Optimal Control Theory for Time-Dependent Quantum Transport

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Optical techniques have been employed to coherently control the quantum transport through nanojunctions. Conventional works on optical control of quantum transport usually applied a tailored electrical pulses to perform specific tasks. In this work, an opposite way is employed and a time-dependent driving field is searched to force the system behave in desired pattern. In order to achieve the goal, an optimal control theory for time-dependent quantum transport is developed. The theory provides a theoretical tool for the design of driving field to control the transient current through a nano junction along a prescribed pattern. The optimal control field is searched by minimizing a control functional. Corresponding equations of motions are derived accordingly to efficiently search for the optimal control field. The development of optimal control theory for time-dependent quantum transport enables the ultra-fast and precise control of current by electrical field.

I. INTRODUCTION

Quantum transport in nanojunctions has been of great research interest. Previous researches in this field were to measure or calculate the current-voltage characteristics. In recent years, time-resolved studies have attracted more and more attentions which give insight on the evolution of transient current upon a given bias voltage or external field. Study of transient transport is of fundamental importance, which helps us understand whether does a steady-state exist and how is it reached. Theoretically, time-dependent approaches have been developed accordingly to uncover the transient phenomena of quantum transport. These approaches are broadly categorized under single-particle approach and many-body theory, including quantum Monte-Carlo (QMC), quantum master equation (QME), hierarchical equation of motion (HEOM), scattering matrix approach, non-equilibrium Green’s function (NEGF) and time-dependent density functional theory (TDDFT) based approaches, etc.

Despite these theoretical methods differ a lot from each other, they share one common feature, transient current or external field, is calculated. However, there is a trend to take a step further and control the current or charge migration by tailoring stimulus. Especially, people are trying to tune laser pulse to coherently control the current by tuning the relative amplitude and phase of two laser pulses. Such ideas have also been applied to control chemical reactions, where chemical reaction are influenced by femto-second laser pulses such that a specific reaction gets enhanced or suppressed. Consequently, optimal control of quantum systems has attracted more and more research efforts due to its fundamental importance and potential applications.

Mathematically, optimal control theory is a general idea which has been used in many problems of classical mechanics. Later it was employed to many other research fields including quantum dynamics. In previous works, Kleinekathöfer and coworkers have combined optimal control theory and QME to control quantum transport with tailored fields. However, the many-particle nature of QME and second-order perturbation treatment of system-lead coupling limit its application to small systems and small coupling regime. In this work, an optimal control theory (OCT) for transient quantum transport is developed by combining optimal control theory with NEGF based time-dependent quantum transport theory. The article is organized as follows. Sec. \textsuperscript{II} introduces time-dependent quantum transport theory. The optimal control theory for time-dependent quantum transport is introduced in details in Sec. \textsuperscript{III}. Finally, Sec. \textsuperscript{IV} summarizes the manuscript.

II. TIME-DEPENDENT QUANTUM TRANSPORT THEORY

The system of interest is a device sandwiched by two leads (extension to multi-lead is formally straightforward). The corresponding Hamiltonian reads

\begin{equation}
H = H_S + \sum_{\alpha} [H_\alpha + H_{\alpha S}],
\end{equation}

where $H_S$ and $H_\alpha$ are the Hamiltonians of the device and lead $\alpha$, respectively; Tight-binding (TB) model Hamiltonians are considered in this work. $H_{\alpha S}$ is the interaction Hamiltonian between device and lead $\alpha$. The Hamiltonian of the device region reads $H_S = \sum_{mn} h_{mn}(t) c^\dagger_m c_n$, where $c^\dagger_m$ and $c_n$ are the electronic creation and annihilation operators in the device region, respectively; $h_{mn}(t)$ is the time-dependent TB Fock matrix. In presence of external field, $h(t) = h_0 - dE(t)$, where $d$ is the dipole matrix. The Hamiltonian of lead $\alpha$ is $H_\alpha = \sum_{k\alpha} \epsilon_{k\alpha}(t) c^\dagger_{k\alpha} c_{k\alpha}$, where $c^\dagger_{k\alpha}$ and $c_{k\alpha}$ are the electronic creation and annihilation operators in the lead $\alpha$, respectively. $\epsilon_{k\alpha}(t)$ is the single-particle energy, the time-dependence of which comes from applied bias voltage or external field. The variation of single-particle energy
in lead $\alpha$ upon time-dependent bias is assumed to be $\epsilon_k(t) = \epsilon_{k}^0 + \Delta_k(t)$, with $\Delta_k(t)$ being the voltage applied on lead $\alpha$. The interaction Hamiltonian between device and lead $\alpha$ reads $H_{\alpha\delta} = \sum_{k_{a,m}}(V_{k_{a,m}} c_{k_{a,m}}^{\dagger} + H.c.)$, where $V_{k_{a,m}}$ is the coupling strength.

To describe the transient transport, we examine the dynamics of reduced single-particle density matrix (RSDM). With the Hamiltonian described above, the equation of motion (EOM) of the RSDM reads:

$$i\dot{\varphi}_\alpha(t) = [h(t), \varphi_\alpha(t)] - \sum_\alpha [\varphi_\alpha(t) - \varphi_\alpha^R(t)], \quad (2)$$

the dissipation matrix $\varphi_\alpha(t)$ in above equation denotes the interaction between the device and lead $\alpha$, which is responsible for the particle dissipation. Within the framework of NEGF approach, $\varphi_\alpha(t)$ is

$$\varphi_\alpha(t) = i \int_{-\infty}^{t} dt'[G^<\alpha(t,\tau)\Sigma^\alpha_>^{\alpha}(\tau, t) - G^>\alpha(t, \tau)\Sigma^\alpha_<(\tau, t)], \quad (3)$$

where $G^<\alpha(t, \tau)$ and $G^>\alpha(t, \tau)$ are the lesser and greater Green’s function of device, respectively. $\Sigma^\alpha_<(t, \tau)$ and $\Sigma^\alpha_>(t, \tau)$ are the lesser and greater self-energies due to the coupling between device and lead $\alpha$, respectively. The lesser and greater self-energy can be obtained from the $G$ propagation of Eq.(2). The complexity now lies in the evaluation of the self-energy. The equation of motion (EOM) of the RSDM reads:

$$\Sigma^\alpha_{<,>}(\tau, t) = \pm \frac{1}{2\pi} \int \frac{d\epsilon}{f^{\pm}\alpha}(\epsilon) \int_{-\infty}^{t} dt'[\epsilon + \Delta_n(t_1)] dt_1 \Lambda_\alpha(\epsilon), \quad (4)$$

where $f^{\pm}\alpha(\epsilon) = 1/(e^{\pm \beta(\epsilon - \mu_\alpha)} + 1)$ is the Fermi distribution, with $\beta$ being the inverse temperature. $\Lambda_\alpha(\epsilon)$ is the line-width function which is related to the density of state (DOS) of lead and device-lead coupling strength $[\Lambda_\alpha(\epsilon)]_{mn} = \pi \sum_k \delta(\epsilon - \epsilon_k) V_{k_{a,m}}^{*} V_{k_{a,n}}$.

Eq.(2) and Eq.(3) are the general formalism for open electronic systems coupled with non-interacting leads. $\varphi_\alpha(t)$ is corresponding to the net rate of electron going through the interface between lead $\alpha$ and device. The transient current can be evaluated by tracing the dissipation matrix $\varphi_\alpha(t)$:

$$I_\alpha(t) = i Tr[\varphi_\alpha(t) - \varphi_\alpha^R(t)] = -2i \text{Im} Tr[\varphi_\alpha(t)]. \quad (5)$$

The RSDM can be obtained by performing time propagation of Eq.(2). The complexity now lies in the evaluation of the dissipation matrix $\varphi_\alpha(t)$. In order to implement this method to simulate realistic systems from first-principles, an efficient method to deal with $\varphi_\alpha(t)$ is desirable. To achieve this, the WBL approximation is employed, which involves the following assumptions for the leads: (i) band widths are assumed to be infinitely large; (ii) line-widths are assumed to be energy-independent, i.e., $\Lambda_\alpha(\epsilon) = \Lambda_\alpha$, where $\Lambda_\alpha = \pi \sum_k |V_k|^{2} \delta(\epsilon_f - \epsilon_k)$ is the line-width function evaluated at Fermi energy $\epsilon_f$ of the unbiased system. To further improve the calculation efficiency, Padé expansion approach is applied to Fermi distribution function. The accuracy of Padé expansion is determined by the expansion order. Based on Padé expansion and WBL approximation, the integration in Eq.(4) can be evaluated analytically through contour integration and residue theorem, the resulting expression of self-energy is rewritten as

$$\Sigma^\alpha_{<,>}(\tau, t) = \pm \frac{1}{2}\delta(t - \tau)\Lambda_\alpha + x \sum_k \Sigma_{\alpha k}(\tau, t), \quad (6)$$

where $x = sgn(t - \tau)$. The sign $x$ corresponds to upper (+) or lower half plane (−) contour integration. $\Sigma_{\alpha k}(\tau, t)$ is defined as $\Sigma_{\alpha k}^{\pm}(\tau, t) = \frac{2}{\beta}\eta_k e^{i \int_{\tau}^{t} \int \Sigma_{\alpha k}(t_1) dt_1} \Lambda_\alpha$, where $\epsilon_{\alpha k}(t) = \pm i\zeta_k / \beta + \mu_\alpha + \Delta_\alpha(t)$. $\pm i\zeta_k / \beta + \mu_\alpha$ are the $k$th Padé poles in the upper and lower half plane, respectively; $\eta_k / \beta$ is the corresponding coefficient. Consequently, the dissipation matrix is rewritten as

$$\varphi_\alpha(t) = i[\rho(t) - 1/2]\Lambda_\alpha + x \sum_k \varphi_{\alpha k}(t). \quad (7)$$

where $\varphi_{\alpha k}(t)$ is the component of the dissipation matrix, which is evaluated through its EOM. Within the WBL approximation, the second term on the RHS of above equation is written as

$$\varphi_{\alpha k}(\tau) = \frac{2\eta_k}{\beta} \int_{-\infty}^{\tau} dt_1 \tilde{U}_{\alpha k}(\tau, t_1) \Lambda_\alpha \quad (8)$$

where $\tilde{U}_{\alpha k}(\tau, t_1)$ can be regarded as the propagator, which is defined as

$$\tilde{U}_{\alpha k}(\tau, t_1) = e^{i \int_{t_1}^{\tau} \Sigma_{\alpha k}(t') dt'}. \quad (9)$$

It is obvious that $\varphi_{\alpha k}(t)$ can be easily calculated from its EOM.

### III. OPTIMAL CONTROL THEORY FOR TIME-DEPENDENT QUANTUM TRANSPORT

The key ingredient of optimal control is to determine the electrical field that can lead to a predefined effect on the current through junctions. This is achieved by using the optimal control theory (OCT) which optimizes a control functional. Considering the optimal control of current, the goal is to search for an optimal control field such that the current follows a target pattern as best as possible. Mathematically, the different between the desired current pattern $P(t)$ and the current obtained from the calculation at each iteration is to be minimized. Hence, we can define a control functional as

$$J_f[E] = \int_{t_0}^{t_f} dt [P(t) - I(t)]^2, \quad (10)$$

where $I(t)$ is the time-dependent current calculated by the method mentioned in previous section. Obviously, an electrical field that makes $J_f[E(t)] = 0$ is the optimal
control field. To ensure the convergence, an additional part is added to the control functional,

$$J[E] = J_1[E] + \frac{\lambda}{2} \int_{t_0}^{t_f} \frac{(E(t) - \tilde{E}(t))^2}{s(t)} dt$$  \hspace{1cm} (11)$$

with $\tilde{E}(t)$ being the electrical field of the previous iteration step. The penalty parameter $\lambda$ is a Lagrange multiplier and a time-dependent function $s(t)$ is introduced to avoid sudden switch-on and switch-off behavior of the control field. For the optimization of the function as described in Eq. (11), the functional derivative with respect to the field $E(t)$ should vanish, i.e., $\frac{\delta J[E]}{\delta E(t)} = 0$. This yields the condition for external fields,

$$E(t) = \tilde{E}(t) - \frac{s(t) \delta J_1[E]}{\delta E(t)}.$$  \hspace{1cm} (12)$$

Therefore, once the fractional derivative of $J_1[E]$ with respect to external field is obtained, the optimal control field is obtained. According to the definition of $J_1[E]$, $\frac{\delta J_1[E]}{\delta E(t)}$ depends on the functional derivative of current, i.e., $\frac{\delta J(t)}{\delta \phi(t)}$. Within NEGF formalism, current is in terms of self-energies and Green’s functions as given by Eq. (6). Hence, the functional derivative of $J_1[E]$ with respect to external field is written as

$$\frac{\delta J_1[E]}{\delta E(t)} = -4 \int_{t_0}^{t_f} dt \{ [I(t) - P(\tau)] \text{Im} \text{Tr} \left[ \frac{\delta \phi_0(\tau)}{\delta E(t)} \right] \}.$$  \hspace{1cm} (13)$$

Because $\phi_0(t)$ is decomposed due to Padé approximation as shown in Eq. (7), the functional derivative of $\phi_0(\tau)$ with respect to field $E(t)$ can be decomposed accordingly,

$$\frac{\delta \phi_0(\tau)}{\delta E(t)} = \frac{\delta \rho(\tau)}{\delta E(t)} \Lambda_\alpha + \sum_k \frac{\delta \varphi_{ak}(\tau)}{\delta E(t)}. \hspace{1cm} (14)$$

The first part on the right hand side (RHS) of above equation requires the detailed knowledge of density matrix within the NEGF formalism. While the second part on the RHS of above equation depends on the propagator as indicated by Eq. (5). The analytical forms of the functional derivatives of $\rho(\tau)$ and $\varphi_{ak}(\tau)$ with respect to $E(t)$ are derived as follows. According to the definition of $\varphi_{ak}(t)$ as shown by Eq. (8), only functional derivative of propagator is needed. Because the single-particle energy $\epsilon_{ak}$ and Fock matrix are dependent on external field, functional derivative of propagator with respect to external field is

$$\frac{\delta \bar{U}_{ak}(\tau, t_1)}{\delta E(t)} = -i \vartheta(\tau - t) \bar{\phi}(t - t_1) \bar{U}_{ak}(\tau, t) \bar{d} \bar{U}_{ak}(t, t_1), \hspace{1cm} (15)$$

where $\bar{d}$ is defined as $\bar{d} = \delta [h(t) - \epsilon_{ak}(t)]/\delta E(t)$, then the functional derivative of $\varphi_{ak}(\tau)$ with respect to field $E(t)$ is expressed as

$$\frac{\delta \varphi_{ak}(\tau)}{\delta E(t)} = -i \vartheta(\tau - t) \bar{U}_{ak}(\tau, t) \bar{d} \bar{\phi}_{ak}(t). \hspace{1cm} (16)$$

Thus, the functional derivative of $\varphi_{ak}(\tau)$ with respect to $E(t)$ is analytically obtained. It should be noticed that if $\epsilon_{ak}(t)$ is not dependent on $E(t)$, then $\bar{d} = \delta [h(t) - \epsilon_{ak}(t)]/\delta E(t)$.

Now, the problem existed in the combination between NEGF-WBL and OCT is the how to get the functional derivative of density matrix $\rho(\tau)$ with respect to external field $E(t)$, i.e., $\frac{\delta \rho(\tau)}{\delta E(t)}$. Within NEGF formalism, density matrix can be evaluated through lesser Green’s function $\rho(t) = -iG^<(t, t)$, while the letter can be expressed in terms of retarded/advanced Green’s functions and self-energies,

$$G^<(t, t) = \int dt_1 \int dt_2 G^r(t, t_1) \Sigma^<(t_1, t_2) G^a(t_2, t). \hspace{1cm} (17)$$

Where $\Sigma^<(t_1, t_2) = \sum_\alpha \Sigma_\alpha(t_1, t_2)$ is the total self-energy. Within WBL approximation, the retarded Green’s function $G^r(t, t_1)$ can be expressed as

$$G^r(t, t_1) = -i \vartheta(t - t_1) U(t, t_1), \hspace{1cm} (18)$$

where $U(t, t_1) = e^{-i \int_{t_1}^{t} [h(t) - \Lambda(t)] dt'}$ is defined with $\Lambda = \sum_\alpha \Lambda_\alpha$ being the total line-width function. Within the Padé approximation to the Fermi distribution function and WBL approximation, the lesser self-energy $\Sigma_\alpha(t_1, t_2)$ is given by Eq. (6). Hence, the density matrix is rewritten as

$$\rho(\tau) = \int dt_1 \sum_\alpha G^r(\tau, t_1) \Lambda_\alpha G^a(t_1, \tau) - i \int dt_1 \int dt_2 \Sigma^r_{\alpha}(t_1, t_2) G^a(t_2, \tau). \hspace{1cm} (19)$$

Thus, after lengthy derivation, the functional derivative of $\rho(\tau)$ with respect to $E(t)$ is

$$\frac{\delta \rho(\tau)}{\delta E(t)} = -i \vartheta(\tau - t) \left\{ U(\tau, t) [d, \rho(t)] U^\dagger(\tau, t) + \left[ U(\tau, t) \bar{d} \sum_\alpha \varphi_{ak}(t) \phi_{ak}(t, \tau) + \text{h.c.} \right] \right\}. \hspace{1cm} (20)$$

where $\phi_{ak}(t, \tau)$ is defined as $\phi_{ak}(t, \tau) = \int dt_1 \Sigma_{\alpha}^r(t_1, t_2) G^a(t_2, \tau)$. Hence, $\frac{\delta \rho(\tau)}{\delta E(t)}$ can be readily evaluated.

Therefore, the functional derivative of $J_1[E]$ with respect to external field is

$$\frac{\delta J_1[E]}{\delta E(t)} = -4 \int_{t_0}^{t_f} dt \vartheta O(\tau) \text{Im} \text{Tr} \left\{ U^\dagger(\tau, t) \Lambda_\alpha U(\tau, t) [d, \rho(t)] + \sum_{\beta k} [\phi_{\beta k}(t, \tau) \Lambda_\alpha U(\tau, t) \bar{d} \phi_{\beta k}(t) + \text{h.c.}] - i \sum_k \bar{U}_{ak}(\tau, t) \bar{d} \bar{\phi}_{ak}(t) \right\}. \hspace{1cm} (21)$$

Where $O(\tau) = I(\tau) - P(\tau)$. Now, the functional derivative of $J_1[E]$ with respect to external field is analytically
obtained. The difficulty of evaluating $\frac{\delta J}{\delta E(t)}$ is the time-integration. Defining

$$\chi_\alpha(t) = \int_0^t d\tau O(\tau)U_\alpha^\dagger(\tau,t)\Lambda_\alpha U(\tau,t)$$

$$\Theta_{\alpha k}(t) = i \int_0^t d\tau O(\tau)\dot{U}_{\alpha k}(\tau,t)$$

$$\Upsilon_{\beta k}(t) = \int_0^t d\tau O(\tau)\phi_{\beta k}(\tau,t)\Lambda_\alpha U(\tau,t) \tag{22}$$

the functional derivative of current with respect to external field, $\frac{\delta J}{\delta E(t)}$, can be rewritten as

$$\frac{\delta J}{\delta E(t)} = -4\text{ImTr} \left\{ \chi_\alpha(t)[d, \rho(t)] - \sum_k \Theta_{\alpha k}(t)d\phi_{\alpha k}(t) \right.$$ 

$$+ \sum_{\beta k} \left[ \Upsilon_{\beta k}(t)d\phi_{\beta k}(t) + h.c. \right] \left\{ \right. \} \tag{23}$$

Hence, analytical expression of $\frac{\delta J}{\delta E(t)}$ is obtained. Density matrix $\rho(t)$ and $\phi_{\alpha k}(t)$ can be evaluated via the time-propagation of their EOMs. Only $\chi_\alpha(t), \Theta_{\alpha k}(t)$ and $\Upsilon_{\beta k}(t)$ remain unknown.

According to the definition of $\chi_\alpha(t), \Theta_{\alpha k}(t)$ and $\Upsilon_{\beta k}(t)$, they can be evaluated through their EOMs,

$$\dot{\Theta}_{\alpha k}(t) = -iO(t) - i\Theta_{\alpha k}(t)[\epsilon_{\alpha k}(t) - h(t) + i\Lambda]$$

$$\Upsilon_{\beta k}(t) = -\frac{2\eta_k}{\beta} \Lambda_\beta \chi_\alpha(t) + i\Upsilon_{\beta k}(t)[\epsilon_{\beta k}(t) + h(t) - i\Lambda]$$

$$\dot{\chi}_\alpha(t) = -O(t)\Lambda_\alpha - i\mathcal{R}(t)\chi_\alpha(t). \tag{24}$$

where $\mathcal{R}(t) \equiv [h(t) + i\Lambda, \cdot ]_+$ and $[A, B]_+ = AB - BA^\dagger$. It is obvious that the boundary conditions for $\chi_\alpha(t), \Theta_{\alpha k}(t)$ and $\Upsilon_{\beta k}(t)$ are at time $t = t_f$ where all the three quantities are zero. Therefore, EOMs of Eq. (24) have to be propagated backwards from $t_f$ to $t_0$ in order to update the control field. In the contrast, the density matrix $\rho(t)$ is propagated forward in time. Eqs. (2) and (24) have to be solved iteratively. In short, the numerical procedure is summarized as follows,

1. Time-propagation of density matrix and dissipation matrices from $t_0$ to $t_f$ with initial guess of external field;
2. Backward propagation of $\chi_\alpha(t), \Theta_{\alpha k}(t)$ and $\Upsilon_{\beta k}(t)$ from $t_f$ to $t_0$ and update the control field;
3. Procedure (1) and (2) can repeated iteratively until convergence is achieved.

However, the procedure (2) requires the storage of density matrix $\rho(t)$ and the component of dissipation matrix $\phi_{\alpha k}(t)$ at each time step, which requires large amount of memory. To reduce the memory requirement, cubic spline interpolation of control field is employed. The electrical field, $E(t)$, is approximated by cubic splines with $N + 1$ equidistant nodes at $t_k = kN/T, k = 0, \cdots, N$. Accordingly, only $N + 1$ snapshots of each quantity at time $t_k, k = 0, \cdots, N$ are needed. Compared to the number of time-step used in the propagation (typical simulation requires thousands of time-steps or tens of thousand time-steps), spline interpolation can efficiently reduce the memory requirement significantly.

IV. SUMMARY

In summary, an optimal control theory for time-dependent quantum transport is developed. The method combines NEGF-WBL method with optimal control theory to achieve the optimal control of transient current. Numerical implementation of present method is also briefly introduced. By employing the method, the optimal control pulse can be found upon desired current pattern. The method can also be employed to find the optimal performance of nano devices, such as optimize Cooper pair splitting efficiency, photovoltaics, thermoelectric, etc. Moreover, the approach is expected to be useful in the control of other observables in quantum transport.

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