Quantum Percolation in Magnetic Fields

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A generalized average inverse participation ratio, for the one-electron wave functions of a dilute tight-binding model on a d-dimensional hypercubic lattice, is studied at finite magnetic fields. Extended wave functions appear above a quantum threshold bond concentration, p_q. This threshold decreases at small magnetic fields, and shows a periodic dependence on the magnetic flux through a basic plaquette, with period $\phi_0 = \hbar c/e$. Extended states appear and disappear periodically even at $d=2$.

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The effects of magnetic fields on the metal-insulator Anderson transition have been the subject of much speculation, some experimental work, and little detailed theoretical understanding.[1-3] In the absence of the field, some wave functions become localized because of destructive interference of waves along parallel routes. These cancellations are eliminated when the phases of the functions are modified by the magnetic flux through loops, and therefore one expects that weak fields may *delocalize* the wave functions, yielding a *negative magnetoresistance*.[1-3] It is also believed that critical exponents may have different values for finite fields.[4] A strong magnetic field, on the other hand, may shrink the wave functions and thus decrease the conductivity.[2]

In an apparently different direction, much recent effort has been invested in the understanding of the periodic dependence of the conductivity of a simple ring on the magnetic flux through it.[5-11] Depending on the size of the ring and on the method of averaging over the randomness, physical properties of the ring show periodicity in the flux with a period of either $\phi_0 = \hbar c/e$ or $\phi_0/2$.[9-11]

In the present paper we combine these two phenomena by studying the effects of a magnetic field, H, on *quantum percolation*.[12-16] Considering a dilute tight-binding one-electron model on a d-dimensional hypercubic lattice, with a concentration p of nonzero nearest-neighbor off-diagonal transfer energy elements, we calculate the quantum threshold $p_q(H)$ above which extended states begin to appear. Our results, shown in Fig. 1 for $d=3$, indicate a periodic dependence of p_q on ϕ, with period ϕ_0. Here and below fields H are measured by their flux $\phi = Ha^2$ through a unit cell, where a is the lattice constant. Although the results are not periodic with period $\phi_0/2$, there is a significant increase in p_q also for half-integral values of ϕ/ϕ_0, when the magnetic phase factors are real.

The oscillation of p_q with H implies a range of concentrations in which a periodic sequence of metal-insulator transitions should be observed as function of H. Unfortunately, if the lattice constant is 1 Å then the period in H is of order 10^9 Oe. Reasonable periods may be realized for larger lattices, e.g., of granular units. In any case, the decrease in p_q for small finite H should be observable experimentally.

Although our results in $d=2$ are somewhat less accurate, we find there, too, finite regions in H (around $\phi/\phi_0 \sim 0.2$) where $p_q(H)$ decreases (from 1) down to about 0.7. Hopefully, this is also observable (at least in computer experiments?).

The usual $H=0$ quantum percolation Hamiltonian is written as[12-16]

$$\mathscr{H} = \sum_i \epsilon_i |i\rangle\langle i| + \sum_{\langle ij\rangle} t_{ij}^0 |j\rangle\langle i| + \text{H.c.}, \tag{1}$$

where $|i\rangle$ is the state on the site i of the lattice, while the nearest-neighbor transfer energy t_{ij}^0 (for the electron to hop from i to j) is equal to 1 (with probability p) or to 0 (with probability $1-p$). Unlike the earlier work,[12-16] we now introduce also very small random diagonal energies, ϵ_i, with zero average. These re-

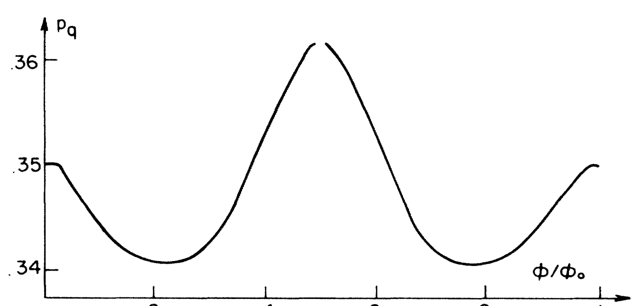

FIG. 1. The quantum threshold p_q as function of the magnetic flux ϕ/ϕ_0, for $d=3$. The graph repeats periodically, with period 1.

move the degeneracies of the eigenstates, and thus simplify the choice of the inverse participation ratio (see below). They have no other effect on the results [except in the close vicinity of $\phi/\phi_0 \sim 0, \frac{1}{2}$, where $\epsilon_i \simeq \sin(2\pi\phi/\phi_o)$].

Earlier work on (1)[15-18] showed that the electronic wave functions are all localized for $p < p_q$, and some extended state appeared above the quantum threshold p_q (which is higher than the geometrical one, p_c). In particular, no extended states were found for any $p < 1$ at $d = 2$. In the present work we present a refinement of Ref. 16, in which the problem with degenerate eigenstates is removed by the diagonal ϵ_i's. We calculate a modified average inverse participation ratio as a power series in p, and show that it diverges for $p \to p_q^-$ as $(p_q - p)^{-\gamma}$. For $H = 0$, our new results agree qualitatively with the previous ones, and we find $p_q \simeq 0.35 \pm 0.02$, 0.22, 0.16, 0.13, 0.11, and 0.09 (with errors of ± 0.01) and $\gamma \simeq 2.2 \pm 0.2$, 1.4, 1.2, 1.1, 1.0, and 1.0 (with errors of ± 0.1) for $d = 3$, 4, 5, 6, 7, and 8, respectively. The values of p_q agree with those of Refs. 15 and 17.

The magnetic field is introduced into the Hamiltonian (1) via phase factors on t_{ij},[19]

$$t_{ij} = t_{ij}^0 \exp(i\mathbf{A}\cdot\mathbf{r}_{ij}/\phi_0), \tag{2}$$

where $\mathbf{A}$ is the magnetic vector potential. In three dimensions, with the magnetic field $\mathbf{H}$ along the z direction, and in the Landau gauge, this becomes

$$t_{ij} = t_{ij}^0 \exp(iHay_i/\phi_0) \tag{3}$$

if $\mathbf{r}_{ij}$ is along the x direction,[19] and $t_{ij} = t_{ij}^0$ otherwise. In two dimensions we take the field to be perpendicular to the xy plane. It is not trivial to generalize these rules to $d > 3$. For the purpose of the present calculation we chose to use the algorithm (3) for all d, i.e., to project loops on a single (xy) plane.

As explained in Ref. 16, we now solve the Hamiltonian (1) on finite clusters, with up to eleven bonds, and find the eigenvalues E and the (normalized) eigenfunctions $\psi_E(i)$ (which are now nondegenerate). These are then used to calculate the inverse participation ratio, defined as

$$y(\Gamma) = \sum_E \left[\sum_i |\psi_E(i)|^4\right]^{-1}, \tag{4}$$

for the cluster Γ. If the eigenstate is extended, $\psi_E(i) \sim 1/\sqrt{N}$ (N is the number of sites on Γ), then $y(\Gamma) \sim N^2$. For a localized state, $\psi_E(i) \sim \delta_{io}$ and $y(\Gamma) \sim N$. We averaged $y(\Gamma)$ over many realizations of the random (small) ϵ_i's, and found a rather fast convergence to a sharp average value. We next weighted the average $y(\Gamma)$ by $p^{N_b}(1-p)^{N_p}$, where N_b and N_p are the numbers of bonds inside and adjacent to Γ, and find the average $\chi(p)$, which is expected to diverge if $y(\Gamma) \sim N^2$.[16]

For $H = 0$ we found eleven terms in the new series for $\chi(p)$, and analyzed them using inhomogeneous differential approximants.[20] In the (L,M,N) approximant we solved the linear equation

$$P_2\, d\chi/dp + P_1\chi = P_0, \tag{5}$$

P_0, P_1, and P_2 being polynomials of degrees L, M, and N. With the assumption that $\chi \sim (p_q - p)^{-\gamma}$, the ratio P_η/P_2 is an approximant for $\gamma/(p_q - p)$. The estimates for $3 < d < 8$ were quoted above. We found no indication of a singularity below $p = 1$ at $d = 2$. We also note that our results are inconclusive as to the identification of the upper critical dimension, at which γ becomes equal to unity (this could happen anywhere for $d \geq 6$).

We now turn to *nonzero fields.* We first note that the phase factors (3) do not affect any physical property of clusters which contain no loops. One can always choose new phases for $\psi_E(i)$, which will absorb those arising from the fields, and $|\psi_E(i)|^2$ will not be affect-

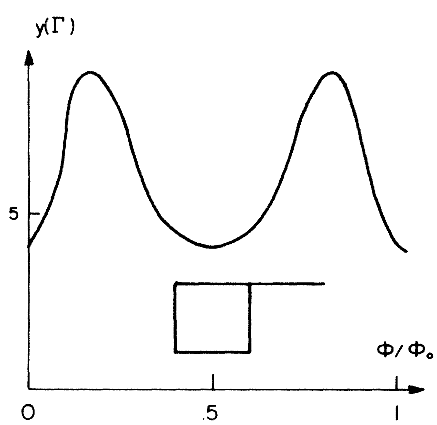

FIG. 2. The inverse participation ratio $y(\Gamma)$ for the cluster shown in the inset.

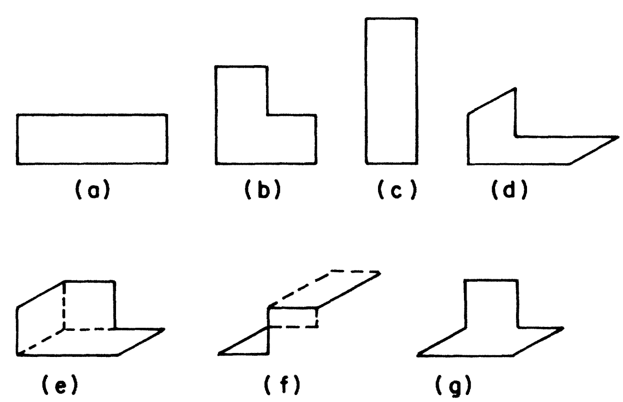

FIG. 3. An example of different clusters which have the same topology.

TABLE I. Coefficients a_k in $\chi(p)=1+6p+5p^2+180p^3-862.15p^4+\sum a_k p^k$ for $d=3$, and estimates for p_q and γ (based on averages over Padé approximants of eight-term series).

ϕ/ϕ_0	a_5	a_6	a_7	a_8	p_q	γ
0	11 500.3	−104 700.0	1093 056.4	−10 945 648.0	0.35 + 0.02	2.2 + 0.2
$\frac{1}{4}$	11 490.0	−104 420.5	1095 779.2	−11 001 494.9	0.32 + 0.03	2.7 + 0.4
$\frac{1}{2}$	11 464.4	−104 628.0	1095 962.9	−10 987 386.0	0.35 + 0.02	2.2 + 0.2

ed. On clusters which contain loops, the phase which accumulates after one goes around a loop is equal to $2\pi\phi/\phi_0$, where ϕ is the magnetic flux through the projection of the loop on the xy plane. For example, if the cluster shown in the inset in Fig. 2 lies in the xy plane then its Hamiltonian is

$$\mathscr{H}=\begin{bmatrix} 0 & t & 0 & 1 & 0 \\ t^* & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 1 \\ 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \end{bmatrix}, \tag{6}$$

with $t=\exp(i_\phi/\phi_0)$. The eigenvalues are 0 and $\pm[5\pm(9+8\cos\phi/\phi_0)^{1/2}]^{1/2}$, and the dependence of $y(\Gamma)$ on H is shown in Fig. 2. Note that $y(\Gamma)$ is periodic in ϕ, with period ϕ_0, and symmetric under $H\rightarrow -H$. The same is true for all $y(\Gamma)$'s, and thus also for $\chi(p)$. We also note that two clusters which are topologically the same, and which have the same projected loop areas on the xy plane, have the same values of $y(\Gamma)$, although their Hamiltonian matrices look different; a unitary transformation always exists to map the wave functions on each other. The results change, of course, if the projections on the xy plane change. Thus, the clusters of Figs. 3(a)–3(c) all have the same $y(\Gamma)$, but those of Figs. 3(e)–3(g) have a different value, and the value changes again (back to the $H=0$ value) if the whole cluster lies in the xz plane.

Since only clusters with loops yield modified values of $y(\Gamma)$, we had to repeat the calculation outlined above only for these clusters. A detailed list of these, up to eight bonds, appears in the work of Aharony and Binder.[21] However, we had to weight the different $y(\Gamma)$'s according to the different orientations of the loops relative to the xy plane. For example, the cluster in Fig. 2 has weight $\binom{d}{2}(8d-8)p^5(1-p)^{10d-10}$, and the fraction of cases in which the loop lies in the xy plane is $1/\binom{d}{2}$.

Table I shows, as an example, the coefficients of our series for $d=3$, for one set of random energies. We analyzed these series using the same method as outlined above, and we show p_q vs ϕ from one of our Padé estimates in Fig. 1. Similar results were found for $d>3$. The exponent γ also showed a periodic variation with H, exhibiting decreasing values as ϕ/ϕ_0 varied from 0 to $\frac{1}{4}$. Since this is an *effective* exponent, in a crossover regime, it is difficult to say if all the points with noninteger ϕ/ϕ_0 belong to a new universality class.[4] If they do, the new value of γ is *lower* than that for $H=0$.

The statements in Ref. 11, which predict an *exact* periodic behavior with period $\phi_0/2$, are not correct for complex loops or for loops with dangling bonds. Our series probes a significant number of these configurations and we see no evidence that such periodicity becomes more nearly realized as the length of the series is increased. However, we note that there is a significant increase in p_q at half-integral values of ϕ/ϕ_0. In particular, we could not trace extended states at $d=2$ for these odd values.

In conclusion, the magnetic field dependence of the localization threshold is found to be periodic, with an anomalous increase in p_q for $\phi\approx\frac{1}{2}\phi_0$, a behavior which is very different from that of random continuum models.[1-3] We hope that the results of this paper will stimulate searches for this anomalous field-dependent behavior.

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