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Physik-Department der Technischen Universität München

H. HOFMANN, R. SOLLACHER

Fluctuations in Nuclear Collective Dynamics

Fluktuacje w kolektywnej dynamice jądrowej

Флуктуации в коллективной ядерной динамике

1) THE GOAL

In nuclear physics collective motion plays an important role. The word "collective" implies the participation of many nucleons in a dynamical process. Hence, in many cases this word is synonimous for "macroscopic". The latter is associated mostly with the notion of classical physics or, at least, with the concept of average motion. However, in many or most examples of nuclear physics, fluctuations around such averages cannot be neglected.

These fluctuations may be entirely quantal. As one of the most exciting cases let us mention ground state fission [1], a process which is not possible within classical physics and where a description in terms of an average motion becomes meaningless.

But in nuclear physics we may have the other extreme of fluctuations becoming entirely statistical. This will be true for high excitations and slow collective processes for which an intrinsic temperature T can be defined. If this T may be considered large compared to the typical collective excitations we are in the regime of classical statistical mechanics, albeit not the one of complete equilibrium. It was no one less than Kramers who pointed out in 1940 already how the dynamics of fission can be described in such a picture.

Thus the problem is set: In nuclear physics we need to understand to describe collective motion including both quantal and statistical aspects. Clearly this has to be non-equilibrium quantum statistical mechanics! But what a tremendous problem: we all know of the high non linearity of nuclear dynamics. The main reason for that can be traced back to the mean field evolving coherently with the collective degrees of freedom; as a first approximation we must describe the nucleon's dynamics with the help of an average potential. To come back to the example of fission one more time: for the mother nucleus this average potential will be very different from the one describing the nascent fragments around the scission region.

How can we handle this problem? Well, TDHF is one answer. But besides the fact that it does not lead to an easy and adequate treatment of fluctuations, it does not account properly for residual interactions (as well as the inclusion of irreversible mechanisms). But such residual interactions are present for the examples to be studied, and the extended version of TDHF just becomes too complicated.

In the last few years there was another suggestion to tackle the task. It bases on the early suggestion of refs. [3] and [4] to apply linear response theory locally. There, one describes large scale collective dynamics in a locally harmonic approximation. In its most general version one may do this by applying successively propagators in phase space. These propagators are valid over a small time interval δt and in a small region of phase-space. Of course, the size of the latter is related to the length of δt through the (local) dynamics. But for this δt there must be a lower limit: it cannot be smaller than the time τ which we must allow to elapse if we want to avoid an <u>explicit</u> description of the intrinsic excitations. This τ is related to a relaxation time for the intrinsic degrees of freedom. We may note that for $\tau = 0$ the description of the dynamics in terms of propagators could be made identical to the path integral formulation. And it would only be in this case that this picture would <u>ensure</u> a complete quantal description. But for finite τ it may still amount to a semiclassical version. (For a somewhat more detailed description of the theory see refs. [4] and [5].

As the main problem then appears to find the equation of motion for the local propagators. But the concept for the perturbation scheme is clear: we linearize locally all forces which are possibly present (within a certain model, see below) and describe the local motion to harmonic order as good as we can. This amounts to a generalization of the RPA in a threefold sense, namely: a) to a finite temperature, b) to include residual interactions, and, finally, c) to treat fluctuations. In this contribution we would like to concentrate fully on the third aspect and wish to refer to refs. [5] and [6] where a close description of points a) and b) can be found.

2) THE THEORY

As our first approximation we take advantage of the picture of Bohr and Mottelson and introduce collective variables Q through a shape dependent shell model potential $V(x_i,Q)$. According to our scheme discussed above we linearize locally like:

$$\hat{V}(\hat{x}_i,Q) \approx \hat{V}(\hat{x}_i,Q_o) + (Q-Q_o)\,\hat{F}(\hat{x}_i,Q_o) \quad . \qquad (1)$$

The first term is a purely intrinsic operator (it "renormalizes" the intrinsic Hamiltonian or energy), whereas the second term defines the effective (local) coupling between the collective motion Q(t) and the intrinsic system.

If we were just to describe average motion, this scheme would do. We could follow a line similar to the one of the conventional "cranking model" and derive an equation of motion for the Q(t), as the representative for the average collective dynamics. It can be seen in ref. [4] and [6] (with further references given there) how the effects of finite temperature and residual interaction can be included, finally leading to an equation having a friction force.

But we are interested in fluctuations. Therefore, we have to "introduce" the Q as a genuine dynamical variable, together with its conjugate momentum. Notice, for a quantal system this "introduction as a dynamical variable" is another word for quantization. A classical dissipative system cannot be quantized. Therefore, we must choose a different way: we have to quantize first and then to perform all the steps necessary to describe dissipative processes. We even have to start "before" eq. (1), in the sense that we should have a two-body force, like

$$V^{(2)} = \frac{k}{2}\,\hat{F}(x_i,Q_0)\,\hat{F}(x_i,Q_0) \quad . \tag{2}$$

Such a force does lead to (1) within the approximation of the mean field. For this we only need to have as a condition:

$$k\langle\hat{F}\rangle_t = Q(t) - Q_0 \quad . \tag{3}$$

How can we get the coupling constant k? Well, it should not depend on time. Therefore we may use a static procedure. We may calculate the total static energy from our Hamiltonian with the (approximate) two body force. This will depend on the coupling constant k. In our locally harmonic approximation we will calculate it to second order in $(Q-Q_0)$. This expression we may identify with total static energy calculated differently, namely by combining the shell model with the liquid drop renormalization according to Strutinsky's procedure. For more details see ref. [7], as well as ref. [6] for possible modifications to include the effects of finite temperature. Clearly, our k will be a function of Q_0.

How can we introduce the dynamical variables $\hat{Q}$ and $\hat{P}$? They have to come as additional, superfluous degrees of freedom. But if we take it serious we then must have a subsidiary condition. Indeed, we found one in eq. (3) already. There it served for the average motion. So we have to generalize it to an operator equation. For the sake of simplicity we shall replace $1/k\ (Q-Q_0)$ by Q. Then this operator equation can be written as:

$$\hat{F}(\hat{x}_i) - \hat{Q} = 0 \quad . \tag{4}$$

All we have to do is to find a Hamiltonian for the extended dynamics (to include both the intrinsic and collective degrees of freedom). Such a Hamiltonian can be obtained by exploiting the method of Bohm and Pines (see ref. [8]) for our nuclear physics problem (see refs. [9] and [10]). It reads:

$$\hat{\mathcal{H}} = \hat{H}_0 + \hat{F}\hat{P} - \beta\hat{Q}\hat{F} + \frac{\hat{P}^2}{2m_0} + \left(\frac{2\beta-k}{2}\right)\hat{Q}^2 \quad .. \tag{5}$$

Here $\hat{H}_0$ is a Hamiltonian which represents the unperturbed intrinsic motion (it includes the potential $V(x_i,Q_0)$. The Operator $\dot{\hat{F}}$ is defined as

$$\dot{\hat{F}} = -i\,[\hat{F},\hat{H}_0] \tag{6}$$

and the unperturbed mass m_0 as

$$\frac{1}{m_0} = i\,\langle[\dot{\hat{F}},\hat{F}]\rangle_0 \quad , \tag{7}$$

where the average is to be calculated with the density distribution $\hat{\rho}_0 = 1/z$

$\exp(-H_0/T)$. To obtain (5) we have been guided by our general scheme to describe (locally) the collective motion to harmonic order, and we have chosen the terms in Q such that the two-body interaction (2) has been cancelled. There is one free parameter β. Fortunately it turns out that the dynamics of the interesting quantities does not depend on its value (see below, in particular section 3).

The Hamiltonian (5) has terms which couple collective and intrinsic motion. They are of linear order in $\hat{Q}$ and $\hat{P}$, and they are essential for the whole dynamics. To understand their influence one may proceed in different ways, depending both on $\hat{H}_0$ as well as on the special question to be answered.

Let's assume for a moment that $\hat{H}_0$ represents simple dynamics of independent particles. In this case we would not expect to find any trace of irreversibility in the final equations of motion. Therefore we would just try to "diagonalize" the Hamiltonian. This may be done by means of canonical transformations as in the original papers by Bohm and Pines. One obtains the usual RPA for undamped motion.

But the $\hat{H}_0$ may represent a more complex situation. It might have, for instance, a quasi-continuous spectrum, or it may have some further residual interaction which couples 1p-1h excitations to more complicated configurations (in a way which is largely independent of Q). Then there will be irreversibility, and a canonical transformation to a new Hamiltonian would not adequately describe all features. It is here where the typical elements of non-equilibrium statistical mechanics show up. The best one can do is to find a transport equation for the reduced density operator $\hat{d}(t)$ for the collective system, or its Wigner tranform $d_w(Q,P,t)$. There, the problem is to treat adequately the coupling terms, such that the dynamical fluctuations are treated on the same footing as the average motion. The latter we know from RPA, or better its extended version to include damping. In this paper there will be no space to describe in more detail the derivation of the transport equation. We refer to [5] as well as to further publications and concentrate once more on the average motion. From this we will then be able to deduce important observation for the fluctuations in equilibrium, at least for somewhat simple cases. Furthermore, it may elucidate the point made about the proper version of perturbation theory.

From (5) the average motion can be obtained via Ehrenfest's equations. They contain $\langle\hat{F}\rangle_t$ and $\langle\dot{\hat{F}}\rangle_t$. Clearly, these averages are functionals of $Q(t) = \langle\hat{Q}\rangle_t$ and $P(t) = \langle\hat{P}\rangle_t$. In linear order one may write:

$$\langle\hat{F}\rangle_t = \beta \int ds\ \tilde{\chi}^{(o)}_{FF}(s)\ Q(t-s) - \int ds\ \tilde{\chi}^{(o)}_{F\dot{F}}(s)\ P(t-s) \tag{8}$$

$$\langle\dot{\hat{F}}\rangle_t = -\int ds\ \tilde{\chi}^{(o)}_{\dot{F}F}(s)\ P(t-s) + \beta \int ds\ \tilde{\chi}^{(o)}_{FF}(s)\ Q(t-s) \tag{9}$$

This form is by no means trivial. It is obtained by treating the influence of the coupling terms on the intrinsic system by low order perturbation theory. Therefore, the response functions for the intrinsic system appear, like

$$\tilde{\chi}^{(o)}_{FF}(t) = 2i\Theta(t)\ \tilde{\chi}''^{(o)}_{FF}(t) = i\Theta(t)\ \langle[\hat{F}^I(t),\hat{F}]\rangle_o \tag{10}$$

and similar expressions for the other functions. In the final equations for Q(t) and P(t) the $\hat{H}_o$ will appear only through this $\tilde{\chi}_{FF}(t)$, and therefore any form of $\hat{H}_o$ is acceptable which allows the computation of this intrinsic response function. With respect to the collective motion the expressions (8) and (9) imply much more than simple perturbation theory. Notice, that the collective factors do not just involve $\hat{Q}$ and $\hat{P}$ in the interaction picture: the Q(t) and P(t) are meant to be the actual solutions of Ehrenfest equations.

Let us not write down these equations but just mention that their solutions may conveniently be described by response functions for the Q,P-motion itself. According to the general definition of the response

$$\delta\langle A_\nu\rangle_\omega = \sum \chi_{\nu\mu}(\omega)\ f^{\mu}_{ext}(\omega) \tag{11}$$

to an external field:

$$\delta H = \sum \hat{A}_\mu\ \bar{f}^{\mu}_{ext}(t)$$

we find for

$$\delta H = -\hat{Q}\ \bar{q}_{ext} - \hat{P}\ \bar{p}_{ext}(t) \quad : \tag{12}$$

$$\chi_{QQ}(\omega) = \frac{\chi_o(\omega)}{1-k\chi_o(\omega)} \tag{13}$$

$$\chi_{QP}(\omega) = -i\ \frac{(1-\beta\ \chi_o(\omega))}{\omega\ \chi_o(\omega)}\ \chi_{QQ}(\omega) = -\chi_{PQ}(\omega) \tag{14}$$

$$\chi_{PP}(\omega) = \frac{(+k-2\beta+\beta^2\chi_o(\omega))}{\omega^2\ \chi_o(\omega)}\ \chi_{QQ}(\omega) \quad . \tag{15}$$

We have used Fouriertransformations and some simple relations among

$$\chi_o(\omega) = \chi^{(o)}_{FF}(\omega)\ ,\quad \chi^{(o)}_{F\dot{F}}(\omega) \quad \text{and} \quad \chi^{(o)}_{\dot{F}F}(\omega) \quad .$$

In the remaining part of this section we would like to comment on these results (13) to (15) and eventually draw some first conclusions.

1) First, we observe that the expressions (13) to (15) turn out to be functions of the frequency ω. Clearly, the frequencies for the actual motion of our system will be found by studying the poles of these expressions. Their values will be different from the frequency ω_0 of the unperturbed case (which can be calculated easily from the last two terms in (5)). This essential feature was obtained only because, above, we did avoid to use simplest perturbation theory. Indeed, had we used the interaction picture to define the time dependence of Q and P appearing in expressions (8) and (9) we would have ended up with expressions with the χ being calculated at ω_0.

2) By looking at $\chi_{QQ}(\omega)$ we encounter the same functional form as known for the quantity $\langle F\rangle_\omega$ from ordinary RPA, i.e. when using just $H_0 + k/2\, F\cdot F$. As a matter of fact it is easy to show that we recover this result as well for our present model, which is to say that (5) guaranties to satisfy (4) on the average for all times, or all frequencies:

$$\langle F\rangle_\omega - Q(\omega) = 0 \quad . \tag{16}$$

We may put it in different words: the form (13) guaranties that the frequency spectrum for the Q-motion to become identical to the frequency spectrum of the $\langle\hat{F}\rangle_t$ motion, when calculated in conventional RPA (provided, of course, we use the same $\hat{H}_0$).

3) This must have implications for the equilibrium values of fluctuations. Let's assume for a moment that we use the form (5) for a situation where we study collective vibrations around a genuine stable point. Then our harmonic solutions represent the true situation for all times, thus also for $t \to \infty$. (For the interpretation of Fouriertransforms in the general case see refs. [5] and [6]). Therefore, we may apply the fluctuation-dissipation theorem to obtain fluctuations in global equilibrium. This theorem, applied to χ_{QQ}, says:

$$\langle(\hat{Q} - \langle Q\rangle_{eq})^2\rangle_{eq} = \int \frac{d\omega}{2\pi} \operatorname{cotgh} \frac{\omega}{2T}\, \chi''_{QQ}(\omega) \quad , \tag{17}$$

with a similar expression for the fluctuations in F. (The χ''_{QQ} is the dissipative part of χ_{QQ}). But since $\chi_{QQ}(\omega) = \chi_{FF}(\omega)$ we obtain the important result

$$\langle\hat{F}^2\rangle_{eq} = \langle\hat{Q}^2\rangle_{eq} \quad . \tag{18}$$

It says that eq. (4) is fulfilled not only in its time-dependent mean but, for the equilibrium, even in second order. Whether or not such a statement is true for the dynamical fluctuations as well is yet unclear. However, for the model represented in section 3) we will be able to fulfill (4) as an operator equation, indeed.

4) Please notice that the statements made so far do not involve the parameter β. From (14) and (15) we see that β appears whenever the momentum is involved. Furthermore, we observe that in the latter case the frequency spectrum has one more solution. These features are hard to understand from the general model. We will be able to clearify it by looking at a schematic case in the next section.

3) A SCHEMATIC MODEL

Suppose we choose H_0 to be a set of coupled oscillators:

$$\hat{H}_0 = \frac{1}{2}\sum_{i=1}^{N}\left[\frac{p_i^2}{m_i} + m_i\omega_i^2 x_i^2\right] \quad , \qquad (19)$$

and F to be a linear function in the x_i,

$$\hat{F} = \sum_{i=1}^{N} \lambda_i \hat{x}_i \quad . \qquad (20)$$

Then our problem allows an analytical solution. However, if we do that for the Bohm-Pines Hamiltonian (5) we encounter a little problem: the secular equation has a solution $\omega = 0$ which makes the diagonalization a little uncomfortable. The reason for that is the subsidiary condition, and in particular the choice of m_0 as given by eq. (7). It is only for this choice that we are able to fulfill the subsidiary condition in the way described in section 2. But then it is clear how we can circumvent the problem: we replace m_0 by $\tilde{m}_0$, do all calculations for a finite

$$\epsilon = (\tilde{m}_0)^{-1} - m_0^{-1} = \tilde{m}_0^{-1} - \sum_{i=1}^{N} \frac{\lambda_i^2}{m_i} \qquad (21)$$

and let ϵ got to zero in the final expressions. In this way the Hamiltonian can be written as

$$\hat{\mathcal{H}} = \sum_{k=0}^{N} \frac{\Omega_k}{2}\,(\hat{c}_k^{+} c_k + \hat{c}_k \hat{c}_k^{+}) \qquad (22a)$$

with the secular equation being given by

$$\epsilon\,[2\beta - k - \beta^2\,\chi_0(\omega)] - \omega^2[1 - k\,\chi_0(\omega)] = 0 \quad . \qquad (23)$$

Clearly, there is one solution, we call it Ω_0, which vanishes in the limit $\epsilon \to 0$ (like $\sqrt{\epsilon}$, provided $2\beta-k-\beta^2\chi(0) \neq 0$). We call this the zero frequency mode. It should be noted that the $\hat{c}_k^{+} + \hat{c}_k$ depend on ϵ as well, so that the term $\kappa = 0$ does not vanish in the limit $\epsilon \to 0$. One obtains:

$$\lim_{\epsilon\to 0} \frac{\Omega_0}{2} (\hat{c}_0^+ \hat{c}_0 + \hat{c}_0 \hat{c}_0^+) = \frac{2\beta-k-\beta^2\chi_0(0)}{1-k\chi_0(\omega)} (\hat{Q}-\hat{F}) \quad . \tag{22b}$$

In this paper we will not go into any further detail of the calculation. We will just mention the most important results and refer to a forthcoming publication [11]:

a) The solution of the Heisenberg equations lead to

$$\hat{Q}(t) - \hat{F}(t) = - \lim_{\epsilon\to 0} \sqrt{\frac{\epsilon}{2\Omega_0}} [\hat{c}_0 + \hat{c}_0^+] = \hat{Q}-\hat{F} \quad \cdot \tag{24}$$

This shows α) that the subsidiary condition is stationary and β) that it is related to the zero frequency mode: the subsidiary condition is a symmetry of our problem. (Notice the close analogy to gauge transformation in quantum field theories).

b) For $\kappa > 0$, and in the limit of $\epsilon \to 0$, all Ω_k are identical to the physical solutions found in the RPA; the secular equation (23) defines the poles of $\chi_{QQ}(\omega)$.

c) As can be seen from (23) the paramter β drops out of the secular equation <u>only</u> in the limit $\epsilon \to 0$.

d) Nevertheless, the parameter β may contribute to solutions for operators or their averages, but only if these operators depend on the momentum $\hat{P}$. We have seen that in section 2) already. But here it is easy to prove that β does not appear, for instance, in the operators for <u>velocities</u> like $d\hat{Q}/dt$ and $d\hat{F}/dt$.

e) We may calculate the fluctuations in thermal equilibrium. If the latter is defined by:

$$\hat{W}_{eq} = \frac{1}{Z} \exp(-\mathcal{H}/T) \quad , \tag{25}$$

we obtain in the limit $\epsilon \to 0$ and among other results:

$$\langle(\hat{Q} - \langle\hat{Q}\rangle_{eq})^2\rangle_{eq} = \frac{(1-\beta\ \chi_0(0))^2}{[1-k\ \chi_0(0)][\alpha-\beta^2\ \chi_0(0)]} T + \sum_k \frac{1}{\mu_k\Omega_k} \operatorname{cotgh} \frac{\Omega_k}{2T} \tag{26}$$

$$\langle((\hat{Q}-\hat{F})^2 - \langle\hat{Q}-\hat{F}\rangle_{eq})^2\rangle_{eq} = \frac{1-k\ \chi_0(0)}{\alpha-\beta^2\ \chi_0(0)} T \tag{27}$$

$$\langle(\frac{d\hat{Q}}{dt} - \langle\frac{d\hat{Q}}{dt}\rangle)_{eq}{}^2\rangle_{eq} = \sum_{k=1}^{N} \frac{\Omega_k}{\mu_k} \operatorname{cotgh} \frac{\Omega_k}{2T} \tag{29}$$

and

$$\langle(\hat{P} - \langle\hat{P}\rangle_{eq})^2\rangle_{eq} = \lim_{\epsilon\to 0} \frac{T}{\epsilon} + \sum_{k=1}^{N} \frac{(\beta-k)^2}{\mu_k \Omega_k^3} \operatorname{cotgh} \frac{\Omega_k}{2} \quad . \tag{30}$$

In (26), (27) and (30) we get a contribution from the zero frequency mode. In the last case this is even divergent, for $T \neq 0$. As stated above the result (29) for the velocity is independent of β, whereas for the momentum $\hat{P}$ β even contributes to the modes $k \neq 0$.

The results (26) and (27) are different from the ones obtained in the previous section by exploiting our response functions (13) to (15). The difference is that (26) and (27) have a contribution from the zero frequency mode, whereas the response functions for the Q and F motion do not have a pole at zero frequency. Looking for possible reasons for this feature, we may notice that these response functions have been derived for ϵ being identically zero from the start, and that certain limits do not commute. We will have to clearify this point further [11]. But in any case we could cure this point simply, and in a physically satisfying way, by using a thermal distribution for the physical solutions $k = 1...N$ and leaving the system in the ground state of the spurious mode $k = 0$. That implies to put $T = 0$ in the terms involving the zero frequency solution.

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STRESZCZENIE

Dyskutujemy potencjalną teorię opisu wielkoskalowej jądrowej dynamiki kolektywnej w skończonych temperaturach. Stwierdzamy, że właściwy opis typowych zjawisk jądrowych wymaga równania opartego o nierównowagową kwantową mechanikę statystyczną. Wskazujemy, jak można wyprowadzić takie równanie i koncentrujemy się na problemie wprowadzenia zmiennych kolektywnych w sposób kwantowy. Sugerujemy użycie metody Bohma i Pinesa, pozwalającej na jawne rozważenie warunku pomocniczego. Dyskutujemy, w jaki sposób warunek pomocniczy może być spełniony w postaci równania operatorowego. Problemy te są objaśnione w ramach uproszczonego modelu pozwalającego uzyskać rozwiązanie analityczne.

Р Е З Ю М Е

Рассматривается потенциальная теория представления крупномасштабной коллективной ядерной динамики при конечных температурах. Доказывается, что правильное представление типичных ядерных явлений требует уравнения базирующегося на неравновесной квантовой статистической механике. Мы показали, как можно вывести такое уравнение, и сосредоточились на проблеме введения коллективных переменных квантовым образом. Полагается применение метода Бома и Пайнеса, позваляющего явно рассматривать воспомогательное условие. Обсуждается, каким образом воспомагательное условие может выполняться как операторное уравнение. Эти ~~про~~ проблемы обясняются в рамках упрощенной модели позваляющей получить аналитическое решение.