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***"Wigner Approach to Quantum Dynamics
Simulations of the Interacting Carriers in
Disordered Systems"***

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Wigner approach to quantum dynamics simulations of the interacting carriers in disordered systems

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The new method for solving Wigner-Liouville's type equations and studying dynamics of quantum particles. has been developed within the Wigner formulation of quantum statistical mechanics. This approach combines both molecular dynamics and Monte Carlo methods and computes traces and spectra of the relevant dynamical quantities. Considering, as an application, the quantum dynamics of an ensemble of interacting electrons in an array of random scatterers clearly demonstrates that the many-particle interaction between the electrons can lead to an enhancement of the electrical conductivity.

1 Introduction It is well known that molecular dynamics method due to its highly efficiency is widely used in treatment of dynamic problems of classical statistical physics. The aim of this work is to develop the 'straight generalization' of classical molecular dynamics methods for rigorous consideration of quantum problems. The words 'straight generalization' mean that in classical limit the developed approach should exactly coincide with molecular dynamics method in the phase space. A generalization molecular dynamics method is possible only in the phase space, so in our work it is naturally to use Wigner formulation of quantum mechanics. In 1932 Wigner proposed joint position and momentum (phase space) representation of quantum mechanics and derived quantum analog of the classical distribution function. This representation contains only the values common both for classical and quantum mechanics, which is especially convenient when one of two interacting subsystems is quantum and another - classical. Wigner's paper has given rise to an extensive literature on formal aspects of quantum theory in phase space.

Noninteracting electrons in an array of fixed random scatterers are known to experience Anderson localization at temperature $T = 0$ in one-dimensional systems [1, 2, 3]. However, it is expected that the many-particle interaction leads to delocalization tendencies which has been confirmed for simple models [4, 5]. To study the influence of the electron-electron Coulomb interaction on kinetic electron properties in a random environment we have simulated the quantum dynamics in a one-dimensional canonical ensemble at finite temperature for both interacting and noninteracting electrons using the developed Quantum-Dynamics-Monte-Carlo scheme. We discovered that the temporal momentum-momentum correlation functions and their frequency-domain Fourier transforms strongly depend on the electron-electron interaction, clearly demonstrating the delocalizing influence of the many-particle interaction at densities

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around $R_s = \bar{r}/a_0 = 5$ (\bar{r} is the mean interparticle distance and a_0 the effective Bohr radius) even at finite temperatures. Our approach also treats the positions of the scattering centers as dynamical variables. We are, therefore, able to generate various initial conditions.

2 Wigner representation of quantum mechanics The basis of our consideration is the Wigner representation of the von Neumann equation – the Wigner-Liouville equation (WLE). To derive the WLE for the full density matrix of the N-particle system $\rho(x_N|y_N)$ we introduce center of mass and relative coordinates in standard manner, $\vec{q} \equiv \vec{q}_N \equiv (\vec{x}_N + \vec{y}_N)/2$ and $\vec{r} \equiv \vec{r}_N \equiv \vec{x}_N - \vec{y}_N$. The Wigner distribution function (WF) is defined by [6]

$$f(\vec{p}, \vec{q}, t) = \frac{1}{(2\pi\hbar)^{6N}} \int \rho \left(\vec{q} - \frac{\vec{r}}{2}, \vec{q} + \frac{\vec{r}}{2} \right) e^{i\vec{p}\vec{r}/\hbar} d\vec{r}. \quad (1)$$

Using this definition it is straightforward to obtain the Wigner transform for the *full* density matrix [6]

$$\frac{\partial f}{\partial t} + \frac{\vec{p}}{m} \frac{\partial f}{\partial \vec{q}} - \frac{\partial V(q)}{\partial \vec{q}} \frac{\partial f}{\partial \vec{p}} = \int_{-\infty}^{\infty} ds f(\vec{p} - \vec{s}, \vec{q}, t) \omega(\vec{s}, \vec{q}), \quad (2)$$

$$\text{where } \omega(\vec{s}, q) = \vec{F}(\vec{q}) \frac{d\delta(\vec{s})}{d\vec{s}} + \frac{4}{\hbar(2\pi\hbar)^{6N}} \int d\vec{q} V(q - \vec{q}) \sin\left(\frac{2\vec{s}\vec{q}}{\hbar}\right), \quad (3)$$

and $\vec{F}(\vec{q}) = -\partial V(q)/\partial \vec{q}$ is the classical force. Obviously, the force term in ω exactly cancels the last term on the lhs of Eq. (2). Retaining these terms allows us to write the WLE as the classical Liouville equation [lhs of Eq. (2)] plus a quantum correction [all terms on the rhs of Eq. (2)] which vanish for $\hbar \rightarrow 0$. This form allows us to identically transform Eq. (2) into an integral equation [6],

$$f(\vec{p}, \vec{q}, t) = f_0(p_0, q_0) + \int_0^t d\tau \int_{-\infty}^{\infty} d\vec{s} f(p_\tau - \vec{s}, q_\tau, \tau) \omega(\vec{s}, q_\tau). \quad (4)$$

The first contribution describes quantum dynamics and is given by the initial WF $f_0(p, q) \equiv f(p, q, 0)$, but taken at arguments $p_0 \equiv \vec{p}(0)$ and $q_0 \equiv \vec{q}(0)$, being classical trajectories $p_\tau \equiv \vec{p}(\tau)$ and $q_\tau \equiv \vec{q}(\tau)$ (solutions of the Hamilton equations associated to the WLE and connecting points (\vec{p}, \vec{q}) at time t and points (p_0, q_0) at time 0). Notice that even the first term may describe the evolution of a *quantum* many-body state if the initial WF $f_0(p, q)$ is chosen appropriately and contains the all powers of the Plank's constant. The integral term in Eq. (4) describes the perturbation of the classical trajectories due to quantum effects, for details we refer to Ref. [7].

The structure of Eq. (4) suggests to construct its solution iteratively, starting with f_0 . Let us, therefore, rewrite Eq. (4) in the following compact form, $f^t = f_0^t + K_\tau^t f^\tau$, where the superscript on the WF denotes the time argument and $K_{\tau_1}^{\tau_2}$ denotes the time integral in Eq. (4). Then, the iteration series has the form :

$$f^t = f_0^t + K_{\tau_1}^t f_0^{\tau_1} + K_{\tau_2}^t K_{\tau_1}^{\tau_2} f_0^{\tau_1} + K_{\tau_3}^t K_{\tau_2}^{\tau_3} K_{\tau_1}^{\tau_2} f_0^{\tau_1} + \dots, \quad (5)$$

where the first term describes the evolution of an initial (classical or quantum) WF f_0 (it may contain any order of Planck's constant). The remaining terms systematically account for all dynamic quantum corrections [trajectories with momentum jumps arising from the shifted momentum arguments in the WF under the integral in (2)] including e.g. tunneling effects and correctly accounting for the Heisenberg uncertainty principle. Thus, the solution of Eq (5) can be understood as a properly weighted sum of classical and quantum phase space trajectories [7].

Using the solution f^t we can compute averages of arbitrary operators in standard way and obtain any dynamic macroscopic property of the correlated quantum particles without approximations on the potential interaction. Naturally, the true particle number N is replaced by a greatly reduced number N_{sim} which is of the order 50 – 100 in the MC cell with periodic boundary conditions. The solution scheme is a combination of Quantum Monte Carlo and classical Molecular Dynamics methods: Quantum MC is used

to generate the correlated initial state, MD generates the $p - q$ trajectories and Monte Carlo methods are applied to perform an importance sampling of the dominant terms of the iteration series (trajectories with momentum jumps).

3 Wigner representation of time correlation functions According to the Kubo formula the conductivity is the Fourier transform of the current–current correlation function. Our starting point is the general operator expression for the canonical ensemble-averaged time correlation function [8]:

$$C_{FA}(t) = Z^{-1} \text{Tr} \left\{ \hat{F} e^{i\hat{H}t_c/\hbar} \hat{A} e^{-i\hat{H}t_c/\hbar} \right\}, \quad (6)$$

where \hat{H} is the Hamiltonian of the system expressed as a sum of the kinetic energy operator, \hat{K} , and the potential energy operator, \hat{U} . Time is taken to be a complex quantity, $t_c = t - i\hbar\beta/2$, where $\beta = 1/k_B T$ is the inverse temperature with k_B denoting the Boltzmann constant. The operators \hat{F} and \hat{A} are quantum operators of the dynamic quantities under consideration and $Z = \text{Tr} \left\{ e^{-\beta\hat{H}} \right\}$ is the partition function. The Wigner representation of the time correlation function in a v -dimensional space can be written as

$$C_{FA}(t) = (2\pi\hbar)^{-2v} \int \int d\mu_1 d\mu_2 F(\mu_1) A(\mu_2) W(\mu_1; \mu_2; t; i\hbar\beta), \quad (7)$$

where we introduce the short-hand notation for the phase space point, $\mu_i = (p_i, q_i)$, ($i = 1, 2$), and p and q comprise the momenta and coordinates, respectively, of all particles in the system. $W(\mu_1; \mu_2; t; i\hbar\beta)$ is the spectral density expressed as

$$W(\mu_1; \mu_2; t; i\hbar\beta) = Z^{-1} \int \int d\xi_1 d\xi_2 e^{i\frac{p_1\xi_1}{\hbar}} e^{i\frac{p_2\xi_2}{\hbar}} \times \\ \left\langle q_1 + \frac{\xi_1}{2} \left| e^{i\hat{H}t_c/\hbar} \right| q_2 - \frac{\xi_2}{2} \right\rangle \left\langle q_2 + \frac{\xi_2}{2} \left| e^{-i\hat{H}t_c/\hbar} \right| q_1 - \frac{\xi_1}{2} \right\rangle, \quad (8)$$

and $A(\mu)$ denotes Weyl's symbol [6] of operator \hat{A} : $A(\mu) = \int d\xi e^{-i\frac{p\xi}{\hbar}} \left\langle q - \frac{\xi}{2} \left| \hat{A} \right| q + \frac{\xi}{2} \right\rangle$, and similarly for the operator \hat{F} . Hence the problem of the numerical calculation of the canonically averaged time correlation function is reduced to the computation of the spectral density.

To obtain the integral equation for W let us introduce a pair of dynamic p, q -trajectories $\{\bar{q}_\tau(\tau; p_1, q_1, t), \bar{p}_\tau(\tau; p_1, q_1, t)\}$ and $\{\tilde{q}_\tau(\tau; p_2, q_2, t), \tilde{p}_\tau(\tau; p_2, q_2, t)\}$ starting at $\tau = t$ from the initial condition $\{q_1, p_1\}$ and $\{q_2, p_2\}$ propagating in 'negative' and 'positive' time direction, respectively:

$$\frac{d\bar{p}_\tau}{d\tau} = \frac{1}{2}F[\bar{q}_\tau(\tau)]; \quad \frac{d\bar{q}_\tau}{d\tau} = \frac{\bar{p}_\tau(\tau)}{2m}, \quad \text{with } \bar{p}_t(\tau = t; p_1, q_1, t) = p_1; \quad \bar{q}_t(\tau = t; p_1, q_1, t) = q_1,$$

$$\frac{d\tilde{p}_\tau}{d\tau} = -\frac{1}{2}F[\tilde{q}_\tau(\tau)]; \quad \frac{d\tilde{q}_\tau}{d\tau} = -\frac{\tilde{p}_\tau(\tau)}{2m}, \quad \text{with } \tilde{p}_t(\tau = t; p_1, q_1, t) = p_1; \quad \tilde{q}_t(\tau = t; p_1, q_1, t) = q_1,$$

where $F(q) \equiv -\nabla\tilde{U}$ with \tilde{U} being the total potential, i.e. the sum of all pair interactions U_{ab} . Then, as has been proven in [9], W obeys the following integral equation

$$W(\mu_1; \mu_2; t; i\hbar\beta) = \bar{W}(\bar{p}_0, \bar{q}_0; \tilde{p}_0, \tilde{q}_0; i\hbar\beta) + \\ + \frac{1}{2} \int_0^t d\tau \int ds W(\bar{p}_\tau - s, \bar{q}_\tau; \tilde{p}_\tau, \tilde{q}_\tau; \tau; i\hbar\beta) \varpi(s, \bar{q}_\tau) \\ - \frac{1}{2} \int_0^t d\tau \int ds W(\bar{p}_\tau, \bar{q}_\tau; \tilde{p}_\tau - s, \tilde{q}_\tau; \tau; i\hbar\beta) \varpi(s, \tilde{q}_\tau), \quad (9)$$

where $\varpi(s, q) = \frac{4}{(2\pi\hbar)^v} \int dq' \tilde{U}(q - q') \sin\left(\frac{2sq'}{\hbar}\right) + F(q)\nabla\delta(s)$, and $\delta(s)$ is the Dirac delta function. Equation (9) has to be supplemented by an initial condition for the spectral density at $t = 0$: $W(\mu_1; \mu_2; 0; i\hbar\beta) = \bar{W}(\mu_1; \mu_2; i\hbar\beta) \big|_{t=0} \equiv \bar{W}$. The τ -integrals connect the points $\bar{p}_\tau, \bar{q}_\tau; \tilde{p}_\tau, \tilde{q}_\tau$ at

time τ of the mentioned above dynamic p,q-trajectories with the points $p_1, q_1; p_2, q_2$ at time t whereas in \bar{W} the trajectories are to be taken at $\tau = 0$ (denoted by the subscript "0"). The function \bar{W} can be expressed in the form of a finite difference approximation of the path integral [9, 7, 10]:

$$\bar{W}(\mu_1; \mu_2; i\hbar\beta) \approx \int \int d\tilde{q}_1 \dots d\tilde{q}_n \int \int dq'_1 \dots dq'_n \Psi(\mu_1; \mu_2; \tilde{q}_1, \dots, \tilde{q}_n; q'_1, \dots, q'_n; i\hbar\beta), \quad (10)$$

with

$$\begin{aligned} \Psi(\mu_1; \mu_2; \tilde{q}_1, \dots, \tilde{q}_n; q'_1, \dots, q'_n; i\hbar\beta) \equiv & \\ \frac{1}{Z} \langle q_1 | e^{-\epsilon\hat{K}} | \tilde{q}_1 \rangle e^{-\epsilon U(\tilde{q}_1)} \langle \tilde{q}_1 | e^{-\epsilon\hat{K}} | \tilde{q}_2 \rangle e^{-\epsilon U(\tilde{q}_2)} \dots & \\ e^{-\epsilon U(\tilde{q}_n)} \langle \tilde{q}_n | e^{-\epsilon\hat{K}} | q_2 \rangle \varphi(p_2; \tilde{q}_n, q'_1) \times & \\ \langle q_2 | e^{-\epsilon\hat{K}} | q'_1 \rangle e^{-\epsilon U(q'_1)} \langle q'_1 | e^{-\epsilon\hat{K}} | q'_2 \rangle e^{-\epsilon U(q'_2)} \dots & \\ e^{-\epsilon U(q'_n)} \langle q'_n | e^{-\epsilon\hat{K}} | q_1 \rangle \varphi(p_1; q'_n, \tilde{q}_1), & \end{aligned} \quad (11)$$

where $\varphi(p; q', q'') \equiv (2\lambda^2)^{v/2} \exp\left[-\frac{1}{2\pi} \left\langle \frac{p\lambda}{\hbar} + i\pi \frac{q'-q''}{\lambda} \left| \frac{p\lambda}{\hbar} + i\pi \frac{q'-q''}{\lambda} \right. \right\rangle\right]$, and $\langle x|y \rangle$ denotes the scalar product of two vectors \vec{x}, \vec{y} . In this expression the original (unknown) density matrix of the correlated system $e^{-\beta(\hat{K}+\hat{U})}$ has been decomposed into $2n$ factors, each at a $2n$ times higher temperature, with the inverse $\epsilon = \beta/2n$ and the corresponding high temperature DeBroglie wave length squared $\lambda^2 \equiv 2\pi\hbar^2\epsilon/m$. This leads to a product of known high-temperature (weakly correlated) density matrices, however, at the price of $2n$ additional integrations over the intermediate coordinate vectors (over the "path"). This representation is exact in the limit $n \rightarrow \infty$, and, for finite n , an error of order $1/n$ occurs. The function Ψ has to be generalized to properly account for spin-statics effects. This gives rise to an additional spin part of the density matrix and antisymmetrization of one off-diagonal matrix element. To improve the accuracy of the obtained expression, we will replace $U_{ab} \rightarrow U_{ab}^{\text{eff}}$ where U_{ab}^{eff} is the proper effective quantum pair potential. For more details on the path integral concept, we refer to Refs. [11]–[13].

Let us now come back to the integral equation (9). For the discussion we note that the integral equation (9) can be exactly converted into an iteration series (which is obtained by successively replacing $W \rightarrow \bar{W}$ under the integrals). This series is, however, not a perturbative expansion in the interaction, neither in the electron-scatterer nor in the electron-electron interaction. It rather is an expansion in terms of corrections to classical trajectories of fully interacting electrons and electrons with scatterers. So multiple scattering effects are fully included. Physically the second order and other terms of the iteration series include corrections to the classical electron trajectories (momentum jumps related to the uncertainty principle between momentum–coordinate and energy–time). A detailed investigation of the conditions for which the contribution of the these terms of the iteration series should be taken into account is presented in [9, 14, 15, 16].

As mentioned above, the first term \bar{W} describes propagation of a correlated quantum initial state along the characteristics of the classical Wigner-Liouville equation. This term, containing all powers of Planck's constant, is the coherent sum of complex-valued contributions of a trajectory ensemble related to \bar{W} . This term allows to describe quantum coherent effects such as Anderson localization, while other terms of iteration series describe deviations from the classical trajectories: the trajectories are perturbed by a finite momentum jump s occurring at arbitrary times τ , $0 \leq \tau \leq t$ [7]. These terms are essential for the recovery of tunneling effects, we expect that they do not give dominant contributions to coherence and localization phenomena. With increasing quantum degeneracy (i.e. decreasing temperature or/and increasing density) the magnitude of these terms will grow. The time correlation functions are linear functionals of the spectral

density, for them the same series representation holds,

$$C_{FA}(t) = (2\pi\hbar)^{-2v} \int \int d\mu_1 d\mu_2 \phi(\mu_1; \mu_2) W(\mu_1; \mu_2; t; i\hbar\beta) \equiv (\phi|W^t) =$$

$$(\phi|\bar{W}^t) + (\phi|K_{\tau_1}^t \bar{W}^{\tau_1}) + (\phi|K_{\tau_2}^t K_{\tau_1}^{\tau_2} \bar{W}^{\tau_1}) + (\phi|K_{\tau_3}^t K_{\tau_2}^{\tau_3} K_{\tau_1}^{\tau_2} \bar{W}^{\tau_1}) + \dots \quad (12)$$

where $\phi(\mu_1; \mu_2) \equiv F(\mu_1)A(\mu_2)$ and the parentheses $(\dots|\dots)$ denote integration over the phase spaces $\{\mu_1; \mu_2\}$, as indicated in the first line of the equation.

Our numerical results below refer to finite temperature and moderate degeneracy $n_e \lambda_e = 0.2 \dots \dots 7$. We, therefore, will include in the following numerical analysis only the first term in this series.

4 Quantum dynamics As an application, in this work we will consider a system composed of heavy particles (called scatterers) with mass m_s and negatively charged electrons with mass m_e . To avoid bound state effects due to attraction we consider in this case study only negatively charged scatterers, assuming a positive background for charge neutrality. The influence of electron-scatterer attraction will be studied in a further publication.

The possibility to convert a iteration series into a form convenient for probabilistic interpretation allows us to apply Monte Carlo methods to its evaluation. According to the general theory of Monte Carlo methods for solving linear integral equations, e.g. [17], one can simultaneously calculate all terms of the iteration series. Using the basic ideas of [17] we have developed a Monte Carlo scheme, which provides domain sampling of the terms giving the main contribution to the iteration series cf. [9]. For simplicity, in this work, we take into account only the first term of iteration series, which is related to the propagation of the initial quantum distribution according to the Hamiltonian equation of motion. This term, however, does not describe pure classical dynamics but accounts for quantum effects [14] and, in fact, contains arbitrarily high powers of Planck's constant. The remaining terms of the iteration series describe momentum jumps [9, 15] which account for higher-order corrections to the classical dynamics of the quantum distribution, which are expected to be relevant in the limit of high density.

This approach allows us to generate, in a controlled way, various kinds of quantum dynamics and initial conditions of the many-body system, in particular (i) those which are characteristic of the fully interacting system [i.e.including scatterer-scatterer (s-s), electron-scatterer (e-s), and electron-electron (e-e)] and (ii) those which result if some aspects of these interactions are ignored.

5 Numerical results We now apply the numerical approach explained above to the problem of an interacting ensemble of electrons and disordered scatterers in one dimension. In all calculations times, frequencies and distances are measured in atomic units. The average distance between electrons, $R_s = 1/(n_e a_0)$, was varied between 12.0 and 0.55, with the densities of electrons and heavy scatterers taken to be equal. The results obtained were practically insensitive to the variation of the whole number of the particles in MC cell from 30 up to 50 and also of the number of high temperature density matrices (determined by the number of factors n), ranging from 10 to 20. Estimates of the average statistical error gave the value of the order 5–7%. We studied two different temperatures: $k_B T/|V_0^{es}| = 0.45$ and 0.28, corresponding to $\lambda_{ee}/a_0 \sim 2.2$ and $\lambda_{ee}/a_0 \sim 3.5$, respectively.

According to the Kubo formula [8] our calculations include two different stages: (i) generation of the initial conditions (configuration of scatterers and electrons) in the canonical ensemble with probability proportional to the quantum density matrix and (ii) generation of the dynamic trajectories on the time scale t' in phase space, starting from these initial configurations. The results presented below are related to two different cases: 1. *with* e-e interaction included in the dynamics (“interacting dynamics”) and 2., *without* e-e interaction (“noninteracting dynamics”). In both cases, the initial state fully includes all interactions.

Fig. 1 presents for our model the real part of the diagonal elements of the electrical conductivity tensor versus frequency (real part of the Fourier transform of the temporal momentum–momentum correlation functions) which characterizes the Ohmic absorption of electromagnetic energy and has the physical

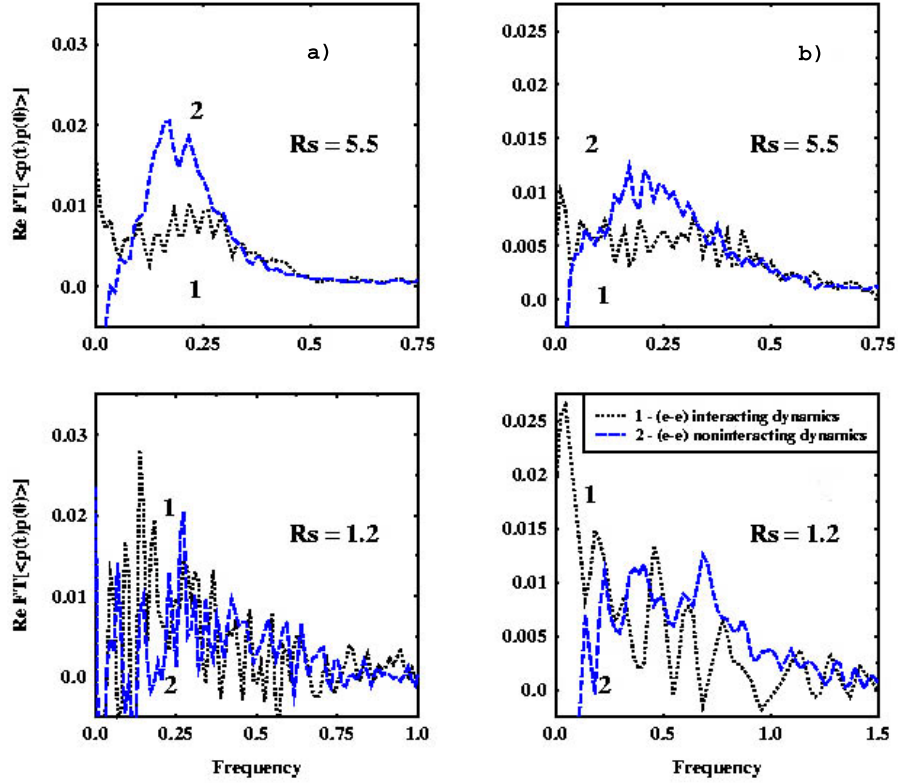


Fig. 1: Real part of the Fourier transform of the temporal momentum-momentum correlation functions for dynamics with (1) and without (2) e-e interaction. Figure parts are for two densities (a,b: $R_s = 5.5$; c,d: $R_s = 1.2$) and temperatures (a,c: $k_B T / |V_0^{es}| = 0.28$; b,d: $k_B T / |V_0^{es}| = 0.45$).

meaning of electron conductivity. To compare influence of electron interactions conductivities are given on Fig. 1 in the same arbitrary units. The first observation is that, in all cases, the conductivity for the noninteracting dynamics (2) has a maximum at some finite frequency related to the coherent oscillations in the time domain and vanishes at low frequency [18]. The latter clearly indicates Anderson localization. The effect of the e-e interaction is, as shown by curves 1, a reduction of the maximum (damping of the coherent oscillations) and, in most cases, an increase of the zero-frequency conductivity. Thus, our calculations confirm the delocalizing effect of the interactions (Figs. a,b,d) at the considered densities. Interestingly, Fig. 1 c) is an exception: even with interactions included, the localization behavior persists. The large oscillations in Fig. 1 c) are not result of numerical noise, they exist inspite of very long simulation duration.

The reason for the observed behavior is an interplay of varying strength of the e-e-interaction (which is weakened with reducing R_s , i.e. from top to bottom figures) and of the magnitude of quantum effects (which grow with temperature reduction, i.e. from right to left figures). Thus, the delocalization tendency observed from Figs. c) to d) is due to thermal activation which, similarly as the interaction, destroys coherence phenomena.

Our simulations qualitatively confirm analytical predictions for the low-frequency and zero temperature limit of the 1D conductivity [19]. Yet our computer power allows us to generate dynamic trajectories up to times t' equal 100 200 in atomic units. Thus for small frequencies of the order 10^{-2} , large fluctuations of the conductivity appear [18], and the accuracy is not yet sufficient to extract an asymptotic frequency behavior. On the other hand, the advantage of our computational method is that it allows to study systematically the influence of finite temperature and of electron correlation effects on localization

phenomena in a wide range of densities. We note that we have also performed simulations at lower densities and found that the delocalizing effect of the e-e-interaction has also been observed at lower density up to $R_s = 12$. At even lower densities, we expect that future simulations will yield a pinned electron Wigner crystal at weak disorder [20] and Coulomb glass behavior at strong disorder.

In summary, we have presented numerical results on the influence of Coulomb interaction on Anderson localization in a one-dimensional system. At low density ($R_s = 5.5$) the interaction is comparatively strong and localization is destroyed. With increasing density $R_s = 1.2$, localization is found to persist even in the presence of Coulomb interaction. For a full understanding of the physical processes additional investigations are needed which are presently under way.

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- [18] In fact, we observe negative values, although, the real part of the conductivity has to be positive. The reason are weakly damped oscillations with a period exceeding the scale t' used in the calculation of the dynamics. To overcome this deficiency of our model one has to increase the time t' and/or to take into account the slow motion of the heavy particles, which will destroy the coherent oscillations of the light electrons trapped by the heavy particles. Additional calculations with increased t' lead to decreasing negative contributions for low frequencies, as expected.
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- [20] In the absence of disorder, Wigner crystallization is clearly found in path-integral MC simulations, see A. Filinov, M. Bonitz, and Yu. Lozovik, Phys. Rev. Lett. **86**, 3851 (2001) and references therein.