Overview of my research interests
(Updated June 2021)

The electronic structure of few-electron atoms (in particular near their critical charge): In most of its electronic states (except the states that correspond to non-vanishing electron affinities), the critical charge of an N-electron atom is $Z_c = N - 1$. Upon approaching this critical charge from above, the outermost electron becomes a diffuse hydrogen-like orbital, with an effective charge $Z - Z_c$. The binding energy of an outermost electron of type $n\ell$ can be written as

$$\epsilon_{n\ell} = -\frac{(Z - Z_c)^2}{2(n - \delta_{n\ell})} ,$$

where $\delta_{n\ell}$ is the "quantum defect". Over the past several years I have reported evidence that

$$\lim_{Z \to Z_c} \delta_{n\ell}(Z) = n_\ell ,$$

where n_ℓ is the number of ℓ-type occupied subshells, in the core. This limiting behavior has a nice heuristic interpretation, but its rigorous derivation remains elusive. In the high Z limit of the N-electron atom (ignoring the onset of relativistic effects) all the orbitals become asymptotically hydrogen-like. These observations imply that, for open-shell isoelectronic sequences the term splitting within a common configuration vanishes at the critical charge and grows linearly in Z for high nuclear charges. Hence, the term splitting divided by the square of the nuclear charge vanishes at both Z_c and at $Z \to \infty$, possessing a maximum in between these two limits. I recently observed (combining the virial and the Helmann-Feynman theorems), that the difference of interelectronic repulsions can be obtained as

$$\Delta C = -Z^3 \frac{\partial}{\partial Z} \left(\frac{\Delta E}{Z^2} \right) .$$

This observation, combined with the non-monotonicity of $\frac{\Delta E}{Z^2}$ pointed out above, sheds new light on an issue that I studied many years ago, establishing the inevitability of the fact that in neutral atoms and moderately charged positive ions the interelectronic repulsion is higher in the lower energy state, within an open-shell configuration (contrary to some speculations offered in the literature, even recently). My work on these issues in the early seventies of the previous century culminated in a revised understanding of the dynamical origin ("interpretation") of Hund's rule ordering in open-shell atoms [that, though sometimes misrepresented, affected the textbook presentation of this topic. In some recent textbooks (e.g., Atkins, *Molecular Quantum Mechanics*, 2003 and further editions) this revised treatment attains the ultimate status of "common knowledge" by being introduced without reference]. An appropriate modification of the relation quoted above accounts for the fact that in flat-bottomed quantum dots no reversal of the interelectronic repulsions takes place. My current interests in this area involve the examination of heavy open-shell atoms, transition metal and lanthanide complex ions, and bulk ferromagnetic materials, looking for observable consequences of the dependence of the spatial wavefunction on the value of the total spin. These include relative magnitudes of transition probabilities and the splitting, due to spin-orbit coupling, of different terms that belong to a common configuration.

Efficient combinatorial algorithms for the characters of the symmetric group and for the structure constants in its group-algebra:
Though these are mathematically solved problems, they become computationally intractable even in applications to systems consisting of a moderate number of identical particles. Some powerful simplifications (some of which also apply to the unitary groups, the quantum unitary groups, and to the Hecke algebra of the symmetric group) were elucidated in a series of articles that I published between the mid eighties and the late ninties [that became textbook items, cf. T. Ceccherini-Silberstein *et al.*, *Representation Theory of the Symmetric Group*, 2010]. A result that can be stated non-technically is that the irreducible representations of the symmetric groups are fully characterized by a small subset of characters of single-cycle conjugacy-classes, and those of the quantum unitary groups are fully characterized by their fundamental ("quadratic") Casimir operator. These results were applied to symmetry adaptation of many-body wavefunctions and to the construction of hyperspherical wavefunctions. They were implemented in a widely applied nuclear shell-model code. I have recently established (joint work with A. Rattan) the equivalence to Kerov's approach (that he only reported in a seminar in Paris shortly before untimely passing away in 2000). Further elucidation of certain rather challenging details of the underlying formalism is definitely called for, and I intend to keep trying for a while.

Combinatorics of boson normal ordering:
A modest study, establishing the role of the Stirling numbers in the normally-ordered expression for the k'th power of the boson number operator, that I published in 1974, was followed, during the quantum group hype of the early ninties, by a generalization to q-bosons (joint work with Maurice Kibler). It triggered a mini-avalanche of activity that is still responsible for a steady output of generalizations [comprehensively reviewed by Mansour, *Combinatorics of set partitions*, 2013]. I have also studied related issues concerning generalized boson operators and generalized coherent and squeezed states. All these are of interest both because of their potential physical applications and because of the rich algebraic combinatorics involved.

Permutational symmetry classification of identical higher-spin particles:
My original interest in this issue was motivated by the fact that the simplicity of the corresponding problem for spin-$\frac{1}{2}$ particles, encapsulated by the Dirac identity that associates a transposition with the scalar product of the individual spin operators of the particles involved, is not shared by higher spins. Specifically, the one-to-one correspondence between the total spin and the label of the irreducible representation does not hold for systems of identical particles with elementary spins $\sigma \geq 1$. The current interest in higher spin Bose-Einstein condensates provides a motivation for further refinement and extension of results concerning the classification of such systems, that I published over a decade ago.

Is there a bound triplet $(1\sigma_g, 1\sigma_u)$ (zero bond order) state of a (heavy hole) biexciton?
Such a state was predicted to be feasible in a polar crystal, where the short-range (high-frequency) dielectric constant is considerably lower than at long distances (low frequency), [thesis by Kamer Murat, that I supervised in the late seventies] but so far never observed.

Recent developments in very low temperature solid state spectroscopy, as well as theoretical progress that suggests a necessary modification of the Haken-potential assumed in that study, call for a more up-to-date treatment of this problem. I may get to doing something about this one of these days.

Some past research highlights that I am unlikely to return to:
Nuclear spectroscopy and thermoluminescnce. Mean-field theory for non-isotropic magnetic materials [a highlight being a generalized Weiss equation

$$\vec{S} = -\frac{\nabla_s H}{|\nabla_s H}\sigma B_\sigma\Big(\beta\sigma|\nabla_s H|\Big) ,$$

that yields the magnetization vector in terms of the gradient of the anisotropic spin-hamiltonian $H(\vec{S})$] and for nematic liquid crystals. Reentrance. Generalization of the Bogolyubov-Tyablikov approximation. The non-linear eikonal approximation [one highlight being the non-linear self-consistency equation

$$n(t) = n\cos^2\left(\epsilon\int_o^t \sqrt{n(\tau)+1}d\tau\right) ,$$

that is analytically soluble in terms of Jacobi elliptic functions (joint work with David Hummer), which is relevant to both four-wave mixing and to bistability in the non-linear Fabry-Perot resonator (joint work with Meir Orenstein and Shammai Speiser)]. The super-hamiltonian formalism for excited states, allowing the formulation of excited-state, degenerate and ensemble Hohenberg-Kohn theorems. Establishing (with Avia Rosenhouse) that in the classical limit the isospectral solutions of the Korteweg de-Vries equation become isochronous potentials. Minor involvement in Amitai Halevi's OCAMS.