PHYSICAL REVIEW B VOLUME 30, NUMBER 11 1 DECEMBER 1984

Periodicity of transport coefficients with half flux quanta in the Aharonov-Bohm effect

Dana A. Browne, John P. Carini, K. A. Muttalib,* and Sidney R. Nagel
The James Franck Institute and The Department of Physics, The University of Chicago, Chicago, Illinois 60637
(Received 23 July 1984)

We prove that all transport coefficients of a dirty normal metal in the Aharonov-Bohm geometry are exactly periodic with a period of a half flux quantum. This special periodicity appears only after performing the ensemble average over a symmetric distribution of random potentials. This result indicates how to improve numerical studies of localization by selectively averaging over the ensemble in such a manner as to preserve the special symmetries of the Hamiltonian.

The Aharonov-Bohm effect with half flux quanta in highly disordered metals, which was first predicted by Al'tshuler, Aronov, and Spivak,[1] has now been verified experimentally by several groups.[2–6] This calculation was based on the maximally crossed (or Langer-Neal) diagrams, and it was not clear how it could be interpreted in terms of the solutions of the one-electron Schrödinger equation although a physical interpretation of the diagrams was given in terms of a path-integral approach.[2,7] In particular it was not obvious from examining the Schrödinger equation why half a flux quantum was the fundamental periodicity.[8] In a recent paper[9] we examined this novel effect in terms of first-order degenerate perturbation theory and offered an explanation of the phenomena including the role of dimensionality and disorder. We showed that the origin of this extra oscillation in the conductivity at the flux value $\phi=\phi_0/2$, where $\phi_0=hc/e$ is the flux quantum, could be traced to the existence of degeneracies and time-reversal invariance occurring at $\phi=\phi_0/2$ in addition to those occurring at $\phi=0$ and ϕ_0. In a ring no degeneracies of this type occur at other values of ϕ. We considered the participation ratio

$$P=\frac{\left[(1/N)\sum_i|\psi(r_i)|^2\right]^2}{(1/N)\sum_i|\psi(r_i)|^4}\ ,$$

where r_i is the position of the ith site of an N-site system, and showed that the quantum correction to the conductivity due to localization has similar behavior at $\phi_0/2$ as at 0 and ϕ_0.

In the present paper we show the generality of this effect for all levels of disorder. We prove for independent electrons in the large system limit that the *total* conductivity, and in fact all transport coefficients, are *exactly* periodic with a period $\phi_0/2$ as long as the random on-site energy is symmetrically distributed about some average value. The proof depends on the observation that an ensemble average[10] over the random potentials restores particle-hole symmetry in a highly disordered system. It is this averaging over ensembles that was not done in the work of Büttiker, Imry, and Landauer[8] and others[11] which pertained to a specific given sample. We also observe that by averaging over appropriate members of the ensemble in pairs before doing the rest of the ensemble average one can significantly reduce the fluctuations in certain numerical simulations of highly disordered systems.

We first note the existence of certain symmetries that appear in the Hamiltonian. We use a gauge-invariant tight-binding version[9] of the single-particle Schrödinger equation on a ring. The electronic energies and eigenvalues can be obtained simply by diagonalizing the matrix:

$$H(\phi)=\begin{pmatrix} V_1 & T_{12} & 0 & \cdots & T_{1N}e^{2\pi i\phi/\phi_0} \\ T_{12} & V_2 & T_{23} & \cdots & 0 \\ 0 & T_{23} & V_3 & & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ \vdots & \vdots & \vdots & & \vdots \\ T_{1N}e^{-2\pi i\phi/\phi_0} & 0 & 0 & \cdots & V_N \end{pmatrix}\ , \quad (1)$$

where V_i is the on-site random potential and T_{ij} the random hopping matrix element between nearest-neighbor sites i and j. The symmetries that are important for the present situation are already apparent for a 3-site and a 4-site ring in the limit of no disorder (all $V_i=0$, all $T_{ij}=\text{const}$). In Fig. 1 we show the eigenvalues as a function of flux ϕ for the two cases. In the 3-site system there is a symmetry between the top and bottom of the band if ϕ is changed by $\phi_0/2$. This "glide plane" symmetry exists for all rings with an odd number of sites. In the 4-site system there is a symmetry between the top and bottom of the band (with no change in ϕ). This particle-hole symmetry exists for all even-numbered rings.

The presence of diagonal disorder (random values for V) destroys these symmetries for any given set $\{V_i\}$. However, we are only interested in the average electronic properties of the ring since in the large-N limit the typical properties should be the same as the average properties. We will show that if V_i is symmetrically distributed about its average value, then the symmetries are restored when an average of the physical quantity is taken over the ensemble of the random $\{V_i\}$. Off-diagonal disorder (random T_{ij}) does not break these symmetries.

To see how the symmetries are restored we construct the average over members of the ensemble by first summing specially related pairs chosen in the following manner. For each member of the ensemble, given by a set of potentials

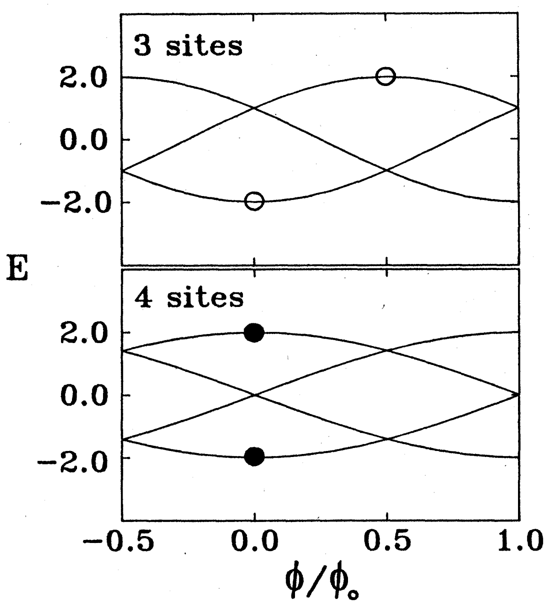

FIG. 1. The energy eigenvalues for a 3-site and a 4-site ring with no disorder. The circles show the points related by the symmetries discussed in the text.

$\{V_i\}$, we also take a second member of the ensemble with Hamiltonian $H'(\phi)$ given by the set of potentials $\{V_i'=-V_i\}$ (where the potential at every site has been multiplied by -1). For a ring with N sites

$$H'\left(\phi+N\frac{\phi_0}{2}\right)=U^+[-H(\phi)]U\ , \tag{2}$$

where we have simply made a unitary transformation by the matrix U on the negative of the Hamiltonian in Eq. (1). The unitary transformation we have used is the one which changes the sign of every wave function on alternate sites, $\psi_{\alpha}'(r_i)=(-1)^i\psi_\alpha(r_i)$ where α labels the eigenstate:

$$U=\begin{pmatrix}1 & 0 & 0 & \cdots & 0\\ 0 & -1 & 0 & \cdots & 0\\ 0 & 0 & 1 & \cdots & 0\\ \vdots & \vdots & \vdots & \cdots & \vdots\\ 0 & 0 & 0 & \cdots & (-1)^{N+1}\end{pmatrix}. \tag{3}$$

Thus, the Hamiltonian $H(\phi)$ is mapped into the matrix $-H'[\phi+N(\phi_0/2)]$ by this transformation. It is clear that any quantity which depends only on $|\psi_\alpha(r_i)|^2$ will have the "glide plane" and particle-hole symmetries when the two systems $H(\phi)$ and $H'(\phi)$ are averaged. Thus, the participation ratio P has these symmetries when averaged. More complicated functions of four wave functions, which are important for the transport coefficients, also obey these symmetries when averaged. An example is

$$\psi_\alpha(r_i)\psi_\beta(r_{i+n})\psi_\gamma(r_j)\psi_\delta(r_{j+n})\ ,$$

which picks up a factor of $(\pm 1)^2=1$ under the transformation.

In the large system limit the physical properties of the system are not expected to be sensitive to whether or not there are an even or an odd number of sites in the ring provided we look at a narrow band of energies rather than a single eigenstate. Thus a large odd- (even-) numbered ring will have exact (approximate) "glide plane" symmetry and approximate (exact) particle-hole symmetry. We expect the approximate symmetries to get proportionally better as the system size is increased. Thus, the average of P over a narrow energy band in a large system will be periodic with flux $\phi_0/2$ (and not ϕ_0 as would be expected from gauge symmetry alone[8,11]) since the states in the upper half of the band at ϕ and $(\phi+\phi_0/2)$ can both be mapped onto the same states in the lower half of the band at ϕ. This argument goes through equally well for a square array of sites that form a two-dimensional cylinder or a cubic array of sites that form a thick-walled cylinder.

The participation ratio is only a portion of the conductivity.[9] We will now show that the conductivity is also periodic with period $\phi_0/2$. The conductivity $\sigma_{a,b}(\phi)$, where a and b denote Cartesian indices, is given by a current-current correlation function[12]

$$i\omega\sigma_{a,b}(\omega,\phi)=\int\frac{d\omega'}{\pi}\frac{\chi''_{J_a,J_b}(\omega',\phi)}{\omega'-\omega-i\delta}-\frac{Ne^2}{m}\delta_{a,b}\ , \tag{4}$$

where

$$\chi''_{J_a,J_b}(\omega,\phi)=\pi\sum_{\alpha,\beta}[f(\epsilon_\alpha)-f(\epsilon_\beta)]\langle\alpha|J_a|\beta\rangle \times\langle\beta|J_b|\alpha\rangle\,\delta(\hbar\omega+\epsilon_\alpha-\epsilon_\beta)\ , \tag{5}$$

where $f(\epsilon)$ is the Fermi-Dirac distribution function. The current operator in the tight-binding model is given by

$$\vec{J}=\sum_i e\frac{d\vec{r}_i}{dt}|r_i\rangle\langle r_i|=\frac{1}{i\hbar}\sum_i[e\,\vec{r}_i|r_i\rangle\langle r_i|,H]\ , \tag{6}$$

where H is given by Eq. (1). Thus,

$$\langle\alpha|J_a|\beta\rangle=\frac{e}{i\hbar}\sum_{\langle ij\rangle}(\vec{r}_i-\vec{r}_j)_a T_{i,j}\psi^*_\alpha(r_i)\psi_\beta(r_j)\ , \tag{7}$$

where the sum is only over nearest-neighbor pairs.

Clearly, under the unitary transformation [Eq. (3)] $\langle\alpha|J_a|\beta\rangle$ changes sign but since the conductivity there is a product of two matrix elements, the conductivity has the same "glide-plane" symmetry for odd-numbered rings and the same particle-hole symmetry for even-numbered rings as does the participation ratio. Thus in the large system limit the conductivity has periodicity of $\phi_0/2$.

This same argument can be extended to any of the other usual transport coefficients, such as the spin susceptibility and dielectric constant. In these cases the matrix elements result in products of wave functions on the same site.

These conclusions evidently apply only to a noninteracting system. However, the leading corrections due to interactions can be included in a random-phase approximation (RPA) expression for the dielectric constant ϵ. Since we have just found that the averaged ϵ also has the same period, $\phi_0/2$, interactions do not effect these results to this level of approximation.

While the transport properties of a ring are exactly periodic with flux $\phi_0/2$ in the limit of infinite system size, it is useful to know the corrections for finite systems. We have studied numerically the approximate particle-hole symmetry of small rings with an odd number of sites at $\phi=0$. A measure of the particle-hole asymmetry is the difference between the average participation ratios in the bottom $\bar{P}_{BOT}$ and top $\bar{P}_{TOP}$ halves of the band when pairs from the ensemble are averaged: $\Delta P = \bar{P}_{BOT} - \bar{P}_{TOP}$. In the limit of low disorder $\Delta P = 2/(3N)$ since all states at $\phi = 0$ are sinusoidal standing waves each of which has $P = \frac{2}{3}$ except for the lowest state in the band which has $P = 1$. For intermediate and large disorder ΔP falls off much faster than $2/(3N)$. We conclude that even in the worst case of small disorder the particle-hole asymmetry in the participation ratio falls off at least as fast as N^{-1}.

In addition to ensemble averages themselves, it is interesting to look at the variance about the average. This can be done by treating each set $\{V_i\}$ separately or by averaging each pair $\{V_i\}$ with $\{-V_i\}$ first and then taking the average over these pairs. We find the remarkable result that if we perform the average in the latter fashion so as to preserve the approximate particle-hole symmetry at each step of the calculation, the noise is much reduced especially at large or small values of disorder. This is shown in Fig. 2 where we plot the variance about the average for a 7-site and a 63-site system. The calculation was done in the two ways mentioned above. We find that the variance is much smaller if the special averaging is done first for all values of disorder except for the region where the localization length at the center of the band is comparable to the system size. At that value of disorder the variance is largest. We see that as the system size is increased the benefit of averaging pairs first is also increased. However, even with only seven sites there is a dramatic savings in the number of different matrices that must be diagonalized to get the same statistics. For an even-site system, where the symmetry is exact, the correct average is given immediately.

In conclusion, we have shown that the transport properties of a disordered material in the Aharonov-Bohm geometry show a periodicity of $\phi_0/2$ instead of the expected ϕ_0. This result is valid only when the ensemble average over the set of random potentials is done. We have shown this by taking the average in a special way which preserves the symmetries of the Hamiltonian at each step. We have also shown that performing the average in this way can be very useful in numerical simulations of localization since it substantially reduces the statistical variations.

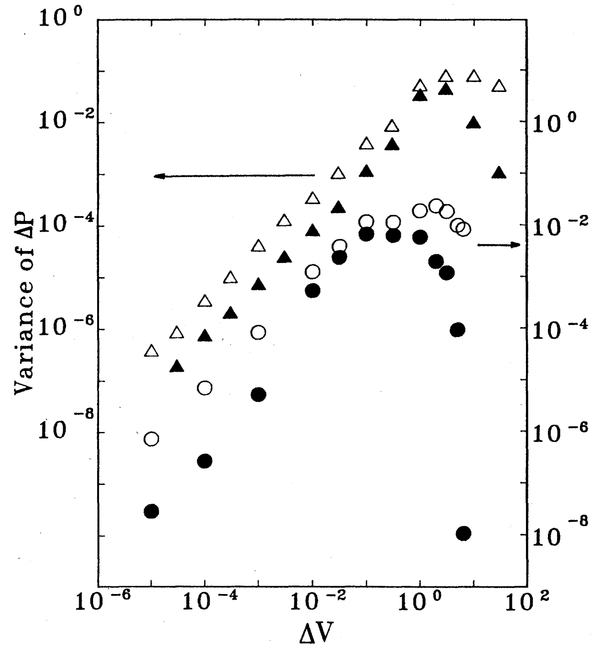

FIG. 2. The variance in the quantity ΔP vs disorder for 7-site (triangles) and 63-site (circles) systems. The triangles are shifted vertically by two decades for clarity. The closed symbols indicate averaging done with the specially selected pairs discussed in the text and the open symbols indicate the average done in the normal fashion. ΔV is the width of the distribution in V where $T_{ij} = -1$.

We wish to thank N. Birge, Y. Jeong, L. Kadanoff, A. Libchaber, and S. H. Shenker for helpful discussions. J.P.C. and S.R.N. were supported by National Science Foundation Grant No. DMR 82-01182. D.A.B. and K.A.M. were supported by National Science Foundation–Materials Research Laboratory Grant No. DMR 82-16892.

*Address after September 1984: Department of Physics, Brookhaven National Laboratory, Upton, NY 11973.

[1]B. L. Al'tshuler, A. G. Aronov, and B. Z. Spivak, Pis'ma Zh. Eksp. Teor. Fiz. **33**, 101 (1981) [JETP Lett. **33**, 94 (1981)].

[2]D. Yu. Sharvin and Yu. V. Sharvin, Pis'ma Zh. Eksp. Teor. Fiz. **34**, 285 (1981) [JETP Lett. **34**, 272 (1981)].

[3]B. L. Al'tshuler, A. G. Aronov, B. Z. Spivak, D. Yu. Sharvin, and Yu. V. Sharvin, Pis'ma Zh. Eksp. Teor. Fiz. **35**, 476 (1982) [JETP Lett. **35**, 588 (1982)].

[4]F. Ladan and J. Maurer, C. R. Acad. Sci. Ser. II **296**, 1753 (1983).

[5]M. Gijs, C. Van Haesendonck, and Y. Bruynseraede, Phys. Rev. Lett. **52**, 2069 (1984).

[6]B. Pannetier, J. Chaussy, R. Rammal, and P. Gandit, Phys. Rev. Lett. **53**, 718 (1984).

[7]G. Bergmann, Phys. Rev. B **28**, 2914 (1983). In this work, which was inadvertantly omitted from the list of references in our Ref. 9, the backscattering contribution to the conductivity of the two time-reversed paths which return to the origin is considered. This leads to an enhanced contribution to the conductivity at $\phi_0/2$. It was not shown why additional structure from multiple paths around the ring do not also occur at $\phi_0/4$, $\phi_0/6$, etc., or why the conductivity is strictly periodic with flux $\phi_0/2$.

[8]M. Büttiker, Y. Imry, and R. Landauer, Phys. Lett. **96A**, 365 (1983). This paper solved the one-dimensional Schrödinger equation and gave ϕ_0, not $\phi_0/2$, as a fundamental period for any given system.

[9]J. P. Carini, K. A. Muttalib, and S. R. Nagel, Phys. Rev. Lett. **53**, 102 (1984).

[10]The idea of taking an ensemble average was independently suggested by Y. Gefen (unpublished).

[11]Y. Gefen, Y. Imry, and M. Ya. Azbel, Phys. Rev. Lett. **52**, 129 (1984); Surf. Sci. **142**, 203 (1984). The transmission coefficient of a ring was calculated and a period of ϕ_0 was deduced. Under very special conditions a higher harmonic at $\phi_0/2$ could become dominant. Those authors claim that their effect is different from that of Refs. 1 and 2.

[12]See, for example, P. C. Martin, in *Many-Body Physics*, edited by C. DeWitt and R. Balian (Gordon and Breach, New York, 1968).