We show and interpret three examples of nontrivial results obtained in numerical simulations of many-body systems: exponential convergence of low-lying energy eigenvalues in the process of progressive truncation of huge shell-model matrices, apparently ordered spectra generated by random interactions, and regular behavior of complex many-body energies in a system with single-particle orbitals in continuum. The possible practical applications and new approaches are suggested.

1 Introduction

As we discussed at the previous conference (S. Agata sui due Golfi, 1998), the ideas of quantum chaos significantly advance our understanding of many-body quantum systems. The new stage of this development is related to the role of incoherent interactions between the constituents. Apart from great theoretical interest, which extends to similar problems in other finite many-body systems as atomic clusters, quantum dots and atomic gases in traps, the progress in this direction would have practical implications for the development of new approaches to the solution of the quantum many-body problem.

Instead of making an attempt to cover recent ideas in a systematic way, we show three examples - puzzles which emerge from numerical modeling of the nuclear many-body problem in restricted Hilbert space. In all three cases, the effect is very clear but its full understanding requires significant theoretical efforts and is not completed until now although below we give plausible explanations.

2 Applying exponential convergence

The dimensions of shell model spaces increase dramatically with the number of single-particle orbitals included. This precludes the full shell model diagonalization in practically interesting regions of the nuclear chart. Even in the $fp$-shell one still awaits for the full calculation for all nuclei. On the other hand, such a full solution would provide too much unphysical information which is not observable and, moreover, unstable with respect to small varia-
tions of the interaction hamiltonian that is never known with high accuracy. In reality we are interested in the properties of relatively few individual states being satisfied with a statistical description for the rest of the spectrum. The average properties of excited states were studied in the shell model framework with the methods of statistical spectroscopy and, with direct diagonalization, in relation to quantum chaos for atoms and nuclei. One can expect that a reasonable truncation of the shell model space could be possible when the influence of the remaining part of the basis is accounted for in some average sense.

Let us consider a behavior of the energy eigenvalue for the ground, or one of low-lying, states, as a function of the matrix dimension used for the exact diagonalization in the process of the progressive truncation of the original huge shell model hamiltonian matrix. The generic picture is shown in Fig. 1, taken from. After the initial steep decline, the ground state energy of \(^{49}\text{Cr}\) monotonously descends to the exact value; the convergence is almost precisely exponential. This is just one of many available examples, both for the realistic shell model and for random Gaussian matrices. The property of
exponential convergence seems to be universal. The full analysis of validity can be performed for tridiagonal matrices with a smooth change of matrix elements along the diagonal.

The underlying physics is based on the saturation property of the energy dispersion of simple, but spin-isospin (JT) projected, basis states. The centroid $\bar{E}_k$ and the width $\sigma_k$ of the basis state $|k\rangle$ can be found prior to the diagonalization in terms of the matrix elements of the shell model hamiltonian:

$$\bar{E}_k = H_{kk}, \quad \sigma_k^2 = \sum_{k \neq l} H_{kl}^2.$$ (1)

The widths $\sigma_k$ are nearly constant for all states of a given JT-class, essentially because of the geometric chaoticity of angular momenta coupling of individual particles. This justifies the recipe of statistical spectroscopy dealing with the centroid $\bar{E}$ and average width $\bar{\sigma}$ of each shell model partition. Expanding states $|k\rangle$ in the eigenbasis $|\alpha\rangle$ of the hamiltonian, $|k\rangle = \sum_{\alpha} C_{\alpha k} |\alpha\rangle$, one can find the strength function $F_k(E) = \sum_{\alpha} C_{\alpha k}^2 \delta(E - E_{\alpha})$ which also reveals the saturation property as a function of $\bar{E}_k$. The generic shape of the strength function evolves, with the interaction strength increasing, from the standard Breit-Wigner to the Gaussian one. Among various consequences of this evolution, one can mention the narrowing of the widths of multiple giant resonances, $\Gamma_n \to \sqrt{n} \Gamma_1$. In the strong coupling limit, the spreading width stabilizes on the level of $\Gamma \approx 2\bar{\sigma}$. The strength fragmented to the states at an energy distance $> \bar{\Gamma}$ should become less and less important. Earlier we have suggested the truncation scheme based on this idea. Now we can complement this with the exponential extrapolation to the exact shell model result.

The detailed shell model analysis has established that the tails of the strength function fall off almost pure exponentially as a function of the energy distance from the centroid. This phenomenon, which reminds the exponential localization of electronic coordinate wave functions in disordered solids, is also related to the nonexponential decay of nonstationary states at the early time stage. Based on this result, we can assume that, in the inverted problem of the composition of the eigenstate $|\alpha\rangle$, the remote basis states $|k\rangle$ give exponentially small contributions. This is indeed seen in numerous examples.

A practical application of the exponential convergence was recently developed for the calculation of ground state energies of nuclei in the $fp$-shell. One starts with the usual partition of the shell model space and calculates the average quantities. The configurations are ordered according to their energy centroids $\bar{E}$ (this order might be very different from that in the particle-hole scheme). After that the diagonalization is performed with progressive inclusion of new partitions in their “natural” order. At an energy distance of $(3 - 4)\bar{\sigma}$
from the original centroid, the exponential regime sets in for low-lying states, see Fig. 1, so that extrapolating the energy dependence on the truncated dimension \( n \) as \( E(n) = C + B \exp(-\gamma n) \), we can go to the limit of \( n = N \), the full space dimension.

Using the FPD6 interaction, we calculated in this way ground state energies, spins and isospins for all the lowest \(|\Delta(N - Z)|\) nuclides from \(^{42}\text{Ca}\) to \(^{56}\text{Ni}\). Spins and isospins are reproduced correctly, except for the case of \(^{45}\text{Ti}\) where the three levels with \( J = 3/2, 5/2 \) and \( 7/2 \) are within 100 keV both in the experiment and in our calculation. As usual for such calculations, the shell model energies (relative to the \(^{40}\text{Ca}\)) require Coulomb corrections and additional monopole corrections taking into account the smooth evolution of the mean field with the valence particle number. These corrections lead to the energy shift without changing the wave functions. The resulting mean square deviation of ground state energies from the data is 0.27 MeV. One can conclude that the exponential convergence method is a powerful tool to be used in the shell model framework for the cases when the full calculation is not feasible. The next step in this direction should extend the method to the calculation of observables and transition probabilities.

3 Apparently ordered spectra from random interactions

The second puzzle was formulated in the paper that triggered an extensive theoretical discussion. Consider a finite shell-model space with a rotationally (or/and isospin) invariant two-body interaction. The interaction is fully characterized by a set of parameters \( V_{L,I}(j_1j_2; j_3j_4) \) corresponding to the scattering \((j_3, j_4) \leftrightarrow (j_1, j_2)\) of the fermion pair in the channel with total spin \( L \) and isospin \( I \) conserved in the process. Let us randomly select these entries from a matrix ensemble which is more or less arbitrary but hermitian, real and symmetric with respect to the sign of the matrix elements \( V_{LI} \). If, for simplicity, the single-particle energies are kept degenerate, what will be the distribution function of the quantum numbers of total spin \( J \) and isospin \( T \) of the many-body ground state generated by this ensemble?

(i) The first idea coming to our mind is that any \( JT \)-set has a chance to have the lowest energy so that the resulting probability is merely determined by the number of available levels with given \( J \) and \( T \) in the Hilbert space. For example, for one kind of particles, according to a traditional consideration of the Fermi-gas level density, the total number \( \mathcal{N}(J) \) of levels with given \( J \) can be estimated as \( \mathcal{N}_{\text{stat}}(J) \propto (2J + 1) \exp[-J(J + 1)/\Theta] \) where \( \Theta \) is related to the statistical moment inertia determined by the average value of \( m^2 \), the squared single-particle angular momentum projection, in the available space.
Figure 2: Fraction $f_J$ of ground states with spin $J$ in the uniform ensemble of random two-body interactions for $N = 6$ particles on the level $j = 15/2$; dashed line shows statistical multiplicities.

The maximum of the statistical distribution corresponds to $2J + 1 = (2\Theta)^{1/2}$.

However, this idea turns out to be wrong. As shown in Ref. and confirmed by many authors, the ground state spin is predominantly (typically with probability exceeding 50%) $J_0 = 0$, although the fraction of states of spin $J = 0$ is usually quite low. The existence of the effect is very robust and insensitive to the peculiarities of the ensemble. Its magnitude depends on the choice of the ensemble and can exceed 90%. The preponderance of $J_0 = 0$ was found also in interacting boson models. In many cases the fraction of the ground states with maximum possible spin, $J_0 = J_m$, is also enhanced (the statistical fraction of such states is very low; in a single-$j$ model, Fig. 2, the state with $J = J_m$ is unique). We know that all even-even nuclei have $J_0 = 0$. Is this fact originated from pairing forces as suggested by the classics of the field, or will the same pattern appear with nearly any physically allowed interaction?

(ii) Statistical spectroscopy teaches us to characterize the general features of the spectra by the lowest moments of the hamiltonian (centroid, width
and so on). Comparing the statistical widths $\sigma(J)$ of the subclasses with various values of spin $J$, we may expect that if a class of states with given $J$ reveals the largest width (even if the deep reason of that is still unclear) the states of this class will be most probably the ground states of the system. However, for a majority of ensembles, this conjecture fails. Fig. 3 shows the widths $\sigma_J$ in the single-$j$-level space for the ensemble of matrix elements $V_L, L = 0, 2, ..., 2j - 1$, uniformly distributed between $-1$ and $+1$ (a system of 6 identical particles). Although the ensemble leads to the dominance of $J_0 = 0$, the statistical width $\sigma_{J=0}$ is not maximum; in some cases even $\sigma_2 > \sigma_0$. Moreover, to get a significant excess of the ground state probability, the corresponding width should be considerably greater than others which almost never happens.

If the level density at energy $E$ for spin $J$ is $\rho_J(E)$, the probability of finding a state of spin $J$ as a ground state can be formally defined as

$$f_J = \int_{-\infty}^{\infty} dE \left[ -\frac{d}{dE} \chi_J(E) \right] \prod_{J' \neq J} \chi_{J'}(E), \quad (2)$$
where, in terms of the level densities normalized to 1, \( g_J(E) = \rho_J(E)/N_J \),

\[
\chi_J(E) = \left( \int_E^\infty dE' g_J(E') \right)^{N_J}.
\]

For uncorrelated densities \( \rho_J \), eq. (3) indeed prefers the class of states with the greatest width. However, this conclusion is not valid since the densities are strongly correlated being determined by the same interaction matrix elements. The task of calculating the many-point correlation function of level densities is very hard.

(iii) Another alluring idea is that the dominance of \( J_0 = 0 \) is related to the time-reversal invariant character of the random hamiltonian. If so, the output could be different for a rotationally invariant, hermitian but complex hamiltonian. Physically this can be associated with the fact that the presence of \( J_z \neq 0 \) acts as if time-reversal symmetry were broken by selecting a sense of rotation; the corresponding quasi-Goldstone mode would be rotation restoring symmetry by the transformation to another projection \( J_z \). This idea in the simplest form (introducing an imaginary part of the random matrix element \( V_L \)) does not work because the ensemble average eliminates all imaginary terms along with the odd powers of \( V_L \). Still, the idea is promising if associated with the spontaneous symmetry breaking which can be accomplished by the consideration of the body-fixed frame, see below.

(iv) In the first paper on the subject, see also, it was suggested that usual pairing correlations and the phonon collectivity emerge somehow from the random forces. This statement is correct in a limited sense. Indeed, each realization of the two-body hamiltonian in a many-level shell model space generates its own mean field. Then it is possible to construct the superposition of the particle-hole operators of a given multipolarity (a generalized phonon) which would maximize the coherence and give an enhanced transition probability. In a similar way one can look for the specially selected generalized seniority operator to enhance the pair transfer processes. Those operators are different in different copies of the ensemble. A comparison with a standard paired state shows that its overlap with the ground states of random interactions is quite small, both in a single \( j \)-case and in a realistic shell model. The phonon collectivity with a fixed multipole operator is also absent.

(v) Currently the only plausible explanation of the preference of \( J_0 = 0 \) ground states in randomly interacting systems is based on the idea of geometric chaoticity. With a random interaction we do not expect any specific shape of the mean field to be singled out. The wave functions are very complicated combinations of shell model basis states. Therefore a statistical approach seems to be suitable which looks for the single-particle density matrix.
with maximum entropy under constraints of fixed particle number $N$ and total spin (isospin). In a single $j$-model, the density matrix is diagonal for the aligned state with the total projection $M = J$ (analog of the body-fixed frame). Its eigenvalues give the single-particle occupation numbers $n_m = [\exp(\gamma m - \mu) + 1]^{-1}$, where the Lagrange multipliers of chemical potential $\mu$ and cranking frequency $\gamma$ fix the average values of $N$ and $M$. The expectation value of the total hamiltonian calculated with such occupation numbers gives the simple approximation for the average yrast line. Depending on the sign of the effective moment of inertia for the given set of $V_L$, this leads to $J_0 = 0$ or $J_0 = J_m$, a normal or inverted band, respectively. Thus we come to a trivial geometric mechanism of the preference for the edge values of the ground state spin. With some improvements, one can reproduce average empirical results.

The energy values estimated with this statistical approach correlate well with the exact numerical values although there is a small systematic discrepancy in the probability $f_J$ for small $J$ (the agreement is almost perfect for high $J$ including $J_m$). One source of the deviation is in the approximation of the expectation value $\langle \hat{n}_m \hat{n}_{m'} \rangle$ by the product of two statistical average values $n_m n_{m'}$. In a given wave function the presence of the mean field makes the occupancies slightly dynamically correlated. Apart from that, there is indeed some coherence generated apparently by the off-diagonal matrix elements of the interaction in higher (even) orders. This brings in a small excess of the overlap of the “random” ground state with the paired one compared to a pure statistical (in the sense of the random matrix theory) estimate. By the same reason, the percentage $f_0$ of the ground states with $J_0 = 0$ increases when going from the single-$j$ case to a more realistic shell model scheme, especially to the set of many spin $1/2$ levels, when the role of the off-diagonal pair transfer elements is the most important. This can be seen also in the fact of the overwhelming percentage of the lowest isospin in the ground states. Another example is given by the specific ensemble which includes only random pairing matrix elements; the sign-independent effect of the off-diagonal pair transfers leads to the percentage $f_0 > 90\%$.

Such dynamical effects are still not fully understood albeit they may be the most interesting and essential for many-body physics in finite quantum systems. The ideas of solving exactly the coherent parts of the interaction (for example, pairing) and accounting in a statistical spirit for incoherent collision-like processes are in the air promising a new interesting development in the near future.
Figure 4: Dynamics of complex energies $E - (1/2)\Gamma$ for a system of 3 fermions on 8 equidistant orbitals interacting via random interaction; the upper orbital has a single-particle width $\gamma$, and the resonances move as $\gamma$ increases.

4 Approaching the continuum

The third puzzle comes from an attempt to generalize the shell-model approach for loosely bound or unbound nuclei where the entire dynamics take place on the edge of or already within the continuum. A progress in this direction is essential both for nuclear physics far from stability and for astrophysics. Since the various versions of the shell model with the discrete spectrum work exceedingly well for stable nuclei, it is tempting to consider a realistic mean field where some single-particle orbitals are resonances in the continuum and include the residual interaction in order to obtain the observable positions and widths of the many-body states.

One example of what happens in such a problem is given by Fig. 4. We assume that the single-particle levels $\epsilon_{\nu}$ have some decay width; for simplicity we attribute here a significant width to one upper level shifting its energy to the complex plane, $\epsilon \to \epsilon - (i/2)\gamma$. Let us switch on a two-body interaction with real random matrix elements $V$ (here we do not observe any conservation laws so that all pairs of orbitals are mutually coupled) and find the eigenvalues of the many-body system. Fig. 4 corresponds to the case of 3 particles on 8 equidistant orbitals; the trajectories of the complex energies $\mathcal{E} = E - (i/2)\Gamma$
are shown as functions of increasing instability $\gamma$ of the upper orbital. Instead of complete chaos, we see a more and more regular pattern as $\gamma$ increases. Interestingly enough, 21 energies move almost parallel to each other into the complex plane whereas 35 states have a very small width.

It is easy to understand this dynamics of complex energies (or poles of the scattering matrix). The total number of many-body states in this truncated space is $8!/3!4! = 56$. In the limit of large $\gamma$, any state which has the upper orbital filled, even with a low probability, will decay very fast. The number of such states corresponds to a number of combinations of the remaining particles within the rest of space, $7!/2!5! = 21$. The increasing original decay width is distributed over the many-body states, since the imaginary part of the trace of the hamiltonian is preserved. As $\gamma$ grows, the “self-organization” occurs: fast and slow decaying states are separated in time. In a reaction populating the system, one would see two distinct time scales, corresponding to direct and compound processes. Thus, coupling to the continuum can bring order in a system governed by a random hamiltonian.

The physics we are looking at here was extensively discussed earlier from a different viewpoint. In that approach one starts with the set of many-body states $|\alpha\rangle$ formed by a normal hermitian interaction hamiltonian $H$. The coupling to the continuum is given by the antihermitian part of the effective energy-dependent hamiltonian,

$$W_{\alpha\beta} = \sum_c A_c^\alpha A_c^{\beta*}.$$  

Here the sum runs over all decay channels $c$ that are open at a given energy, and $A_c^\alpha$ is the decay vertex of an intrinsic state $|\alpha\rangle$ into a channel $c$. The factorizable form of eq. (4) comes from the on-shell contribution of the effective propagator for intrinsic states coupled through the continuum and unitarity requirements. The complex eigenvalues of the total effective hamiltonian $\mathcal{H} = H - (i/2)W$ give the resonance energies. In the weak continuum coupling regime, $W$ is a perturbation providing narrow resonance widths. As this coupling becomes strong, a phase transition occurs to the overlap regime with Ericson fluctuations of cross sections and separation of the time scales. A number of states (equal to the number of open channels) gives rise to broad short-lived resonances absorbing the lion’s share of the total width while the remaining compound states become long-lived and reveal internal thermalization and equilibration. This phenomenon, being an analog of the Dicke superradiance in optics, has interesting applications to physics of giant resonances.

In the example above, strictly speaking, all many-body states are nonsta-
tonary. In reality there exists a set of threshold energies $E^{(c)}$ determined by the $Q$-values of a reaction in channel $c$. The amplitudes $A_{\alpha}^{c}$ depend on running energy $E$ and have a branching point at threshold $E^{(c)}$ for example in the case of decay into an $s$-wave in the continuum, $A_{\alpha}^{c} \propto (E - E^{(c)})^{1/2}$. Therefore, in principle, the hybrid approach combining the shell model with the effective nonhermitian hamiltonian allows for a self-consistent calculation of discrete levels, resonances and reaction cross sections. Being technically very difficult, this problem is of vital importance for physics of weakly bound nuclei. Far away of thresholds, the method of a nonhermitian hamiltonian was used for the microscopic derivation and analysis of the kinetics of resonance population and decay. Two phenomena, the loss of the collective strength, and the restoration of isospin purity at high excitation energy naturally follow from this consideration.

5 Conclusion

Three “puzzles” briefly discussed above show significant gaps in current theory of nuclear structure and reactions. The blunt diagonalization of huge shell-model matrices cannot be an optimal way of solving the nuclear many-body problem. Even randomly taken but geometrically correct interactions generate some features of observed regular spectra. The presence of continuum aligns the intrinsic states along the new “axis” related to their ability to decay. Those are just particular examples of new avenues which should be actively studied.

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