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Quantum versus Statistical Fluctuations in Mean-Field Theories

J. L. Egido
Departmento de Física Teórica, Universidad Autónoma, 28049 Madrid, Spain
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General, separate formulas are derived for the quantum and the statistical fluctuations of any operator. The formalism is applied to the study of these fluctuations for the particle-number as well as the angular-momentum operators in a realistic case.

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The finite-temperature mean-field theories (Bardeen-Cooper-Schriefer,[1] Hartree-Fock,[2] and Hartree-Fock-Bogoliubov[3]) have become a common tool in many branches of physics. The success of mean-field theories is based, to some extent, on the breaking of symmetries which allows a considerable enlargement of the variational Hilbert space so as to include the appropriate correlations. The breaking of the particle-number symmetry in the BCS theory and of the rotational invariant in deformed nuclei are two well-known examples. The symmetry breaking is usually related to phase transitions, superfluid to normal fluid in the particle-number case, and spherical to deformed shape in the angular momentum one.

The use of symmetry-breaking wave functions induces (quantum) fluctuations (QF) in the related operators. At finite temperature, because of the thermal averaging, there are (statistical) fluctuations (SF) associated with any operator. In general, both of these will be present, and I shall call them total fluctuations (TF). Imagine a temperature-induced superfluid–normal-fluid phase transition which is being investigated in the BCS approximation. At zero temperature, the particle-number fluctuations are of quantum origin; at temperatures T below the critical temperature T_c, we shall have quantum as well as statistical fluctuations; at temperatures T larger than T_c only statistical fluctuations remain.

In some situations one has to go beyond the mean-field approach, in a phase transition, for example. Normally, one[4] *assumes* that, at the temperature that the phase transition takes place, the statistical fluctuations are the most important. Therefore, the corrections[4] that one applies to the mean-field theory are purely statistical. This assumption has, however, no well-founded reason since there are no calculations that justify it; i.e., some kind of evaluation is needed. Also, for the comparison of the theoretical results with the experiments, it is important to know the roles of both kinds of fluctuations. The aim of this Letter is to propose general formulas for the quantum and the statistical fluctuations of any operator in mean-field theories.

Our starting point[5] is the finite-temperature Hartree-Fock-Bogoliubov equation

$$[\mathcal{H}(\mathcal{R}^0),\mathcal{R}^0]=0\,, \tag{1}$$

where $\mathcal{H}$ and $\mathcal{R}$ are the Hartree-Fock-Bogoliubov approximation to the Hamiltonian H and the density matrix, respectively, i.e.,

$$\mathcal{H}=\begin{bmatrix}\langle\{[a_m,H],a_n^\dagger\}\rangle_T & \langle\{[a_m,H],a_n\}\rangle_T\\ \langle\{[a_m^\dagger,H],a_n^\dagger\}\rangle_T & \langle\{[a_m,H],a_n\}\rangle_T\end{bmatrix},\quad \mathcal{R}=\begin{bmatrix}\langle a_n^\dagger a_m\rangle_T & \langle a_n a_m\rangle_T\\ \langle a_n^\dagger a_m^\dagger\rangle_T & \langle a_n a_m^\dagger\rangle_T\end{bmatrix}, \tag{2}$$

where the subscript T means, as usual, the thermal average expectation value and the a_m are arbitrary quasiparticle operators. In the self-consistent basis determined by Eq. (1), which I shall continue denoting by $(a_m,a_m^\dagger)$, $\mathcal{H}$ and $\mathcal{R}$ are both diagonal with matrix elements $(E_m,-E_m)$ and $(f_m,1-f_m)$, respectively. E_m are the quasiparticles energies and

f_m the quasiparticle occupation factors. In this basis, a one-body Hermitean operator can be written as

$$F=F^0+\sum_m F^{11}_{mm}\alpha^\dagger_m\alpha_m+\sum_{(m,n)}[F^{11}_{mn}\alpha^\dagger_m\alpha_n+F^{20}_{mn}\alpha^\dagger_m\alpha^\dagger_n+\text{H.c.}]\,, \tag{3}$$

where (m,n) means sum over ordered pairs, i.e., $(m,n$ with $m<n)$. The total fluctuations associated with this operator are defined by

$$\Delta F^2=\langle F^2\rangle_T-\langle F\rangle_T^2\,. \tag{4}$$

This expression can be easily evaluated by means of the generalized Wick theorem; one obtains

$$\Delta F^2=\tfrac{1}{2}\sum_{m,n}\{|F^{11}_{mn}|^2(f_m+f_n-2f_mf_n)+|F^{20}_{mn}|^2[1-(f_m+f_n-2f_mf_n)]\}\,. \tag{5}$$

In the last expression for the total fluctuations, one cannot disentangle which part corresponds to the QF and which to the SF in the sense mentioned above.

In order to obtain some insight into the meaning of the different contributions to the total fluctuations, an expression shall now be worked out whose terms do have a physical interpretation. Since all the calculations can be expressed in terms of the density matrix, Eq. (2), we shall find it convenient to work with pairs of fermions. These possible pairs are $(\alpha_m\alpha_n)$, $(\alpha^\dagger_m\alpha_n)$, with $m<n$, and their Hermitean conjugates; ordering of the states by growing energy $E_m\le E_{m+1}$ guarantees that the pairs $(\alpha^\dagger_m\alpha_n)^\dagger$ correspond to excitations of positive energy. To evaluate the fluctuations, one has to calculate $\langle F^2\rangle_T$ and $\langle F\rangle_T^2$. If we take into account that the density matrix is diagonal, the generalized Wick theorem guarantees that the only nonzero expectation values are those with an even number of creator and annihilation operators, i.e.,

$$\langle F\rangle_T=F^0+\sum_m F^{11}_{mm}f_m\,, \tag{6}$$

$$\begin{aligned}\langle F^2\rangle_T=&F^{0^2}+2F^0\sum_m F^{11}_{mm}f_m+\sum_{k,m}F^{11}_{kk}F^{11}_{mm}\langle(\alpha^\dagger_k\alpha_k)(\alpha^\dagger_m\alpha_m)\rangle_T\\&+\sum_{(k,l)(m,n)}\{F^{11}_{kl}F^{11}_{nm}\langle(\alpha^\dagger_k\alpha_l)(\alpha^\dagger_m\alpha_n)^\dagger\rangle_T+F^{11}_{lk}F^{11}_{mn}\langle(\alpha^\dagger_k\alpha_l)^\dagger(\alpha^\dagger_m\alpha_m)\rangle_T\\&+F^{20}_{kl}F^{20*}_{mn}\langle(\alpha^\dagger_k\alpha^\dagger_l)(\alpha_n\alpha_m)\rangle_T+F^{20*}_{kl}F^{20}_{mn}\langle(\alpha_l\alpha_k)(\alpha^\dagger_m\alpha^\dagger_n)\rangle_T\}\,.\end{aligned} \tag{7}$$

Because of the sum on ordered pairs, only one contraction is nonzero in the last four terms whereas in the third term on the right-hand side there is one additional contraction; i.e., one can write

$$\sum_{k,m}F^{11}_{kk}F^{11}_{mm}\langle(\alpha^\dagger_k\alpha_k)(\alpha^\dagger_m\alpha_m)\rangle_T=\Big(\sum_k F^{11}_{kk}f_k\Big)^2+\sum_{k,m}{}'F^{11}_{kk}F^{11}_{mm}\langle(\alpha^\dagger_k\alpha_k)(\alpha^\dagger_m\alpha_m)\rangle_T\,. \tag{8}$$

The prime on the sum is just to indicate that the contraction inside one pair has been extracted; in this way all pairs are treated on an equal footing. From the four factors enclosed in the curly brackets in Eq. (7), the first and fourth terms can be related to the second and third terms just by commuting the pairs. Taking into account these two considerations in Eq. (7), one obtains from Eq. (4)

$$\begin{aligned}\Delta F^2=&\sum_{(k,l)(m,n)}\{F^{11}_{kl}F^{11}_{nm}\langle[(\alpha^\dagger_k\alpha_l),(\alpha^\dagger_m\alpha_n)^\dagger]\rangle_T+F^{20*}_{kl}F^{20}_{mn}\langle[(\alpha_l\alpha_k),(\alpha^\dagger_m\alpha^\dagger_n)]\rangle_T\}\\&+2\sum_{(k,l)(m,n)}\{F^{11}_{lk}F^{11}_{mn}\langle(\alpha^\dagger_k\alpha_l)^\dagger(\alpha^\dagger_m\alpha_n)\rangle_T+F^{20}_{kl}F^{20*}_{mn}\langle(\alpha^\dagger_k\alpha^\dagger_l)(\alpha_n\alpha_m)\rangle_T\}\\&+\sum_{k,m}{}'F^{11}_{kk}F^{11}_{mm}\langle(\alpha^\dagger_k\alpha_k)(\alpha^\dagger_m\alpha_m)\rangle_T\,.\end{aligned} \tag{9}$$

The first two terms of this expression are identified with the quantum fluctuations ΔF_Q^2, and the last three with the statistical fluctuations ΔF_S^2. The evaluation of the expectation values leads finally to

$$\Delta F_Q^2=\sum_{(m,n)}[|F^{11}_{mn}|^2(f_m-f_n)+|F^{20}_{mn}|^2(1-f_m-f_n)]\,, \tag{10}$$

$$\Delta F_S^2=\sum_m|F^{11}_{mm}|^2f_m(1-f_m)+2\sum_{(m,n)}[|F^{11}_{mn}|^2f_n(1-f_m)+|F^{20}_{mn}|^2f_mf_n]\,. \tag{11}$$

The reasons for these identifications are the following: (1) The processes taking place in the SF [see the last three terms of Eq. (9)] are the thermal average of the dispersion of pairs with energy $E\le 0$. (2) In the high-temperature limit, $T\to\infty$ and $f_n=0.5$, the QF vanish as they are supposed to do. (3) In the zero-temperature limit, $f_n\to 0$, the SF go to zero and the QF to $\sum_{(m,n)}|F^{20}_{mn}|^2$ as one expects. (4) In the case that a given symmetry (for example, the particle number) is conserved in the mean-field approximation, and the density matrix is invariant to rotations in the associated gauge space, i.e.,

$$\bar{\mathcal{R}} = e^{i\alpha F}\mathcal{R}\, e^{-i\alpha F} = \mathcal{R}\,. \qquad (12)$$

Obviously, this is also true for an infinitesimal rotation where $\bar{\mathcal{R}}$ can be expanded. To first order in α, one obtains

$$\bar{\mathcal{R}} \approx \mathcal{R} + i\alpha[F,\mathcal{R}] = \mathcal{R} \Longrightarrow (f_m - f_n)F^{11}_{mn} = (1 - f_m - f_n)F^{20}_{mn} = 0\,. \qquad (13)$$

Condition (13) guarantees [see Eq. (10)], that the QF of the operator associated with the conserved symmetry are zero. In the same way in a phase transition, from a superfluid to a normal fluid, for example, the QF of the particle-number operator will vanish after the transition has taken place.

To illustrate the formulas, I shall study the behavior of the fluctuations of some operators for the nucleus ^{164}Er at high excitation energy and angular momenta. For deformed superfluid nuclei, one finds, in mean-field theories, a phase transition to normal fluid induced by two parameters, the temperature (excitation energy), and the angular frequency (angular momentum). The finite-temperature Hartree-Fock-Bogoliubov equations were solved with the configuration space and Hamiltonian of Baranger and Kumar.[6] The results for deformation parameters, gaps, and other quantities are given in Ref. 7; in particular, one finds that for temperatures $T \geq 0.5$ MeV (≥ 0.6 MeV) the gap of the neutrons (protons) vanishes for high angular momenta even at lower temperatures. For temperatures smaller than 1 MeV, investigated in Ref. 7, one does not find any shape transition.

In Fig. 1 the QF are shown for the particle-number operators for neutrons and protons as a function of the angular frequency ω for different temperatures. One sees a structure strongly correlated with the behavior (see Ref. 7) of the gap parameters at the given temperatures and angular frequencies. As expected, they go to zero when the gap parameter (the cause for the base states not being eigenstates of the number operator) vanishes. In Fig. 2 the total particle-number fluctuations are shown in a display similar to Fig. 1. At zero temperature, they are exactly the same as in Fig. 1, since there are no SF. At $T = 0.2$ MeV and small ω values, we find almost no difference between the total and the quantum fluctuations; i.e., the SF are very small, for medium angular frequencies (still $T = 0.2$ MeV) the TF are larger than the QF, and for high frequencies the TF are rather constant. What is observed here is that the SF are ω dependent as long as the QF are not zero. The reason for this is the ω dependence of the gap parameter. A large gap causes large quasiparticle energies and therefore small quasiparticle occupation factors f_m. The pairing correlations which induce the QF inhibit the SF! At $T = 0.4$ MeV and small ω values, the TF are already larger than the QF; the structure they show is just caused by the latter. For T values 0.6, 0.8, and 1.0 MeV, the TF are flat and parallel to each other as one

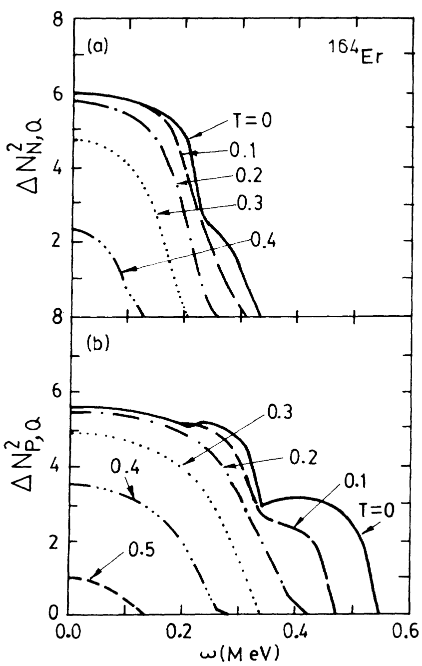

FIG. 1. The quantum fluctuations of the particle-number operators for neutrons (upper part) and protons (lower part).

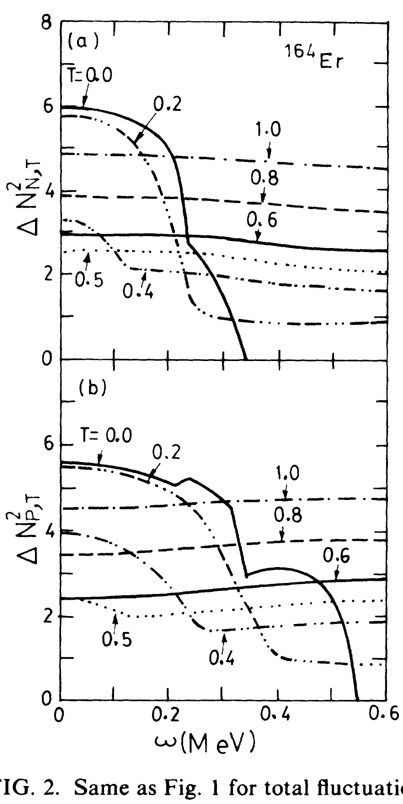

FIG. 2. Same as Fig. 1 for total fluctuations.

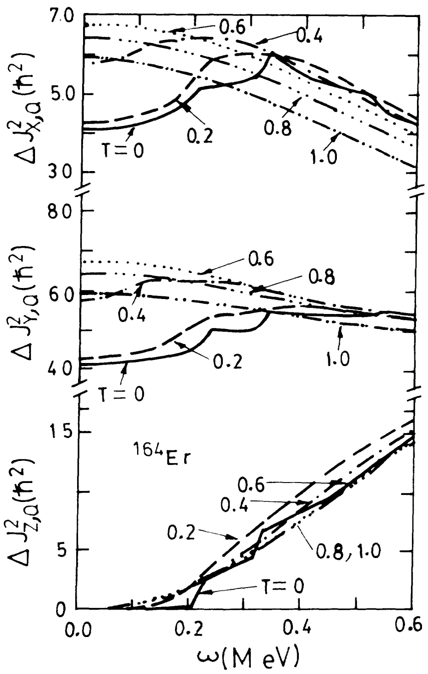

FIG. 3. The quantum fluctuations for the angular-momentum components.

would expect for SF.

To illustrate the behavior of the fluctuations for an operator not related to a phase transition, at least in the temperature range we are looking at, in the next two figures the fluctuations of the angular momentum are shown. Figure 3 displays the QF of the $J_x J_y$, and J_z operators. The fluctuations in J_x and J_y are similar in magnitude because the nucleus remains,[7] for all T and ω values, approximately axially symmetric; this is also the reason why $\Delta J^2_{z,Q}$ is that small. It is interesting to observe that the QF in J_z are zero at $\omega = 0$ for all temperatures: The reason is that the mean-field approach for the Hamiltonian, at this ω value, commutes with J_z. At higher angular frequencies, when we work with the Hamiltonian $H' = H - \omega J_x$, this is not the case anymore.

For small ω values and $T \geq 0.4$ MeV, an increase in the QF of J_x and J_y is observed; this is due to an increase of the deformation parameter caused by the quenching of the pairing correlations by the temperature. The structure at $T = 0$ in all the three cases is produced by the alignment of particles during the cranking. At higher temperature, when the shell effects are less important, rather smooth curves are obtained. The general increase of the J_z fluctuation with ω is due to the fact that the nucleus becomes somewhat triaxial. The general decline of the QF for $T > 0.8$ MeV is due to a decrease of the total deformation for those temperatures. In Fig. 4 the total fluctuations for the same three operators are shown. We see that in this case of no phase transition, the TF always grow with increasing temperature. We also notice that the relative increase in the TF with respect to the QF is much larger for the J_z operator than for the J_x and J_y operators; this is due to the fact that the QF in the case of the J_z operator were inhibited by the approximately conserved axial symmetry.

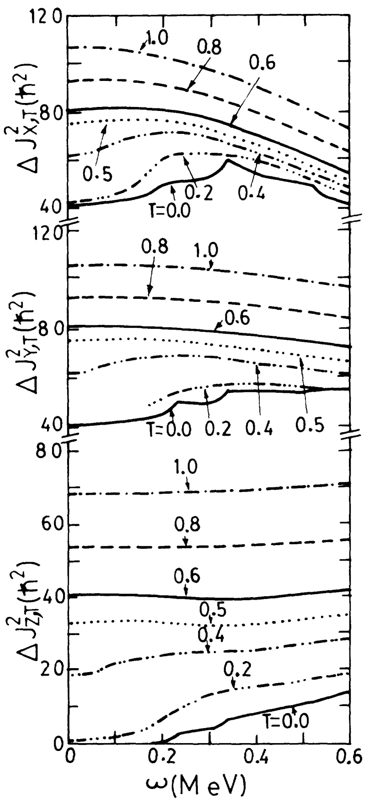

FIG. 4. Same as Fig. 3 for the total fluctuations.

In conclusion, I have derived formulas for the quantum as well as the statistical fluctuations of a system described by a finite-temperature mean-field theory. The formulas have been applied to investigate the fluctuations of the particle-number and the angular-momentum operators for a well-deformed superfluid nucleus.

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