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Field Theory of Collective Excitations.

II. – Large-Amplitude Phenomena.

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In this letter we would like to draw attention to the fact that for a general many-fermion system, large-amplitude collective excitations, their quasi-classical quantization, and barrier penetration processes are described by the extrema of the effective action $\Gamma[\varrho]$ which is a functional of the density matrix ϱ (including pair correlations). In contrast with an earlier path integral approach to the same phenomena in which the Hartree approximation is the starting point, the expansion of $\Gamma[\varrho]$ according to fermion loops amounts to the time-dependent Hartree-Fock-Bogoljubov (TDHFB) equations and their systematic improvements.

Some years ago, in part I of this paper, the direct use of collective Bose fields was proposed as a powerful tool in the description of nuclear collective phenomena ([1-3]). The ideas were illustrated in a simple solvable model with pure pairing forces. Since then, much effort has been spent on attempts to make the same ([4]) or a slightly modified ([5,6]) technique applicable to the general many-body situation. The particular advantage of collective Bose fields consists in a direct access to semi-classical phenomena ([7,8]) which apparently play an important role in low-energy nuclear physics.

In the model, the main simplification derives from an immediate introduction of a fluctuating collective pair field for which a semi-classical expansion is readily available. When trying to apply the same formalism to a realistic nuclear problem, however, difficulties arise. The collective field is a hybrid object, as far as $\hbar$ is concerned, and there is no simple way of extracting a semi-classical expansion in powers of $\hbar$; in particular, the first order in $\hbar$ corresponds only to the Hartree approximation and the exchange

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([3]) H. KLEINERT: *Fortschr. Phys.*, **26**, 565 (1978), in particular p. 644-665.
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([7]) H. KLEINERT and H. REINHARDT: *Nucl. Phys. A*, **332**, 331 (1979).
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forces (Fock terms), which are so important in many nuclear calculations, can only be collected after summing up an infinite number of loops in the collective quantum field. In fact, this difficulty was the motivation for attempts to use alternative collective fields based on coherent states ([5,6]).

It is the purpose of this note to point out that the natural solution of this problem is provided by the effective action functional $\Gamma[\varrho]$, whose extrema give the density matrix ϱ of the full quantum system (*). This object is well known in quantum field theory and statistical mechanics ([9]) and its history goes back to the extremal principles of Lee and Yang ([10]).

$\Gamma[\varrho]$ is specified in terms of a graphical expansion according to the number of fermion loops. The lowest contributions lead directly to the time-dependent Hartree-Fock Bogoljubov (TDHFB) equations. The higher corrections are all simple expressions of ϱ and can easily be incorporated into the usual iterative procedure of solving the equations. Large-amplitude collective excitations follow from extremizing $\Gamma[\varrho]$.

Let

$$\mathscr{A}[\psi] = \psi^+(i\partial_t - \xi)\,\psi - \tfrac{1}{2} v\psi^+\psi\psi^+\psi \tag{1}$$

be the action of an arbitrary many-fermion system with two-body forces. All indices are suppressed since they can immediately be reconstructed if desired. Also the time variable is treated as an index. The parameter ξ denotes the single-particle energies measured from some chemical potential. Because of the fermion nature of ψ all Green's functions involving an odd number of fields vanish. We may then generate all nonzero ones from the functional (**)

$$Z[K] \equiv \int \mathscr{D}\psi\, \mathscr{D}\psi^+ \exp\left[i\mathscr{A}[\psi] + \frac{i}{2}\varphi K \varphi\right] \tag{2}$$

by forming derivatives with respect to the auxiliary source (***)

$$K = \begin{pmatrix} \lambda^+ & -\mu^{\mathrm{T}} \\ \mu & \lambda \end{pmatrix} = -K^{\mathrm{T}}.$$

(*) For notational simplicity, the single symbol ϱ is supposed to include particle- as well as pair-correlation functions

$$\varrho(t,t') \equiv \begin{pmatrix} \langle T\psi_\alpha(t)\psi_\beta(t')\rangle & \langle T\psi_\alpha(t)\psi_\beta(t')\rangle \\ \langle T\psi^+_\alpha(t)\psi_\beta(t')\rangle & \langle T\psi^+_\alpha(t)\psi^+_\beta(t')\rangle \end{pmatrix}.$$

More economically, we use doubled fields $\varphi_a \equiv \begin{pmatrix} \varphi_{\alpha\uparrow} \\ \varphi_{\alpha\downarrow} \end{pmatrix} \equiv \begin{pmatrix} \psi_\alpha \\ \psi^+_\alpha \end{pmatrix}$ such that

$$\varrho_{ab}(t,t') \equiv \langle T\varphi_a(t)\varphi_b(t')\rangle\,.$$

If the potential is instantaneous, only the part of ϱ which is diagonal in the time « index » will enter the effective action.

(9) See any modern textbook on quantum field theory, *e.g.* D. J. AMIT: *Field Theory, the Renormalization Group, and Critical Phenomena* (New York, N. Y., 1978); C. NASH: *Relativistic Quantum Fields* (London, 1978).

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(**) In our notation, $\varphi K\varphi$ stands short for

$$\int dt\, dt'\, \varphi_a(t) K_{ab}(t,t')\varphi_b(t')\,.$$

(***) The symbol T denotes functional transposition, *i.e.* $K^{\mathrm{T}}_{ab}(t,t') = K_{ba}(t',t)$, $\mu^{\mathrm{T}}_{\alpha\beta}(t,t') = \mu_{\beta\alpha}(t',t)$. The potential V with doubled indices is antisymmetric and equals $V_{\alpha\downarrow\beta\uparrow\gamma\downarrow\delta\uparrow} = 2v_{\alpha\beta\gamma\delta}$.

Formally, $Z[K]$ can be calculated by rewriting the exponent in (2) as

$$\mathscr{A}[\varphi] + \frac{1}{2}\varphi K\varphi = \frac{1}{2}\varphi\begin{pmatrix} \lambda^{+} & i\partial_t + \xi - \mu^{\mathrm{T}} \\ i\partial_t - \xi + \mu & \lambda \end{pmatrix}\varphi - \frac{1}{4!}V\varphi\varphi\varphi\varphi \equiv \tag{3}$$

$$\equiv \frac{1}{2}\varphi i G_K^{-1}\varphi - \frac{1}{4!}V\varphi\varphi\varphi\varphi$$

and by removing the interacting part from the integral

$$Z[K] = \exp\left[-\frac{i}{6}V\frac{\delta}{i\,\delta K}\frac{\delta}{i\,\delta K}\right]Z_0[K] \tag{4}$$

in such a way that the remaining functional integral is Gaussian and can be performed to give

$$Z_0[K] = \int \mathfrak{D}\varphi \exp\left[\frac{i}{2}\varphi i G_K^{-1}\varphi\right] = \exp\left[\frac{1}{2}\operatorname{tr}\log i G_K^{-1}\right]. \tag{5}$$

This is the generating functional of the free theory. The notation G_K^{-1} has been chosen for the (2×2)-matrix in (3), (5) since the inverse G_K is the conventional Green's function of the fermions in the presence of an external field K.

Expanding Z in powers of V results in the standard perturbation series which can be evaluated in terms of diagrammatic rules. If we form the logarithm (*)

$$iW[K] = \log Z[K], \tag{6}$$

then $iW[K]$ consists of the sum of all connected vacuum graphs involving the propagator G_K. Due to the fermion nature of φ these are one-particle irreducible (OPI). They are pictured in fig. 1, each vertex standing for $iV/4!$, and each line for $\overline{\varphi\varphi} = G_K$.

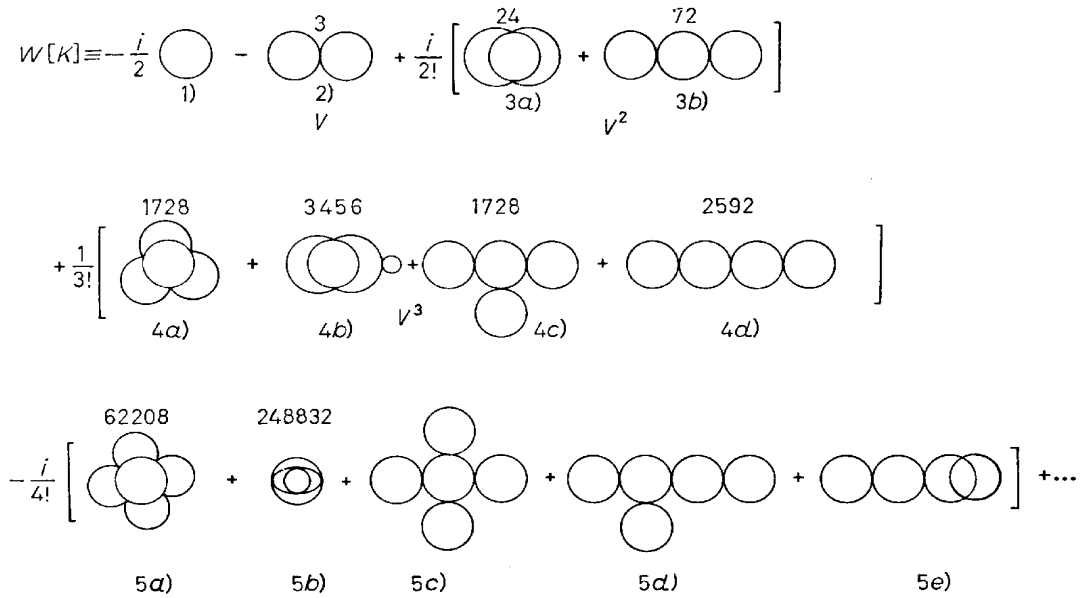

Fig. 1. – ———: $G_K \equiv i\left[\begin{pmatrix} 0 & i\partial_t + \xi \\ i\partial_t - \xi & 0 \end{pmatrix} + K\right]^{-1}$; ×: $V/4!$

(*) We neglect constant factors in Z, *i.e.* additive constants in W.

Given $W[K]$, it is easy to find the exact density matrix of the system

$$\frac{1}{2}\varrho_{ab} = \delta W[K]/\delta K_{ab} = -\left(\frac{\delta}{\delta K}\right)_{ab} W[K] \tag{7}$$

as follows from (2) and the general definition of ϱ:

$$\varrho_{ab} \equiv \langle T\varphi_a\varphi_b\rangle \equiv \int \mathcal{D}\varphi\, \varphi_a\varphi_b \exp\left[i\mathcal{A}[\varphi] + \frac{i}{2}\varphi K\varphi\right]. \tag{8}$$

We may therefore introduce the effective action $\Gamma[\varrho]$ of the system as the Legendre transform

$$\Gamma[\varrho] \equiv W[K] - \tfrac{1}{2}\,\mathrm{tr}\,(K^T\varrho)|_{K=K[\varrho]} \tag{9}$$

such that (7) amounts to

$$\frac{\delta\Gamma[\varrho]}{\delta\varrho_{ab}} = -\frac{1}{2}K_{ab}\,. \tag{10}$$

Certainly, the auxiliary source K was employed only for the technical reason of deriving $\Gamma[\varrho]$. The physical situation is recovered by setting $K = 0$. Thus we conclude that a physical density matrix extremizes $\Gamma[\varrho]$ just as mechanical orbits extremize classical actions. The important difference is, however, that now all quantum corrections are included. That is why $\Gamma[\varrho]$ is called the effective action [9].

Let us evaluate the lower contributions explicitly: At the one-loop level we have

$$W^{(1)}[K] = -\frac{i}{2}\,\mathrm{tr}\log iG_K^{-1} \tag{11}$$

such that from (7)

$$\varrho = G_K\,, \qquad K = i\varrho^{-1} - \begin{pmatrix} 0 & i\partial_t + \xi \\ i\partial_t - \xi & 0 \end{pmatrix} \equiv i\varrho^{-1} - iG_0^{-1}\,. \tag{12}$$

Inserting this into (9), we obtain

$$\Gamma[\varrho] \equiv \Gamma^{(0)}[\varrho] + \Gamma^{(1)}[\varrho] = \frac{i}{2}\,\mathrm{tr}\,(G_0^{-1}\varrho^T) - \frac{i}{2}\,\mathrm{tr}\log i\varrho^{-1}\,. \tag{13}$$

The extremum of this is the density matrix of the free fermion system

$$\varrho = G_0 = i\begin{pmatrix} 0 & i\partial_t + \xi \\ i\partial_t - \xi & 0 \end{pmatrix}^{-1}. \tag{14}$$

Consider now the two-loop correction 2 in fig. 1:

$$W^{(2)}[K] = -\tfrac{1}{8}\,V_{abcd}(G_K)_{ab}(G_K)_{cd}\,. \tag{15}$$

Written in terms of upper and lower components, this contains Hartree, Fock, and Bogoljubov contributions

$$(16) \qquad -\tfrac{1}{2} v_{\alpha\beta\gamma\delta}[(G_K)_{\alpha\downarrow\beta\uparrow}(G_K)_{\gamma\downarrow\delta\uparrow} - (G_K)_{\alpha\downarrow\delta\uparrow}(G_K)_{\gamma\downarrow\beta\uparrow} - (G_K)_{\alpha\downarrow\gamma\downarrow}(G_K)_{\beta\uparrow\delta\uparrow}] .$$

Now

$$(17a) \qquad \varrho = G_K - \frac{i}{2} G_K (V G_K) G_K ,$$

$$(17b) \qquad K = i\varrho^{-1} - iG_0^{-1} + \tfrac{1}{2} V\varrho ,$$

such that we obtain

$$(18) \qquad \Gamma^{(2)}[\varrho] = -\tfrac{1}{8} V_{abcd}\varrho_{ab}\varrho_{cd} \equiv -\tfrac{1}{8} V\varrho\varrho .$$

Extremizing this gives (17*b*) for $K = 0$, *i.e.*

$$(19) \qquad \varrho = i[iG_0^{-1} - \tfrac{1}{2} V\varrho]^{-1} ,$$

which is just the TDHFB equation.

It is possible but tedious to proceed in this fashion to higher-loop corrections. More directly we may use the obvious functional identity

$$(20) \qquad \int \mathfrak{D}\varphi \frac{\delta}{\delta\varphi} \varphi \exp\left[i\mathscr{A}[\varphi] + \frac{i}{2}\varphi K\varphi\right] = 0 ,$$

work out the differentiations and derive (*)

$$(21) \qquad (iG_0^{-1} + K) W_K + \frac{i}{3} V(W_{KK} + iW_K^2) - \frac{i}{2} = 0 ,$$

which becomes with (7) and $-iW_{KK} = \varrho_K/2 = K_\varrho^{-1}/2 = -\Gamma_{\varrho\varrho}^{-1}/4$

$$(22) \qquad (iG_0^{-1} - 2\Gamma_\varrho)\varrho - \frac{1}{3!} V(\varrho^2 + i\Gamma_{\varrho\varrho}^{-1}) - i = 0 .$$

By separating out the trivial parts

$$(23) \qquad \Gamma[\varrho] \equiv \Gamma^{(0)}[\varrho] + \Gamma^{(1)}[\varrho] + \Gamma^{\mathrm{int}}[\varrho] ,$$

the interacting part satisfies the coupled equations

$$(24) \qquad \Gamma_\varrho^{\mathrm{int}}[\varrho]\varrho = -\frac{1}{4} V\varrho\varrho + \frac{i}{12} V\varrho^4\alpha ,$$

$$(25) \qquad \alpha = -4\Gamma_{\varrho\varrho}^{\mathrm{int}}(1 - 2i\varrho\varrho\Gamma_{\varrho\varrho}^{\mathrm{int}})^{-1} = -4\Gamma_{\varrho\varrho}^{\mathrm{int}} + 2i\Gamma_{\varrho\varrho}^{\mathrm{int}}\varrho\varrho\alpha .$$

(*) Functional differentiation is indicated by a subscript, *i.e.* $W_K \equiv (\delta/\delta K)W$.

We have found it convenient to introduce the quantity α, since it can easily be verified to be the exact four-particle vertex function of the theory. The index contractions in these equations are pictured in fig. 2. The solution can be found by iteration. For the bookkeeping of the indices, this is best done graphically with lines representing the density matrix ϱ and vertices the potential V. We see that in this way we generate precisely those vacuum graphs which do not fall into pieces by cutting two lines. These are called two-particle irreducible (TPI). In fig. 1 the graphs 2), 3*a*), 4*a*), 5*a*), *b*), ... are TPI.

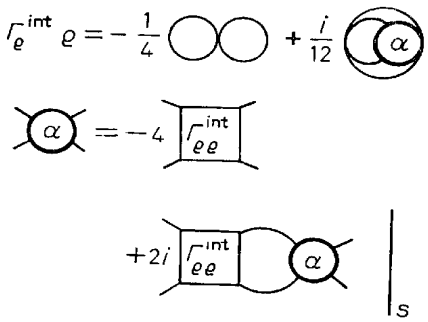

Fig. 2. – ———: ϱ; ×: V.

Notice that this expansion is nonpertubative even though $n-1$ counts also the number of explicit V's in each term (for $n > 1$). But the lines are the fully interacting density matrices which themselves contain V to all orders.

By means of (23) the extremality condition $\Gamma_\varrho[\varrho] = 0$ becomes

$$\varrho = i\{iG_0^{-1} - \Sigma[\varrho]\}^{-1}, \tag{26}$$

where $\Sigma[\varrho]$ stands short for

$$\Sigma[\varrho] = -2\Gamma_\varrho^{\text{int}}[\varrho] = \frac{1}{2}V\varrho - \frac{i}{6}V\varrho^3\alpha \tag{27}$$

Equation (26) was first used by DYSON [9] with the prescription that $\Sigma[\varrho]$ contains all those self-energy graphs which are one-particle irreducible (OPI), *i.e.* which do not fall apart when cutting one line. But this agrees exactly with our result: differentiating $(\delta/\delta\varrho)\Gamma[\varrho]$ corresponds to removing a single line from a TPI vacuum graph. What remains is a self-energy graph which, moreover, must be OPI.

We are now ready to study large amplitude collective excitations. For any periodic orbit one chooses some initial density matrix and solves the eigenvalue equation

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\{iG_0^{-1} - \Sigma[\varrho]\}\chi^l(t) = \varkappa^l\chi^l(t), \tag{28}$$

where $\chi^l(t)$ are antiperiodic wave functions and $\varkappa^l$ the corresponding Bloch-Floquet indices. Then one determines

$$\varrho_{ab}(t,t') = \sum_l\sum_n \frac{i}{\omega_n - \varkappa^l}\exp[-i\omega_n(t-t')]\,\chi_a^l(t)\,\chi_{b'}^{l}(t')\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}_{b'b} = \tag{29}$$

$$= \sum_l (\exp[i\varkappa^l T] + 1)^{-1}\exp[-i\varkappa^l(t-t')]\,\chi_a^l(t)\,\chi_{b'}^{l}(t')\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}_{b'b},$$

where the Fermi distribution with imaginary temperature comes from summing the frequencies $\omega_n = 2\pi(n+\frac{1}{2})/T$ ($T \equiv$ period). This ϱ may again be used in (28) for a next iteration. (The static case follows from $T \to \infty$ where the sum reduces to the states below the Fermi surface and $\chi(t)$ are time-independent wave functions.)

The resulting ϱ can be inserted into the effective action $\Gamma[\varrho]$ for a quantization of the large-amplitude oscillating orbits (or for a determination of the energy in the case of static ϱ configurations, $E = -\Gamma[\varrho]/T$). For this purpose one only has to form the full quantum propagator as the Fourier transform ([7])

$$\int \frac{\mathrm{d}T}{2\pi} \exp\left[i\Gamma[\varrho] + ET\right] \equiv \frac{\partial W(E)}{\partial E} \exp\left[iW(E)\right], \tag{30}$$

where T is the period. Running through the same orbit many times gives a Green's function

$$\partial W/\partial E \sum_{n=1}^{\infty} \exp\left[inW(E)\right] = \partial W/\partial E \exp\left[iW(E)\right](1 - \exp\left[iW(E)\right])^{-1}$$

which has pole at $W(E_n)$ ($n+\frac{1}{2}$ if the orbit has turning points) ([7]).

Notice that if imaginary-time solutions are known passing through a potential barrier, $\exp[-TE] = \exp[i\Gamma[\varrho]]$ gives the amplitude of penetration ([8]).

It goes without saying that the partial derivatives of $\Gamma[\varrho]$ provide directly for all Green's functions via (9), (10). For example

$$-\frac{1}{4} G^{(4)} = W_{KK} = \frac{i}{2} \varrho_K = \frac{i}{2} K_\varrho^{-1} = -\frac{i}{4} \Gamma_{\varrho\varrho}^{-1} \tag{31}$$

gives the four-point functions.

It may be useful to point out the connection with the collective action employed in I. Using (19), we may express the effective action in a two-variable form as

$$\Gamma[\Sigma, \varrho] = -\frac{1}{2} \operatorname{tr}(\Sigma\varrho) - \frac{i}{2} \operatorname{tr} \log(iG_0^{-1} - \Sigma) - \frac{1}{8} V_{\varrho\varrho} + \sum_{n \geqslant 3}^{\infty} \Gamma^{(n)}[\varrho]. \tag{32}$$

Neglecting $n \geqslant 3$ terms and bringing ϱ to the extremum $\varrho[\Sigma]$ we obtain

$$\Gamma[\Sigma] \equiv \Gamma[\Sigma, \varrho[\Sigma]] = \frac{1}{2} V^{-1} \Sigma\Sigma - \frac{i}{2} \operatorname{tr} \log(iG_0^{-1} - \Sigma), \tag{33}$$

which is precisely the quasi-classical limit of the action discussed in I except that there Hartree and Fock parts of the potential were absent.

Further developments will be published elsewhere ([11]).

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([11]) H. Kleinert: *Phys. Lett. A* (in press); *Fortschr. Phys.* (in press).

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