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Level broadening and quantum interference effects in insulators

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We study quantum interference effects in the context of the Nguyen-Spivak-Shklovskii (NSS) model including level broadening due to inelastic events. Improving on a recent mean-field approach, we incorporate path correlations and study both the log-conductance and its fluctuations. In contrast with mean field, we find that all changes in the conductance, due to broadening, imply *corrections to the localization length*. Furthermore, the change in the magnetoconductance sign, predicted by mean field, is not borne out by direct solution of the NSS model within reasonable broadening parameters. We compute a phase diagram for the magnetoconductance in the broadening parameter space and propose a replica theory for weak inelastic events.

The effects of inelastic events on quantum interference in insulators was recently addressed within the independent path approximation[1] by Entin-Wohlman, Levinson, and Aronov (ELA).[2] Phonons are introduced by adding an imaginary part in the off-resonant local energies. ELA report the surprising conclusion that level broadening can bring about a change of sign in the magneto conductance (MC) depending on the relation between broadening width and level average. They also find that the sign of the MC may be temperature dependent. Such behaviors are important in determining different experimental regimes as a function of temperature, disorder, and magnetic field strength. For example, does the reported change in the MC preempt wave function shrinkage producing the same effect?

The shortcoming of the ELA approach, addressed here, is the exclusion of path correlations permitting proper accounting of localization length effects.[3,4] By correlation we mean path sections shared by different electron paths on the lattice or path intersections. Such effects should become more important as temperature decreases and hops become longer ranged. Path correlations are also unaccounted for by the minimal three-site Holstein model as different paths do not overlap. It is then worthwhile to ask whether the predicted changes in the MC sign survive proper account of path correlations, and if so, are they amplitude effects or exponential changes in the conductance?[4,5]

We have assessed this question by numerically solving the Nguyen, Spivak, and Shklovskii (NSS) model of quantum interference effects.[6] At weak phonon scattering and zero field, we find a small exponential enhancement of the conductance as opposed to the prefactor effect predicted in Ref. 2. When a magnetic field is applied, regions of positive and negative MC are found. Nevertheless, negative MC regions only occur for unreasonably large broadening, and should rule them out in experiments. We also inquire into the conductance fluctuations and find that they continuously decrease, as broadening increases, until a saturation sets in. Finally, we propose a replica analysis, including path correlations, to justify some of the features described above at weak broadening.

To study quantum interference (QI) processes for a single electron hop in the insulating regime, the NSS model places the impurities on the sites of a regular lattice. The initial and final sites for the hop are chosen at the edges of a square. The overall tunneling amplitude is computed by summing all (virtual) paths between the two points, each contributing an appropriate quantum mechanical complex weight.[6,7] These weights are obtained from an Anderson tight-binding Hamiltonian with on-site energies taking random values from a symmetric distribution of width W and hopping matrix elements V. To describe strong localization, the Anderson parameter is taken to be much smaller than one $(V/W \ll 1)$,[6] which consequently favors forward-scattering paths. The effective hopping matrix element is computed using a locator expansion.[8]

To add inelastic events at intermediate sites, we consider that local energies are broadened so that $\epsilon_{i_\Gamma} = \epsilon_1 + i\epsilon_2$.[2] Neglecting backscattering and for paths of length t, the overlap amplitude (Green's function) between the initial and final sites is given by

$$\langle i|G(E)|f\rangle = V\left(\frac{V}{W}\right)^t J(t), \quad J(t) = \sum_\Gamma e^{i\phi_\Gamma} \prod_{i_\Gamma} \eta_{i_\Gamma}, \quad (1)$$

where ϕ_Γ is the phase picked up on the directed path Γ and $|i\rangle, |f\rangle$ the initial and final sites, respectively. The interference information is captured by the function $J(t)$, while the factor $(V/W)^t$ is the leading contribution to the expected exponential decay of the localized wavefunction. In Ref. 2 the interference term has the form $\Pi_{i_\Gamma}\eta_{i_\Gamma} = j_r + i j_i$, where the $j_{r,i}$ are uncorrelated. We take the broadening model literally, so strictly speaking one should use

$$\eta_{i_\Gamma} = \frac{\gamma + i\epsilon_2/W}{1 + (\epsilon_2/W)^2}, \quad (2)$$

where $\gamma = \epsilon_1/W$ takes values ± 1 on the bonds with equal probability. This choice correlates real and imaginary parts in the expression for the overlap amplitude on the bonds. The imaginary part of the local energy levels, ϵ_2, is chosen from a flatop distribution with a finite positive mean. The width of

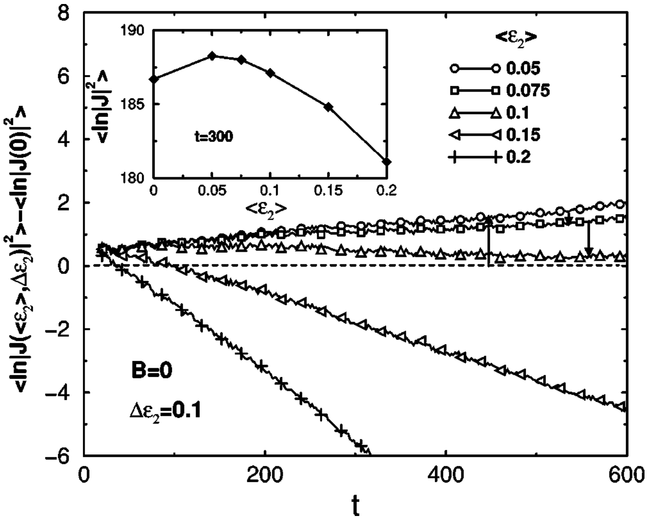

FIG. 1. The figure shows the change in log-conductance as a function of system size for different values of the broadening average, $\Delta\epsilon_2=0.1$ and $B=0$. The linear dependence evidences asymptotic exponential changes in the conductance implying correction to the localization length. Arrows indicate sequence of curves. The inset shows the data for a fixed size $t=300$. The conductance is first enhanced and then reduced by level broadening.

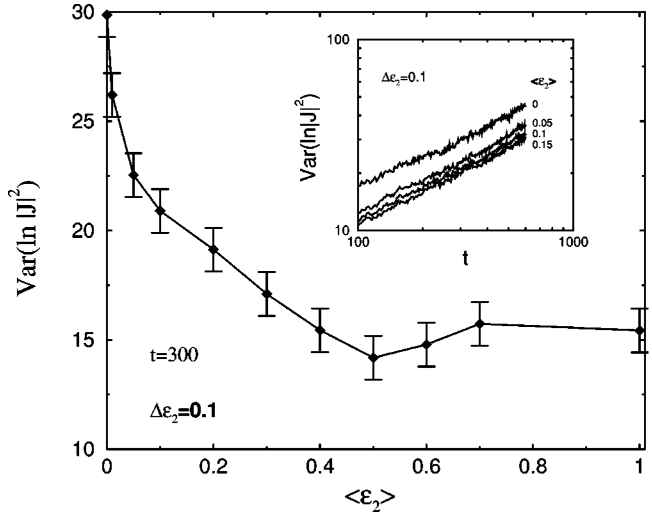

FIG. 2. Change of the fluctuations of $\ln|J|^2$ as a function of the average broadening for the same parameters of Fig. 1. The variance exhibits only a monotone decay as a function of $\langle\epsilon_2\rangle$, in agreement with the behavior of path intersections in the replica argument (see text). The inset shows the variance as a function of system size t.

the flatop, $\Delta\epsilon_2$, is such that ϵ_2 remains positive definite. The level average should also be smaller than the energy difference to the Fermi level so that in summary $\Delta\epsilon_2/2\leqslant\langle\epsilon_2\rangle\ll W$. We have set $W=1$ in the numerics. For any particular realization of randomness, all paths and their correlations are evolved using the transfer matrix algorithm.[4]

We performed extensive transfer matrix computations for the two-dimensional NSS model using Eqs. (1) and 2. Lattice sizes of up to $t=600$ and 2000 realizations of randomness were typically used. The magnetic field only changes the phase of hopping electrons in the model.

At zero field, we find that a small amount of level broadening enhances conductance *exponentially*, i.e., changes in the slope of $\log|J|^2$, which increase linearly with size t. Figure 1 shows the difference between the log-conductance at finite and zero broadening (at $\Delta\epsilon_2=0.1$ fixed). The dotted line represents the zero broadening reference. At $\langle\epsilon_2\rangle=0.05$ (full circles) the conductance is enhanced for all system sizes shown. As one sweeps through $\langle\epsilon_2\rangle=0.075-0.1$ (full squares and up triangles), the conductance is still increased but less so, as compared to 0.05. Finally beyond $\langle\epsilon_2\rangle=0.1$ (full up triangles), the conductance decreases. Note that there is a size dependence, i.e., for $\langle\epsilon_2\rangle=0.15$ we observe an enhanced conductance for $t<100$, while above, the conductance is reduced. The value of system size t for which the crossover occurs decreases as $\langle\epsilon_2\rangle$ increases. The inset of Fig. 1 shows a followup of the conductance sequence for a fixed value of t. As explained by ELA, the increase in the conductance is due to the fact that, at zero field and no broadening, randomly signed paths result in an interference minimum. Any small added phase due to broadening of the field, will result in increasing the transmission.

The fluctuations, on the other hand, exhibit a monotone reduction in the same range described above, as depicted in Fig. 2. The inset in the figure shows the $V\,\mathrm{ar}(\ln|J|^2)$ as a function of system size, for increasing values of the average broadening. Further increase of level broadening results in a continuously decreasing conductance while, concurrently, the *conductance fluctuations decrease* until a saturation is reached at around $\langle\epsilon_2\rangle=0.5$. Phase memory is only lost in such saturation range. Before that, the system still responds to the magnetic field.

Figure 3 shows the phase diagram for the sign of the MC, in broadening parameter space. The first region (region I) corresponds to a positive MC. This region extends further than the enhancement region at $B=0$ (see Fig. 1). In region II, the MC is negative. In both ranges the conductance changes are exponential (Fig. 3 inset), implying a change in the localization length ξ, i.e., first an increase then a decrease in ξ. We note that the broadening is already very strong

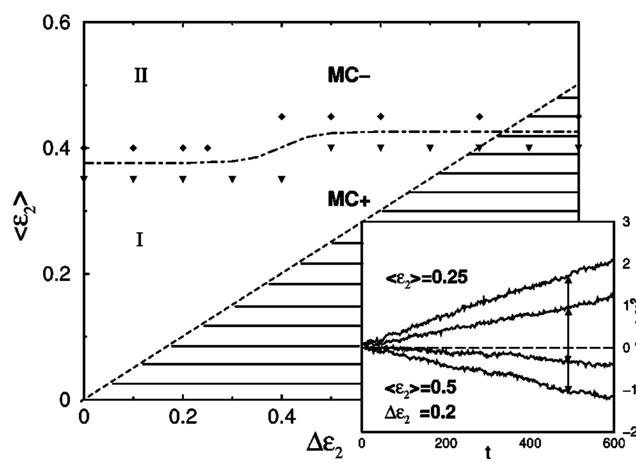

FIG. 3. Phase diagram showing the two MC regimes as a function of level broadening in the physical parameter range. The *dot-dashed* curve, separating the phases, is drawn as a guide to the eye. Points above (below) the curve denote negative MC (positive MC) conductance regions found numerically. The hatched region corresponds to $\Delta\epsilon_2/2>\langle\epsilon_2\rangle$. The inset shows evidence of exponential corrections to the conductance for $+$MC and $-$MC regimes (curves above and below dotted line, respectively).

($\langle\epsilon_2\rangle \sim W=1$ in simulations) when one enters the negative MC region. This would imply level widths so large that one would no longer be in the insulating state. Consequently, we believe the limit of negative MC, predicted by mean field, is never reached in experimental conditions.

As expected, the response to the field gets weaker as broadening is increased within region I. This is manifest both in the log-conductance and its fluctuations. In region II, while the MC is negative, there is no change in the fluctuations within the error bars (and within physical parameter range). The border of region I coincides with the random phase limit studied in Ref. 4. It is only in this limit that we obtain the unitary symmetry in the presence of path correlations. We note that, in the region where there is a negative MC, the fluctuations, again, decrease sharply with broadening (after having saturated for $0.5<\epsilon_2<1$). Nevertheless, the fluctuations now increase with the field in correlation with the log-conductance.

We now present a replica argument accounting for the observed numerical results. The correspondence between discrete and continuum replica arguments has been developed in previous papers[9,4] and will only briefly be accounted here.

The quantity J is a sum of all single paths between the initial and final impurities. As we have complex numbers on the bonds of the lattice model, we must consider the moments $\langle (JJ^*)^n\rangle)$ corresponding to the characteristic function $\exp(n \ln|J|^2)$. To distinguish between paths from J and J^* we label them as forward (J) or backward (J^*) propagating in ''time.'' The moment $\langle (JJ^*)\rangle$ will represent all paths pairs, one from J and one from J^* going between the initial and final impurities. To analyze the averages over disorder, we focus on the bonds, which carry independent random variables.[9]

If a single path crosses a bond, the contribution from that bond after averaging is given by $\langle\eta\rangle = \langle(\gamma + i\epsilon_2/W)/(1+(\epsilon_2/W)^2)\rangle$. Here $\gamma=\pm 1$ with equal probability according to the NSS model. The brackets $\langle\cdot\rangle$, denote both average over $\pm$ disorder and broadening. This quantity is strictly less than one in absolute value. Crossing of different sets of t bonds for each term in $\langle JJ^*\rangle$ has the form $\langle\eta\rangle^t\langle\eta^*\rangle^t$ and implies an exponential decay with the length of the system. On the other hand, if *two paths* cross a particular bond (pairing), there are three possibilities; $\langle\eta\eta\rangle = \langle\eta^*\eta^*\rangle$ and $\langle\eta\eta^*\rangle$. The first of these averages involves either two forward or backward paths propagating together (crossing the same bond). These we label *charged paths* because they are field sensitive. On the other hand the second expression involves one forward and one backward path propagating together. The latter we label as *neutral paths* and do not respond to the field.

Neutral paths make the largest contribution to $\langle (JJ^*)^n\rangle$, decaying much slower with length t than charged paths. Furthermore, for small level broadening ($\langle\epsilon_2\rangle << 1$), both neutral and charged paths decay much slower than single, unpaired, paths. As in the analysis of Ref. 4, averaging then encourages *paths pairing*.[10]

Averaging implies combinatorial interactions between path pairs. In the absence of broadening, there is a combinatorial attraction factor of three per intersection. As neutral paths decay much slower than charged paths they will give the dominant contribution. Nevertheless, charged paths can occur for short lengths in between two neutral path intersections. The multiplicity is then $4\langle\eta\eta^*\rangle + (\langle\eta\eta\rangle + \langle\eta^*\eta^*\rangle)$. When broadening is zero $\langle\eta\eta^*\rangle = 1$ and $\langle\eta\eta\rangle = \langle\eta^*\eta^*\rangle = 1$ so we have a factor of six (three per crossing), while if broadening is nonzero the charged terms decrease more rapidly than their neutral counterparts, and the effective attraction is reduced.

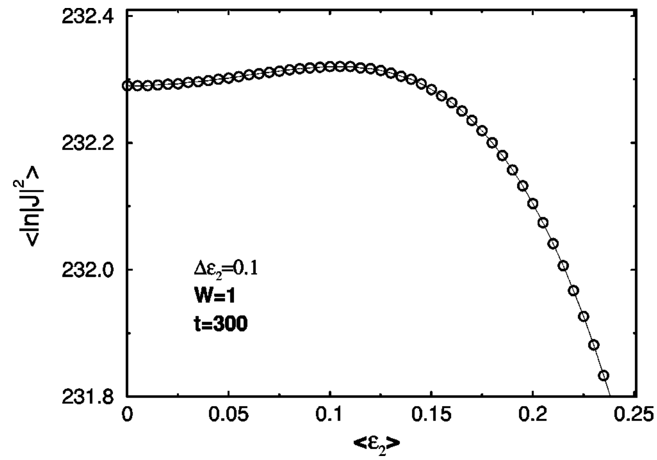

FIG. 4. Interplay between local and global (path interaction) contributions, according to replicas, giving the conductance enhancement with broadening. As explained in the text, the figure has a single adjustable parameter for the behavior of ρ in Eq. (3). We have taken $W=1$ and $t=300$ as in Fig. 1.

In order to obtain analytical expressions we go to the continuum limit, where discrete paths are seen as world lines of bosons with contact interactions.[9] In the continuum, the presence of broadening results in

$$\langle \ln|J(t)|^2\rangle = (\ln 2 + \ln\langle\eta\eta^*\rangle - \rho)t,$$

$$C_3(\ln|J(t)|^2) = 6\rho t. \tag{3}$$

$C_3(\ln|J(t)|^2)$ denotes the third cummulant of the argument, the leading measure of fluctuations to order of t, and ρ is proportional to the attraction factor between paths (or multiplicity discussed above[4]). With the previous expressions in mind, we can explain the features described previously; Eq. (3) implies a monotonous decay, with broadening parameters, of the path interactions (or ρ in continuum theory). This results in a monotonous decay of the fluctuations according to $C_3(\ln|J(t)|^2)$. This is indeed what is observed in the transfer matrix studies (see Fig. 2) up to $\langle\epsilon_2\rangle = 1$.

In order to simultaneously explain the initial increase and then decrease of the log-conductance, we must take into account the term $\ln\langle\eta\eta^*\rangle$ in Eq. (3). Such a term gets reduced continuously with broadening. Nevertheless, at small broadening the reduction of ρ is strong winning over $\ln\langle\eta\eta^*\rangle$ and thus increasing $\ln|J|^2$. At larger broadening the reduction of ρ begins to saturate (see Fig. 2) and the term $\ln\langle\eta\eta^*\rangle$ dominates, reducing the conductance monotonically. Although the mapping between the discrete model and the continuum does not permit deriving ρ explicitly we have plotted Eq. (3) for $\langle \ln|J(t)|^2\rangle$ with one free parameter, i.e., taking $\rho = C(4\langle\eta\eta^*\rangle + (\langle\eta\eta\rangle + \langle\eta^*\eta^*\rangle))$. Using $W=1$ and fixing $\Delta\epsilon_2 = 0.1$ we obtain Fig. 4. Although the agreement is not quantitative the interplay between intersections and the local contribution explained above is borne out. The replica approach outlined here takes only the leading contribution assuming that neutral paths go together always except, only briefly, at intersections.

Regarding the field dependence, previous replica arguments[4] have shown that the field couples through two consecutive path intersections (bubble diagram). The intersection now has the form $4\langle\eta\eta^*\rangle+(\langle\eta\eta\rangle\exp(2i\phi)+\langle\eta^*\eta^*\rangle\exp(-2i\phi))=4\langle\eta\eta^*\rangle+2\langle\eta\eta\rangle\cos(2\phi)$, where ϕ is the flux enclosed by the diagram. As the field increases, for any fixed broadening, the attraction is reduced ($\cos\phi$ gets smaller as ϕ increases, increasing $\ln|J|^2$ and reducing $Var(\ln|J|^2)$ [see Eq. (3)].

We have not been able to explain, through replicas, the change in the MC sign for large broadening. Although the parameter range in which it occurs is unphysical, it implies a change in the localization length (according to numerics) and should be related to the path crossings.

In conclusion, we have studied the effects of level broadening on the NSS model for quantum coherence in the strongly localized regime. Our approach in contrast with that of ELA, includes path correlations and takes the level broadening model literally. We found that path correlations turn amplitude effects, implied by mean field, into exponential effects, suggesting important corrections to the localization length. Furthermore, we find that fluctuations always get reduced by broadening in a nontrivial way.

With the tools of replica theory we are able to explain the above features in terms of an interplay between reduction of the effective path interactions and the local bond average due to broadening. The effective path interaction always decreases and governs the fluctuations. The log-conductance depends both on the path interactions and local bond averages $\langle\eta\eta^*\rangle$. Departing from Eq. (3) one identifies a local ξ_0 and a global (interference) ξ_g contribution to the localization length[4]

$$\xi_0^{-1}=2\ln\frac{W}{\sqrt{2\langle\eta\eta^*\rangle}V}, \tag{4}$$

$$\xi_g^{-1}=\rho. \tag{5}$$

Obviously, the phonon model used here is the simplest possible approach and does not consistently describe contact with a thermal reservoir. Such a consistent model, preserving unitarity, would involve absorption and re-injection of probability amplitude as done by Entin-Wohlman *et al.*[11] in the context of the Holstein model and D'Amato and Pastawski[12] for one-dimensional systems. Work in this direction is in progress.

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[1] U. Sivan, O. Entin-Wohlman, and Y. Imry, Phys. Rev. Lett. **60**, 1566 (1988); Phys. Rev. B **40**, 8342 (1989).
[2] O. Entin-Wohlman, Y. Levinson, and A.G. Aronov, Phys. Rev. B **49**, 5165 (1994).
[3] Y. Shapir and X.R. Wang, Europhys. Lett. **4**, 1165 (1987); Mod. Phys. Lett. B **4**, 1301 (1990).
[4] E. Medina and M. Kardar, Phys. Rev. B **46**, 9984 (1992).
[5] J.L. Pichard, M. Sanquer, K. Slevin, and P. Debray, Phys. Rev. Lett. **65**, 1812 (1990).
[6] V.L. Nguyen, B.Z. Spivak, and B.I. Shklovskii, Pis'ma Zh. Éksp. Teor. Fiz. **41**, 35 (1985) [JETP Lett. **41**, 42 (1985)]; Zh. Éksp. Teor. Fiz. **89**, 11 (1985) [Sov. Phys. JETP **62**, 1021 (1985)].
[7] H.L. Zhao, B.Z. Spivak, M.P. Gelfand, and S. Feng, Phys. Rev. B **44**, 10 760 (1991).
[8] I.M. Lifshits and V. Ya. Kirpichenko, Pis'ma Zh. Éksp. Teor. Fiz. **77**, 989 (1979) [Sov. Phys. JETP **50**, 499 (1979)].
[9] M. Kardar, Nucl. Phys. B **290**, 582 (1987).
[10] For zero broadening and field, $\langle\eta\eta\rangle^t=\langle\eta^*\eta^*\rangle^t=\langle\eta_i\eta_i^*\rangle^t=1$ and $\langle\eta\rangle^t=0$ so pairing is mandated.
[11] O. Entin-Wohlman, Y. Imry, A.G. Aronov, and Y. Levinson, Phys. Rev. B **51**, 11 584 (1995).
[12] J.L. D'Amato and H.M. Pastawski, Phys. Rev. B **41**, 7411 (1990).