Quantum dynamics in canonical and micro-canonical ensembles. Part I. Anderson localization of electrons.

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The new numerical approach for consideration of quantum dynamics and calculations of the average values of quantum operators and time correlation functions in the Wigner representation of quantum statistical mechanics has been developed. The time correlation functions have been presented in the form of the integral of the Weyl's symbol of considered operators and the Fourier transform of the product of matrix elements of the dynamic propagators. For the last function the integral Wigner-Liouville's type equation has been derived. The initial condition for this equation has been obtained in the form of the Fourier transform of the Wiener path integral representation of the matrix elements of the propagators at initial time. The numerical procedure for solving this equation combining both molecular dynamics and Monte Carlo methods has been developed. An application of the developed approach to the micro canonical ensemble has been also considered in the second part of this paper.

For electrons in disordered systems of scatterers the numerical results have been obtained for series of the average values of the quantum operators including position and momentum dispersions, average energy, energy distribution function as well as for the frequency dependencies of tensor of electron conductivity and permittivity according to quantum Kubo formula. Zero or very small value of static conductivity have been considered as the manifestation of Anderson localization of electrons in 1D case. Independent evidence of Anderson localization comes from the behaviour of the calculated time dependence of position dispersion. Nevertheless for localized electrons the energy distribution function obtained has the long exponentially decaying tail, which is the reason of exponentially rare appearance of large values of quantum particle virtual energy that strongly affects the behaviour of the position dispersion.

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I. INTRODUCTION

It is known that crystalline materials have been studied intensively by physicists for a long time since the beginning of quantum physics. Practically the same is valid for investigations of the disorder state of the matter. Disorder exist in varying degree, ranging from the a few impurities or interstitials in an otherwise perfect crystalline host to the strongly disordered limit of alloys or glassy structures. In the past few years there has been growing realization that for understanding the disordered materials new concepts must be introduced which treat the disorder from the very beginning. The new understanding is based on advances in two different areas. The first is the problem of Anderson localization, which deals with the nature of the wave function of single electron in the presence of the random potential. A scaling description of the Anderson localization problem has greatly deepened understanding of the problem. The second aspect of the problem is the interaction among electrons in the presence of a random potential. The fact that the electrons are diffusive instead of freely propagating leads to a profound modification of the traditional view based on the Fermi-liquid theory of metals.

In this paper we treat the first of the mentioned above problem. In 1958, Anderson pointed out that if disorder is strong enough, the electron wave function may become localized, in that the its envelope decays exponentially from the initial electron position in space. The characteristic space scale of this decay is called as localization length. The energy and density dependence of localization length results in the metal-insulator transition and the concepts of the mobility energetic edge. Despite of significant advances the mentioned and a lot of other related problem are unsolved now due to thire complexity. For investigation of the problem of Anderson localization we have applied the developed in [2], [3] numerical approach allowing rigorous calculations of the quantum time correlation functions and average values of quantum operators in the Wigner formulation of quantum statistical mechanics.

Within Wigner formulation of quantum mechanics the time correlation function can be presented in the form of the integral of Weil’s symbols of the operators $\hat{F}$ and $\hat{A}$ and so called spectral density, which is the Fourier transform of the product of the dynamic propagator matrix elements arising due to Heisenberg representation of the operator $\hat{A}(t)$. For spectral density the integral equation of the Wigner-Liouville’ type has been derived. The developed approach for solving this equation combines both molecular dynamics and Monte Carlo methods and allows to combine the existing molecular dynamics and Monte Carlo codes after small modernization. Efficiency of the developed method is high enough to use for calculations not very fast computers. The explicit expression of the initial condition for this integral equation is convenient to obtain as Fourier transform of the propagator matrix elements presented in the form of Wiener path integrals.

The numerical results have been obtained for series of the average value of the quantum operators as well as for the frequency dependencies of tensor of electron conductivity and permittivity according to quantum Kubo formulas for electrons in disordered systems of scatterers. Zero or very small value of static conductivity have been obtained as the manifestation of Anderson localization of electrons in 1D case. Independent evidence of Anderson localization comes from the behaviour of the calculated time dependence of position dispersion. Nevertheless for localized electrons the energy distribution function obtained has the long exponentially decaying tail, which is the reason of exponentially rare appearance of large values of quantum particle virtual energy that strongly affects the behaviour of the position dispersion.

II. WIGNER REPRESENTATION OF QUANTUM STATISTICAL MECHANICS

The time correlation functions $C_{FA}(t) = \langle \hat{F}(0)\hat{A}(t) \rangle$ for different dynamic properties are among the most interesting quantities in studying dynamics of electrons in disordered systems of scatters, transport coefficients, chemical reaction rates, consideration of equilibrium and transient spectroscopy and so on. Our starting point is the general operator expression for canonical ensemble averaged time correlation functions $\hat{F}, \hat{A}$:

$$C_{FA}(t) = Z^{-1} Tr \left( \hat{F} \exp \left( i\hat{H}t_{c}/\hbar \right) \hat{A} \exp \left( -i\hat{H}t_{c}/\hbar \right) \right)$$

Here $\hat{H}$ is the Hamiltonian of the system, $\hat{H} = \hat{K} + \hat{U}$, $\hat{K}$ is the kinetic energy operator, $\hat{U}$ is the potential energy operator, $t_{c} = t - i\hbar\beta/2$, $\beta = 1/k_{B}T$, $\hat{F}$ and $\hat{A}$ are quantum operators of the considered dynamic quantities, $Z = Tr \left( \exp \left( -\beta\hat{H} \right) \right)$ is the partition function. Wigner representation of the time correlation function can be written as:

$$C_{FA}(t) = \frac{1}{(2\pi\hbar)^{3v}} \int \int dp_{1} dq_{1} dp_{2} dq_{2} F(p_{1}, q_{1}) A(p_{2}, q_{2}) \times \times W(p_{1}, q_{1}; p_{2}, q_{2}; t; i\hbar\beta)$$
where the spectral density \( W(p_1, q_1; p_2, q_2; t; i\hbar\beta) \) is defined by:

\[
W(p_1, q_1; p_2, q_2; t; i\hbar\beta) = Z^{-1} \int d\xi_1 d\xi_2 \exp \left( i\frac{p_1 \xi_1}{\hbar} \right) \exp \left( i\frac{q_1 \xi_1}{2} \right) \times \left\langle q_1 + \frac{\xi_1}{2} \bigg| \exp \left( i\hbar t_c / \hbar \right) \right| q_2 + \frac{\xi_2}{2} \bigg| \exp \left( -i\hbar t_c / \hbar \right) \right| q_1 - \frac{\xi_1}{2} \bigg\rangle
\]

and \( F(p_1, q_1) \) and \( A(p_2, q_2) \) are Weyl's symbols of operators \( \hat{F} \) and \( \hat{A} \):

\[
A(p, q) = \int d\xi \exp \left( -i\frac{p \xi}{\hbar} \right) \left\langle q - \frac{\xi}{2} \bigg| A \bigg| q + \frac{\xi}{2} \right\rangle
\]

where \( \left\langle q \bigg| A \bigg| q' \right\rangle \) are the matrix elements and \( v \) is the space dimension. So the problem of numerical calculation of the canonically averaged time correlation function can be reduced to the consideration of the spectral density evolution describing as can been proved by the following integral equation:

\[
W(p_1, q_1; p_2, q_2; t; i\hbar\beta) = \tilde{W}(\tilde{p}_0, \tilde{q}_0; \tilde{p}_0, \tilde{q}_0; i\hbar\beta) + \int_0^t dt \int ds dq W(\tilde{p}_r - s, \tilde{q}_r; \tilde{p}_r - \eta, \tilde{q}_r; \tau; i\hbar\beta) \gamma(s, \tilde{q}_r; \eta, \tilde{q}_r)
\]

where \( \gamma(s, \tilde{q}_r; \eta, \tilde{q}_r) = \frac{1}{2} \{ \varpi(s, \tilde{q}_r) \delta(\eta) - \varpi(\tilde{q}_r, \eta) \delta(s) \} \), \( \delta(s) \) is Dirac delta function, \( \varpi(s, q) \) is defined by the expression

\[
\varpi(s, q) = \frac{4}{(2\pi \hbar)^2} \int dq' U(q - q') \sin \left( \frac{2\pi q'}{\hbar} \right) + \tilde{F}(q) \frac{d\delta(s)}{ds}
\]

\( \tilde{F}(q) \) is the classical force, \( \{\tilde{q}_r(\tau; p_1, q_1, t), \tilde{p}_r(\tau; p_1, q_1, t)\} \) and \( \{\tilde{q}_r(\tau; p_2, q_2, t), \tilde{p}_r(\tau; p_2, q_2, t)\} \) are the pair of dynamic \( pq \)-trajectories for 'negative and positive time direction' respectively and initial condition at \( \tau = t \):

\[
\begin{align*}
\frac{d\tilde{p}}{dt} &= \tilde{F}(\tilde{q}_r(\tau))/2; \quad \tilde{q}_r(t; p_1, q_1, t) = q_1 \\
\frac{d\tilde{q}}{dt} &= \tilde{p}_r(\tau)/2m; \quad \tilde{p}(t; p_1, q_1, t) = p_1 \\
\end{align*}
\]

The spectral density initial condition \( \tilde{W}(p_1, q_1; p_2, q_2; 0; i\hbar\beta) \) can be written in the form of the finite difference approximation of the path integral \( \tilde{W} \) :

\[
\tilde{W}(p_1, q_1; p_2, q_2; i\hbar\beta) \approx W(p_1, q_1; p_2, q_2; 0; i\hbar\beta)
\]

\[
\Psi(p_1, q_1; p_2, q_2; \tilde{q}_1, ..., \tilde{q}_M; q_1', ..., q_M'; i\hbar\beta) = Z^{-1} \left\langle q_1 \bigg| \exp \left( -\epsilon \tilde{K} \right) \right| \tilde{q}_1 \bigg\rangle \left\langle \tilde{q}_1 \bigg| \exp \left( -\epsilon U(\tilde{q}_1) \right) \right| \tilde{q}_1 \bigg\rangle \exp \left( -\epsilon \tilde{U}(\tilde{q}_2) \right) \times
\]

\[
\times \exp \left( -\epsilon U(\tilde{q}_M) \right) \left\langle \tilde{q}_M \bigg| \exp \left( -\epsilon \tilde{K} \right) \right| \tilde{q}_2 \bigg\rangle \varphi(p_2; q_2', q_2) \left\langle q_2 \bigg| \exp \left( -\epsilon U(q_2) \right) \right| q_2 \bigg\rangle \exp \left( -\epsilon U(q_2) \right) \times
\]

\[
\times \exp \left( -\epsilon U(q_1) \right) \left\langle q_1 \bigg| \exp \left( -\epsilon \tilde{K} \right) \right| q_1 \bigg\rangle \varphi(p_1; q_1', q_1) \left\langle q_1 \bigg| \exp \left( -\epsilon U(q_1) \right) \right| q_1 \bigg\rangle \exp \left( -\epsilon U(q_1) \right) \times
\]

\[
\varphi(p; q', q'' \rangle = (2\lambda^2)^{v/2} \exp \left( -\frac{(p\lambda + i\pi(q' - q''))}{\lambda^2} \right) \left( \frac{\lambda}{2\pi} \int \frac{d\lambda}{\lambda} \right)
\]

where \( \epsilon = \frac{\beta}{2M}, M \gg 1 \) and \( \lambda^2 = 2\pi\hbar^2\beta/2mM \).

Let us rewrite the integral equation (1) and the iteration form of its solution in symbolic form: \( W^t = \tilde{W} + K^t_1 W^\tau \) and

\[
W^t = \tilde{W}^t + K^t_1 \tilde{W}^\tau + K^t_2 \tilde{K}^\tau_1 \tilde{W}^\tau + K^t_2 \tilde{K}^\tau_2 \tilde{K}^\tau_1 \tilde{W}^\tau + ...
\]

Here \( \tilde{W}^t \) and \( \tilde{W}^\tau \) is the quantum initial density evolving classically in intervals \( [0, t] \) and \( [0, \tau_1] \), while \( K^\tau_i \) are operators, which describe propagation between times \( \tau_i \) and \( \tau_{i+1} \). The time correlation functions are the linear functionals of the spectral density.
\[ C_{FA}(t) = \frac{1}{(2\pi\hbar)^{2n}} \int \int dp_1 dq_1 dp_2 dq_2 F(p_1, q_1) A(p_2, q_2) \times \]
\[ \times W(p_1, q_1; p_2, q_2; t; i\hbar\beta) = \]
\[ (\phi|\hat{W}^t) + (\phi|K_{r_1}^t\hat{W}^{r_1}) + (\phi|K_{r_2}^t K_{r_1}^{r_2} \hat{W}^{r_1}) + ... \]

where brackets (|) for functions \( \phi(p_1, q_1; p_2, q_2) = F(p_1, q_1) A(p_2, q_2) \) and \( \tilde{W}(\tilde{p}_0, \tilde{q}_0; \tilde{p}_0, \tilde{q}_0; i\hbar\beta) \) or \( K_{r_1}^t, K_{r_2}^{r_1}, ... K_{r_1}^{r_2} \hat{W}^{r_1} \) mean the integration over the phase spaces \( \{p_1, q_1; p_2, q_2\} \).

Note that average values of quantum operators \( \tilde{F}(t) \) can be formally presented in the form analogous to (3):

\[ \tilde{F}(t) = \tilde{Z}^{-1} Tr \left( \exp \left(i\hat{H}t/\hbar \right) \tilde{F} \exp \left(-i\hat{H}t/\hbar \right) \rho(0) \right) = \]
\[ \frac{1}{(2\pi\hbar)^{2n}} \int \int dp_1 dq_1 dp_2 dq_2 \frac{1}{2} \{ F(p_1, q_1) + F(p_2, q_2) \} \times \]
\[ \times W(p_1, q_1; p_2, q_2; t; i\hbar\beta) \]

where \( \rho(0) \) is the initial density matrix and \( \tilde{Z} = Tr(\rho(0)) \). To obtain the explicit expression of the terms of series (3), while the dynamic evolution has been performed according to equations (6), we have developed the Monte Carlo scheme, which provides domain sampling of the terms giving the main contribution to the series (3). This sampling reduces also numerical expenses for calculations of integrals of each term. Ensemble averaging on the configuration of interacting quantum particles and classical heavy scatterers has been performed according to the probability distribution proportional to \( |\Psi| \) (3), while the dynamic evolution has been realized according to equations (3).

### III. QUANTUM DYNAMICS

The possibility to convert series like (3) into the form convenient for probabilistic interpretation allow us to develop the Monte Carlo method for its calculation (3), (4). According to the general theory of the Monte Carlo methods for solving linear integral equations one can simultaneously calculate all terms in the iteration series like (3), (4). So using the basic ideas of (3) we have developed the Monte Carlo scheme, which provides domain sampling of the terms giving the main contribution to the series (3). This sampling reduces also numerical expenses for calculations of integrals of each terms. Ensemble averaging on the configuration of interacting quantum particles and classical heavy scatterers has been performed according to the probability distribution proportional to \( |\Psi| \) (3), while the dynamic evolution has been realized according to equations (3).

### IV. SYSTEM OF UNITS

Numerical calculations are more convenient to perform for dimensionless equations. Let the quantum system considered have the following characteristic energy \( E_0 \) and time \( T_0 \) scales. The dimensionless combination \( E_0 T_0/\hbar \) may be considered as a measure of quantum behaviour of a system. However in our quantum dynamics studies it is more convenient to fix the maximum value of the considered time \( t' \) and to take it as a unit of dynamic time \( t \) of the
system. So dimensionless time $\tau = t/t'$ will always vary from 0 up to 1. As unit of a length we take the reciprocal wavenumber $k^{-1}$, determined by the ratio $k^2 = 2mE_0/\hbar^2$, where $m$ is characteristic mass of quantum particle. So, for example, for one electron in the external potential field $V_0U(q)$ the operator exponent of the time propagator can be rewritten in the form:

$$\hat{H}t/\hbar = \left\{-\frac{\hbar^2}{2m}\nabla^2 + V_0U(q)\right\}t/\hbar = \left\{-\frac{1}{2M}\nabla^2 + \xi_0U(q)\right\}\tau$$

Here $\triangle$ is Laplace operator, $V_0$ is characteristic constant of interaction of potential field, $M = \hbar^2/2E_0t'$, $\xi_0 = V_0/2E_0M = V_0t'/\hbar$, $t = t'/t$. The similar expressions and system of units were made use of for one electron in a field of chaotic classical scatterers. In this system of units all the above mentioned formulas take more simple form as the developed approach. According to quantum Kubo formulas in one electron approximation the tensor of electrical conductivity has been performed as the first example of application of the developed approach. According to quantum Kubo formulas in one electron approximation the tensor of electrical conductivity is $\sigma_{\alpha\gamma}(\omega) = n\int_0^\infty \exp (i\omega t - \epsilon t) \int_0^\beta \left\langle \hat{J}_{\alpha}(t + i\hbar\lambda) \right\rangle d\lambda dt$ where $\epsilon \to 0$, $n$ is the electron density, $\hat{J}_\alpha = e\hat{q}_\alpha(t) = e\hat{p}_\alpha/m$ is the electrical current operator, $\hat{q}_\alpha$ is the $\alpha$ component of electron velocity operator. Wigner representation of this tensor may be written in the form:

$$\sigma_{\alpha\gamma}(\omega) = n\int_0^\infty \exp (i\omega t - \epsilon t) \int_0^\beta \phi_{\alpha\gamma}(t, \lambda) d\lambda dt$$

where $\phi_{\alpha\gamma}(t, \lambda) = \left\langle \hat{J}_{\alpha}(t + i\hbar\lambda) \right\rangle$.

Here $\phi_{\alpha\gamma}(t, \lambda)$ is the dimensionless tensor of electrical conductivity. In the model of independent electrons in the medium of chaotic classical scatterers (one particle approximation) the Hamiltonian of the system can be written in the form:

$$\hat{H} = \hat{H}_{es} + \hat{H}_{ss}^{cl}$$

$$\hat{H}_{es} = -\triangle/2M + \sum_{j=1}^N \xi_0^{es} U_{es}(|q - Q_j|/\sigma')$$

$$\hat{H}_{ss}^{cl} = \sum_{j=1}^N p^2 m_j/2M m_j + \sum_{i \neq j}^N \xi_0^{ss} U_{ss}(|Q_i - Q_j|/\sigma'')$$

where $m_j$ is the mass of scatterer ($m/m_j \ll 1$), $\hat{H}_{ss}^{cl}$ is the classical Hamiltonian of scatterers, $\xi_0^{es} = V_0^{es}t'/\hbar$ and $\xi_0^{ss} = V_0^{ss}t'/\hbar$ are constant of interaction of pair wise electron-scatterer $U_{es}(|q - Q_j|/\sigma')$ and scatterer-scatterer $U_{ss}(|Q_i - Q_j|/\sigma'')$ potentials respectively, $Q_j$ are the scatterers positions ($j = 1, ..., N$), $\sigma$ is the characteristic length of potential.

Ensemble averaging on the configuration of interacting electron and classical heavy scatterers in quantum Kubo formulas has been performed according to the probability distribution proportional to $|\Psi|^2$, while the dynamic evolution has been realized according to recurrent relations (3)
The potential barrier of real type for electron-scatterer and scatterer-scatterer interaction has been taken in the Gaussian form:

\[ U(|q - q'|/\sigma) = \exp\left(-|q - q'|^2/\sigma^2\right) \]  

(7)

with equal to each other the all constants of interaction (\(\xi_0^{ss} = \xi_0^{ss} > 0\) and \(\sigma' = \sigma''\)).

### V. NUMERICAL RESULTS

Anderson localization of electrons have been investigated for one, two- and three dimensional disordered systems of scatterers. For 1D case the results of our simulation and their brief description are presented below. In all calculations the dimensionless density of classical scatterer is approximately equal to unity (\(n\sigma \approx 1\)), while \(k\sigma \approx 1\) and \(k^{-1}n \approx 1\).

#### A. Electron conductivity of disordered systems of scatterers

For the two small ratios of temperature to the height of a potential barrier \((kT/V_0)\) equal to 0.04 and 0.0025 the Fig. 1 and Fig. 2 present 1D results for diagonal elements of the tensor of the electrical conductivity, which are the momentum-momentum time correlation functions. Curves 1 on both figures relate to calculations taking into account only one term of iteration series (5), while curve 2 present results allowing for all terms of iteration series (5). So curves 1 on both figures have been obtained by using only the classical trajectories without momentum jumps. The curve 1 on the Fig. 1 have practically the traditional fast decay.

Curves 2 on both figures present momentum-momentum time correlation function obtained for dynamic trajectories with momentum jumps. The difference between these two correlation functions is larger at lower temperatures. Analyzing Fig. 2 one can conclude that curves 1 and 2 show undamped oscillations. Appearing of the undamped oscillations at very low temperature results from shortcomings of our model, in which the classical slow heavy scatterers are treated as non-moving particles on the time scale of the order of characteristic dynamic time of electrons.

However as is known from the literature the undamped oscillations results in unphysical behaviour of the Fourier transform of the momentum-momentum time correlation function. The next Fig. 3, 4, 5 and 6 show the significant difference of the Fourier transforms for correlation function with damped and undamped oscillations. Fig. 3, 4 and 5, 6 demonstrate the real and imaginary parts of its Fourier transforms versus the dimensionless frequency \(\bar{\hbar}\omega/V_0\). The real part of Fourier transform characterizes the Ohmic absorption of electromagnetic energy and has the physical meaning of electron conductivity, while the imaginary part presents \((\epsilon - 1)\omega\), where \(\epsilon\) is permittivity of the system. The curve 2 (quantum trajectories) on Fig. 3 is higher than the curve 1 (classical trajectories) but both curves are going to zero at small frequency pointing out that the static conductivity at zero frequency is equal to zero or is very small. Note that points of curve 2 are going to zero faster than the same value obtained in approximation of classical trajectories (curve 1). This behaviour of conductivity in the vicinity of zero frequency is the characteristic manifestation of the electron Anderson localization.

At lower temperatures the undamped oscillations with the proper phase shift of the momentum-momentum time correlation function may result in appearance of the negative values of real part of Fourier transform on Fig. 4. To overcome this shortcomings of our model at very low temperature it is necessary to take into account the slow motion of heavy particles, which should destroy the coherence oscillation of the light electrons trapped by heavy particles and cancel these negative values.

#### B. Position and momentum dispersions

The Fig. 7 presents the 1D results for quantum position dispersion versus the dimensionless time \(tV_0/\bar{\hbar}\) at the mentioned above two ratios of temperature to the height of a potential barrier \((kT/V_0)\). Curves 1 and 2 correspond to \(kT/V_0\) equal to 0.04 and 0.0025 respectively.

In one dimensional case quantum electrons is known should be localized at any temperatures but the length of localization is function of the particle energy. Analyzing data, submitted on the Fig. 7, it is possible to note that at lower temperature the curve 2 is very flat and the localization length (\(\lambda\)) can be estimated as the squared root of the characteristic value of the position dispersion (\(\lambda \leq 0.7\)). At higher temperature the behaviour of curve 1 is more complicated. At the initial stage \((tV_0/\bar{\hbar} \leq 100)\) curve 1 has a very flat part, which can be also considered as a characteristic manifestation of localization.
However when the time is more than 100 the curve 1 shows behaviour, which is typical for particle diffusion. This characteristic change in behaviour may be connected with momentum jumps of quantum trajectories. The virtual energy of the trajectories due to momentum jumps may be large. So the exponentially rare fast trajectories with very large value of localization length can give the exponentially large contribution to position dispersion as the difference in positions of fast trajectories may be exponentially large at large enough time. The similar problem connected with the exponentially large contribution of the exponentially rare events arises at the consideration of the classical wave propagation in random media. It is known for one dimensional case that the dispersion of wave intensity is not self-averaging value as the exponentially rare configurations of scatterers can give the exponentially large contribution of intensity at large enough distances from the wave source. Assuming that the initial flat part of curve 2 indicates the particle localization we can estimate the localization length as equal to 1.2.

The Fig. 8 presents momentum dispersion of quantum particle in disordered systems of scatterers. Curves 1 and 2 are stabilized and it is interesting to note that the lower temperature curve 2 are stabilized at larger value than curve 1. This may be connected with the uncertainty momentum-position principle and related fast oscillation of the localized quantum particles.

C. Energy distribution function

Quantum average energy of the system has been calculated according to the easily derived formula:

$$\bar{H}(t) = \frac{1}{(2\pi\hbar)^{2\nu}} \int dp_1 dq_1 dp_2 dq_2 \frac{1}{2} \{H(p_1, q_1) + H(p_2, q_2)\} \times W(p_1, q_1; p_2, q_2; t; i\hbar\beta)$$

Our calculations have shown that this function versus time variable is practically constant. To analyze the energy fluctuations during quantum dynamic evolution of the system the more interesting energy distribution function has been also calculated. The simple semi classical approximation of this function is defined by the following expression:

$$\rho(E, \beta) =$$

$$\frac{1}{(2\pi\hbar)^{2\nu}} \int_0^1 dt \int dp_1 dq_1 dp_2 dq_2 \frac{1}{2} \left\{ \delta(E - H(p_1, q_1)) + \delta(E - H(p_2, q_2)) \right\} \times W(p_1, q_1; p_2, q_2; t; i\hbar\beta)$$

The function $\ln(\rho(E, \beta))$ versus $E/V_0$ has been presented by curves 1 and 2 on the Fig. 8 and 9 for higher and lower temperatures respectively. Curves 1 present results obtained in approximation of classical trajectories (only first term in iteration series), while curves 2 show results allowing for all terms of iteration series. At $E/V_0 \leq 4$ curves 1 and 2 practically coincide both at higher and lower temperatures. However at the $E/V_0 \geq 4$ the distinction in curves 1 and 2 is large due to momentum jumps resulting in appearance of trajectories with large virtual energy. So the asymptotic behaviour of the curves 1 and 2 is quite different. These asymptotics in logarithmic scale may be fitted by the straight lines with different slope. The existence of the long exponentially decreasing tail of the energy distribution function supports our explanation of the peculiarity in the behaviour of position dispersion of quantum particles. For detailed investigations the additional consideration is needed to analyze this effect.

Lowering temperatures results also in splitting the main peak in energy distribution function into two sharper peaks. As it follows from Fig. 8 and 10 the energy gap at the edge of the energy spectrum a bit increases with the lowering temperature.

VI. CONCLUSION

In the Wigner formulation of quantum statistical mechanics for canonical and micro canonical ensembles we have presented a new computational technique allowing quantum dynamics simulations for systems including subsystems of quantum interacting particles and subsystems of classical heavy scatterers as well as the system of quantum particles.
in external potential field. The developed approach for quantum dynamics includes a sophisticated combination of well known molecular dynamics method and Monte Carlo technique.

For electrons in disordered systems of scatterers the numerical results have been obtained for series of the average values of the quantum operators including position and momentum dispersions, average energy, energy distribution function as well as for the frequency dependencies of tensor of electron conductivity and permittivity according to quantum Kubo formula. Zero or very small value of static conductivity have been considered as the manifestation of Anderson localization of electrons in 1D case. Independent evidence of Anderson localization comes from the behaviour of the calculated time dependence of position dispersion. Nevertheless for localized electrons the energy distribution function obtained has the long exponentially decaying tail, which is the reason of exponentially rare appearance of large values of quantum particle virtual energy that strongly affects the behaviour of the position dispersion.

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FIG. 1. Momentum-momentum time correlation function versus $tV_0/\hbar$ for higher temperature ($kT/V_0 = 0.04$): 1- approximation of the classical trajectories; 2- quantum trajectories

FIG. 2. Momentum-momentum time correlation function versus $tV_0/\hbar$ for lower temperature ($kT/V_0 = 0.0025$): 1- approximation of the classical trajectories; 2- quantum trajectories

FIG. 3. The real part of Fourier transform of the momentum-momentum time correlation function versus $\hbar\omega/V_0$ for higher temperature ($kT/V_0 = 0.04$): 1- approximation of the classical trajectories; 2- quantum trajectories

FIG. 4. The real part of Fourier transform of the momentum-momentum time correlation function versus $\hbar\omega/V_0$ for lower temperature ($kT/V_0 = 0.0025$): 1- approximation of the classical trajectories; 2- quantum trajectories

FIG. 5. The imaginary part of Fourier transform of the momentum-momentum time correlation function versus $\hbar\omega/V_0$ for higher temperature ($kT/V_0 = 0.04$): 1- approximation of the classical trajectories; 2- quantum trajectories

FIG. 6. The imaginary part of Fourier transform of the momentum-momentum time correlation function versus $\hbar\omega/V_0$ for lower temperature ($kT/V_0 = 0.0025$): 1- approximation of the classical trajectories; 2- quantum trajectories

FIG. 7. Position dispersion: 1- higher temperature ($kT\omega/V_0 = 0.04$); 2- lower temperature ($kT/V_0 = 0.0025$)

FIG. 8. Momentum dispersion: 1- higher temperature ($kT/V_0 = 0.04$); 2- lower temperature ($kT/V_0 = 0.0025$)

FIG. 9. Energy distribution in logarithmic scale versus $E_0/V_0$ for higher temperature ($kT/V_0 = 0.04$): 1- approximation of the classical trajectories; 2- quantum trajectories

FIG. 10. Energy distribution in logarithmic scale versus $E_0/V_0$ for lower temperature ($kT/V_0 = 0.0025$): 1- approximation of the classical trajectories; 2- quantum trajectories
