SCIENTIFIC ACTIVITY OF LORENZO RESCA

(Updated on 6-6-2018**)**

Since the mid 1980's, I have been mostly interested and contributed to six different areas of research: (A) Electronic structure of semiconductor heterostructures and superlattices; (B) Electrical response in heterogeneous systems and electrorheological fluids; (C) First-principles theory of ferroelectricity; (D) Psychophysical measurements and computer simulations of eye movements in visual search; (E) Theory, computation, and engineering of thermoelectric materials; (F) Coarse-grained entropy studies of microscopic reversibility and macroscopic irreversibility based on lattice-gas models; (G) Space, time and space-time curvatures and geodesics in general relativity and Schwarzschild's geometry.

With regard to the first area (A), mainly in collaboration with R. D. Graft, M. Fornari, D. J. Lohrmann, and G. Pastori Parravicini, we have applied recursion-renormalization methods to study the microscopic structure of heterostructures and superlattices. We have studied in particular HgCdTe quantum wells and superlattices, with technological applications to infrared detectors. Accurate microscopic wavefunctions have been obtained, allowing a more detailed study of interface states, semiconductor-semimetal transitions, and valence-band offset. We have also applied Green's function and recursion methods to study localized defects and impurities in semiconductors, demonstrating relative contributions of Coulomb tails, central cell potential, and intervalley interference, resulting in a "shallow-deep instability" that has been subsequently found and demonstrated in many other systems. Previously, we had used quantum defect methods to study excitons in rare-gas and other molecular solids, including fullerides.

With regard to the second area (B), mainly in collaboration with L. Fu, we have developed an analytical method to calculate exactly the classical electrical response of heterogeneous systems. Our method is based on a multipolar re-expansion, and includes all the multipolar images generated in the experimental configuration of parallel electrode plates, as well as in other substrate configurations. We also applied this multipolar method to the mean field theory of disordered systems, including two-particle distributions of all multipolar orders. We studied in particular clusters of spheres and inclusions with permanent multipoles, solving problems of anomalous infrared absorption in composites and resolving ambiguities in the original models of Debye and Onsager. A major application of our multipolar method has been to electro-rheological fluids (ERF), allowing to calculate exactly the electrostatic interactions and forces among the suspended particles, and between the particles and the electrodes. We have demonstrated rigorously that dipole approximations, often used in calculations and simulations, yields only a few percent of the exact forces at typical ERF densities. We have shown in particular that an ERF consisting of metal spheres coated with a thin insulating layer exhibits largely enhanced electrostatic forces. Another major application of our multipolar method has involved nonlinear composites. We have shown that the effective nonlinear (third order) susceptibility for disordered systems of coated spherical particles can be enhanced by five to seven orders of magnitude, and that the peak frequency can be largely shifted, through the combined effects of the particle structure and the inter-particle interactions. As a result, the nonlinear spectrum can be sensitively tuned by varying a given concentration-distribution parameter. We have extended our theory to all ranges of applied fields, producing both the weak- and strong-field nonlinearities as particular limits. Striking and unexpected results have been found at intermediate fields, consisting of multiple solutions in certain frequency ranges. This may still have major implications for optical communications and laser technologies.

With regard to the third area (C), mainly in collaboration with L. Fu, E. Yaschenko, and R. Resta, we have contributed to seminal research in the theory of ferroelectricity. Ferroelectric materials have unusual properties in their structural, electrical, and electromechanical behavior. Such properties stem from the electronic structure of these materials, where the highly variable hybridization of the relevant orbitals plays a critical role. We elucidated in particular the relationships between electronic levels, crystal structure, and electrical properties. Namely, we have explained underlying microscopic mechanisms, understood general trends, and interpreted various experiments. In dealing with these materials and properties, a quantum-mechanical first-principles approach is essential. Our approach has consisted in performing first-principles calculations using methods of modern electronic-structure theory and state-of-the-art technical ingredients. An important characteristic of our work has been the use of both Hartree-Fock and density-functional methods, which provide results having the same overall quality, but with errors typically providing opposite bounds to the experimental results. In another fundamental development, we have shown that the very fact that insulators have a finite bulk polarization originates from the essential localization of the electronic wavefunction. We have thus provided a novel definition of electronic localization, and demonstrated the value of this concept not only for “non-exotic” insulators, but even for a highly correlated model material. Furthermore, we have studied several surface properties of ferroelectric perovskites, and pointed out those properties ─such as dynamical charges─ where a naive extrapolation of the bulk results leads to even qualitatively incorrect values. Other inquiries of ours have delved into non-ferroelectric oxides, where we have predicted some unexpected polarization features. From the technological point of view, ferroelectric materials are currently used in the most effective acoustic transducers. Our research has contributed to an understanding at the fundamental level that fosters a more rational and systematic search of better materials for such transducers.

With regard to the fourth area (D), mainly in collaboration with T. D. Keech, we have conducted psychophysical measurements of eye movements in young and older adults performing conjunctive visual search tasks, and thus determined corresponding elements of perception, selection, attention, and memory. We have found age-related differences in various measures of eye movements, consistently indicating slightly reduced conspicuity areas for older adults - hence, correspondingly reduced processing and memory capacities. Most importantly, we have demonstrated the formation of spiraling or circulating patterns in the eye movement trajectories and developed a corresponding computational model and simulations. The relation of attention, memory and spatial constraints to pattern formation in eye movement trajectories has been demonstrated through studies of saccade autocorrelations and power spectra that confirm a bias to progress forwardly, while turning at the display boundaries, plus a long-range memory component for the search path. Analyses of certain measures of circulation and imbalance in the eye trajectories, and their relations with the display area correspondingly subtended, also bear signatures of spiraling or circulating patterns. We have interpreted their prevalence as mainly due to the interactions between three basic psycho-neural mechanisms (conspicuity area, forward bias, long-range memory) and two task-specific geometric-spatial constraints on the eye trajectories (central start and display confinement). Conversely, computer simulations of random walks in which all psycho-neural mechanisms are eliminated, while geometric-spatial constrains are maintained, show no prevalence of circulating patterns by those measures. We did find certain peculiarities of some individual participants in their pattern selections, but they appear too casual and incidental to suggest more systematic or complex search strategies in our randomized displays of uninformative stimuli. Most notably, we have developed a computational model and corresponding computer simulations that mimic phenomenologically the eye movement trajectories observed in a conjunctive visual search task. The element of randomness is captured in the model through a Monte Carlo selection of a particular eye movement based on its probability, which depends on three factors, adjusted to match the observed saccade amplitude distribution, forward bias in consecutive saccades, and return rates. Memory is assumed to operate through tagging of objects already recognized as non-target, which in turn requires their processing within the attentional area of conspicuity (AC). That AC is adjusted so that computer simulations reproduce optimally the distribution of the number of saccades, the failure rate to capture the target, and the return rate to previously inspected locations. For their viability, computer simulations critically depend on memory to be long-ranged. In turn, the simulations confirm the formation of circulating or spiraling patterns in the observed eye trajectories. We have also related consistently the average number of saccades per trial to the saccade amplitude distribution by modeling analytically the combined roles of the AC in attention and memory.

With regard to the fifth area (E), mainly in collaboration with N. A. Mecholsky, I. L. Pegg and M. Fornari, we have developed a theory of angular effective mass and band structure warping to study electronic and thermal properties of materials, using first-principles calculations and computer simulations to apply and support it. That should guide the engineering of thermoelectric materials so to optimize their thermoelectric performance and transport properties. That includes subjecting materials to perturbations such as strain or doping, or fabricating them as heterostructures, superlattices, nanostructures or nanowires, thus tailoring their electronic band structures and warping to affect transport coefficients and figures of merit as optimally desired.

With regard to the sixth area (F), mainly in collaboration with F. C. Pérez-Cárdenas and I. L. Pegg, we have developed coarse-grained descriptions and computations of the time evolution of a lattice gas system of indistinguishable particles, whose microscopic laws of motion are exactly reversible, in order to investigate how or what kind of macroscopically irreversible behavior may eventually arise. With increasing coarse-graining and number of particles, relative fluctuations of entropy rapidly decrease and apparently irreversible behavior unfolds. Although that behavior becomes typical in those limits and within a certain range, it is never absolutely irreversible for any individual system with specific initial conditions. Irreversible behavior may arise in various ways. We have illustrated one possibility by replacing detailed integer occupation numbers at lattice sites with particle probability densities that evolve diffusively. We have further shown that the entropy of a system with normal density fluctuations in coarse-grained cells evolves toward an equilibrium average and narrowly fluctuates around it, typically remaining well below the maximum entropy. We have derived a power law that relates coarse-graining to that entropy gap. Another power law relates the noise range of entropy fluctuations to coarse-graining. We tested these power laws with numerical calculations based on our two-dimensional lattice-gas model. As theoretically expected, these power law effects diminish with increasing coarse-graining, eventually disappearing in the thermodynamic limit, where the maximum-entropy principle is reasserted.

With regard to the seventh area (G), I have shown that geodesic orbit equations in Schwarzschild’s geometry of general relativity reduce to ordinary conic sections of Newtonian mechanics and gravity for material particles in the non-relativistic limit. On the contrary, geodesic orbit equations for a proper spatial submanifold of Schwarzschild’s metric at any given coordinate-time correspond to an unphysical gravitational repulsion in the non-relativistic limit. This demonstrates at a basic level the centrality and critical role of relativistic time and its intimate pseudo-Riemannian connection with space. Correspondingly, a commonly popularized depiction of geodesic orbits of planets as resulting from the curvature of space produced by the sun, represented as a rubber sheet dipped in the middle by the weighing of that massive body, is mistaken and misleading for the essence of relativity, even in the non-relativistic limit. In collaboration with R. T. Eufrasio and N. A. Mecholsky, we have investigated at a deeper level geodesic orbits and manifolds for all three metrics associated with Schwarzschild’s geometry. For “a-temporal” space, we have solved my central geodesic orbit equation in terms of elliptic integrals and functions. We have shown that the intrinsic geometry of a two-sided equatorial plane corresponds to that of a full Flamm's paraboloid. Two kinds of geodesics thus emerge. Both kinds may or may not encircle the hole region any number of times, crossing themselves correspondingly. Regular geodesics reach a periastron greater than Schwarzschild’s radius, thus remaining confined to a half of Flamm's paraboloid. Singular or s-geodesics tangentially reach the circular horizon. These s-geodesics must then be regarded as funneling through the “belt” of the full Flamm's paraboloid. Infinitely many geodesics can possibly be drawn between any two points, but they must be of specific regular or singular types. We have made their precise classification in terms of impact parameters. We have conveyed geodesic structure and completeness with computer-generated figures depicting either Schwarzschild’s equatorial plane or Flamm's paraboloid. For the “curved-time” metric, devoid of any spatial curvature, we have shown that geodesic orbits have the same apsides as in Schwarzschild’s space-time. We focused on null geodesics in particular. For the limit of light grazing the sun, we have confirmed that “spatial bending” and “time bending” become essentially equal, adding up to the total light deflection of 1.75 arc-seconds predicted by general relativity. However, for a much closer approach of the periastron to Schwarzschild's radius, we have demonstrated that "time bending" largely exceeds "spatial bending" of light, while their sum remains substantially below that of Schwarzschild's space-time.

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Positions:

-SNS student fellow, 1966-1970.
-National Research Council (CNR) postdoctoral fellow, Department of Physics, University of Pisa, 1971-1973.
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TEACHING AT THE CATHOLIC UNIVERSITY OF AMERICA

I have taught all the core courses of both the undergraduate and graduate curriculum, plus numerous advanced courses on continuum mechanics, chaotic dynamics, quantum field theory, many-body theory, relativity and cosmology. For all of these courses, I have prepared and provided to the students extensive and detailed notes, problems, and solutions. A partial list of courses that I have taught at CUA since 1980 follows:

PHYS 215 (4) University Physics I, S(pring)81, F(all)83.
PHYS 216 (4 Credit Hours) University Physics II, S84, S89.
PHYS 611 (4) Math. Meth. Theoretical Phys. I, F81, F82, F01.
PHYS 612 (4) Math. Meth. II, S82, S83, S84, S95, S99, S01, S04, S07, S11.
PHYS 615 (3) Adv. Mechanics I, F80, F81, F84, F95, F97, F99, F01.
PHYS 616 (3) Adv. Mechanics II, S81, S82, S83, S91, S93, S02.
PHYS 616 (3) Adv. Mech. II: Chaos in Dynamical Systems, S96, S05.
PHYS 618 (3) Continuum Mechanics, S96.
PHYS 621 (3) Stat. Mech. I, F89, F90, F93, F94, S96, S98, F00, F02, F04, F05, F06, F08.

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