High-fidelity modeling of nanosystems: Novel methods and paradigms

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High-Fidelity Modeling of Nanosystems: Novel Methods and Paradigms

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Abstract — Recent scientific and technological developments have stimulated basic, applied, and experimental research in nanoelectronics, nanoscience, and nanotechnology advancing fundamental paradigms. Contemporary results in nonlinear quantum electrodynamics and mechanics, advances in modeling and simulation of complex nanosystems, biomimicking and prototyping, discovery of new phenomena and effects, as well as rapid engineering/technological advances in fabrication (molecular wires, carbon nanotubes, thin films, etcetera), provide enabling benefits and capabilities to devise and fabricate new nanostructures, nanodevices, and nanoelectromechanical systems (NEMS). Critical problems that remain to be addressed and solved are the fundamental research to model, simulate, and analyze NEMS. High-fidelity modeling, heterogeneous simulation and data-intensive analysis must be performed. Using the developed paradigms, we examine these problems for NEMS and report the promising solution of the Schrödinger equation using the optimality principle.

I. INTRODUCTION

The ability to find equations (mathematical models), which adequately describe nanosystems properties, phenomena and effects, is a key problem in modeling, analysis, synthesis, optimization, control, fabrication, manufacturing, and commercialization of NEMS [1, 2]. In this paper, using classical and quantum mechanics, functional density concept [3–5], and electromagnetic theory we document the nanoelectromechanical theory to model, analyze, and simulate nanosystems. The reported developments support the existing setups in modeling, analysis, and design of NEMS. The proposed fundamental results allow the designer to solve a broad spectrum of problems. The reported theoretical and applied results are verified and demonstrated. In this paper, we study complex phenomena in nanosystems using quantum, classical, and optimization theories. This research is critical to overcome current obstacles in complete understanding of processes and phenomena in nanoscale, with long-standing goal to develop fundamental and experimental tools to design and fabricate NEMS using synthesis and design methods devised.

II. MATHEMATICAL MODELS: ENERGY-BASED QUANTUM AND CLASSICAL MECHANICS

To perform the comprehensive modeling and analysis of NEMS in the time domain, there is a critical need to develop and apply advanced theories using fundamental physical laws. Classical and quantum mechanics are widely used, and this paper illustrates that the Schrödinger equation can be found using Hamilton’s concept (it is well known that the Euler-Lagrange equations, given in terms of the generalized coordinates and forces, can be straightforwardly derived applying the variational principle). The quantum mechanics gives the system evolution in the form of the Schrödinger equations.

Newton’s second law

\[ \sum \vec{F}(\vec{r}) = m\ddot{\vec{r}} \]

in terms of the linear momentum \( \vec{p} = m\dot{\vec{r}} \) is given by

\[ \sum \vec{F} = \frac{d\vec{p}}{dt} = \frac{d(m\dot{\vec{r}})}{dt} = m\ddot{\vec{r}}. \]

Using the potential energy \( \Pi(\vec{r}) \), for the conservative mechanical system we have

\[ \sum \vec{F}(\vec{r}) = -\nabla \Pi(\vec{r}). \]

Hence,

\[ m\ddot{\vec{r}} + \nabla \Pi(\vec{r}) = 0. \]

For the system of \( N \) particles, the equations of motion are
The total kinetic energy of the particle is \( \Gamma = \frac{1}{2} m v^2 \), and for \( N \) particles, one has

\[
\Gamma = \frac{1}{2} \sum_{i=1}^{N} m_i \left( \frac{dx_i}{dt} \right)^2 + \frac{1}{2} \sum_{i=1}^{N} \sum_{j=i+1}^{N} m_i m_j \left( \frac{dx_i}{dt} - \frac{dx_j}{dt} \right)^2 .
\]

Using the generalized coordinates \( q_i \) and generalized velocities \( \frac{dq_i}{dt} \), one finds the total kinetic \( \Gamma(q_1, ..., q_n) \) and potential \( \Pi(q_1, ..., q_n) \) energies.

Thus, Newton's second law of motion can be given as

\[
\frac{d}{dt} \left( \frac{\delta \Pi}{\delta \dot{q}_i} \right) - \frac{\partial \Pi}{\partial q_i} = \frac{\partial F}{\partial q_i} .
\]

That is, the generalized coordinates \( q_i \) are used to model multi-body systems, and \( (q_1, ..., q_n) = (x_1, y_1, z_1, ..., x_N, y_N, z_N) \).

The obtained results are connected to the Lagrange equations of motion. Using the total

1. kinetic \( \Gamma(t, q_1, ..., q_n, \frac{dq_1}{dt}, ..., \frac{dq_n}{dt}) \),
2. dissipation \( D(t, q_1, ..., q_n, \frac{dq_1}{dt}, ..., \frac{dq_n}{dt}) \),
3. potential \( \Pi(t, q_1, ..., q_n) \) energies,

the Lagrange equations of motion are found as

\[
\frac{d}{dt} \left( \frac{\delta \Pi}{\delta \dot{q}_i} \right) - \frac{\partial \Pi}{\partial q_i} = F_i .
\]

Here, \( q_i \) and \( F_i \) are the generalized coordinates and the generalized forces (applied forces and disturbances).

The Hamilton concept allows one to model the system dynamics, and the differential equations are found using the generalized momenta \( p_i \),

\[
p_i = \frac{\partial L}{\partial \dot{q}_i} .
\]

The Lagrangian function

\[
L(t, q_1, ..., q_n, \frac{dq_1}{dt}, ..., \frac{dq_n}{dt})
\]

for the conservative systems is the difference between the total kinetic and potential energies.

We have

\[
L(t, q_1, ..., q_n, \frac{dq_1}{dt}, ..., \frac{dq_n}{dt}) = \Gamma(t, q_1, ..., q_n, \frac{dq_1}{dt}, ..., \frac{dq_n}{dt}) - \Pi(t, q_1, ..., q_n).
\]

Thus, \( L(t, q_1, ..., q_n, \frac{dq_1}{dt}, ..., \frac{dq_n}{dt}) \) is the function of \( 2n \) independent variables, and

\[
dL = \sum_{i=1}^{n} \left( \frac{\partial L}{\partial q_i} dq_i + \frac{\partial L}{\partial \dot{q}_i} \dot{q}_i \right) = \sum_{i=1}^{n} (p_i dq_i + p_i \dot{q}_i).
\]

Define the Hamiltonian function as

\[
H(t, q_1, ..., q_n, p_1, ..., p_n)
\]

\[
= -L(t, q_1, ..., q_n, \frac{dq_1}{dt}, ..., \frac{dq_n}{dt}) + \sum_{i=1}^{n} p_i \dot{q}_i,
\]

\[
dH = \sum_{i=1}^{n} \left( -\dot{p}_i dq_i + \dot{p}_i d\dot{q}_i \right),
\]

where

\[
\sum_{i=1}^{n} p_i \dot{q}_i = \sum_{i=1}^{n} \frac{\partial L}{\partial q_i} \dot{q}_i = \sum_{i=1}^{n} \frac{\partial \Gamma}{\partial q_i} \dot{q}_i = 2 \Gamma.
\]

Thus,

\[
H(t, q_1, ..., q_n, \frac{dq_1}{dt}, ..., \frac{dq_n}{dt}) = \Gamma(t, q_1, ..., q_n, \frac{dq_1}{dt}, ..., \frac{dq_n}{dt}) + \Pi(t, q_1, ..., q_n),
\]

or

\[
H(t, q_1, ..., q_n, p_1, ..., p_n) = \Gamma(t, q_1, ..., q_n, p_1, ..., p_n) + \Pi(t, q_1, ..., q_n)
\]
One concludes that the Hamiltonian, which is equal to the total energy, is expressed as a function of the generalized coordinates and generalized momenta. The equations of motion are governed by the following equations
\[ \dot{p}_i = \frac{\partial H}{\partial q_i}, \]
\[ \dot{q}_i = \frac{\partial H}{\partial p_i}, \]
which are called the Hamiltonian equations of motion.

The Hamiltonian function
\[ H = \frac{-\hbar^2}{2m} \nabla^2 \text{one-electron kinetic energy} + \Pi \text{potential energy} \]
can be used to derive the one-electron Schrödinger equation. To describe the behavior of electrons in a medium, one must use N-dimensional Schrödinger equation to obtain the N-electron wavefunction \( \psi(t, r_1, r_2, ..., r_N) \).

The Hamiltonian for an isolated N-electron atomic system is
\[ H = \sum_{i=1}^{N} \frac{-\hbar^2}{2m} \nabla_i^2 - \frac{\hbar^2}{2M} \nabla_q^2 - \sum_{i=1}^{N} \frac{1}{4\pi e} \frac{e_q}{|r_i - r_k|} + \sum_{i=1}^{N} \frac{1}{4\pi e} \frac{e^2}{|r_i - r_j|} + \sum_{k=m}^{N} \frac{1}{4\pi e} \frac{q_k q_m}{|r_i - r_m|} \]
where \( q \) is the potential due to nucleus; \( e = 1.6 \times 10^{-19} \text{ C} \).

For an isolated N-electron, Z-nucleus molecular system, the Hamiltonian function (Hamiltonian operator) is found to be
\[ H = \sum_{i=1}^{N} \frac{-\hbar^2}{2m} \nabla_i^2 - \sum_{k=1}^{N} \frac{\hbar^2}{2m_k} \nabla_k^2 \]
\[ - \sum_{i=1}^{N} \sum_{k=1}^{Z} \frac{1}{4\pi e} \frac{e_q}{|r_i - r_k|} + \sum_{i=1}^{N} \frac{1}{4\pi e} \frac{e^2}{|r_i - r_j|} + \sum_{k=m}^{N} \frac{1}{4\pi e} \frac{q_k q_m}{|r_i - r_m|} \]
where \( q_k \) are the potentials due to nuclei.

Terms of the Hamiltonian function \( \frac{-\hbar^2}{2m} \sum_{i=1}^{N} \nabla_i^2 \) and \( - \sum_{k=1}^{N} \frac{\hbar^2}{2m_k} \nabla_k^2 \) are the multi-body kinetic energy operators.

The term \( - \sum_{i=1}^{N} \sum_{k=1}^{Z} \frac{1}{4\pi e} \frac{e_q}{|r_i - r_k|} \) maps the interaction of the electrons with the nuclei at \( R \) (the electron-nucleus attraction energy operator).

In the Hamiltonian, the fourth term \( \sum_{r_j} \frac{1}{4\pi e} \frac{e^2}{|r_i - r_j|} \) gives the interactions of electrons with each other (the electron-electron repulsion energy operator).

The term \( \sum_{k=1}^{Z} \sum_{m=1}^{N} \frac{1}{4\pi e} \frac{q_k q_m}{|r_i - r_m|} \) describes the interaction of the Z nuclei at \( R \) (the nucleus-nucleus repulsion energy operator).

For an isolated N-electron Z-nucleus atomic or molecular systems in the Born-Oppenheimer nonrelativistic approximation, we have \( H\Psi = E\Psi \).

The Schrödinger equation is
\[ \left[ \frac{-\hbar^2}{2m} \sum_{i=1}^{N} \nabla_i^2 - \sum_{i=1}^{N} \frac{\hbar^2}{2m_i} \nabla_i^2 - \sum_{i=1}^{N} \frac{1}{4\pi e} \frac{e_q}{|r_i - r_k|} + \sum_{i=1}^{N} \frac{1}{4\pi e} \frac{e^2}{|r_i - r_j|} + \sum_{m=1}^{Z} \sum_{n=1}^{N} \frac{1}{4\pi e} \frac{q_k q_m}{|r_i - r_m|} \right] \Psi(t, r_1, r_2, ..., r_N) = E(t, r_1, r_2, ..., r_N) \Psi(t, r_1, r_2, ..., r_N). \]

The total energy \( E(t, r_1, r_2, ..., r_N) \) must be found using the nucleus-nucleus Coulomb repulsion energy as well as the electron energy.

It is very difficult, or impossible, to solve analytically or numerically the nonlinear partial differential equation (1). Taking into account only the Coulomb force (electrons and nuclei are assumed to interact due to the Coulomb force only), the Hartree approximation is applied. In particular, the N-electron wavefunction \( \Psi(t, r_1, r_2, ..., r_N) \) is expressed as a product of N one-electron wavefunctions as
\[ \Psi(t, r_1, r_2, ..., r_N) = \psi_1(t, r_1) \psi_2(t, r_2) ... \psi_N(t, r_N). \]

The one-electron Schrödinger equation for \( j \)th electron is
\[ \left[ \frac{-\hbar^2}{2m} \nabla_j^2 + \Pi(t, r) \right] \psi_j(t, r) = E_j(t, r) \psi_j(t, r). \]

In equation (2), the first term \( \frac{-\hbar^2}{2m} \nabla_j^2 \) is the one-electron kinetic energy, and \( \Pi(t, r) \) is the total potential.
energy. The potential energy includes the potential that \( j \)th electron feels from the nucleus (considering the ion, the repulsive potential in the case of anion, or attractive in the case of cation). It is obvious that \( j \)th electron feels the repulsion (repulsive forces) from other electrons.

Assume that the negative electrons charge density \( \rho(r) \) is smoothly distributed in \( \mathbb{R} \). Hence, the potential energy due interaction (repulsion) of an electron in \( \mathbb{R} \) is

\[

\Pi_{rj}(r,r') = \int_{\mathbb{R}} \frac{\epsilon \rho(r')}{4\pi \epsilon_0 |r - r'|} dr'.

\]

### III. HAMILTON-JACOBI OPTIMIZATION THEORY AND QUANTUM MECHANICS

The Hamiltonian for a particle is

\[

\Delta \int_{t_0}^{t_f} [p v - H(t,x,p)] dt = 0,

\]

where \( \Delta \) is the variation of the succeeding expression with respect to \( v \) and \( p \).

Using the optimal (stationary) value of the integral

\[

\int_{t_0}^{t_f} [p v - H(t,x,p)] dt,

\]

as denoted by \( \mathbf{V}(t,x) \), one has [6]

\[

\mathbf{S} \left[ \int_{t_0}^{t_f} \frac{dV}{dt} + pv - H(t,x,p) \right] dt = 0,

\]

where \( \mathbf{S} \) is the optimal (stationary) value obtained by varying \( v \) and \( p \).

Therefore, one has

\[

p = -\frac{\partial V}{\partial x},
\]

\[

\dot{p} = -\frac{\partial V}{\partial x} \frac{\partial V}{\partial t} + v \frac{\partial^2 V}{\partial x^2} = -\frac{\partial H}{\partial x} + \frac{\partial H}{\partial p} \frac{\partial p}{\partial x},
\]

\[

v = \frac{\partial H}{\partial p},
\]

\[

H = \frac{\partial V}{\partial t}.
\]

The variables \( x \) and \( p \) are independent, and therefore, the Hamiltonian equations of motion

\[

\dot{p} = -\frac{\partial H}{\partial x},
\]

and

\[

\dot{x} = \frac{\partial H}{\partial p}
\]

results.

The complex functions are used in quantum mechanics, and we replace the displacement \( x \) by the complex variable \( q \), and instead of velocity \( v \) we have \( dq = vdt + ndz \), where \( n \) is complex, \( n = -i \frac{\hbar}{m} \), and \( z \) is the white noise (normalized Wiener process). Therefore, one obtains

\[

\Delta \mathbf{E} \left[ \int_{t_0}^{t_f} [p v - H(t,q,p)] dt \right] dt = 0,
\]

where \( \mathbf{E} \) denotes the expectation.

Making use of the dynamic programming (variational principle), from

\[

E dz^2 = dt \quad \text{and} \quad E dq^2 = n^2 dt,
\]

we have

\[

\mathbf{S} \left[ \frac{dV}{dt} + pv + \frac{\partial V}{\partial q} + \frac{1}{2} n^2 \frac{\partial^2 V}{\partial q^2} - H(t,q,p) \right] = 0.
\]

The minimization gives the following Hamiltonian equations

\[

p = -\frac{\partial V}{\partial q},
\]

\[

v = \frac{\partial H}{\partial p},
\]

\[

H = \frac{\partial V}{\partial t} - \frac{i\hbar}{2m} \frac{\partial^2 V}{\partial q^2}.
\]

Letting

\[

V = i\hbar \log \Psi
\]

and taking note of

\[

p = -i\hbar \frac{\partial}{\partial q},
\]

one finds
Thus, finally we obtain the Schrödinger equation
\[ E\Psi = i\hbar \frac{\partial}{\partial t} \Psi(t, q) = \left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial q^2} + \Pi(q) \right] \Psi(t, q) = \hbar \Psi. \]

The wavefunction \( \Psi = e^{i\phi} \) is the solution of the Schrödinger equation. The Schrödinger equation was derived using Hamilton's principle. Furthermore, it was illustrated that the Schrödinger equation was found minimizing the functional. It is very important that the Schrödinger equation was derived from the closed-loop solution through optimization of the functional because it establishes the relationship between the Hamilton theory and quantum mechanics. The Schrödinger equation leads to the solution in the form of wavefunctions, while the Hamiltonian concept results in the optimal cost function. Furthermore, it was shown that the Schrödinger equation results from a closed-loop solution of the Hamiltonian equation:
\[ \Delta E \left[ L_{q} - H(t, q, p) \right] dt = 0, \]
and the closed-loop solution represents the goal-seeking behavior (dynamics) of nature.

**IV. CONCLUSIONS**

This paper studies several key problems in modeling, analysis, simulation, and optimization of nanoscale systems. Using quantum and functional density theories as well as electromagnetics, a novel energy-based avenue in modeling and analysis of nanostructures and nanodevices is developed. From the optimization perspective and standpoint, it is illustrated that the Schrödinger equation can be derived using Hamilton's principle. The importance of the results is that the Schrödinger equation was obtained from the closed-loop solution through optimization of the functional. This establishes the relationship between the Hamilton theory and quantum mechanics. The Schrödinger equation leads to the solution in the form of wavefunctions, while the Hamiltonian concept results in the optimal cost function. Furthermore, it was shown that the Schrödinger equation results form a closed-loop solution of the Hamiltonian equation.

**REFERENCES**