Brief Reports

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Dephasing and quantum localization in disordered systems

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Two self-consistent Green-function theories of quantum localization [the theory of Abou-Chacra, Anderson, and Thouless (AAT) and the effective dephasing approximation] are compared. It is shown that, in contrast to recent claims, the self-energy of the AAT equation represents population relaxation (T_1 processes) rather than pure dephasing (T_2 processes).

The effective dephasing approximation (EDA) developed recently[1-3] provides a new way of interpreting and calculating the localization of a quantum particle in a disordered medium, in terms of a frequency-dependent dephasing rate. The dephasing rate is introduced as a self-energy in the tetradic (Liouville-space) Green function. The theory of Anderson localization developed by Abou-Chacra, Anderson, and Thouless[4] (AAT) focuses, on the other hand, on the calculation of an energy-dependent self-energy of the dyadic (ordinary, Hilbert-space) Green function. In this report the EDA and AAT equations are compared in order to clarify a recent confusion[5] regarding the role of dephasing in quantum localization.

In order to calculate quantum transport in disordered systems and to introduce correctly the concept of pure dephasing, we shall consider the ensemble-averaged density matrix of a quantum particle at time t which is given by

$$\langle \rho_{jk}(t) \rangle = \sum_{m,n} \langle \mathcal{G}_{jk,mn}(t) \rangle \rho_{mn}(0) \ . \tag{1}$$

We are using here a tight-binding basis set, and j, k, m, and n denote states, where the particle is localized at sites j, k, m, and n, respectively. The angular brackets denote an average over the disorder. $\mathcal{G}(t)$ is a Liouville-space (*tetradic*) propagator.[6] Its Fourier transform $\mathcal{G}(E)$ is the Liouville-space Green function:

$$\langle \mathcal{G}(E) \rangle = \left\langle \frac{1}{E-L} \right\rangle \equiv \frac{1}{E-L_{\text{eff}}(E)} \ . \tag{2}$$

L is the Liouville operator, defined by its action on an arbitrary operator A, $LA \equiv [H, A]$, H being the Hamiltonian, and L_{eff} is an *effective Liouville operator,* which determines the time evolution of the ensemble-averaged density matrix of the particle. A proper treatment of transport processes requires calculating the tetradic matrix element $\langle \mathcal{G}_{kk,jj}(E) \rangle$, whose Fourier transform is the time-dependent probability of the particle to occupy the site k at time t when it started at site j at $t=0$.[1-3] This probability is necessary for calculating the frequency-dependent diffusion constant and the ac conductivity.

The EDA is based on the physical intuition that L_{eff} can be expressed in terms of a generalized frequency-dependent dephasing rate $\Gamma(\epsilon)$, where ϵ is the Laplace transform variable conjugate to the time, and $\epsilon = -iE$. $\Gamma(\epsilon)$ describes the loss of phase coherence between different sites and is determined self-consistently. The transport properties at long times are determined by the behavior of $\Gamma(\epsilon)$ for small ϵ. The signature of the Anderson localization transition is the crossover from a dephasing rate that is finite at small frequencies to one that displays an infrared divergence.

The self-consistent equation of AAT provides an approximation for the distribution of diagonal elements $G_{jj}(E)$ of the ordinary *dyadic* Green function

$$G_{jj}(E) = \left[\frac{1}{E-H} \right]_{jj} \ . \tag{3}$$

This Green function is expressed in terms of an energy-dependent self-energy $\gamma_j(E)$. The imaginary part of $\gamma_j(E)$ vanishes for localized states, and it becomes finite when the states are delocalized.

In order to compare the two formulations we recall that the dyadic and tetradic Green functions are formally related by[6]

$$\langle \mathcal{G}_{jk,mn}(E) \rangle = \frac{1}{2\pi i} \int d\omega \langle G_{jm}(\omega) G^{\dagger}_{kn}(\omega - E) \rangle \ . \tag{4}$$

The dyadic Green function $G_{jj}(E)$ allows the calculation of the density of states, and the onset of localization. Using Eq. (4), we see that the distribution of $G_{jj}(E)$, obtained from the AAT formulation, allows only the calculation of $\langle \mathcal{G}_{jj,jj}(E=0)\rangle$. Using a Tauberian theorem, this quantity gives the probability that the particle remains at site j for a long time $t\rightarrow\infty$, when it started at the same site at $t=0$. Therefore the AAT equation does not carry enough microscopic information to calculate the conductivity or transport properties other than $\langle \mathcal{G}_{jj,jj}(E=0)\rangle$. The conductivity may, of course, be estimated, using the AAT analysis by introducing some additional external assumptions (such as scaling arguments). In contrast, the EDA provides an approximation for the full tetradic Green function $\langle \mathcal{G}_{jk,mn}(E)\rangle$ and allows the direct calculation of transport properties. In addition, the AAT equation with nearest-neighbor interactions is virtually independent of the dimensionality d of the problem. As clearly stated by AAT, it is exact on a Cayley tree. Consequently, its predictions in one, two, and three dimensions are basically the same (apart from a simple dependence of the critical disorder on the number of neighbors). In contrast the EDA predicts the absence of transition in $d=1$ and $d=2$ dimensions and the existence of the Anderson transition in $d=3$ dimensions, in agreement with scaling theories of Anderson localization.

In recent articles,[5] Logan and Wolynes (LW) developed an approximate solution to the self-consistent equation of AAT and applied it to Anderson localization in topologically disordered systems and to the dynamics of dipolar excitons. In these articles it was stated that the self-energy of AAT can be interpreted as pure dephasing. LW introduced a damping rate, $\eta=\hbar(2\tau)$, in the dyadic Green function [Eq. (3)] by replacing E with $E+i\eta$, and state that τ might represent a time scale characterizing pure dephasing processes. This statement is incorrect. It is impossible to incorporate pure dephasing processes, which do not affect the populations of the levels, just their phase, by simply adding a damping term to the dyadic Green function. As is well known,[7] pure dephasing may be introduced via the *effective Liouville operator* [Eq. (2)], since pure dephasing is related to the damping of off-diagonal elements of the density matrix. The matrix element of the tetradic Green function, which describes the dephasing process, is[1,6]

$$\langle \mathcal{G}_{jk,jk}(\epsilon)\rangle=\frac{1}{2\pi i}\int d\omega\langle G_{jj}(\omega)G^{\dagger}_{kk}(\omega-E)\rangle\ , \qquad (5)$$

where j and k represent two different sites. The evaluation of the average in the right-hand side of Eq. (5) requires the *joint probability distribution* of G_{jj} and G_{kk}. The distribution of G_{jj} (or G_{kk}) alone, obtained from the AAT formulation, does not allow the calculation of pure dephasing processes. This is to be expected since the dephasing is related to the loss of coherence (phase) between two sites, and is determined by the correlated dynamics of both sites. Any attempt to represent pure dephasing using single-site information is conceptually incorrect. The parameter η of LW is, therefore, simply an inelastic scattering rate corresponding to a finite lifetime of the particle, as pointed out by Thouless and Kirkpatrick.[8] In the language of optical line shapes, η is related to T_1 and not to pure dephasing T_2 processes.[6,7] Since η is an imaginary part of the self-energy of all levels, its dynamical role is trivial. The total density matrix of the system is multiplied by $\exp(-2\eta t)$. Therefore, in contrast to the analysis of LW, η does not have any profound effect on the dynamics of the system, and consequently, it does not influence in any way the Anderson localization. On the other hand, the addition of a dephasing rate Γ to the tetradic Green function does affect the nature of the dynamics. As was shown by Haken and Strobl,[9,10] a coherent exciton motion will turn incoherent as the dephasing rate is increased.

Finally, it should be noted that dephasing processes play a major role in condensed-matter spectroscopy.[6,7,11] The interpretation of quantum localization in terms of dephasing establishes therefore an interesting and potentially useful link between optical and transport properties of disordered systems. The EDA constitutes a general treatment of transport in disordered systems with which coherent motion, incoherent motion, and localization are treated in a unified fashion using the concept of pure dephasing. It is essential to use the Liouville-space, tetradic Green function rather than the Hilbert-space dyadic Green function in order to incorporate pure dephasing processes.

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