ($E = 0$), for simplicity.

First, we carry out a finite-size scaling analysis [24] of the Anderson transition and estimate the critical exponent $\nu$. We consider a quasi-one dimensional system $(M \times M \times L)$ with $L \gg M$ whose cross section is composed of an $M \times M$ two-dimensional lattice with a periodic boundary condition. We calculate the localization length $\xi_M$ along such a quasi-one dimensional system with the transfer matrix method, in which we adopt the quaternion-real representation of the Hamiltonian so as to carry out numerical multiplications efficiently. The system-sizes treated here are $M = 6, 8, 10$ and $12$ with $L$ up to $5 \times 10^4$. An average over four independent realizations of random potentials has been performed in order to reduce the error of raw data, resulting in relative errors smaller than 1%. In Fig. 1, the renormalized localization length $\Lambda_M$ defined by $\Lambda_M \equiv \xi_M/M$ is plotted as a function of the disorder parameter $W$ for $\theta = \pi/6$. It is clear that the Anderson transition takes place at $W_c/V = 19.0 \pm 0.2$ for this $\theta$. The standard analysis for the critical exponent $\nu$ of the localization length defined as $\xi(W) \sim |W - W_c|^{-\nu}$ ($W \to W_c$) yields $\nu = 1.3 \pm 0.2$. This value of $\nu$ is close to those obtained for the orthogonal and the unitary symmetry classes in 3D [3, 4]. The value of the renormalized localization length at the critical point $\Lambda_c$ is $\Lambda_c = 0.56 \pm 0.02$ (Fig. 1), slightly smaller than those obtained for the orthogonal and the unitary classes [3, 4]. A similar calculation for $\theta = \pi/4$ leads to $W_c/V = 19.9 \pm 0.2$ with $\nu = 1.3 \pm 0.2$ and $\Lambda_c = 0.55 \pm 0.02$. The fact that both $\nu$ and $\Lambda_c$ are insensitive to the strength of the spin-orbit coupling $\theta$ supports the single-parameter scaling behavior of $\xi_M/M$. By introducing the scaling parameter $\xi$, we have demonstrated that $\xi_M/M$ is indeed a single parameter function of $M/\xi$ (Fig. 1, inset).

Now we focus on the level statistics at the critical point. Clarifying the relationship between the statistics at the critical point and the critical behavior of the localization length and of the conductivity is one of the important open problems in the theory of the Anderson transition. It has been proposed in refs. [25] and [26] that the asymptotic form of the critical spacing distribution $P_c(s)$ of neighboring energy levels is related to the critical exponent $\nu$. The proposed form for $P_c(s)$ is

$$P_c(s) \sim \exp(-Cs^{2-\gamma}), \quad s \gg 1,$$

where $\gamma$ is related to the critical exponent $\nu$ of the localization length

$$\gamma = 1 - \frac{1}{d \nu}.$$  

Here $C$ is a positive constant, which may depend on the symmetry of the system, and $d$ denotes the dimensionality. For $s \ll 1$, the form of $P_c(s)$ is expected to be $P_c(s) \sim s^{\beta}$, where $\beta$ is equal to 1, 2 and 4 for the orthogonal, the unitary and the symplectic universality classes, respectively. It has also been suggested that the overall shape of $P_c(s)$ can be described by the form $[24]$

$$P_c(s) = As^\beta \exp(-Bs^{2-\gamma}).$$

The constants $A$ and $B$ are determined by the two constraints $\int P(s)ds = 1$ and $\int sP(s)ds = 1$. For a 3D system with orthogonal symmetry the above formula [24], with $\nu \approx 1.3$, describes reasonably well the numerical data for $P_c(s)$ [4, 5, 7].

We have investigated the level spacing distribution $P_c(s)$ at the critical point for our 3D symplectic system, by numerically diagonalizing the Hamiltonians of the $M \times M \times M$ systems with $M = 6, 8, 10$ and $12$. The numbers of realizations of random potentials are 2000 for $M = 6$ and 1000 for $M = 8, 10$ and $12$. One-tenth of the unfolded spectra around $E = 0$ ($|E| \lesssim V$) is used for calculating the spacing distribution $P_c(s)$. This is justified if $W_c$ does not vary considerably for energies $E$ close to the band center. In fact, the critical disorder $W_c$ for $E = 2V$ and $\theta = \pi/6$ is estimated to be $W_c/V = 18.9 \pm 0.5$, which is almost the same as that for $E = 0$. 

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The spacing distributions $P_c(s)$ at the critical point $W_c = 19V(\theta = \pi/6)$ for $M = 6, 8, 10$ and $12$ are shown in Figs. 2 and 3. It is seen that $P_c(s)$ is independent of the size of the system $M$ confirming the existence of a critical spacing distribution.

First we consider the limiting behavior of $P_c(s)$ as $s \to 0$. Here we find $P_c(s) \sim s^\beta$ with $\beta \simeq 4$ (see inset Fig. 2). This quartic limiting behavior is characteristic of systems with symplectic symmetry and is a clear indication that the breaking of spin rotation symmetry is relevant at the critical point.

Next we consider the behavior of $P_c(s)$ in the limit $s \gg 1$. A fit to (3) for $s > 2$ yields $\gamma = 1.0 \pm 0.15$. Making use of (4) this yields $\nu > 2.2$ which is inconsistent with the value of $\nu = 1.3 \pm 0.2$ we obtained earlier. In fact the data are well fitted by a simple exponential law $P_c(s) \sim \exp(-\alpha s)$ with $\alpha \simeq 1.7$ (Fig. 2, solid line). We note that a good fit to data for 3D orthogonal [21] and 2D symplectic systems [21,23] has also been obtained with a simple exponential.

Finally we consider a fit to the entire spacing distribution. If we take equation (3) with $\beta = 4$ and $\gamma = 0.75$, a value obtained by substituting $\nu \simeq 1.3$ into (4), we find a very poor fit to $P_c(s)$ (dashed line Fig 2). On the other hand if we vary $\gamma$ so as to obtain the best fit (see Fig 3) we find $\gamma = 1.43 \pm 0.01$ which corresponds to $\nu < 0$ which is physically unacceptable. We conclude that the proposed form, corresponding to equations (3) and (4), is not consistent with our numerical data. For comparison, we also plot in Fig. 3 $P_c(s)$ for a 2D symplectic system [21,23] where the exponent $\nu$ is estimated to be $\nu \simeq 2.7$ [11,12]. It is worth noting that although the estimated critical exponent $\nu$ in 2D is roughly twice our estimate for $\nu$ in 3D the corresponding values of $\gamma$ obtained from (4) are close to each other. If the formulae (3) and (4) were valid, $P_c(s)$ in 2D would have to look similar to that in the 3D system. We see in Fig. 3 that this is clearly not so.

In summary, we have analyzed the Anderson transition in a 3D system with symplectic symmetry. The critical exponent $\nu$ of the localization length is estimated to be $\nu = 1.3 \pm 0.2$, which is rather close to the values found in 3D unitary and orthogonal systems. On the other hand, we have demonstrated that the energy level spacing distribution $P_c(s)$ at the critical point is sensitive to the breaking of spin rotation symmetry. In particular for $s < 1$ we find $P_c(s) \sim s^\beta$ with $\beta \simeq 4$ which is characteristic of the symplectic symmetry class. The sensitivity of $P_c(s)$, at small $s$, to the breaking of spin rotation symmetry is consistent with the conventional classification of the critical behavior according to symmetry.

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FIG. 1. The renormalized localization length $\Lambda_M$ as a function of the disorder $W$ for $\theta = \pi/6$. Open triangles, open diamonds, open squares and open circles correspond to $M = 6$, 8, 10 and 12, respectively. Inset: One-parameter scaling behavior of $\Lambda_M$ for $\theta = \pi/6$ and $\pi/4$. Filled triangles, filled diamonds, filled squares and filled circles represent the data in the case of $\theta = \pi/4$ for $M = 6$, 8, 10 and 12, respectively, while open marks are for $\theta = \pi/6$.

FIG. 2. The spacing distribution $P_c(s)$ at the critical point $W = W_c (= 19V)$ for $\theta = \pi/6$. Open triangles, open diamonds, open squares and open circles stand for the data for $M = 6$, 8, 10 and 12, respectively. Dashed curves represent the result by the formula (5) with $\gamma = 0.75$ and $\beta = 4$. Solid line is a function $\propto \exp(-1.68s)$. Inset: Double logarithmic plot of $P_c(s)$ for $s \ll 1$. The solid line expresses the behavior $\propto s^4$ whereas the dashed lines express $\propto s$.

FIG. 3. The spacing distribution $P_c(s)$ at the critical point $W = W_c (= 19V)$ for $\theta = \pi/6$ is shown in the linear-scale. For comparison, the data of the critical spacing distribution for the 2D symplectic system, which is taken from Ref. [22], are also plotted (crosses). The dashed curve represents the Wigner surmise for the Gaussian symplectic ensemble. The solid one represents the best fit based on the formula (5) with $\gamma = 1.43$ and $\beta = 4$. 