Основной показатель точности и достоверности: с вероятностью 0,95 ошибка определения координат утечек не более 0,5 м на участках трубопроводов теплосетей длиной до 600 м и диаметром до 1200 мм при условии применения оригинальной методики комплексного использования течеискателей К-10 и А-10. Другие характеристики течеискателя приведены в табл.1.

Таблица 1. Технические характеристики течеискателя К10-3М.

№	Наименование характеристики		Значение
1	Дальность действия радиоканалов (в городских условиях)		900 + 900 м
2	Время работы радиоканала без подзарядки аккумуляторов прием/передача		30/6 часов
3	Температурный диапазон	Вибродатчик	-30 … +85°С
4		Выносные радиоблоки	-10 … +65°С
5		Системный блок	+10 … +65°С
6	Длина кабеля	Катушки	25 м
7		Вибродатчика	10 м

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THE KELDYSH FORMALISM IN THE TIME-DEPENDENT DENSITY-FUNCTIONAL THEORY

We have considered application the Keldysh formalism in time-dependent density functional theory. It is shown that effects of electron-electron interaction can be taken systematically into account in the framework of the Kadanoff-Baym equations for Green functions determined on the Keldysh contour for the second-order

self-energy approximation. With the help of these Green functions we have derived the time-dependent Kohn-Sham potential from an action functional. The Keldysh formalism in a similar way leads to response functions that obey the causality principle that is illustrated on the case of the time-dependent optimized effective potential equations.

1. Introduction

We will consider the Keldysh formalism [1], which is an extremely useful tool for firstprinciples studies of nonequilibrium many-particle systems. Of particular interest to time-dependent density functional theory (TDDFT) is the relation to non-equilibrium Green functions (NEGF), which allows to construct exchange-correlation potentials with memory by the variational derivative method [2]. For many problems, such as, e.g., quantum transport or atoms in intense laser pulses, one needs exchange-correlation functionals with memory, and Green function techniques offer a systematic method for developing these.

The Keldysh formalism is also necessary for defining response functions in TDDFT and for defining an action functional needed for deriving TDDFT from a variational principle. The formalism does not differ much from ordinary equilibrium theory, the main difference being that all time-dependent functions are definied for time-arguments on a contour, known as the Keldysh contour.

The Green function, $G(r,t;r't')$ is a function of two space- and time-coordinates, and is obviously more complicated than the one-particle density $n(r,t)$, which is the main ingredient in TDDFT. However, the advantage of the NEGF methods is that we can systematically improve the approximations by taking into account particular physical processes. The Green function provides us directly with all expectation values of one-body operators (such as the density and the current), and also the total energy, ionization potentials, response functions, spectral functions, etc. In relation to TDDFT, this is useful not only for developing orbital functional and exchange-correlation functionals with memory, but also for providing insight in the exact properties of the non-interacting Kohn-Sham system [5,6].

In the following, we shall focus on systems that are initially in thermal equilibrium. We will start by introducing the Keldysh contour and the nonequilbrium Green functions, and then explain how to combine and manipulate functions with time variables on the contour. While we in TDDFT take exchange- and correlation-effects into account through $v_{xc}(n)$, the corresponding quantity in Green function theory is the self-energy $\Sigma(G)$. Just like $v_{xc}(n)$, the self-energy functional must be approximated. For a given functional $\Sigma(G)$, it is important that the resulting observables obey the macroscopic conservation laws, such as, e.g., the continuity equation. These approximations are known as conserving, and will be discussed briefly. In the last part of this section we will discuss the applications of the Keldysh formalism in TDDFT, including the relation between Σ and v_{xc}, the

derivation of the Kohn-Sham equations from an action functional, and the derivation of an f_{xc} functional. As an illustrative example, we will discuss the time-dependent exchange only optimized effective potential approximation.

In quantum mechanics we associate with any observable quantity $\overline{O}$ a hermitean operator O . The expectation value $Sp\{\rho_0 O\}$ gives the value of O when the system is described by the density operator ρ and the trace denotes a sum over a complete set of states in Hilbert space. For an isolated system the Hamiltonian H_0 does not depend on time, and the expectation value of any observable quantity is constant, provided $[\rho_{0,} H_0] = 0$. In these notes we want to discuss how to describe systems that are isolated for times $t < 0$, such that $H(t < 0) = H_0$, but disturbed by an external time-dependent field at $t > 0$. The expectation value of O at $t > 0$ is then given by the average on the initial density operator ρ_0 of the operator O in the Heisenberg representation,

$$\overline{O}(t) = Sp\{\rho_0 O_H(t)\} = Sp\{\rho_0 S(0,t) O_H S(t,0)\}, \qquad (1)$$

where the operator in the Heisenberg picture has a time-dependence according to $O_H(t) = S(0,t) O S(t,0)$. The evolution operator $S(t,t')$ is the solution of the equations

$$i\frac{d}{dt}S(t,t') = H(t)S(t,t'), \quad i\frac{d}{dt'}S(t,t') = -S(t,t')H(t'),$$

with boundary condition S(t,t)=1, and which can be formally written as

$$S(t,t') = \theta(t,t')T\exp\left(-i\int_{t'}^{t} dt_1 H(t_1)\right) + \theta(t',t)\overline{T}\exp\left(-i\int_{t'}^{t} dt_1 H(t_1)\right).$$

where the function $\theta(t,t')$ is defined to be 1 if t is later than t'; T is the time-ordering operator that rearranges the operators in chronological order with later times to the left; $\overline{T}$ is the anti-chronological time-ordering operator. The evolution operator satisfies the group property $S(t;t_1)S(t_1;t') = S(t:t')$ for any t_1. Notice that if the Hamiltonian is time-independent in the interval between t and t′, then the evolution operator becomes $S(t;t') = \exp\left(-iH(t-t')\right)$. If we now let the system be initially in thermal equilibrium, with an inverse temperature $\beta = 1/k_B T$ and chemical potential μ, the initial density matrix is $\rho_0 = \exp\left(-\beta(H_0 - \mu N)\right)/Sp\left(-\beta(H_0 - \mu N)\right)$. Inserting this expression in (1), we find

$$\overline{O}(t) = \frac{\mathrm{Sp}\left\{\exp(\beta\mu N)S(-i\beta\mu)S(0;t)OS(t;0)\right\}}{\mathrm{Sp}\left\{\exp(\beta\mu N)S(-i\beta\mu)\right\}}. \qquad (2)$$

Reading the arguments in the numerator from the right to the left, we see that we

can design a time-contour γ with a forward branch going from 0 to t, a backward branch coming back from t and ending in 0, and a branch along the imaginary time-axis from 0 to $-i\beta$. This contour is illustrated in Fig. 1.

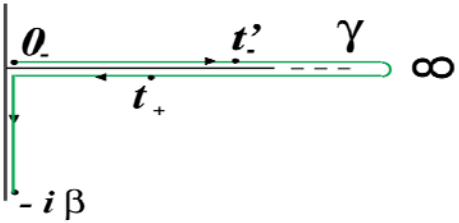

Fig. 1. The Keldysh contour, starting at $t = 0$, and ending at $t = -i\beta$, with t on the backward branch and t' on the forward branch. By definition, any point lying on the vertical track is later than a point lying on the forward or backward branch.

Note that the group property of S means that we are free to extend this contour up to infinity. We can now generalize (2), and let z be a time-contour variable on γ. Letting the variable z run along this same contour, (2) can be formally recast as

$$\overline{O}(z) = \frac{\mathrm{Sp}\left\{\exp(\beta\mu N)T_C \exp\left(-i\int_\gamma dzH(z)\right)O(z)\right\}}{\mathrm{Sp}\left\{\exp(\beta\mu N)T_C \exp\left(-i\int_\gamma dzH(z)\right)\right\}} \qquad (3)$$

The contour ordering operator T_C moves the operators with "later" contour variable to the left. In (3), $O(z)$ is not the operator in the Heisenberg representation (the latter is denoted with $O_H(t)$). The contour-time argument in O is there only to specify the position of the operator O on γ. A point on the real axis can be either on the forward (we denote these points t_-, or on the backward branch (denoted t_+), and a point which is earlier in real time, can therefore be later on the contour, as illustrated in Fig. 1.

To summarize, in (5) the variable z lies on the contour γ; the r.h.s. gives the time-dependent statistical average of the observable O when z lies on the forward or backward branch, and the statistical average before the system is disturbed when z lies on the vertical track.

2. NONEQUILIBRIUM GREEN FUNCTIONS

We now introduce the nonequilibrium Green function (NEGF), which is a function of two contour time-variables. In order to keep the notation as light as possible, we here discard the spin degree of freedom; the spin index may be restored later as needed. The field operators $\psi(r)$, $\psi^+(r)$ destroy and create an

electron in r r and obey the anticommutation relations $[\psi(r),\psi^+(r)]=\delta(r-r')$. We write the Hamiltonian $H(t)$ as the sum of a quadratic term

$$h(t)=\int drdr'\psi^+(r)<r\,|\,h(t)\}r'>\psi^+(r') \tag{4}$$

and the interaction operator

$$H_{in}(t)=\frac{1}{2}\int drdr'\psi^+(r)\psi^+(r')<r\,|\,\omega(r,r')\}\psi(r')\psi(r)\,. \tag{5}$$

Here, when describing electrons in electro-magnetic field, the quadratic term is given by $<r\,|\,h(t)\,|\,r'>=\delta(r-r')\left([\nabla/i+A(r,t)]^2/2+v(r,t)\right)$.

The definition of an expectation value in (3) can be generalized to the expectation value of two operators. Then Green function is defined as

$$G(r,z;r',z')=-i\left\langle T_C\psi_H(r,z)\psi_H^+(r',z')\right\rangle,$$

where the contour variable in the field operators specifies the position in the contour ordering. The operators have a time-dependence according to the definition of the Heisenberg picture, e.g. $\psi_H(r,z)=S(0;z)\psi^+(r)S(z;0)$. The Green function can be written

$$G(z;z')=\theta(z,z')G^>(z;z')+\theta(z',z)G^<(z;z'). \tag{6}$$

From the definition of the time-dependent expectation value in Eq. (2), it follows that the greater Green function $G^>(z,z')$), where z is later on the contour than z' is

$$G^>(r,z;r',z')=\frac{1}{i}\frac{\mathrm{Sp}\left\{\exp(\beta\mu N)S(-i\beta;0)\psi_H(r,z)\psi_H^+(r',z')\right\}}{\mathrm{Sp}\left\{\exp\left(\beta\mu N\right)S(-i\beta\mu)\right)\}}\,. \tag{7}$$

If z'' is later on the contour than z, then the Green function equals

$$G^<(r,z;r',z')=-\frac{1}{i}\frac{\mathrm{Sp}\left\{\exp(\beta\mu N)S(-i\beta;0)\psi_H^+(r',z')\psi_H(r,z)\right\}}{\mathrm{Sp}\left\{\exp\left(\beta\mu N\right)S(-i\beta\mu)\right)\}}\,. \tag{8}$$

The extra minus sign on the right hand side comes from the contour ordering. More generally, rearranging the field operators ψ and ψ^+ (later arguments to the left), we also have to multiply by $(-1)^{\mathrm{P}}$, where P is the parity of the permutation. From the definition of the Green function, it is easily seen that the electron density, $n(r,z)=<\psi_H^+(r,z)\psi_H(r,z)>$ and current is obtained according to

$$n(r,z)=-G(r,z;r,z^+),$$

$$j(r,z)=-i\left\{\left[\frac{\nabla}{2i}-\frac{\nabla'}{2i}+A(r,z)\right]G(r,z;r',z')\right\}_{z'=z^+}\,.$$

where z^+ indicates that this time-argument is infinitesimally later on the contour.

The Green function $G(z;z')$ obeys an important cyclic relation on the Keldysh contour. Choosing $z = 0_-$, which is the earliest time on the contour, we find $G(0_-;z') = G^<(0;z')$, given by (8) with $\psi_H(r,0) = \psi_H(r)$. Inside the trace we can move $\psi(r)$ to the left. Furthermore, we can exchange the position of $\psi(r)$ and $\exp(\beta\mu N)$ by noting that $\psi(r)\exp(\beta\mu N) = \exp(\beta\mu(N+1))\ \times\psi(r)$. Using the group identity $S(-i\beta;0)S(0;-i\beta) = 1$, we obtain

$$G(r,0;r',z') = -\frac{1}{i}\frac{\mathrm{Sp}\left\{\psi_H(r)\exp(\beta\mu N)S(-i\beta;0)\psi_H^+(r',z')\right\}}{\mathrm{Sp}\left\{\exp\left(\beta\mu N\right)S(-i\beta;0)\right\}} =$$

$$= \frac{\exp(-\beta\mu)}{i}\frac{\mathrm{Sp}\left\{\exp(\beta\mu N)S(-i\beta;0)\psi_H(r,-i\beta)\psi_H^+(r',z')\right\}}{\mathrm{Sp}\left\{\exp\left(\beta\mu N\right)S(-i\beta;0)\right\}}.$$

The r.h.s. equals $-\exp(-\beta\mu) < r \mid G(-i\beta;z' \mid r') >$. Together with similar analysis for $G(z;0_-)$, we include that $G(0_-;z') = -\exp(\beta\mu)G(-i\beta;z')$. These equation constitute the so called Kubo-Martin-Schvinger (KMS) conditions [3,4]). It is easily seen that $G^>(z;z) = G^<(z;z) - i1$.

3. RELATIONS FOR KELDYSH FUNCTIONS

The Green function belongs to a larger class of functions of two time-contour variables that we will refer to as Keldysh space. These functions can be written on the form

$$k(z;z') = \delta(z,z')k^\delta(z) + \theta(z,z')k^>(z,z') + \theta(z',z)k^<(z,z'), \qquad (9)$$

where the δ-function on the contour is defined as $\delta(z,z') = d\theta(z,z')/dz$. These functions are somewhat complicated due to the fact that each of the time-arguments can be located on three different branches of the contour γ. Below we systematically derive a set of identities that are commonly used for dealing with such functions and will be used extensively in the following sections.

For any $k(z;z')$ in the Keldysh space we define the greater and lesser functions on the physical time axis $k^>(t;t') \equiv k(t_+;t'_-)$ and $k^<(t;t') \equiv k(t_-;t'_+)$. We also define the following two-point functions with one argument t on the physical time axis and the other τ on the vertical track $k^{\urcorner|}(t;t') \equiv k(t_\pm;\tau)$ and $k^{\urcorner|}(t;t') \equiv k^{|\urcorner}(\tau;t_\pm)$. In the definition of $k^{\urcorner|}$ and $k^{|\urcorner}$ we can arbitrarily choose t_+ or t_- since τ is later than both of them. The symbols "$^{\urcorner|}$" and "$^{|\urcorner}$" have been chosen in order to help the visualization of the time arguments. For instance, "$\urcorner$" has a horizontal segment followed by a vertical one; correspondingly, $k^{\urcorner|}$ has a first argument which is real (and thus lies on the horizontal axis) and a second argument which is imaginary (and thus lies on the vertical axis). We will also use

the convention of denoting the real time with latin letters and the imaginary time with greek letters.

The above mentioned k -functions obey the relations

$$k^{>}(t,t') = k(t_+,t'_-),\ \ k^{<}(t,t') = k(t_-,t'_+),$$
$$k^{R}(t,t') = \delta(t-t')k^{\delta}(t) + \theta(t-t')[k^{>}(t,t') - k^{<}(t,t')],$$
$$k^{A}(t,t') = \delta(t-t')k^{\delta}(t) - \theta(t'-t)[k^{>}(t,t') - k^{<}(t,t')],$$
$$k^{\urcorner}(t;\tau) \equiv k(t_\pm;\tau),\ \ k^{\ulcorner}(t;\tau) \equiv k(\tau;t_\pm),$$
$$k^{M}(\tau;\tau') = k(z=\tau;z'=\tau'),$$

which occur also for the mentioned Green functions.

It is straightforward to show that if $a(z;z')$ and $b(z;z')$ belong to the Keldysh space, then

$$c(z;z') = \int_\gamma dz_1 a(z;z_1)b(z_1;z') \tag{10}$$

also belongs to the Keldysh space. Such contour integrals is contained in equations for the Green functions. Therefore we will consider its calculation. If we write out the contour integral in (10) in detail, we see with the help of Fig. 1, that the integral consists of four main parts. First, we must integrate along the real axis from $z_1 = 0_-$ to $z_1 = t'_-$, for which $a = a^{>}$ and $b = b^{<}$. Then, the integral goes from $z_1 = t'_-$ to $z_1 = t_+$, where $a = a^{>}$ and $b = b^{>}$. The third part of the integral goes along the real axis from $z_1 = t_+$ to $z_1 = 0_+$, with $a = a^{<}$ and $b = b^{>}$. The last integral is along the imaginary track, from 0_+ to $-i\beta$, where $a = a^{\urcorner}$ and $b = b^{\ulcorner}$. In addition, we have the contribution from the singular parts, a^{δ} and b^{δ}, which is trivial since these integrals involve a δ-function. With these specifications, we can drop the $\pm$ -subscripts on the time-arguments and write

$$c^{>}(t;t') = a^{>}(t,t')b^{\delta}(t') + a^{\delta}(t)b^{>}(t,t') + \int_0^{t'} dt_1 a^{>}(t,t_1)b^{<}(t_1,t')$$
$$+\int_{t'}^{t} dt_1 a^{>}(t,t_1)b^{>}(t_1,t') + \int_{t}^{o} dt_1 a^{<}(t,t_1)b^{>}(t_1,t') + \int_{t'}^{t} d\tau_1 a^{\urcorner}(t,\tau_1)b^{\ulcorner}(\tau_1,t').$$

The second integral on the r.h.s. is an ordinary integral on the real axis of two well defined functions and may be rewritten as

$$\int_{t'}^{t} dt_1 a^{>}(t,t_1)b^{>}(t_1,t') = \int_{t'}^{0} dt_1 a^{>}(t,t_1)b^{>}(t_1,t') + \int_{0'}^{t'} dt_1 a^{>}(t,t_1)b^{>}(t_1,t')$$

Using this relation, the expression for $c^{>}$ becomes

$$c^{>}(t;t') = a^{>}(t,t')b^{\delta}(t') + a^{\delta}(t)b^{>}(t,t') + \int_0^{t'} dt_1 a^{>}(t,t_1)[b^{>}(t_1,t')$$
$$-b^{>}(t_1,t')] + \int_0^{t} dt_1[a^{>}(t,t_1) - a^{>}(t,t_1)]b^{>}(t_1,t') + \int_0^{-i\beta} d\tau_1 a^{\urcorner}(t,\tau_1)b^{\ulcorner}(\tau_1,t').$$

Taking into account into account above entered retarded and advanced functions Next, we introduce two other functions on the physical time axis

$$k^R(t,t') = \delta(t-t')k^\delta(t) + \theta(t-t')[k^>(t,t') - k^<(t,t')],$$
$$k^A(t,t') = \delta(t-t')k^\delta(t) - \theta(t'-t)[k^>(t,t') - k^<(t,t')],$$

We can rewrite the function $c^>$ in a more compact form

$$c^>(t;t') = a^>(t,t')b^\delta(t') + a^\delta(t)b^>(t,t') + \int_0^\infty dt_1[a^>(t,t_1)b^A(t_1,t')$$
$$+a^R(t;t_1)b^>(t_1,t')] + \int_0^{-i\beta} d\tau_1 a^\urcorner(t,\tau_1)b^\ulcorner(\tau_1,t').$$

Introducing a short hand notation for integral along the physical time axis and for those between 0 and $-i\beta$, namely

$$f\cdot g \equiv \int_0^\infty dt f(t)g(t) \text{ and } f*g \equiv \int_0^{-i\beta} d\tau f(\tau)g(\tau),$$

we obtain

$$c^> = a^>b^A + a^Rb^> + a^\urcorner * b^\ulcorner$$

Similarly, one can prove that

$$c^< = a^<b^A + a^Rb^< + a^\urcorner * b^\ulcorner,\ c^R = a^R\cdot b^R,\ c^A = a^A\cdot b^A,$$
$$c^\urcorner = a^R\cdot b^\urcorner + a^\urcorner * b^{\urcorner M},\quad c^\ulcorner = a^\ulcorner\cdot b^{A\urcorner} + a^{M\urcorner} * b^\ulcorner,$$

were $k^M(\tau;\tau') = k(z=\tau;z'=\tau')$.

4. THE KADANOFF-BAYM EQUATIONS

The Green function, as defined in (6), satisfies the equation of motion

$$i\frac{d}{dz}G(z;z') = 1\delta(z,z') + h(z)G(z,z') + \int_\gamma dz_1\Sigma(z,z_1)G(z_1z'),$$
$$-i\frac{d}{dz'}G(z;z') = 1\delta(z,z') + G(z,z')h(z') + \int_\gamma dz_1 G(z;z_1)\Sigma(z_1,z').$$

The external potential is included in h, while the self-energy Σ _ is a functional of the Green function, and describes the effects of the electron interaction. The self-energy belongs to Keldysh space and can therefore be written on the form $\Sigma(z,z') = \delta(z,z')\Sigma^\delta(z) + \theta(z,z')\Sigma^>(z) + \theta(z',z)\Sigma^<(z)$. The singular part of the self-energy can be identified as the Hartree–Fock potential, $\Sigma^\delta(z) = U_H(z) + \Sigma_x(z)$. The self-energy obeys the same anti-periodic boundary conditions at $z = 0_-$ and $z = -i\beta$ as G. We will discuss self-energy approximations in more detail below. Calculating the Green function on the time-contour now consists of two steps: 1) First one has to find the Green function for imaginary times, which is equivalent to

finding the equilibrium Matzubara Green function $G^M(\tau;\tau')$. This Green function depends only on the difference between the time-coordinates, and satisfies the KMS boundary conditions according to $G^M(\tau+i\beta,\tau') = -e^{\beta\mu N}G^M(\tau,\tau')$. Since the self-energy depends on the Green function, this amounts to solving the finite-temperature Dyson equation to self-consistency. 2) The Green function with one or two time-variables on the real axis can now be found by propagating according to the above mentioned equations of motion. Starting from $t=0$, this procedure corresponds to extending the time-contour along the real time-axis. The process is illustrated in Fig. 2. Writing out the equations for the components of G using the above mentioned relations for Keldysh functions, we obtain the equations known as the Kadanoff-Baym equations [2],

$$i\frac{d}{dz}G^{<}(z;z') = h(t)G^{<}(t,t') + \left[\Sigma^R \cdot G^{<}\right](t,t') + \left[\Sigma^{<} \cdot G^A\right](t,t') + \left[\Sigma^{\lceil} \cdot G^{\lfloor}\right](t,t'), \tag{11}$$

$$i\frac{d}{dt}G^{\lceil}(t,\tau) = h(t)G^{\lceil}(t,\tau) + \left[\Sigma^R \cdot G^{\lceil}\right](t,\tau) + \left[\Sigma^{\lceil} \cdot G^M\right](t,\tau). \tag{12}$$

It is easily seen that if we denote by T the largest of the two time-arguments t and t', then the right hand side of (11) and (12) depend on $G^{<}(t_1,t_2)$, $G^{\lfloor}(\tau_1,t_2)$, $G^{\lceil}(t_1,\tau_2)$ for t_1, $t_2 \le T$. When propagating the Kadanoff-Baym equations one therefore starts at $t=t'=0$, with the initial conditions given by $G^{<}(0,0) = \lim_{\eta\to 0} G^M(-i\eta,0)$, $G^{\lfloor}(\tau,0) = G^M(\tau,0)$. One then calculates $G^{<}(t,t')$ for time-arguments within the expanding square given by $t,t' \le T$. Simultaneously, one calculates $G^{\lfloor}(t,\tau)$ and $G^{\lceil}(\tau,t)$ for $t \le T$.

5. ACTION FUNCTIONAL AND TDDFT

We defined the action as $A = i\ln \mathrm{Sp}\left\{e^{\beta\mu N}S(-i\beta;0)\right\}$, where the evolution operator S is the same as defined above. The action functional is a tool for generating equations of motion, and is not interesting per se. Nevertheless, one should notice that the action $i\ln Z$, where Z is the thermodynamic partition function. It is easy to show that if we make a perturbation $\delta V(z)$ in the Hamiltonian, the change in the evolution operator is given by

$$i\frac{d}{dt}\delta S(z;z') = \delta V(z)S(z;z') + H(z)S(z;z') \tag{13}$$

A similar equation for the dependence on z', and the boundary condition $\delta S(z;z')=0$ gives

$$\delta S(z;z') = -i\int_{z'}^{z} dz_1 S(z;z_1)\delta V(z_1)S(z_1;z'). \qquad (14)$$

We stress that the time-coordinates are on a contour going from 0 to $-i\beta$. The variation in, e.g., $V(t_+)$ is therefore independent of the variation in $V(t_-)$ (t−). If we let $\delta V(z)=\int dr\delta v(r,z)n(r)$, a combination of (13) and (14) yields the expectation values of the density,

$$\frac{\delta A}{\delta v(r,z)} = \frac{i}{\mathrm{Sp}\left(e^{\beta\mu N}S(-i\beta;0)\right)}\frac{\delta}{\delta v(r,z)}\mathrm{Sp}\left\{e^{\beta\mu N}S(-i\beta;0)\right\}$$

$$= \frac{\mathrm{Sp}\left(e^{\beta\mu N}S(-i\beta;0)S(0;z)n(r)S(z;0)\right)}{\mathrm{Sp}\left(e^{\beta\mu N}S(-i\beta;0)\right)} = n(r,z).$$

A physical potential is the same on the positive and on the negative branch of the contour, and the same is true for the corresponding time-dependent density, $n(r,t)=n(r,t_\pm)$. A density response function defined for time-arguments on the contour is found by taking the functional derivative of the density with respect to the external potential. Using the compact notation $1=(r_1,z_1)$, the response function is written

$$\chi(1,2)=\frac{\delta n(1)}{\delta v(2)}=\frac{\delta^2 A}{\delta v(1)\delta v(2)}=\chi(2,1). \qquad (15)$$

This response function is symmetric in the space and time-contour coordinates. We again stress that the variations in the potentials at t+ and t− are independent. If, however, one uses this response function to calculate the density response to an actual physical perturbing electric field, we obtain

$$\delta n(r,t)=\delta n(r,t_\pm)=\int_\gamma dz'\int dr'\,\chi(r,t_\pm;r',z')\delta v(r',z'), \qquad (14)$$

where γ indicates an integral along the contour. In this expression, the perturbing potential (as well as the induced density response) is independent of whether it is located on the positive or negative branch, i.e. $\delta v(r',t_\pm')=\delta v(r',t')$. We consider a perturbation of a system initially in equilibrium, which means that $\delta v(r',t_\pm')\neq 0$ only for $t>0$, and we can therefore ignore the integral along the imaginary track of the time-contour. The contour integral then consists of two parts: 1) First an integral from $t'=0$ to $t'=t$, in which $\chi=\chi^>$, and 2) an integral from $t'=0$ to $t=0$, where $\chi=\chi^<$. Writing out the contour integral in (14) explicitly then gives $\delta n(r,t)=\int_0^t dt'\int dr'\,\chi^R(rt;r't')\delta v(r't')$. The response to a perturbing field is

therefore given by the retarded response function, while $\chi(1,2)$ defined on the contour is symmetric in $(1 \leftrightarrow 2)$.

If we now consider a system of non-interacting electrons in some external potential v_s, we can similarly define a non-interacting action-functional A_s. The steps above can be repeated to calculate the non-interacting response function. The derivation is straightforward, and gives

$$\chi_s(1,2) = \frac{\delta^2 A_s n(1)}{\delta v_s(1)\delta v_s(2)} = -iG_s(1;2)G_s(2;1)\,, \qquad (16)$$

were G_s is non-interactive Green function.

Having defined the action functional for both the interacting and the non-interacting systems, we now make a Legendre transform, and define

$$A[n] = -A[v] + \int d(1)n(1)v(1)\,,$$

which has the property that $\delta A[n]/\delta n(1) = v(1)$. Similarly, we define the action function $A_s[n]$ with property $\delta A_s[n]/\delta n(1) = v_s(1)$. The Legendre transforms assume the existence of a one-to-one correspondence between the density and the potential. From these action functionals, we now define the exchange-correlation part to be

$$A_{xc}[n] = A_s[n] - A[n] - \frac{1}{2}\int d(12)\delta(z_1,z_2)\frac{n(1)n(2)}{|r_1 - r_2|}\,.$$

Taking the functional derivative with respect to the density gives $v_s[n](1) = v(1) + v_H(1) + v_{sc}[n](1)$, where $v_H(1)$ is the Hartree potential and $v_{xc} = \delta A_{xc}/\delta n(1)$. Again, for time-arguments on the real axis, these potentials are independent of whether the time is on the positive or the negative branch. If we, however, want to calculate the response function from the action functional, then it is indeed important which part of the contour the time-arguments are located on.

We already described how to define response function on the contour, both in the interacting (15) and the non-interacting (16) case. Given the exact Kohn-Sham potential, the TDDFT response function should give exactly the same density change as the exact response function $\delta v_s(1) = \int d(2)\chi_s(1;2)\delta v_s(2)$. The change in the Kohn-Sharm potential is given by

$$\chi^R(r_1,t_1;r_2,t_2) = \chi_s^R(r_1,t_1;r_2,t_2) + \int dt_3 dt_4 dr_3 dr_4 \chi_s^R(r_1,t_1;r_3,t_3)$$
$$\times f_s^R(r_3,t_3;r_4,t_4)\chi^R(r_4,t_4;r_2,t_2).$$

The time-integrals in the last expression go from 0 to ∞. As expected, only the retarded functions are involved in this expression. We stress the important result that while the function $f_{Hxc}(1,2)$ is symmetric under the coordinate permutation $(1 \leftrightarrow 2$, it is the retarded function $f_{Hxc}^R(r_1,t_1;r_2,t_2) = \delta(t_1,t_2)/|r_1 - r_2| + +f_{xc}^R(r_1,t_1;r_2,t_2)$, which the response to a perturbing potential.

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ВИКОРИСТАННЯ ГЕНЕТИЧНИХ АЛГОРИТМІВ ДЛЯ ВИЯВЛЕНЯ ВТОРГНЕННЯ В КОМП'ЮТЕРНІ МЕРЕЖІ

This paper describes how it is possible to apply Genetic Algorithm in Intrusion Detection Systems. A brief overview of the Intrusion Detection System, genetic algorithm, and related detection techniques is presented. Compare with other implementations of the same problem, this implementation considers both temporal and spatial information of network connections in encoding the network connection information into rules in IDS. The main system architecture and diagram of GA are shown.

Вступ

Генетичні алгоритми широко застосовуються в системах виявлення вторгнення. Генетичні алгоритми використовуються для створення правил поведінки системи в разі вторгнення. Мережне з'єднання та його характер можна представити так, щоб у відповідність йому можливо було поставити правило для прийняття рішення про те розцінювати дане з'єднання як вторгнення або ні. Ці правили моделюються як хромосоми певної популяції. Популяція перебуває в розвитку до тих пір поки вона не буде задовольняти встановленим критеріям. Сформовані правили використовуються системою для прийняття рішення про характер з'єднання (вторгнення або ні). Генетичні алгоритм не є самостійною системою безпеки, а являють собою механізм формування правил для використання в системах безпеки [1-3]. Останнім часом найбільш досліджуваною сферою комп'ютерної безпеки є системи виявлення вторгнення. Ця технологія виявлення використовується як

