Dynamics of short-time-scale energy relaxation of optical excitations due to electron-electron scattering in the presence of arbitrary disorder

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A nonequilibrium occupation distribution relaxes towards the Fermi-Dirac distribution due to electron-electron scattering even in finite Fermi systems. The dynamic evolution of this thermalization process assumed to result from an optical excitation is investigated numerically by solving a Boltzmann equation for the carrier populations using a one-dimensional disordered system. We focus on the short-time-scale behavior. The logarithmically long time scale associated with the glassy behavior of interacting electrons in disordered systems is not treated in our investigation. For weak disorder and short range interaction we recover the expected result that the relaxation rate is enhanced by disorder. For sufficiently strong disorder, however, we find an opposite trend due to the reduction of scattering probabilities originating from the strong localization of the single-particle states. Long-range interaction in this regime produces a similar effect. The relaxation rate is found to scale with the interaction strength, however, the interplay between the implicit and the explicit character of the interaction produces an anomalous exponent.

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The interplay of strong disorder and electron-electron interaction is one of the major issues of contemporary condensed matter physics. This problem may well be behind the insulator metal transition in two dimensions[1] or behind the unexpectedly large persistent current observed in experiments as compared to theoretical predictions.[2] Similarly this interplay is responsible for the glassy behavior of the electrons recently investigated both experimentally[3] and theoretically.[4] Since theoretically the nonperturbative treatment of both disorder and interaction is still a very demanding task, numerical simulations may yield important insight into the problem. In this paper we present results of such a numerical simulation.

For photoexcited ordered semiconductors, it is known that Coulomb scattering is a rapid process.[5] In the presence of a weak disorder, i.e., in dirty metals in the diffusive regime such process may become even faster[7] because the particles diffusively can spend more time close to each other, which results in an enhanced probability of scattering. This enhancement can in other words be attributed to the absence of k vector selection rules in the scattering process.

Very little is known about the Coulomb scattering for the case of a strong disorder. In this paper we show that with increasing disorder the localization length of the single-particle states reduces drastically and hence the scattering probabilities as well. Our result is obtained from numerical investigations of the dynamical energy relaxation due to electron-electron scattering in a system modeling a disordered metal in the localized regime. Our model is related to the quantum Coulomb-glass model introduced and studied in detail in Ref. 8. In these and subsequent studies this model has been used to determine stationary and equilibrium properties of interacting electrons in a disordered environment. The interplay of strong interaction with strong disorder is also responsible for the emergence of glassy behavior[3,4] which results in logarithmically slow relaxation processes with time scales of the order of a day.

Here we are interested in the short-time-scale relaxation of an initially nonequilibrium occupation number distribution which is assumed to be a result of an optical excitation. Ultimately we are interested in optical phase relaxation due to Coulomb interactions in a strongly disordered system. These particular relaxation processes will take place around a local minimum of the free energy of the Coulomb glass. They are completed long before the system moves from one minimum to a lower one. Therefore the logarithmic relaxation times arising due to the slow process of finding the global minimum of the free energy is beyond the scope of the present study. The treatment of optical relaxation due to interactions is not a trivial subject even in ordered semiconductors.[5] In order to gain some insight into these processes we here study first the population relaxation in this time regime, typical for processes within a given minimum. We are aware, however, that phase and population relaxations are not identical. Nevertheless, the dependence of the relaxation rates on disorder and interaction strength in the situation envisaged is interesting in itself as far as optical phenomena are considered.

In order to investigate the diffusive and the localized regimes as well, we use both Hubbard-type short-range interactions and Coulomb-type long-range interactions. We already anticipate that the former is more appropriate in the diffusive regime as it roughly incorporates the screening effect of the other electrons, although, both types of interactions yield qualitatively similar results in the localized regime.

In order to investigate the population relaxation due to the particle-particle scattering we consider a simplified model of a strongly disordered system described by the Hamiltonian that consists of two parts, $H=H_1+H_2$, where the single-particle part H_1 reads as

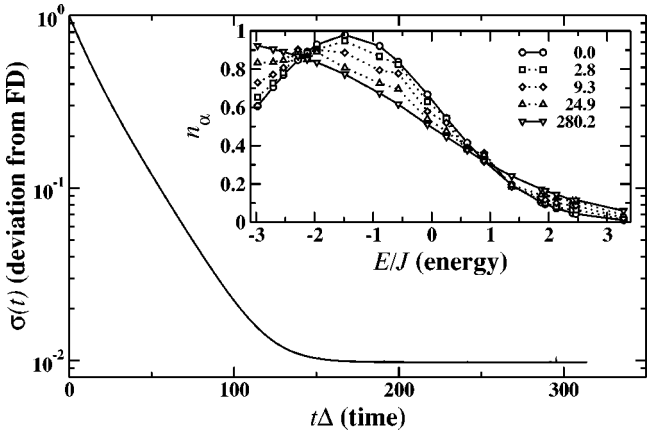

FIG. 1. Typical time evolution of the root-mean-squared deviation of an initially nonequilibrium occupation from the Fermi-Dirac distribution for the case of long-range Coulomb interaction. The inset shows the n_α distribution at different time instants. Time is measured in units of Heisenberg-time Δ^{-1} energy in units of nearest neighbor hopping, J.

$$H_1=\sum_i \varepsilon_i c_i^\dagger c_i+\sum_{i,j} J_{ij} c_i^\dagger c_j, \tag{1}$$

where c_i ($c_i^\dagger$) annihilates (creates) an electron on site i, (i.e., a state $|i\rangle$). We consider electrons without spin. The atomic energy levels ε_i are taken randomly from a box distribution of width W around zero mean value. J_{ij} describe the hopping amplitude from site i to site j. Nearest neighbor approximation has been used with a constant hopping rate J taken as the unit of energy. The sites are assembled in a regular one-dimensional lattice of unit lattice spacing with periodic boundary conditions.

The second part of the total Hamiltonian contains the two-particle interaction which in site representation reads as

$$H_2=\frac{1}{2}\sum_{ij} V_{ij}(c_i^\dagger c_i-K)(c_j^\dagger c_j-K), \tag{2}$$

where for the sake of charge neutrality we have already included a compensating charge of Ke at each lattice site where K is the filling factor. The interaction matrix element is either of short-range or long-range type. In the former case $V_{ij}=U_0$ when two electrons are on the neighboring sites, $|i-j|=1$, and zero otherwise. For long-range interaction, $V_{ij}=U_0/|i-j|$, $U_0>0$ characterizes the strength of the repulsion between electrons located at neighboring sites. In any case due to the Pauli principle the electrons are not allowed to occupy the same site.

The electron-electron scattering is evaluated in an effective single particle basis. This basis is obtained from the diagonalization of the Hamiltonian H_1 including the ''diagonal'' part of the interaction, i.e., as a first step we self-consistently obtain the Hartree–Fock (HF) solution of the Hamiltonian (1) by replacing the parameters ε_i and J_{ij} as $\varepsilon_i+\frac{1}{2}\Sigma_j V_{ij} n_{jj}$ and $J\delta_{\langle i,j\rangle}-\frac{1}{2}V_{ij}n_{ji}$, respectively. In the HF basis our original Hamiltonian can be expressed as

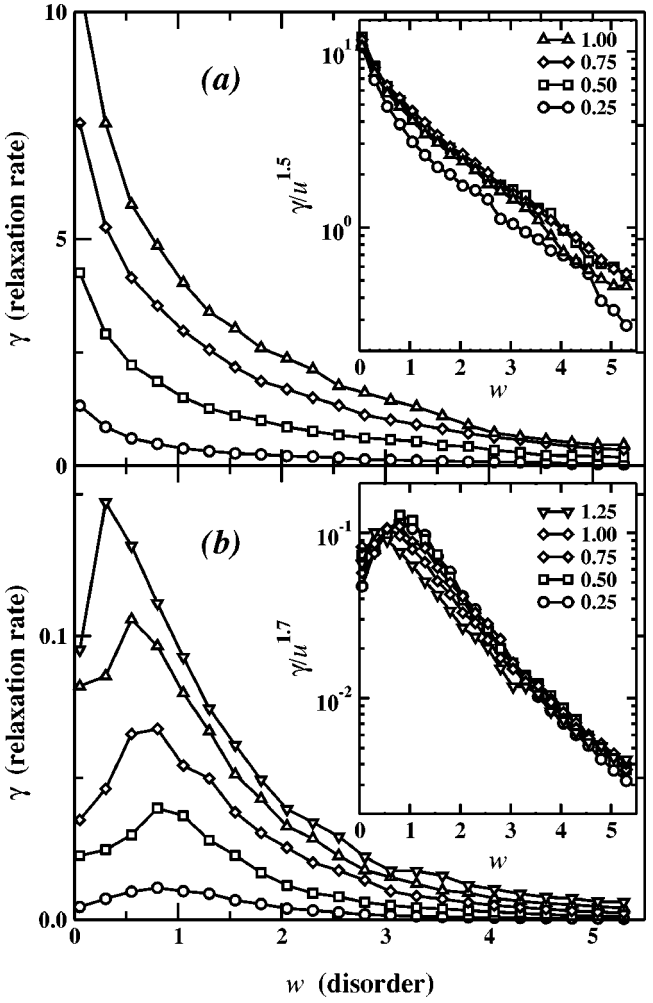

FIG. 2. Dimensionless relaxation rate in units of the mean level spacing for the case $\gamma=\Gamma/\Delta$ of (a) long-range Coulomb interaction and (b) short-range Hubbard interaction as a function of the dimensionless disorder strength $w=W/J$. The initial occupation is similar as in the inset of Fig. 1. The different curves are labeled according to $u=U_0/J$. The insets show the curves which are rescaled with the dimensionless interaction parameter u. The system size is $N=20$.

$$H=\sum_\alpha \varepsilon_\alpha c_\alpha^\dagger c_\alpha+\sum_{\alpha\beta\gamma\delta} U_{\alpha\beta}^{\gamma\delta} c_\alpha^\dagger c_\beta^\dagger c_\gamma c_\delta, \tag{3}$$

where the single-particle part is obviously diagonal in the HF basis with the ε_α's being the HF eigenvalues. In the residual interaction

$$U_{\alpha\beta}^{\gamma\delta}=\sum_{ij} V_{ij} C_{i\alpha}^* C_{j\beta}^* C_{i\gamma} C_{j\delta}, \tag{4}$$

where the $C_{i\alpha}$ numbers represent the HF states in site representation. This model is in fact the standard two-body random interaction model (TBRIM) of fermions. Within the TBRIM, for example, $U_{\alpha\beta}^{\gamma\delta}$ values are chosen randomly from a Gaussian distribution assuming that the single-particle states are sufficiently chaotic, i.e., delocalized. The typical matrix element $\overline{U}\approx\Delta/g$, where g is the dimensionless conductance of the system and Δ is the mean HF-level spacing. In our case these interaction matrix elements contain the

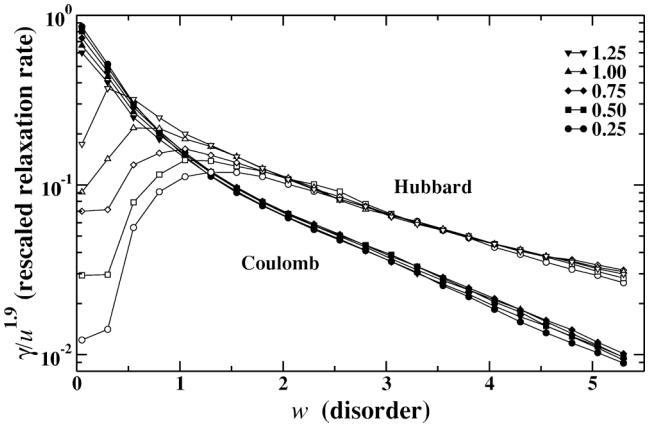

FIG. 3. Average dimensionless relaxation rate $\gamma=\langle\Gamma_\alpha\rangle/\Delta$ as a function of the dimensionless disorder strength $w=W/J$ as obtained from the exponential ansatz for short times. The different curves are labeled according to $u=U_0/J$. Open symbols stand for Hubbard type interaction and filled symbols for Coulomb type interaction. The data for the Coulomb interaction has been scaled down by a factor of N, where $N=20$ is the size of the system.

information about the microscopic details of the original model, e.g., the long-range correlations due to the Coulomb interaction and the presence of a disorder potential. Hence, especially in the case of strong disorder we are not allowed to use the TBRIM model. Also note that Eq. (4) depends on the interaction strength U_0 explicitly through V_{ij} and implicitly through the coefficients $C_{i\alpha}$.

This HF basis corresponds to a zero-temperature equilibrium distribution of the occupation numbers $n_\alpha=\langle c_\alpha^\dagger c_\alpha\rangle$ that equals 1 (0) for $\varepsilon_\alpha\leqslant E_F$ ($\varepsilon_\alpha>E_F$).

We assume that an excitation process has somehow generated an initial, nonequilibrium n_α distribution of the form $n_\alpha=Z^{-1}\exp[-(\varepsilon_\alpha-E_c)^2/2w^2]$, where E_c is the center of the ''excitation'' and w is its energy spread. Z is fixed by the condition $\Sigma_\alpha n_\alpha=N$. The center of the excitation is chosen in the lower half of the energy band, typically at its middle or at the band edge. The width w is typically chosen to be one fourth of the bandwidth with which one could more or less avoid the possibility of the non physical situation of $n_\alpha>1$. During the numerical simulation this initial distribution is assumed to relax[6] towards equilibrium via electron-electron scattering. This process is described by the Boltzmann equation[7]

$$\frac{d}{dt}n_\alpha=-\frac{2\pi}{\hbar}\sum_{\beta,\gamma,\delta}|U_{\alpha\beta}^{\gamma\delta}|^2\delta(\varepsilon_\alpha+\varepsilon_\beta-\varepsilon_\gamma-\varepsilon_\delta)\times[n_\alpha n_\beta(1-n_\gamma)(1-n_\delta)-(1-n_\alpha)(1-n_\beta)n_\gamma n_\delta]. \tag{5}$$

As we have noted already, in the localized regime we cannot apply assumptions of ergodic wave functions in order to estimate the typical value of $U_{\alpha\beta}^{\gamma\delta}$. Also our spectra are discrete therefore the δ function in Eq. (5) is not possible to be satisfied exactly. However, we may approximate it with a box of finite width of the order of the mean level spacing Δ. This approximation enables us to call the relaxation described in Eq. (5), in fact an inelastic process because the finite width effectively results in loss of energy.

Integration of the above equation using a standard fourth order Runge–Kutta procedure gives the time evolution of $n_\alpha(t)$. The form of a Fermi–Dirac distribution $n_{FD}(E)=1/(1+\exp[\beta(E-\mu)])$ is fitted at every time step. This fit provides a ''chemical potential'' μ and an ''inverse temperature'' β. However, we are more interested in the error of this fit, $\sigma^2(t)=\Sigma_\alpha[n_\alpha-n_{FD}(\varepsilon_\alpha)]^2$. This quantity characterizes how close the distribution n_α is to n_{FD}. An example for one single realization over $N=20$ sites with half filling is presented in Fig. 1 where we can clearly see an approximately exponential decrease that initially characterizes the relaxation process. From these initial exponentials a relaxation rate Γ can be obtained through $\sigma(t)\approx\sigma_0\exp(-\Gamma t)$.

The scattering probability between the pairs of single-particle states $\{\alpha,\beta\}$ and $\{\gamma,\delta\}$ is $(U_{\alpha\beta}^{\gamma\delta})^2$ which is explicitly proportional to U_0^2. Therefore for small enough U_0 when the Hartree-Fock states differ very little from the noninteracting basis we expect $\Gamma\sim U_0^2$. The power of two should, however, be an approximate value, since for strong enough interaction and also for strong enough disorder we expect a different exponent due to the implicit character of the interaction encoded in the coefficients $C_{i\alpha}$.

The relaxation rate obtained from the exponentials as shown in Fig. 1 has been collected and averaged over many realizations. In Fig. 2 we show the data obtained for several interaction strength U_0 and disorder W. We can clearly identify qualitatively that for the case of short-range interactions, weak disorder produces an increase of the relaxation rate.[7] As disorder is increased, however, the rate decreases. Note that a long-range interaction induces a much faster relaxation as compared to a short range one.

As we can see in the insets of Fig. 2 the relaxation rate grows as a power of U_0 that is smaller than two. This is due to the strong perturbation the interaction makes on the HF states as compared to the noninteracting basis. One may also detect a slight difference in the exponents between the two types of interactions.

We may summarize that the error of the occupation number distribution decays for short times roughly as an exponential (Fig. 1) therefore we may expect that the solution of Eq. (5) is also an exponential whose derivative is $\dot{n}_\alpha\approx-\Gamma_\alpha n_\alpha$. If we substitute this ansatz into Eq. (5) we can calculate the Γ_α values from the initial derivatives. This allows obviously for a much better statistics, however, will still strongly depend on the initial n_α distribution. An average over the individual rates Γ_α and obviously over many realizations of the disordered potential is presented in Fig. 3. We can observe that the effective U_0 dependence here is roughly two owing to the simple approximation of the exponential ansatz for short times.

In summary our numerical results show that weak disorder indeed causes the energy relaxation of an initially nonequilibrium occupation number distribution towards a Fermi-Dirac distribution to become faster for the case of short-range interactions. On the other hand with an increase of

disorder the single-particle localization volume decreases hence the quasiparticles have smaller chance to effectively scatter and therefore the relaxation rate decreases considerably. Note that the long-range type interaction is more effective, therefore Γ is orders of magnitude larger than in the case of short-range interaction. However, qualitatively both of them produce a similar tendency as a function of large enough disorder, W.

From the results presented here one could expect that coherent phenomena at elevated density of particles may be more robust with respect to dephasing processes in strongly disordered systems. Thus one could suspect that these systems may serve as a testing ground of coherent phenomena even at elevated carrier densities, especially in the case when these phenomena do require the presence of strong disorder anyway. One such phenomenon is for instance the current echo.[9]

The loss of coherence, i.e., dephasing, following interband photoexcitation has been widely studied in semiconductor systems, where the optically induced coherence is monitored in the time domain by ultrafast nonlinear optical techniques.[10,11] Using many-body theory it has, however, been shown that the dephasing of the interband polarization due to the Coulomb many-body interaction cannot be estimated directly from the carrier-carrier scattering rates but it is a rather complicated phenomenon. So-called *in* scattering contributions largely compensate the dephasing provided by the usual *out* scattering terms.[5,10–12] As a result the dependence of the dephasing rate of the interband polarization on the carrier density n is rather weak, see Ref. 11, where for two- and three-dimensional systems a dependence of $\propto n^{1/3}$ was found. It would be very interesting to include coherent contributions in our type of approach and to investigate up to what extent such results are altered in the presence of disorder.

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[6] The single particle basis is fixed throughout the simulation even though selfconsistency should be enforced at every timestep in the relaxation process. For the considered scenario we believe that our treatment yields at least a reasonable approximation of the description of the short time dynamics, provided the initial perturbation is not too strong.

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