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Control of Charge Carriers in Molecular Devices

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Abstract – This paper focuses on control of electron transports and switching of molecular devices ($^M$-devices). To accomplish these objectives one should control motion of charge carriers. Various phenomena and transitions, exhibited by $^M$-devices (microscopic systems) and microscopic particles, can be utilized only if specific effects, evolutions and events are controlled ensuring device functionality and required capabilities. Concentrating on molecular electronics, our objective is to develop sound and practical solutions. Molecular (nano) electronics is fundamentally distinct and cannot be compared to solid-state microelectronics due to: (1) Distinct phenomena exhibited and utilized; (2) Device physics and functionality differences; (3) Distinct device-physics centered control principles and mechanisms; etc. We examine dynamics and control of microscopic charge carriers in $^M$-devices. In particular, for solid and fluidic $^M$-devices, the controlled motion of electrons, ions and molecules is studied. Applying sound device physics, we report theoretical and applied developments in analysis and control of $^M$-device transitions with a primary focusing on: (i) Device physics and analysis consistency; (ii) Device physics and control coherency; (iii) Device physics and technology soundness. It is possible to control the transitions and motion of microscopic particles (charge carriers) thereby control tunneling, transport, characteristics and other evolutions exhibited by $^M$-device variables (quantities of interest). The processing and memory transitions at the device level are defined by the device physics, control principles, behavior of microscopic system (device) and particles, etc. The ability to control microscopic particles means guaranteeing the overall device functionality. We examine the device physics and demonstrate that the device functionality, performance requirements and specified capabilities can be achieved by controlling principles. The results are validated by examining device transitions by applying quantum mechanics. We perform high-fidelity modeling and carry out heterogeneous simulations. The quantifying and qualifying studies are reported.

I. INTRODUCTION

Molecular electronics and molecular processing platforms ($^M$-PPs) have become a topic of intensive research in recent years [1-5]. For three-dimensional (3D) molecular integrated circuits ($^M$ICs) and $^M$PPs, various 3D-topology solid and fluidic $^M$-devices were introduced [4]. The overall feasibility and soundness of $^M$-PPs was established examining superb biomolecular information processing and memory platforms. Though molecular and biomolecular solutions can be fundamentally different, promising results in devising $^M$ICs and $^M$PPs were reported. The bottom-up synthesis of $^M$-PPs was covered typifying the neuronal organization/architecture and aggregating neuronal hypercells which comprised from $^M$-devices. It is a hope that sound technologies will be developed to progress beyond theoretical studies at the systems ($^M$PPs and $^M$ICs) and device levels.

For $^M$-devices, a number of fundamental problems are examined in the literature. The most notable recent developments were performed by:

- Devising sound $^M$-devices which are based on novel well-defined device physics;
- Examining phenomena, effects, evolutions and transitions exhibited and utilized to guarantee functionality;
- Analyzing dynamic and steady-state characteristics and capabilities which provide baseline performance measures.

With a focus on the device-level research, we study the controlled behavior and motion of microscopic particles. These transitions and phenomena exhibited ultimately:

1. Result in functionality and operationability of $^M$-devices;
2. Define and affect the overall device characteristics.

For multi-terminal molecular electronic devices ($^M$E-devices), the solution of problems associated with the controlled motion of electrons, tunneling, electron transport and other phenomena may ensure the specified performance. The device performance and capabilities are assessed by examining dynamic and steady-state characteristics, controllability, switching, losses, robustness, noise immunity, etc.

Dynamics and control of microscopic particles (molecules, atoms, ions, electrons, etc.) in electromagnetic, thermal and hydrodynamic fields are important problems in various applications. These studies directly contribute to microscopic systems including cellular units and organelles, nanoscaled actuators and sensors, etc. A coherent analysis and control of particles in electromagnetic field allows one to study confinement of particles by magnetic traps, dynamics of particles in fluidic channels, control of plasma, etc. Open fundamental problems in analysis and control of microscopic particles limit the applied research, experimental studies as well as technological developments in biotechnology, neuroscience, medicine and engineering.

II. DEVICE PHYSICS: QUANTUM-EFFECT MOLECULAR ELECTRONIC DEVICE

A 3D-topology multi-terminal $^M$E-device, engineered using cyclic molecules with a carbon interconnecting framework, was proposed in [4]. Figure 1 documents $^M$E-devices which have the input, control and output terminals. The device physics is based on the quantum interaction and controlled electron tunneling (transport) which result in the transitions and controlled characteristics allowing one to consider these devices as possible molecular primitives for envisioned $^M$ICs.
The applied \( V_{\text{control}}(t) \) changes the charge distribution \( \rho(t,\mathbf{r}) \) and electric field \( E_{\text{field}}(t,\mathbf{r}) \) affecting the electron transport. These M\(^{\text{M}}\) devices operate in the controlled electron-exchangeable environment due to quantum phenomena and interactions. The controlled super-fast potential-assisted tunneling is achieved. The electron-exchangeable environment interactions affect phenomena exhibited and transitions observed in a device. These phenomena qualitatively and quantitatively modify the device dynamic behavior and its steady-state characteristics. In particular, the multiple-valued device controllability is achieved by varying \( \partial_{\mathbf{r}} V(t,\mathbf{r}) \) and other characteristics. The electron transport in the time- and spatial-varying metastable potentials \( \Pi(t,\mathbf{r}) \) is studied. The changes in the Hamiltonian result in: (1) Changes of tunneling \( T(E) \) and controllable device characteristics; (2) Quantum interactions due to variations of \( \rho(t,\mathbf{r}), E_{\text{field}}(t,\mathbf{r}) \) and \( \Pi(t,\mathbf{r}) \); (3) Varying the charge carriers velocity. These transitions, effects and phenomena ensure overall device functionality.

Due to the well-known challenges [1-5], only analytic and basic results currently are available for multi-terminal solid and fluidic \(^{\text{M}}\) devices. Up to date, the results have not been obtained for three-terminal M\(^{\text{M}}\) devices [1-5]. However, the quantum-effect induced transitions have been verified and experimentally characterizes in various molecules and molecular assemblies. The interconnect, aggregation and interfacing of M\(^{\text{M}}\) devices are expected to be achieved departing from conventional microelectronics solutions [4].

### III. EVOLUTION OF MICROSCOPIC SYSTEMS

Quantum mechanics is applied to describe and examine the motion, evolution and transitions of microscopic particles and microsystems (molecular device). Studies of device behavior ultimately results in the analysis of functionality and capabilities. To model microscopic systems, including M\(^{\text{M}}\) devices, we consider evolutions and behavior due to the controlled motion of microscopic particles. The time-dependent Schrödinger equation to be solved is

\[
\frac{-\hbar^2}{2m} \nabla^2 \Psi(t,\mathbf{r}) + \Pi(t,\mathbf{r}) \Psi(t,\mathbf{r}) = i\hbar \frac{\partial \Psi(t,\mathbf{r})}{\partial t},
\]

where \( m \) is the mass; \( \Psi(t,\mathbf{r}) \) is the wave function; \( \Pi(t,\mathbf{r}) \) is the potential energy function.

We study the time-varying and time-invariant problems. For a free particle in the Cartesian coordinate system, one has \( E(r) = p^2/2m \). For a time-independent \( \Pi(t,\mathbf{r}) \), we obtain \( E(r) = p^2/2m + \Pi(r) \).

In a magnetic field, the interaction of a magnetic moment \( \mu \) with a magnetic field \( \mathbf{B} \) changes the energy by \( -\mu \cdot \mathbf{B} \). The external electromagnetic field, which can be controlled, affects the Hamiltonian. For a particle in a uniform magnetic field \( \mathbf{B} \), one has

\[
H = \frac{1}{2m} p^2 + \Pi(x) - \frac{q}{2\mu} \mathbf{B} \cdot \mathbf{L} + \frac{q^2}{8\mu^2} \left[ B^2 r^2 - (\mathbf{B} \cdot \mathbf{r})^2 \right].
\]

where \( \mu \) is the angular momentum; \( \mathbf{L} \) is the orbital angular momentum.

Consider a microscopic particle with a charge \( q \) and mass \( m \) in a one-dimensional potential \( \Pi(x) \). Let a particle propagates under an external time-varying electric field \( E_{\text{field}}(t) \). The particle Hamiltonian is \( H = \frac{1}{2m} p^2 + \Pi(x) + qE_{\text{field}}(t)x \).

For example, \( E_{\text{field}}(t) = E_{\text{field}}0 \sin \omega t \), where \( E_{\text{field}}0 \) is the filed amplitude.

Using the Hamiltonian \( H(t,\mathbf{r}) \), one solves the Schrödinger equation

\[
H(t,\mathbf{r})\Psi(t,\mathbf{r}) = i\hbar \frac{\partial \Psi(t,\mathbf{r})}{\partial t}.
\]

We consider a microscopic particle which moves in an external time-dependent electromagnetic field. The vector and scalar potentials of the electromagnetic field are \( \mathbf{A}(t,\mathbf{r}) \) and \( V(t,\mathbf{r}) \). The Hamiltonian is

\[
H(t,\mathbf{r},p) = \frac{1}{2m} \left( p - \frac{q}{c} \mathbf{A} \right)^2 + qV.
\]

For a microscopic particle, the time rate of change of the expectation value of \( \mathbf{r} \) is

\[
\frac{d}{dt} \langle \mathbf{r} \rangle = \frac{1}{i\hbar} \left\langle [\mathbf{r}, H] \right\rangle = \frac{1}{m} \left( p - \frac{q}{c} \mathbf{A} \right),
\]

yielding the velocity operator

\[
\mathbf{v} = \frac{1}{m} \left( p - \frac{q}{c} \mathbf{A} \right).
\]

Newton’s second law in quantum mechanical form is

\[
\frac{d}{dt} \langle \mathbf{v} \rangle = \frac{i}{\hbar} \left\langle [\mathbf{v}, H] \right\rangle + \frac{\partial \mathbf{v}}{\partial t} = \frac{i}{\hbar} \left\langle [\mathbf{v}, q\mathbf{A}] \right\rangle + \frac{i}{\hbar} \left\langle [\mathbf{v}, qV] \right\rangle - \frac{q}{mc} \frac{\partial \mathbf{A}}{\partial t}.
\]

Hence, equation

\[
\frac{d}{dt} \langle \mathbf{v} \rangle = \frac{q}{2mc} (\mathbf{v} \times \mathbf{B} - \mathbf{B} \times \mathbf{v}) - \frac{q}{m} \left\langle \nabla V \right\rangle - \frac{q}{mc} \frac{\partial \mathbf{A}}{\partial t}
\]

describes the dynamics of charge carriers in M\(^{\text{M}}\) devices.
Using $E = -\nabla V - \frac{1}{c} \frac{\partial A}{\partial t}$, we have

$$\frac{d}{dt} \langle \mathbf{v} \rangle = \frac{q}{2mc} (\mathbf{v} \times \mathbf{B} - \mathbf{B} \times \mathbf{v}) - \frac{q}{m} \langle E \rangle. \quad (9)$$

Equation (9) describes the evolution of $\langle \mathbf{v} \rangle$ of the controlled carriers in devices by changing the electromagnetic field. The time-dependent Schrödinger equations of two distinct device states with

$$H_1 = \frac{1}{2m} \left( \mathbf{p} - \frac{q}{c} \mathbf{A}_1 \right)^2 + \Pi_1 + qV_1$$

and

$$H_2 = \frac{1}{2m} \left( \mathbf{p} - \frac{q}{c} \mathbf{A}_2 \right)^2 + \Pi_2 + qV_2$$

are

$$-\frac{\hbar^2}{2m} \left( \nabla - i \frac{q}{\hbar c} \mathbf{A}_1 \right)^2 \Psi_1(t, \mathbf{r}) + \left( \Pi_1 + qV_1 \right) \Psi_1(t, \mathbf{r}) = i\hbar \frac{\partial \Psi_1(t, \mathbf{r})}{\partial t},$$

$$-\frac{\hbar^2}{2m} \left( \nabla - i \frac{q}{\hbar c} \mathbf{A}_2 \right)^2 \Psi_2(t, \mathbf{r}) + \left( \Pi_2 + qV_2 \right) \Psi_2(t, \mathbf{r}) = i\hbar \frac{\partial \Psi_2(t, \mathbf{r})}{\partial t}, \quad (10)$$

where $\mathbf{A}_1 + \nabla f(t, \mathbf{r})$ and $\Pi_2 = V_1 - \frac{1}{c} \frac{\partial f(t, \mathbf{r})}{\partial t} = f(t, \mathbf{r})$ is the continuous differentiable Lipshitz function.

For the wave function, which is the physical state for the system, we have $\Psi(t + \Delta t, \mathbf{r}) = \Psi(t, \mathbf{r}) + \frac{i\hbar}{2m} (\nabla \Psi(t, \mathbf{r}))^2$.

For a one-dimensional case, the expectation value of the charged particle position and momentum at time $t$ are

$$\langle x \rangle = \int \Psi^*(t, x) \Psi(t, x) dx,$$

$$\langle p \rangle = -i\hbar \int \Psi^*(t, x) \frac{\partial \Psi(t, x)}{\partial x} dx. \quad (11)$$

Equations (11) provide the expectation value of the observable variables in the state $\sigma$.

Correspondingly, one examines the motion (behavior) using $\langle \mathbf{v} \rangle$, $\langle \mathbf{p} \rangle$, $\langle \mathbf{v} \rangle$ and other observable variables of our interest. The application of Ehrenfest principle yields

$$\frac{d}{dt} \langle \mathbf{r} \rangle = \frac{\partial H}{\partial \mathbf{p}},$$

$$\frac{d}{dt} \langle \mathbf{p} \rangle = -\frac{\partial H}{\partial \mathbf{r}}. \quad (12)$$

Furthermore,

$$\langle \mathbf{p} \rangle = m \frac{\partial}{\partial t} \langle \mathbf{r} \rangle. \quad (13)$$

The charge carriers must be controlled. The controlled tunneling and transport of microscopic particles can be achieved by developing a sound control concept with must be coherent with the device physics and technologies. For example, it is unlikely that the conventional feedback control techniques can be applied.

IV. STOCHASTIC DYNAMICS OF MICROSCOPIC PARTICLES

The Schrödinger equation is applied to quantitatively examine the quantities of interest, e.g., expectation values, energies, transmission, reflection, etc. The evolution of the average position $r$ of $i$th particles is

$$\frac{d}{dt} \langle r_i \rangle = \frac{1}{m} \langle \mathbf{p}_i \rangle. \quad (14)$$

For the momentum $\mathbf{p}$ and spin $\mathbf{S}$ we have

$$\frac{d}{dt} \langle \mathbf{p}_i \rangle = \frac{\mu}{\hbar} \langle (\nabla (\mathbf{S}_i \cdot \mathbf{B}_i)) \rangle - \sum_{j,i,j \neq i} N \langle \nabla V_j \rangle, \quad (15)$$

$$\frac{d}{dt} \langle \mathbf{S}_i \rangle = \frac{\mu}{\hbar} \langle \mathbf{S}_i \times \mathbf{B}_i \rangle, \quad (16)$$

where $V$ is the interacting potential which includes the interacting, external, control and stochastic forces.

Due to the stochastic potential, one obtains the nonlinear stochastic differential equations. Hence, the dynamics of the microscopic particles is described by stochastic nonlinear differential equations. The stochastic Ornstein-Uhlenbeck process is expressed by the following stochastic differential equation [6]

$$dz_i = -a(z_i - b)dt + \sigma dw_i, \quad (17)$$

where $a$, $b$ and $\sigma$ are parameters; $w_i$ denotes the Wiener process.

The considered stochastic process has a bounded variance and admits a stationary probability distribution in contrast to the Wiener process. The stationary variance is $0.5a^2/\sigma$.

Example 4. 1.

Let the magnetic field is

$\mathbf{B} = B_0 \mathbf{a}_z + B_{\text{rms}} \cos \left( \frac{2\pi}{\lambda} x \right) + \cos \left( \frac{2\pi}{\lambda} y \right) \mathbf{a}_z$,\]

where $B_0$ is the uniform component of the magnetic field; $B_{\text{rms}}$ is the amplitude of the magnetic field modulation.

One obtains $H(r, \mathbf{p}) = \frac{1}{2m} \left( \mathbf{p} - \frac{q}{c} \mathbf{A} \right)^2$, where $\mathbf{A}$ is the vector potential

$$\mathbf{A} = -\frac{1}{\pi} \left[ B_0 y + \frac{aB}{\pi} \sin \left( \frac{2\pi}{\lambda} x \right) \right] \mathbf{a}_x + \frac{1}{2} \left[ B_0 x + \frac{aB}{\pi} \sin \left( \frac{2\pi}{\lambda} x \right) \right] \mathbf{a}_y.$$

The equations of motion are

$$dv_x = \left[ \frac{qB_{\text{rms}}}{mc} + \frac{qB_0}{mc} \cos \left( \frac{2\pi}{\lambda} x \right) + \cos \left( \frac{2\pi}{\lambda} y \right) \right] v_x dt + D_x dw_x, \quad dx = v_x dt,$$

$$dv_y = \left[ \frac{qB_{\text{rms}}}{mc} + \frac{qB_0}{mc} \cos \left( \frac{2\pi}{\lambda} x \right) + \cos \left( \frac{2\pi}{\lambda} y \right) \right] v_y dt + D_y dw_y, \quad dy = v_y dt.$$
Example 4.2.
Consider stochastic differential equations which govern the velocity and position of a charged particle in a uniform magnetic field. This problem is of a significant importance in the molecular switches, control of plasma, etc. The uncontrolled stochastic differential equations which describe the dynamics of a charged particle in the \( xy \) plane are

\[
dv_x = \left( -\frac{1}{T} v_x + \frac{qB_z}{mc} v_y \right) dt + D_x dw_x, \quad dx = v_x dt,
\]

\[
dv_y = \left( -\frac{1}{T} v_y - \frac{qB_0}{mc} v_x \right) dt + D_y dw_y, \quad dy = v_y dt,
\]

where \( T \) is the collision relaxation time constant; \( D_x \) and \( D_y \) are the diffusion constants.

Utilizing the Langevin equation the dynamic analysis can be performed. Taking note of Lorentz force, one obtains the following equation

\[
dv = \left( -A v + \frac{q}{m} E + \frac{q}{mc} v \times B \right) dt + D dw.
\]  

(18)

Example 4.3.
Assume that the magnetic field is directed along the \( z \) axis. That is, \( B=[0 \ 0 \ B_z]^T \). If \( B_z \) is constant, we have the following equation for the uncontrolled microscopic particle velocity vector

\[
dv = \begin{bmatrix}
\frac{1}{T} v & \frac{qB_z}{mc} v & 0 \\
-\frac{qB_z}{mc} v & -\frac{1}{T} v & 0 \\
0 & 0 & -\frac{1}{T} v
\end{bmatrix} dt + D dw.
\]

V. CONTROL OF ELECTRONS IN MOLECULAR DEVICES

We consider the controller transport of electrons in a solid \( M \) device which is documented in Figure 1. The analytic and numerical results are found by utilizing the derived equations of motion, studying control and performing numerical studies. We have \( q = 1.6 \times 10^{-19} \) C, \( m = 9.1 \times 10^{-31} \) kg, \( a = 1 \times 10^{-9} \) m and \( T = 5 \times 10^{-15} \) sec. Figure 2 illustrates the controlled motion of an electron. We achieve the specified velocities \( v_x \) and \( v_y \).

The settling time is \( \approx 5 \times 10^{-16} \) sec, and the single-electron transit time is \( \approx 1 \times 10^{-14} \) sec. This does not imply that the switching frequency could be \( f = 1/(2\pi\tau) \) because one should examine the device physics features (number of electrons, heating, interference, potential, energy, noise, etc.), system-level functionality, circuit specifications, etc. For example, one strives to ensure the specified physical quantities (current, voltage, field, etc.), minimize losses, ensure robustness, accomplish noise immunity, etc.

VI. CONCLUSIONS

We examined the controlled dynamics of microscopic particles in \( M \) devices in order to guarantee the functionality, ensure optimal achievable performance, attain controllability, maximize switching frequency, etc. Coherent fundamental, applied and numerical results were reported as applied to solid and fluidic \( M \) devices. The simulation studies are documented. It is found that the motion of microscopic particles in \( M \) devices can be controlled. In particular, one may control the momentum, velocity, position and other variables which define the device transition quantities. It is illustrated that quantum mechanics, stochastic differential equations, heterogeneous simulations and data-intensive analysis methods must be applied. We report a theoretical foundation in dynamic analysis, control and optimization of microscopic particles and \( M \) devices. The qualitative and quantitative results are reported.

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