Quantum and classical connections in modeling atomic, molecular and electrodynamic systems

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STATIONARY SYSTEMS:

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SYSTEMS COMPOSED OF PARTICLES AND FIELDS:

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Theory of Quantum and Classical Connections in Modeling Atomic, Molecular and Electrodynamic Systems
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Applications of Quantum and Classical Connections in Modeling Atomic, Molecular and Electrodynamic Systems
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Figure: 1

I. STATIONARY SYSTEMS

- 1) N electrons and N' nuclei.
  2) The system is closed and stationary (E is constant and U does not depend explicitly on time).
  3) The behavior of the system is completely described by the Schrödinger equation.
- The analysis is made in the space R^{3N} of the electron coordinates $q = (q_1, q_2, ..., q_{3N})$.

The equivalence between the Schrödinger and wave equation.

$$-i\hbar\frac{\partial\Psi}{\partial t}-\frac{\hbar^2}{2m}\sum_j\frac{\partial^2\Psi}{\partial q_j^2}+U\Psi=0(1)\Longleftrightarrow\begin{cases}\sum_j\frac{\partial^2\Psi}{\partial q_j^2}-\frac{1}{v_w^2}\frac{\partial^2\Psi}{\partial t^2}=0 & (2)\\ \Psi=\Psi_0\exp(-iEt/\hbar) & (3)\end{cases}$$

$v_w=\pm|E|/\sqrt{2m(E-U)}$ (4)
$\Psi=\Psi(q,t,E,c)$ $\Psi_0=\Psi_0(q,E,c)$ where $c=(c_1,c_2,\ldots,c_S)$

Calculation of the characteristic surfaces, which are identical to the wave surfaces (Courant and Hilbert or Smirnov).

- Equation of the characteristic surfaces (χ is the charactertistic function):
  $\chi(q, t, E, c) = 0 \ (5)$
- Characteristic equation:
  $\sum_j \left(\frac{\partial \chi}{\partial q_j}\right)^2 - \frac{1}{v_w^2}\left(\frac{\partial \chi}{\partial t}\right)^2 = 0 \quad (6)$
- Solution of (5) leads to the equation of the wave surfaces:
  $f(q, E, c) = |E|t - p\pi/k \ (7)$
  where f is the single valued function which verifies the time independent Hamilton-Jacobi equation

Proof of the properties of the characteristic surfaces and of their normals.

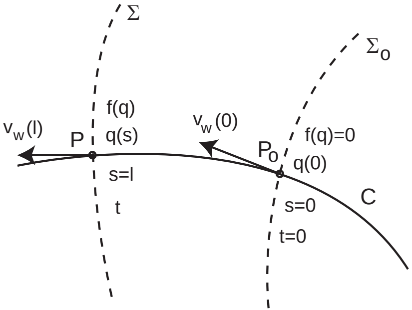

Figure: 2

- Two Σ surfaces never intersects each other.
- The velocity v_w never passes through zero and the point P moves always in the same direction.

- The motion of the Σ surface is periodic, and the C curve is closed.

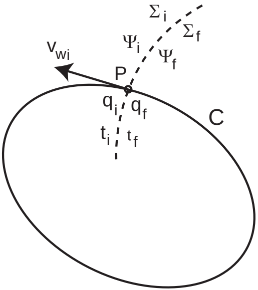

Figure: 3

Equations which characterize the periodical motion of the wave.

1) Motion equation of the Σ surface:
$f(q, E, c) = |E|t - p|E|\tau_w$ for $p\tau_w \leq t < (p+1)\tau_w$ (8)
$0 \leq f(q, E, c) < f_M$ where $f_M = |E| \cdot \tau_w$ (9)
2) Equations of the reduced action function and its variation along the C curve:
$S_0(q, E, c) = f(q, E, c) + pf_M$ and $\Delta_C S_0 = f_M$ (10)
3) Relation between the velocities of the two motions which are associated with the C curve.
$vv_w = |E|/m$ (11)

Properties resulting from the integral relation of the time independent Schrödinger equation on the C curve.

- Substitution $\Psi_0 = \exp(i\sigma/\hbar)$ (12) in the time independent Schrödinger equation leads to:
  $\frac{1}{2m}\sum_j \left(\frac{\partial\sigma}{\partial q_j}\right)^2 + U - E - \frac{i\hbar}{2m}\sum_j \frac{\partial^2\sigma}{\partial q_j^2} = 0$ (13)
- The integral relation of (13) on the C curve:
  $\int_C \sum_j \left(\frac{\partial\sigma}{\partial q_j}\right)^2 dt - i\hbar \int_C \left(\sum_j \frac{\partial^2\sigma}{\partial q_j^2}\right) dt = \int_C \sum_j \left(\frac{\partial S_0}{\partial q_j}\right)^2 dt$ (14)
- Solution of (14) is $\sigma_g = S_0$ (15)
- From (2), (12) and (15) obtain
  $\Psi_{0g} = A\exp(iS_0/\hbar)$ (16) and
  $\Psi_g = A\exp(iS/\hbar)$ where $S = S_0 - Et$ (17)

Generalized relations.

- The single valued property of Ψ_{g0} leads to the generalized Bohr quantization relation:
  $\Delta_C S_0 = nh$ (18)
- From (9)-(11) and (18) obtain the generalized de Broglie relations:
  $\overline{p} = n\hbar\overline{k}_w$ (19)
  $|E| = n\hbar\omega_w$ (20)
  where $\lambda_w = \tau_w \cdot v_w$ and $\omega_w = 2\pi/\tau_w$.

The principle of our method. The wave function and the characteristic surfaces and curves are mathematical objects which describe the same physical system and depend on its constants of motion. It follows that any of these mathematical objects can be used to study the properties of the system.

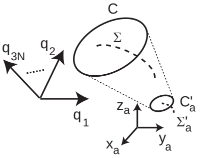

Figure: 4

- A central field method leads to the calculations of the projections of the motion from the space R^{3N} to the spaces of the electrons coordinates, and to the calculation of the energy of the system.

Exact connection between Schrödinger and Hamilton-Jacobi equation

- 1) Discontinuities of the partial second derivatives of the wave functions propagate following the trajectories determined by the Hamilton-Jacobi equation:
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- 2) Characterictic surfaces of the wave equation are solutions of Hamilton-Jacobi equation:
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II. SYSTEMS COMPOSED OF PARTICLES AND FIELDS

- We consider a system composed of an electron interacting with an elliptic polarized electromagnetic field in the general case, when the electron velocity and the phase of the field are arbitrary.
- We proved [Phys. Rev. A, 84, 023824, 2011] that the Klein-Gordon equation, written for this system
  $\left[c^2\left(-i\hbar\nabla + e\overline{A}\right)^2 - \left(i\hbar\partial/\partial t\right)^2 + \left(mc^2\right)^2\right]\Psi = 0$ (21)
  is verified exactly by
  $\Psi = A\exp(iS/\hbar)$ (22)
  where S is the solution of the relativistic Hamilton-Jacobi equation.

PROPERTY RELATED TO CLASSICAL SOLUTION (22)

- The relations are used to prove the connection between Klein-Gordon and relativistic Hamilton-Jacobi equation, lead also to a periodicity property which simplifies significantly the modeling interactions between very intense laser beams and:
  (1) electron plasmas
  (2) relativistic electron beams
  (3) atoms
  PERIODICITY PROPERTY: All the physical quantities, which are involved in the generation of harmonics, in the interactions (1), (2), (3), are periodic functions of only one variable, that is the phase of the incident electromagnetic field. The property is valid also for the physical quantities which describe the radiation damping effect, using the Landau and Lifschitz model, for the above interactions.

II.1. MODELING INTERACTION BETWEEN LASER BEAM AND ELECTRONS

- System composed of an electron interacting with an elliptic polarized electromagnetic field in the general case. Three step solution.
- First step. The solution of the relativistic motion equations. We obtain: $\overline{\beta} = \overline{\beta}\,(\sin\eta, \cos\eta, constants)$ and $\dot{\overline{\beta}} = \dot{\overline{\beta}}\,(\sin\eta, \cos\eta, constants)$.
- Second step. We introduce $\overline{\beta}$ and $\dot{\overline{\beta}}$ in Liènard-Wiechert equation and obtain $\overline{E} = \overline{E}\,(\sin\eta, \cos\eta, constants, \theta, \varphi)$ and intensity of the scattered radiation: $I_{av} = \epsilon_0 c \frac{1}{2\pi} \int_0^{2\pi} \overline{E}^2 d\eta$.
- Third step. The Fourier series development leads to the spectral components of the electrical field: $\overline{E}_j = \overline{E}_j\,(\sin j\eta, \cos j\eta, constants, \theta, \varphi)$ and to the intensity of the harmonic of order j: $I_j = \epsilon_0 c \frac{1}{2\pi} \int_0^{2\pi} \overline{E}_j^{\,2} d\eta$.

- Spectral distribution of the scattered radiation:

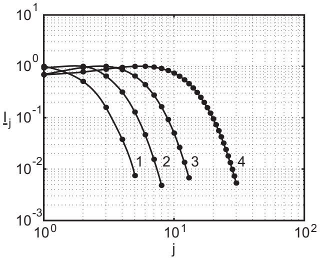

Figure: 5. Spectral distribution for elliptic polarized field, having $a_2 = 5$. The curves 1, 2, 3 and 4 correspond, to $a_1 = 2, 4, 6, 8$.

- Angular distributions of the scattered radiation.

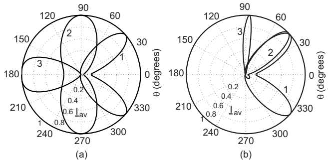

Figure: 6. Polar plots of $\underline{I}_{av}$ in the case of the interaction between a circular polarized field, having $a_1 = a_2 = 2$, which propagate in the *oz* direction, and relativistic electrons which move (a) in the opposite direction and (b) which move in the *ox* direction.

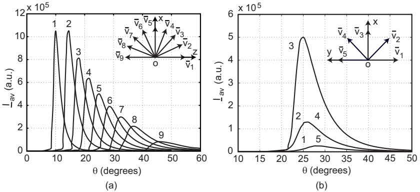

Figure: 7. Typical angular distributions of $\underline{I}_{av}$ versus θ, when the laser field interact with nine electrons whose velocities are situated (a) in the the plane *xz* and (b) in the the plane *xy*.

I.2. MODELING COLLISIONS BETWEEN VERY INTENSE LASER BEAMS AND RELATIVISTIC ELECTRON BEAMS

- We consider the head-on collision between laser and electron beams. The analysis is identical to that from the previous case, but it is made in the inertial system S' in which the velocity of the electron is zero.
- Spectral distribution of the scattered radiation:

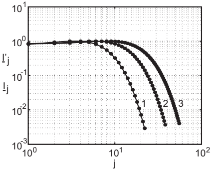

Figure: 8. Typical spectral distributions, namely variations of $\underline{I}'_j$ and $\underline{I}_j$ in the inertial systems S' and S. The spectra from curves 1, 2 and 3 correspond, respectively, to $a = 3$, $a = 5$ and $a = 7$.

- Angular distributions of the scattered radiation.

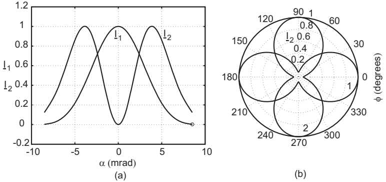

Figure: 9. (a) Variations of $\underline{I}_1$ and $\underline{I}_2$ with $\alpha = \pi - \theta$; (b) Variations of $\underline{I}_2$ with ϕ when the field is linearly polarized in the *ox* direction for curve 1, and in *oy* direction for curve 2.

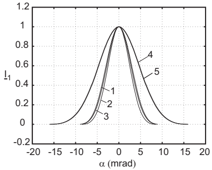

Figure: 10. Variations of $\underline{I}_1$, with α for different experiments.

II.3. MODELING INTERACTION BETWEEN LASER BEAM AND ATOMS

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Figure: 11. The three sequences of the harmonic generation.

- Three sequences mechanism of harmonic generation:
  1) Multiphoton absorption followed by leaving the atom by tunneling.
  2) Oscillation in the ionization domain.
  3) The electron returns in the vicinity of the atom; it transfers the kinetic energy to the electromagnetic field by electric dipole transition.

Two dominant effects involved in the harmonic generation

- 1. The behavior of the system in the second phase can be approximated by classical motion of the electron. The solution identical to that from I.1.
- 2. The emission of the harmonics is due to the electric dipole transition. An accurate rate of electric dipole transition, is calculated by Lewenstein et al (Phys.Rev.A 49, 2117, 1994), in the frame of the theory of Bethe and Salpeter.

- Typical harmonic spectra.

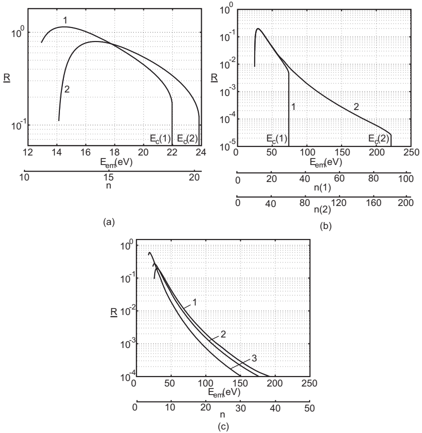

Figure: 12. Typical harmonic spectra. (a) For low values of I_L, of the order 10^{13} W/cm^2 the spectrum has the well known plateau shape; (b) When I_L is increased to the order 10^{15} W/cm^2, the slope of the plateau is increased; (c) When I_L is of the order 10^{17} W/cm^2, the domain of the high harmonics is strongly diminished.

CONCLUSIONS:

- Despite the fact that the stationary atomic and molecular (AM) systems and the nonstationary electrodynamic (ED) systems are very different, they have common properties.
- The connection between quantum and classical equations results directly, without any supplementary postulate or approximation, from the properties of quantum equations, in both cases.
- A classical solution of the type $A \exp iS/\hbar$ results, without any approximation, from the mathematical properties of both, the Schrodinger and Klein-Gordon equations
- The existence of connections between quantum and classical equations is accompanied by the existence of periodicity properties in both cases, for AM and ED systems. This property has a practical importance, because it leads to accurate models for the calculation of properties of AM and ED systems.