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GRASSMANN INTEGRATION IN STOCHASTIC QUANTUM PHYSICS: THE CASE OF COMPOUND–NUCLEUS SCATTERING

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Abstract:

Using a stochastic model for N compound–nucleus resonances coupled to the channels, we calculate in the limit $N \to \infty$ the ensemble average of the S-matrix (the "one-point function"), and of the product of an S-matrix element with the complex conjugate of another, both taken at different energies (the "two-point function"). Using a generating function involving both commuting and anticommuting integration variables, we evaluate the ensemble averages trivially. The problem of carrying out the remaining integrations is solved with the help of the Hubbard–Stratonovitch transformation. We put special emphasis on the convergence properties of this transformation, and on the underlying symmetries of the stochastic model for the compound nucleus. These two features together completely define the parametrization of the composite variables in terms of a group of transformations. This group is compact in the "Fermion–Fermion block" and non-compact in the "Boson–Boson block". The limit $N \to \infty$ is taken with the help of the saddle-point approximation. After integration over the "massive modes", we show that the two-point function can be expressed in terms of the transmission coefficients. In this way we prove that the fluctuation properties of the nuclear S-matrix are the same over the entire spectrum of the random Hamiltonian describing the compound nucleus. The integration over the saddle-point manifold is carried out using symmetry properties of the random Hamiltonian. We finally obtain a closed-form expression for the two-point function in terms of a threefold integral over real variables. This expression can be easily evaluated numerically.

1. Introduction and overview

Random Hamiltonians are widely used in theoretical physics for the modelling of statistical phenomena. The implementation of such concepts often poses serious problems, however, because observables usually depend in a highly non-linear fashion on the random Hamiltonian, this making the calculation of ensemble averages very difficult. In the present paper, we present the exact (non-perturbative) solution to a long-standing problem in the statistical theory of nuclear reactions, which dates back to Niels Bohr's model of the compound nucleus. This problem, too, has been formulated in terms of a random Hamiltonian. The solution is here obtained by combining the use of a generating function with the method of integration over anticommuting or Grassmann variables. There are other problems in statistical nuclear theory which have previously been solved exactly. We recall the celebrated results of Dyson and Mehta on spectral fluctuation properties [1]. The method of solution presented in this paper differs from earlier approaches in that we use methods which are widely applied in statistical physics and elsewhere. Our solution will therefore be of interest beyond the confines of nuclear physics, and it may serve as a case study in stochastic quantum physics. We believe that two issues in particular deserve general interest. One issue relates to the parametrization of the composite variables. After taking the ensemble average of the two-point function, we introduce these variables via the Hubbard–Stratonovitch transformation in the usual fashion. In the context of the replica trick, where one proceeds similarly, the problem of how to parametrize the composite variables also arises. For ordinary (commuting) integration variables, this problem has been thoroughly discussed, and solved, by Schäfer and Wegner [2]. These authors demonstrated the necessity to parametrize the composite variables in terms of a non-compact group. We are not aware of an investigation of the same problem in the presence of both commuting and anticommuting integration variables, and we believe that our results relating to this point [3] are novel. The commuting composite variables form two classes. For one class (the "Boson–Boson block"), the arguments of Schäfer and Wegner prevail, and the parametrization must make use of a non-compact group. For the other class (the "Fermion–Fermion block") we show that it is mandatory in contradistinction to parametrize the variables in terms of a compact group. We are led to this conclusion using arguments of convergence and symmetry which are perfectly general and independent of the specific nuclear-physics problem which we solve. The second issue relates to the manner in which the exact solution is derived. It turns out that the nuclear-physics problem here investigated is comparatively simple: After introduction of the composite variables and integration over the "massive modes", the problem is mapped onto a non-linear σ-model of dimensionality zero. Nevertheless, the evaluation of the remaining 16 integrals is not trivial. It becomes possible only by tenaciously using the symmetry properties of the model. It is for this reason that we believe that also this second issue, and the methods used to calculate the answer, are of general interest and hopefully useful in another context. In writing the paper, we have therefore aimed at a compact but full account of all steps taken.

The problem which we consider concerns the calculation of average compound–nucleus cross sections. After early work by N. Bohr, Bethe and Weisskopf, and motivated by Wigner's idea of describing properties of highly excited nuclear levels in terms of a random Hamiltonian, various authors in the 1950's and 60's defined this problem in terms of an ensemble of random matrices coupled to a (fixed) number of channels [4]. The random matrices of dimension N (we here eventually take the limit $N\to\infty$) simulate the presence of N compound-nucleus resonances. Following Wigner, one usually chooses the ensemble as the Gaussian Orthogonal Ensemble (GOE). In spite of numerous efforts, this model could not be solved exactly, and only partial answers in terms of series expansions (valid when the number of open channels is either very small, or very large) have been obtained [4]. We only mention in passing that this model is of interest not only as a problem of theoretical physics but also in nuclear-science applications.

Using the GOE to simulate the stochastic properties of highly excited nuclear levels may seem pure phenomenology, and even arbitrary. Recent developments in the theory of non-integrable classical systems and their quantum counterparts suggest that this is not the case, and have greatly enhanced our enthusiasm for this work. Numerical studies of particularly simple classical chaotic systems, and of the distribution and fluctuation properties of the eigenvalues of their quantum counterparts, have shown [5] that these fluctuation properties coincide (within statistical accuracy) with those found experimentally in high-lying parts of nuclear spectra, and with those predicted by the GOE. This observation suggests that nuclear fluctuation properties are a universal feature of microscopic quantum systems: They should surface for any system in which a resolution of properties down to an energy scale given by the average level spacing is experimentally feasible, and they should hence be generic, expressing a property which in the analogous classical system would be identified as chaotic behaviour. The use of the GOE to simulate these fluctuation properties is not arbitrary. The GOE can be derived [6] from the assumption of minimal information content of the Hamiltonian (an assumption which intuitively relates to classical chaotic motion); fluctuation properties obtained from the GOE are statistically indistinguishable from those generated by related matrix ensembles [1]; and the GOE is much more suitable for analytical treatment than are these other ensembles. For these reasons, we believe that the GOE encapsulates a very essential aspect of the nuclear dynamics, which is complementary to the description of regular features and of average nuclear properties as furnished by the shell model, the collective model, and similar approaches based on a mean-field description. We use the GOE with confidence for the description of *fluctuation* properties although it is known to fail badly for the description of *average* properties like the average level density. We also believe that our results are generally valid and insensitive to specific details of the GOE. This belief is supported by a recent and yet unpublished comparison (suggesting complete agreement) which we have carried out between numerical results obtained in the framework of our approach, and those obtained by the Mexican group [7]. These latter authors derived the probability distribution function of the nuclear S-matrix elements directly from a maximum entropy principle for the S-matrix, avoiding the introduction of a Hamiltonian altogether. In this sense we feel that the problem studied in the present paper lies at the interface between the classical mechanics of non-integrable systems and their quantum counterparts (these systems furnish the justification for our model), the statistical mechanics of disordered systems (these systems furnish much of the theoretical framework which we use although the disorder studied there is usually of geometrical rather than inherently dynamical origin), and fluctuation properties of microscopic quantum systems.

It goes without saying that our method can also be used to calculate other statistical properties of nuclei than the compound–nucleus cross section studied here. We hope in fact that it will be used widely. The method clearly provides a unified description of the fluctuation properties of nuclear spectra, and of the stochastic aspects of nuclear reactions. It is more powerful than the replica trick which we used previously [8, 9, 10], the latter only being able to yield asymptotic expansions [3]. In this paper, we focus attention mainly on the two-point function which we evaluate in the limit $N \to \infty$. The same method (when applied to the one-point function) yields simple integral representations for every finite N. This may be of interest in some cases. The calculation of n-point functions for $n > 2$ in the framework of the present approach poses problems which seem to grow quickly with increasing n.

The main body of the paper involves fairly technical manipulations of sets of both commuting and anticommuting integration variables. Except for parts of appendix L, we have aimed at a presentation which is self-contained. We felt that this would be desirable especially for nuclear theorists who are largely unfamiliar with the techniques used here, but also for a wider group of readers since we are not aware of any sufficiently detailed work on the use of anticommuting integration variables. In order to cope with a fairly sizeable amount of mathematical detail, in order to make the main body of the paper easy reading for the experts, and in order to clearly display the main line of reasoning, we have relegated all technical details to a number of appendices.

The model for the nuclear S-matrix is defined in section 2. The generating function defined in terms of commuting and anticommuting variables is introduced in section 3; cf. also appendices A and B. The ensemble average is calculated in section 4 and appendix C. In the same section, we also introduce the Hubbard–Stratonovitch transformation. Questions of convergence of this transformation, of the symmetry of a fundamental quadratic form, and of the proper parametrization of the composite variables form the subject of the central section 5 and appendices D and E. The integration over "massive modes" (possible in the limit $N \to \infty$) is carried out in section 6 and appendix F. In appendix G we show that the unitarity of the S-matrix is preserved by the steps taken up to and including section 6. In section 7 and appendix H, we show that the average two-point function can be expressed in terms of the transmission coefficients. In section 8 and appendices I, K and L, we carry out the remaining 8 integrations over anticommuting variables, and 5 of the remaining 8 integrations over commuting variables, finally arriving at an integral representation for the two-point function in terms of a threefold integral which is easily evaluated numerically. Section 9 contains a summary, and our conclusions.

In dealing with anticommuting variables, we received much stimulation from a recent paper by Efetov [11]. Although pretending to be a review, this paper unfortunately contains so little detail that we found it of no help for our actual calculations. This situation furnished us with yet another motivation to write our paper in its present form.

2. The model

For fixed spin and parity, we consider a nuclear scattering problem involving compound-nucleus formation. The physical channels (denoted by small latin letters $a, b, c, \ldots$) are characterized, as usual, by the internal states of the two fragments, the channel spin, and the relative angular momentum. We denote by E the total energy of the system. The channel wave functions are called $|\chi_a(E)\rangle$, and we use the normalization that $\langle \chi_a(E_1)|\chi_b(E_2)\rangle = \delta_{ab}\,\delta(E_1 - E_2)$. The compound-nucleus resonances are caused by a large number $N \gg 1$ of bound states $|\mu\rangle$, $\mu = 1, \ldots, N$ with $\langle \mu|\nu\rangle = \delta_{\mu\nu}$. We shall later take the limit $N \to \infty$. In the space spanned by the functions $\{|\mu\rangle, |\chi_a(E)\rangle\}$, the model Hamiltonian $\mathcal{H}$ has the form