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On the Stability of the Hartree-Fock Solution in Many-Body Problem

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A necessary condition for the stability of the Hartree-Fock solution in many-body problem is presented. If this condition is not satisfied, then the solution becomes no longer stable as was discussed by Overhauser in connection with the one-dimensional spin wave model. A variational method is proposed in this case to construct a stable solution which has definitely a lower energy than the Hartree-Fock value. The workability of our method is tested in some realistic examples like the B.C.S.-Bogolyubov theory of superconductivity. Then the method is applied to field theory which seems to be inconsistent in view of the presence of "ghost states". A canonical transformation leads to a new vacuum state with lower energy, but the high momentum part of the coupling is not damped.

§ 1. Introduction

Recently, a serious question has been raised concerning the stability of the Hartree-Fock solution by Overhauser[1] who treated the one-dimensional system of interacting fermions and found a new solution which gives a lower energy than the Hartree-Fock value. In such a system, the free ground state is not connected with the true one adiabatically, but rather with some kind of excited state. The B.C.S. theory of superconductivity[2] is another example where the ground state is far from the Fermi distribution.

Now in the Overhauser model, one can show that the propagator for a pair of particle and hole with spin either parallel or antiparallel according to the sign of force has an imaginary pole, the corresponding excitation being completely unstable. In the B.C.S. theory, the propagator for a pair of particle or of hole with opposite momenta and spins has also an imaginary pole at the momentum close to the Fermi value.[3] One may expect that this difficulty is intimately connected with the instability of the Fermi distribution, that is, the Hartree-Fock solution against the deformation in accordance with such an excitation.

Following this observation, one will introduce in § 2 an approximate collective operator by applying the method of normal mode,[4] calculate the variational energy with respect to the deformed state corresponding to thier collective excitation, and then show that the second derivative of this energy at the Hartree-Fock state is actually positive if the eigenfrequency is real, but is zero if this is imaginary. In the former case the Hartree-Fock state is stable within the family of variations employed and in the latter case it is unstable.

Then a family of variational functions are suggested which would make the energy lower than the Hartree-Fock value. In order to assure the absolute stability, one will in principle have to look for a complete set of these excited modes, but from physical grounds lower excited states will usually play an important role.

In the following three sections, the criterion of instability is applied to the three-dimensional model of Overhauser, to the B.C.S. theory of superconductivity, and to the Bogolyubov Hamiltonian of liquid He^4 with negative scattering length.[5] It is then shown that our new variational solution will actually turn out to be the lower energy state. The new excited eigenmodes, phonon spectrum, for instance, based on this ground state now have real frequencies.

In § 6, the method is applied to field theory by taking the meson-nucleon system as an illustration. The meson spectrum now includes an imaginary frequency which is made use of to derive a new ground state with lower energy. The canonical transformation leading to this state has two effects. One is to change the effective coupling between the meson and nucleon which becomes weaker than the original one. The high frequency part of the coupling is however not altered. The other effect is that the eigenfrequencies of the meson are now all real.

§ 2. Stability condition for the Hartree-Fock solution of a Fermi gas

As an orientation of our basic idea, let us first consider a Fermi gas in which particles are interacting through ordinary two-body forces. The Hamiltonian of our system is given in the second quantized form as

$$H=\Sigma_p C_p^* C_p \frac{p^2}{2m}+\frac{1}{2}\Sigma_{p,p',q} v(q) C_p^* C_{p'}^* C_{p'+q} C_{p-q}, \qquad (2\cdot1)$$

where $\boldsymbol{p}$'s are the momentum and spin of a particle, C_p's and C_p^*'s are annihilation and creation operators of a particle, respectively, and $v(q)$ the Fourier transform of the potential. In the hole theory formulation in which the Fermi distribution is taken as a vacuum, C_p's are replaced by

$$C_p=\begin{cases} a_p, & \text{for } |\boldsymbol{p}|>p_F, \\ b_p^*, & \text{for } |\boldsymbol{p}|<p_F, \end{cases} \qquad (2\cdot2)$$

where a_p and b_p are the annihilation operators of a "particle" and a "hole", respectively, and p_F the Fermi momentum.

It is one of the most important objects in the recent many-body problem to find some kind of approximate normal modes in the interacting system which are usually called collective oscillations. The condition for the normal mode is given by the presence of operators A_c and A_c^* which satisfy an equation

$$[A_c^*,\ H]_- = -\omega_c A_c^*, \tag{2·3}$$

where ω_c is the frequency of the collective oscillation. These A_c's are a function of original operators a's and b's, and obey the canonical commutation relation, plus or minus according to the Fermion and Boson type collective motion. One of the typical examples is the plasma oscillation at high density discussed by us and others.[4] In some cases, however, the collective frequency ω_c becomes imaginary as will be shown in the following sections, which turns out to be connected with the instability of the Hartree-Fock solution.

A theorem concerning this instability can be formulated as follows. Suppose there is an operator S which is an n-th order ordered polynormial of a's and b's and satisfies

$$[S^*,\ H]_- = -\omega S^* + C \tag{2·4}$$

where C is composed of products of more than n ordered operators.* ω may be real or imaginary. Denoting the free vacuum, that is, the Fermi distribution by Φ_0 which is known to be the Hartree-Fock solution of our system, we will consider a family of variational functions defined by

$$\Psi(\lambda) = e^{i\lambda(S^*+S)}\Phi_0,\ \Psi(0) = \Phi_0. \tag{2·5}$$

Then the variational energy is given by

$$E(\lambda) = \langle \Psi(\lambda),\ H\Psi(\lambda)\rangle = \langle \Phi_0,\ e^{-i\lambda(S^*+S)} H e^{i\lambda(S^*+S)}\Phi_0\rangle, \tag{2·6}$$

which is of course equal to the Hartree-Fock energy for $\lambda=0$. If one takes the first derivative of Eq. (2·5) with respect to λ and makes λ tend to zero, one has

$$\frac{\partial}{\partial\lambda}E(\lambda)\Big|_{\lambda=0} = (-i)\langle \Phi_0,\ [S^*+S,\ H]_-\Phi_0\rangle \tag{2·7}$$

which is zero on account of Eq. (2·4). This is the ordinary statement that the Hartree-Fock solution is the variational one. If one takes a_p or b_p itself as S, one will have the Hartree-Fock single particle energy as ω.

In order to see whether the solution is really stable, one has to look into the sign of the second derivative of $E(\lambda)$ at $\lambda=0$ which is given by

$$\begin{aligned}\frac{\partial^2}{\partial\lambda^2}E(\lambda)\Big|_{\lambda=0} &= (-i)^2\langle \Phi_0,\ [S^*+S[S^*+S,\ H]_-]_-\Phi_0\rangle \\ &= (\omega+\omega^*)\langle \Phi_0,\ [S,\ S^*]_-\Phi_0\rangle,\end{aligned} \tag{2·8}$$

since the commutators of S's and C's have the zero expectation value. In the case where all ω's are real and positive,[6] one can show that the expectation value of $[S,\ S^*]_-$ is positive and one has

* S and C are assumed to have no constant terms.

$$\frac{\partial^2}{\partial\lambda^2}E(\lambda)\Big|_{\lambda=0}>0, \quad \text{for } \omega>0. \tag{2·9}$$

The Hartree-Fock solution satisfies, therefore, the minimum condition within the family of variations employed here. However, if some of ω's are imaginary ($\omega=i\Gamma$), then one has

$$\frac{\partial^2}{\partial\lambda^2}E(\lambda)\Big|_{\lambda=0}=0, \quad \text{for } \omega=i\Gamma, \tag{2·10}$$

and the minimum condition is usually violated.* It will be shown in the following sections that there exists in this case another ground state solution with lower energy which is to be obtained by the variational principle by making use of trial functions similar to Eq. (2·5):

$$\Psi(\alpha)=e^{i(S^*(\alpha)+S(\alpha))}\Phi_0, \tag{2·11}$$

where the function $S(\alpha)$ has the same structure as S with respect to operators, a's and b's, but the coefficients contain some variational parameters.

§ 3. Spin wave model of Overhauser—*Three-dimensional case*—

As an application of our stability condition, let us consider in this section a model discussed by Overhauser[1] where the potential is assumed to be of the δ-function. For the sake of convenience, one will separate the spin index and employ the two-component operator defined by

$$\boldsymbol{C}_p=\begin{pmatrix}C_{p\uparrow}\\ C_{p\downarrow}\end{pmatrix}. \tag{3·1}$$

Then the total Hamiltonian is written as

$$H=\Sigma_p \boldsymbol{C}_p^* \boldsymbol{C}_p E_p+\frac{\gamma}{2}\Sigma_{pp'q}\boldsymbol{C}_p^*(\boldsymbol{C}_{p'}^*\boldsymbol{C}_{p'+q})\boldsymbol{C}_{p-q},$$
$$E_p=p^2/2m, \tag{3·2}$$

where γ is the strength of the potential and is positive for repulsion and negative for attraction.

Now one takes as the operator S^* a form suggested by the study of collective oscillations in a Fermi gas,[4] in particular the plasma oscillation, and puts

$$S^*=\Sigma_p(\Phi^\sigma_{p;q}\boldsymbol{a}^*_{p+q}\sigma\boldsymbol{b}_p^*+\Theta^\sigma_{p;q}\boldsymbol{b}_{-p}\sigma\boldsymbol{a}_{-p-q}+\chi^\sigma_{p;q}\boldsymbol{a}^*_{p+q}\sigma\boldsymbol{a}_p+\Xi^\sigma_{p;q}\boldsymbol{b}_{-p}\sigma\boldsymbol{b}^*_{-p-q}), \tag{3·3}$$

where σ is 1 or any of the Pauli matrices, σ_x, σ_y and σ_z, and q is an arbitrary

* We will put the special case out of consideration in which $E^{III}(0)=0$ and $E^{IV}(0)>0$.

momentum. The meaning of $\boldsymbol{a}$ and $\boldsymbol{b}$ is clear from Eqs. (2·2) and (3·1). The coefficients Φ's are to be determined from Eq. (2·4), where the operator C now consists of products of more than three ordered operators. Putting

$$\omega_{p;q}=E_{p+q}-E_p, \tag{3·4}$$

and taking $\sigma=1$ one has the following coupled integral equations for Φ's;

$$\begin{aligned}
&(\omega-\omega_{p;q})\Phi^1_{p;q}=\gamma\,\Sigma_{p'}(\Phi^1_{p';q}-\Theta^1_{p';q}),\\
&(\omega+\omega_{p;q})\Theta^1_{p,q}=\ \text{,,}\quad\ \text{,,}\quad\ \text{,,}\quad\ ,\\
&(\omega-\omega_{p;q})\,\chi^1_{p;q}=\ \text{,,}\quad\ \text{,,}\quad\ \text{,,}\quad\ ,\\
&(\omega-\omega_{p;q})\,\Xi^1_{p;q}=\ \text{,,}\quad\ \text{,,}\quad\ \text{,,}\quad\ ,
\end{aligned} \tag{3·5}$$

from which the secular equation for ω is obtained as

$$1-\gamma\sum_{\substack{p\\|p+q|>p_F\\|p|<p_F}}\left(\frac{1}{\omega-\omega_{p;q}}-\frac{1}{\omega+\omega_{p;q}}\right)=0. \tag{3·6}$$

If one takes $\sigma=\sigma_x$, σ_y or σ_z, the sign in front of γ is changed and one has, instead of (3·6), an equation

$$1+\gamma\sum_{\substack{p\\|p+q|>p_F\\|p|<p_F}}\left(\frac{1}{\omega-\omega_{p;q}}-\frac{1}{\omega+\omega_{p;q}}\right)=0. \tag{3·7}$$

From the stability conditions, Eqs. (2·8) and (2·9), one can conclude that if the coupling is sufficiently large, either Eq. (3·6) or Eq. (3·7) according to the sign of γ has an imaginary root for ω and the Hartree-Fock solution becomes unstable. In the one-dimensional case, this instability always occurs for q equal to $2P_F$ irrespective of the strength and sign of γ as pointed out by Overhauser. More specifically, for the repulsive case ($\gamma>0$), Eq. (3·6) leads only to real ω, whereas Eq. (3·7) has always an imaginary solution in the one-dimensional problem. For the attractive case ($\gamma<0$), the role of Eqs. (3·6) and (3·7) is interchanged.[7]

In order to get the Overhauser solution for the one-dimensional repulsive case ($\gamma>0$) according to our procedure, Eq. (2·11), one puts

$$S=-i\sum_k \boldsymbol{C}_k^*\frac{\sigma_x+i\sigma_y}{2}\boldsymbol{C}_{k+q}\alpha_k, \tag{3·8}$$

which generates the transformations

$$\begin{aligned}
&e^{i(S+S^*)}\,C_{k\uparrow}\,e^{-i(S+S^*)}=\cos\alpha_k\cdot C_{k\uparrow}-\sin\alpha_k\cdot C_{k+q\downarrow},\\
&e^{i(S+S^*)}\,C_{k\downarrow}\,e^{-i(S+S^*)}=\cos\alpha_{k-q}\cdot C_{k\downarrow}+\sin\alpha_{k-q}\cdot C_{k-q\uparrow}.
\end{aligned} \tag{3·9}$$

The minimum condition for the expectation value with respect to $\Psi(\alpha)$ determines the function α_k by

$$2\alpha_k=\tan^{-1}\frac{\beta_q}{\omega_{k,q}};\ 1=\gamma\sum_l((|l|<p_F)-(|l+q|<p_F))\frac{\omega_{l;q}/|\omega_{l;q}|}{\sqrt{\omega_{l;q}^2+\beta_q^2}}. \quad (3\cdot10)$$

The transformed Hamiltonian takes the form, disregarding the constant term which is actually lower than the Hartree-Fock energy,

$$H_{Overhauser}=\sum_k E_{k\uparrow}C_{k\uparrow}^*C_{k\uparrow}+\sum_k E_{k\downarrow}C_{k\downarrow}^*C_{k\downarrow}+(4\text{ operators ordered}), \quad (3\cdot11)$$

with

$$E_{k\uparrow}=\frac{E_k+E_{k+q}}{2}-\frac{\sqrt{\omega_{k;q}^2+\beta_q^2}}{2}\frac{\omega_{k;q}}{|\omega_{k;q}|},$$
$$E_{k\downarrow}=\frac{E_k+E_{k+q}}{2}+\frac{\sqrt{\omega_{k;q}^2+\beta_q^2}}{2}\frac{\omega_{k;q}}{|\omega_{k;q}|}. \quad (3\cdot12)$$

There is another form of $S(\alpha)$ in this case given by

$$S=i\sum_k \boldsymbol{C}_k^*\sigma_z\boldsymbol{C}_{k+q}\alpha_k, \quad (3\cdot13)$$

which however leads to a higher ground state energy than the value obtained above.

The above result is identical with what Overhauser has already obtained, but our criterion seems to work in more general cases in finding the variational trial functions. It should be noticed that the Hartree-Fock solution will be stable in the three dimensional case within the family of variations employed here, if the coupling is sufficiently weak.[8]

§ 4. B.C.S. theory of superconductivity

Let us now turn to the difficulty which one encounters in dealing with the B.C.S. model Hamiltonian of superconductors. In this case, one can sum up all ladder type diagrams up to infinite order following the technique of Gell-Mann and Brueckner,[3] the remaining diagrams being inversely proportional to the total volume to be neglected, but the propagator for a pair of electrons has an imaginary pole.[8] This situation can be easily reproduced in our language and is shown, as expected, to lead to the instability of the Hartree-Fock solution.

The B.C.S. Hamiltonian is written as

$$H_{BCS}=\sum_{k;s}a_{k,s}^*a_{k,s}E_k-\sum_{k;s}b_{k,s}^*b_{k,s}E_k$$
$$+\gamma\sum_k(a_{k\uparrow}^*+b_{k\uparrow})(a_{-k\downarrow}^*+b_{-k\downarrow})\cdot\sum_{k'}(a_{-k'\downarrow}+b_{-k'\downarrow}^*)(a_{k'\uparrow}+b_{k'\uparrow}^*), \quad (4\cdot1)$$

where E_k's ($\lesseqgtr0$ according as $|\boldsymbol{k}|\lesseqgtr p_F$) are measured from E_F. Consider the operator S defined by

$$S=\sum_k(A_k a_{k\uparrow}^*a_{-k\downarrow}^*+B_k b_{k\uparrow}b_{-k\downarrow}). \quad (4\cdot2)$$

Then the coefficients A's and B's are to be determined from Eq. (2·4), where the operator C now consists of products of four ordered operators. One has

in this way

$$(\omega-2E_k)A_k=\gamma\sum_{k'}(A_{k'}-B_{k'}),$$
$$(\omega-2E_k)B_k=\gamma\sum_{k'}(A_{k'}-B_{k'}). \tag{4·3}$$

From which follows the eigenvalue equation for ω:

$$1=\gamma\left(\sum_{k(>|p_F|)}\frac{1}{\omega-2E_k}-\sum_{k(<|p_F|)}\frac{1}{\omega-2E_k}\right). \tag{4·4}$$

This result is identical with what was obtained in the diagram method.[10]

For the repulsive case ($\gamma>0$), all the eigenvalues ($\omega\gtrless0$) shift from zero to the outer side with respect to zero and are of course real, but for the attractive case ($\gamma<0$), this shift occurs to toward zero and the eigenvalue adjacent to zero goes over into an imaginary value. According to our criterion, the Hartree-Fock solution Φ_0 becomes unstable in the latter case and the new trial functions should be looked for in the form of Eq. (2·10), namely

$$\Psi(\lambda)=e^{i(\Sigma_k h_k(\lambda)\, c_{k\uparrow}{}^* c_{-k\downarrow}{}^*+\text{H.C.})}\Phi_0, \tag{4·5}$$

which generates the Bogolyubov transformation.[2] Thus one sees that our criterion works also in this case.

It should be noticed at this point that the collective mode discussed here is a special kind of scattering mode for a pair of opposite momenta and spins. The general treatment of scattering modes for the full Hamiltonian (2·1) has been presented elsewhere by one of the authors (K.S.),[11] which will serve as the instability criterion for the Hartree-Fock solution when the interaction includes an appreciable attractive part.

§ 5. Liquid helium with negative scattering length

Another example to which our instability criterion can be applied will be found in the model Hamiltonian derived by Bogolyubov and others for the discussion of a dilute Boson gas.[5] This is written as

$$H=\sum_k\beta_k{}^*\beta_k E_k+\frac{1}{2}n_0{}^2\alpha+\sum_q n_q 2\alpha n_0+\left(\frac{1}{2}\sum_q\beta_q{}^*\beta_{-q}^*\alpha\beta_0\beta_0+\text{H.C.}\right), \tag{5·1}$$

where β_q and $\beta_q{}^*$ are the annihilation and creation operators for a Boson with momentum $\boldsymbol{q}$, respectively, and the constant α is proportional to the scattering length. The sum in Eq. (5·1) does not include $\boldsymbol{q}=0$. The Hartree solution is in this case the state in which all the particles are degenerate in the state $\boldsymbol{K}=0$. If this solution is stable, then one will obtain, following Bogolyubov, the excitation energy of the form

$$\sqrt{E_k{}^2+2\alpha NE_k}=\omega_k, \tag{5·2}$$

where N is the total number of the particles.

In the language of normal mode, one can equivalently obtain the result by choosing the operators S in Eq. (2·4) as[10]

$$S_k^* = A_k \beta_k^* + B_k \beta_{-k}. \tag{5·3}$$

Then, putting $n_0 = N - \sum_q n_q$ and $\beta_0^* \beta_0 = N$, one has, omitting $(\sum_q n_q)^2$ term compared to N,

$$\begin{aligned}[S_k^*, H]_- &= A_k\{-(E_k+\alpha N)\beta_k^* - \alpha N \beta_{-k}\} + B_k\{(E_k+\alpha N)\beta_{-k} + \alpha N \beta_k^*\} \\ &= -\omega_k (A_k \beta_k^* + B_k \beta_{-k}),\end{aligned} \tag{5·4}$$

from which follow the equations to determine the coefficients A and B:

$$\begin{aligned}&\{\omega_k - (E_k+\alpha N)\} A_k + \alpha N B_k = 0, \\ &-\alpha N A_k + \{\omega_k + (E_k+\alpha N)\} B_k = 0.\end{aligned} \tag{5·5}$$

The solubility condition for this leads to the eigenfrequency ω_k given by Eq. (5·2).

If the scattering length (α) is negative, then ω_q becomes imaginary for low momentum $\boldsymbol{q} \sim 0$ and the Hartree solution is unstable. One may expect in this case to obtain a stable solution by adopting the variational trial functions,

$$\Psi(\lambda) = e^{i\Sigma_k (\alpha_k(\lambda) \beta_k^* \beta_0 + \text{H.C.})} \Phi_0. \tag{5·6}$$

One of the authors (K.S.) and Vasudevan[9] have recently determined the parameter α from the variational principle and actually obtained the ground state energy lower than the Hartree value. It was shown moreover that the real excitation energy was derived in this way.

§ 6. Application to field theory

It is anticipated also in field theory that some of the approximate eigenmodes of strongly interacting elementary particles may be imaginary and the free vacuum state becomes unstable according to our criterion. Then one may choose some appropriate variational trial functions to obtain the stable vacuum state with the real eigenmodes for excitation. The effective coupling will be changed in this case.

Let us consider, as a typical example, a system of the nucleon and the pseudoscalar neutral meson which are interacting each other through pseudoscalar coupling. The Hamiltonian is given by

$$\begin{aligned}H = &\sum_k \varphi_k^* \varphi_k \nu_k + \sum_{p;s} C_p^{*s} C_p^s \varepsilon_p \\ &+ \sum_k g_k (\varphi_k + \varphi_{-k}^*) \sum_{pss'} C_p^{*s} (u_p^{*s} \rho_2 u_{p-k}^{s'}) C_{p-k}^{s'},\end{aligned} \tag{6·1}$$

where φ_k's are the meson operators and C's the nucleon operators with positive

and negative energy, s being the spin index.* The function u is the ordinary Dirac spinor and

$$g_k=\frac{g}{(2\nu_k\Omega)^{1/2}},$$
$$\nu_k=\sqrt{\boldsymbol{k}^2+\mu^2},\quad \varepsilon_p=\pm\sqrt{\boldsymbol{p}^2+m^2}, \tag{6·2}$$

where Ω is the normalization volume, and μ and m the masses of meson and nucleon, respectively. In the hole theory, one usually puts

$$C_p^{\ s}=\begin{cases} a_p^{\ s} & \text{for } \varepsilon_p>0, \\ b_p^{s*} & \text{for } \varepsilon_p<0, \end{cases} \tag{6·3}$$

where a is the annihilation operator for the nucleon and b for the anti-nucleon. In order to avoid the divergence difficulty, one will occasionally introduce the high momentum cutoff.

Let us first look for approximate eigenmodes for the meson by choosing the function S in Eq. (2·4) as

$$S^*=\sum_k A_k\varphi_k^*+\sum_k B_k\varphi_{-k}+\sum_{pkss'} D_{p,p-k}^{s,s'}C_p^{*s}C_{p-k}^{s'}. \tag{6·4}$$

Then the coefficients A's are to be determined from Eq. (2·4) where C now consists of products of three ordered operators. One gets in this way

$$(\omega-\nu_k)A_k=-g_k\sum_{p,s,s'}D_{p,p-k}^{s,s'}\{(u_{p-k}^{*s'}\rho_2 u_p^{s-})-(u_{p-k}^{*s'-}\rho_2 u_p^{s})\},$$
$$(\omega+\nu_k)B_k=-g_k\sum_{p,s,s'}\ \text{(same as above)},$$
$$(\omega-(\varepsilon_p-\varepsilon_{p-k}))\,D_{p,p-k}^{s,s'}=g_k(u_p^{*s}\rho_2 u_{p-k}^{s'})(A_k+B_k), \tag{6·5}$$

where $\boldsymbol{p}^-$'s (or $\boldsymbol{p}^+$'s) refer to the negative (or positive) energy state hereafter. The eigenvalue equation for ω becomes

$$\omega^2-\nu_k^{\ 2}+2g_k^{\ 2}\nu_k\sum_{p,s,s'}\left\{\frac{|(u_{p^-}^{s*}\rho_2 u_{p-k^+}^{s'})|^2}{\omega+|\varepsilon_p|+|\varepsilon_{p-k}|}+\frac{|(u_{p^+}^{s*}\rho_2 u_{p-k^-}^{s'})|^2}{-\omega+|\varepsilon_p|+|\varepsilon_{k-k}|}\right\}=0,$$

namley,

$$1=-\frac{4g_k^{\ 2}\nu_k}{\omega^2-\nu_k^{\ 2}}\sum_p\frac{2(|\varepsilon_{p+(k/2)}|+|\varepsilon_{p-(k/2)}|)\{|\varepsilon_p|^2-(1/4)(|\varepsilon_{p+(k/2)}|-|\varepsilon_{p-(k/2)}|)^2\}}{\{-\omega^2+(|\varepsilon_{p+(k/2)}|+|\varepsilon_{p-(k/2)}|)^2\}\,|\varepsilon_{p+(k/2)}|\,|\varepsilon_{p-(k/2)}|}, \tag{6·6}$$

from which one sees that if the cutoff for the sum is large enough, an imaginary solution is obtained and the free vacuum becomes unstable. This situation will be seen clearly in the Appendix for the special case $\boldsymbol{k}=0$.

The following variational trial functions are now tenable from our criterion to obtain the stable solution:

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* The unit $\hbar=c=1$ is taken. The Dirac operator ρ_2 is equal to $i\gamma_4\gamma_5$ in terms of the ordinary γ-matrices.

$$\Psi=\exp[\sum_k(A_k\varphi_k{}^*-A_k{}^*\varphi_k)+i\sum_{p,p',s,s'}D^{s,s'}_{p,p'}C^{*s}_{p}C^{s'}_{p'}]\cdot\Phi_0 \tag{6·7}$$

which generates the transformations

$$\varphi_k{}^*\to\varphi_k{}^*+A_k{}^*,\quad \varphi_k\to\varphi_k+A_k,$$
$$C^{*s}_{p}\to\sum_{p',s'}C^{*s'}_{p'}(e^{-iD})^{s',s}_{p',p}. \tag{6·8}$$

The new Hamiltonian has the form

$$\begin{aligned}
&H\to H_{transf.}=H_1+H_2+E_0,\\
&H_1=\sum_k\varphi_k{}^*\varphi_k\nu_k+\sum_{\substack{p',p''\\ s',s''}}:C^{*s'}_{p'}\{\sum_{ps}(e^{-iD})^{s's}_{p'p}\varepsilon_p(e^{iD})^{ss''}_{pp''}\\
&\quad+\sum_k g_k(A_k+A^*_{-k})\sum_{pts}(e^{-iD})^{s's}_{p'p}(u^{*s}_{p}\rho_2u^{t}_{p-k})(e^{iD})^{t}_{p-k\,p''}{}^{s''}\}C^{s''}_{p''}:\\
&\quad+\sum_k g_k(\varphi_k+\varphi^*_{-k})\sum_{\substack{p'p''p\\ s's''st}}:C^{*s'}_{p'}(e^{-iD})^{s's}_{p'p}(u^{*s}_{p}\rho_2u^{t}_{p-k})(e^{iD})^{t}_{p-k\,p''}{}^{s''}C^{s''}_{p''}:\\
&H_2=\sum_k\varphi_k{}^*\{\nu_kA_k+g_k\sum_{p's'pst}(e^{-iD})^{s's}_{p'-p}(u^{*s}_{p}\rho_2u^{t}_{p+k})(e^{iD})^{t}_{p+k\,s'p'}-\}+\text{H.C.}\\
&E_0=\sum_k A_k{}^*A_k\nu_k+\sum_{\substack{pp'\\ ss'}}(e^{-iD})^{s's}_{p'-p}\varepsilon_p(e^{iD})^{ss'}_{pp'}-\\
&\quad+\sum_k g_k(A_k+A^*_{-k})\sum_{p's'pst}(e^{-iD})^{s's}_{p'-p}(u^{*s}_{p}\rho_2u^{t}_{p-k})(e^{iD})^{t}_{p-k\,s'p'}-.
\end{aligned} \tag{6·9}$$

The stationary condition for E_0 with respect to A and A^* leads to the equations

$$\begin{aligned}
&\nu_kA_k+g_k\sum_{p's'pst}(e^{-iD})^{s's}_{p'-p}(u^{*s}_{p}\rho_2u^{t}_{p+k})(e^{iD})^{t}_{p+k\,s'p'}-=0,\\
&\nu_{-k}A^*_{-k}+g_{-k}\sum_{p's'pst}\ (\text{same as above})=0,
\end{aligned} \tag{6·10}$$

which makes H_2 vanish. To make variation with respect to D, one must take into account the condition

$$\sum_{p,s}(e^{-iD})^{s's}_{p'p}(e^{iD})^{ss'}_{pp'}=1. \tag{6·11}$$

By introducing the Lagrange indefinite multiplier, one obtains another equation

$$(\delta_{p',p''}\varepsilon_p-\lambda^{s'}_{p''})(e^{iD})^{ss'}_{pp'}+\delta_{p',p''}-\sum_k g_k(A_k+A^*_{-k})\sum_t(u^{*s}_{p}\rho_2u^{t}_{p-k})(e^{iD})^{t}_{p-k\,s'p'}=0, \tag{6·12}$$

from which it follows that

$$\lambda^{s'}_{p'}=0,\quad (e^{iD})^{s\,s'}_{pp'}-=\text{arbitrary}. \tag{6·13}$$

For the sake of convenience, one may therefore replace Eq. (6·12) by

$$(\varepsilon_p-\lambda^{s'}_{p'})(e^{iD})^{ss'}_{pp'}+\sum_k g_k(A_k+A^*_{-k})\sum_t(u^{*s}_{p}\rho_2u^{t}_{p-k})(e^{iD})^{t}_{p-k\,s'p'}=0. \tag{6·14}$$

Multiplying this with $(e^{-iD})^{s'''s}_{p'''p}$ and taking sum over s and p, one gets

$$\begin{aligned}
&\sum_{ps}(e^{-iD})^{s'''s}_{p'''p}\varepsilon_p(e^{iD})^{ss'}_{pp'}-\lambda^{s'}_{p'}\delta_{s's'''}\delta_{p'p'''}\\
&\quad+\sum_k g_k(A_k+A^*_{-k})\sum_{pss''}(e^{-iD})^{s'''s}_{p'''p}(u^{*s}_{p}\rho_2u^{s''}_{p-k})(e^{iD})^{s''}_{p-k\,p'}{}^{s'}=0.
\end{aligned} \tag{6·15}$$

One can now rewrite the transformed Hamiltonian, Eq. (6·9), and Eqs. (6·10) and (6·14) in terms of the function

$$v_q^t(\boldsymbol{p}) = \sum_{s(\pm\varepsilon_p)} u_p^s (e^{tD})_{pq}^{st}, \tag{6·16}$$

where $(\pm\varepsilon_p)$ means the sum over the sign of the energy with momentum $\boldsymbol{p}$. Namely, one has

$$\begin{aligned} H_{transf.} &= \sum_k \varphi_k^* \varphi_k \nu_k + \sum_{ps} : C_p^{*s} C_p^s : \lambda_p^s \\ &+ \sum_k g_k (\varphi_k + \varphi_{-k}^*) \sum_{\substack{ps \\ p's'}} : C_p^{*s} \sum_{p''} (v_p^{*s}(\boldsymbol{p}'') \rho_2 v_{p'}^{s'}(\boldsymbol{p}''-\boldsymbol{k})) C_{p'}^{s'} : \\ &+ \sum_k A_k^* A_k \nu_k + \sum_{p,s} \lambda_{p^-}^s ; \end{aligned} \tag{6·17}$$

$$\nu_k A_k + g_k \sum_{pp's} (v_{p^-}^{*s}(\boldsymbol{p}') \rho_2 v_{p^-}^s(\boldsymbol{p}'+\boldsymbol{k})) = 0, \tag{6·18}$$

$$(\boldsymbol{\alpha p} + \beta m - \lambda_q^t) v_q^t(\boldsymbol{p}) + \sum_k g_k (A_k + A_{-k}^*) \rho_2 v_q^t(\boldsymbol{p}-\boldsymbol{k}) = 0. \tag{6·19}$$

In deriving Eq. (6·17), use has been made of Eq. (6·15). The last two equations lead to a non-linear equation for v, the general solution of which is difficult to obtain, and one is obliged to content oneself with the following particular solution. Let us put

$$v_q^t(\boldsymbol{p}) = \delta_{q,p} w_q^t. \tag{6·20}$$

Then Eqs. (6·18) and (6·19) become

$$\begin{aligned} &\nu_k A_k + \delta_{k;0} g_k \sum_{qt} (w_{q^-}^{*t} \rho_2 w_{q^-}^t) = 0, \\ &(\boldsymbol{\alpha q} + \beta m + 2 g_0 A_0 \rho_2 - \lambda_q^t) w_q^t = 0, \end{aligned} \tag{6·21}$$

which has a solution

$$w_q^t = \frac{1}{(1 + \{2g_0 A_0/(\lambda_q + \varepsilon_q)\}^2)^{1/2}} \left(1 + \frac{2g_0 A_0}{\lambda_q + \varepsilon_q} \rho_2\right) u_q^t, \tag{6·22}$$

where u_q^t is the ordinary Dirac amplitude and

$$\begin{aligned} \lambda_q &= \sqrt{\varepsilon_q^2 + (2g_0 A_0)^2}, \quad \text{for } \varepsilon_q > 0, \\ &= -\sqrt{\varepsilon_q^2 + (2g_0 A_0)^2}, \quad \text{for } \varepsilon_q < 0. \end{aligned} \tag{6·23}$$

The function A_k is zero for $\boldsymbol{k} \neq 0$ and A_0 satisfies

$$1 + \frac{4g_0^2}{\nu_0} \sum_q \frac{(-1)}{|\lambda_q|} = 0, \tag{6·24}$$

which has the solution if the cutoff is sufficiently large.[12] Our transformed Hamiltonian (6·17) has now the form

$$\begin{aligned} H_{transf.} &= \sum_k \varphi_k^* \varphi_k \nu_k + \sum_{ps} : C_p^{*s} C_p^s : \pm \sqrt{\varepsilon_p^2 + (2g_0 A_0)^2} \\ &+ \sum_k g_k (\varphi_k + \varphi_{-k}^*) \sum_{pss'} : C_p^{*s} \cdot \frac{1}{(1 + \{2g_0 A_0/(\lambda_p + \varepsilon_p)\}^2)^{1/2}} \end{aligned}$$

$$\times\frac{1}{(1+\{2g_0A_0/(\lambda_{p-k}+\varepsilon_{p-k})\}^2)^{1/2}}\cdot\left(u_p^{*s}\cdot\left\{\rho_2\left(1+\frac{(2g_0A_0)^2}{(\lambda_p+\varepsilon_p)(\lambda_{p-k}+\varepsilon_{p-k})}\right)\right.\right.$$

$$\left.\left.+2g_0A_0\left(\frac{1}{\lambda_p+\varepsilon_p}+\frac{1}{\lambda_{p-k}+\varepsilon_{p-k}}\right)\right\}u_{p-k}^{s'}\right)\times C_{p-k}^{s'}:-2\sum_p|\varepsilon_p|+\Delta E_0,\quad(6\cdot25)$$

with

$$\Delta E_0=-\sum_p\frac{(\sqrt{\varepsilon_p^2+(2g_0A_0)^2}-|\varepsilon_p|)^2}{\sqrt{\varepsilon_p^2+(2g_0A_0)^2}}\ (<0),\qquad(6\cdot26)$$

which is the energy decrease on account of our transformation.

It should be noticed here that the solubility of Eq. (6·24) leads to the condition for the cutoff momentum and the coupling constant, which is consistent with the condition that Eq. (6·6) has an imaginary solution. The reasonable values for these quantities adopted in the cutoff theory give

$$\frac{4g_0^2}{\nu_0}\sum_q\frac{1}{|\varepsilon_q|}>1,\qquad(6\cdot27)$$

which is the condition that Eq. (6·6) with $\boldsymbol{k}=0$ has an imaginary solution for ω (see the Appendix) and is at the same time the condition that Eq. (6·24) has a real solution for $2g_0A_0$. Thus our criterion seems really to work. The effective coupling in Eq. (6·26) has now a scalar term in marked contrast to the original coupling in Eq. (6·1), but these interaction terms becomes always smaller with respect to the positive-negative component and vanishes in the strong coupling limit.

After the transformation, one can construct the eigen-value equation corresponding to Eq. (6·6) again, but in this case on account of the deformation of vacuum (or mathematically due to Eq. (6·24)) there is no imaginary root (see the Appendix), and the free vacuum defined by our new Hamiltonian Eq. (6·25) is now stable against the deformation considered.

§ 7. Conclusion

A criterion has been presented to see the stability of the Hartree-Fock solution for the given dynamical system. If one can construct any kind of approximate collective modes which may have an imaginary frequency, then the Hartree-Fock solution becomes unstable in the sense that a state deformed in accordance with this collective oscillation will give a lower ground state energy. A method of choosing appropriate variational trial functions is proposed in this case and is actually shown to give stable solutions in some examples, that is, the three-dimensional spin wave model of Overhauser, the theory of Liquid He^4 with negative scattering length and the B.C.S. theory of superconductivity. This method is then applied to field theory, in particular a meson-nucleon system which in fact shows the instability mentioned above, and one sees that the

"zeroth order" vacuum is deformed into another which now includes virtual pairs and mesons and that the effective coupling is changed in such a way that the new eigenfrequencies of the meson and nucleon become real. The high frequency part of the original coupling is not altered, but there might be some collective modes, e.g. nucleonic level strucutre, arising from this part, just like the plasma oscillation which screens the long-range tail of the Coulomb force.

Appendix

The eigenvalues of the meson

The eigenvalue equation, Eq. (6·6), can be evaluated explicity. As an illustration, let us consider the special case $\boldsymbol{k}=0$. Then one has to solve the equation

$$1=-\frac{4g_0^2\nu_0}{\omega^2-\nu_0^2}\sum_{\boldsymbol{p}}\frac{|\varepsilon_p|}{|\varepsilon_p|^2-\omega^2/4}.$$

The right-hand side is shown as a function of ω^2 in Fig. 1, on the assumption that the instability condition Eq. (6·27) is satisfied, which means the point B lies above 1. (ν_0 is, of course, smaller than m.) The point A corresponds to an imaginary eigenvalue. If the stability condition is satisfied, one has Fig. 2 in which the point B lies below 1 and a collective mode of excitation associated with the point C appears which lies between 0 and $Min(\nu_0^2, 4m^2)$. But as stated in the text, any reasonable cutoff momentum and coupling strength can hardly satisfy the stability condition.

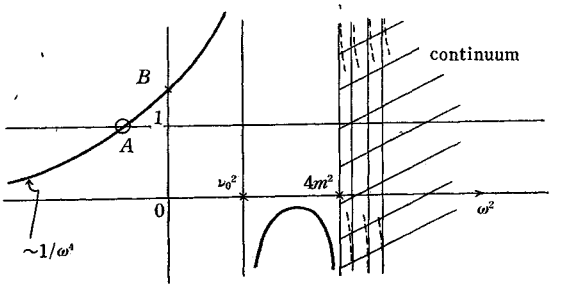

Fig. 1.

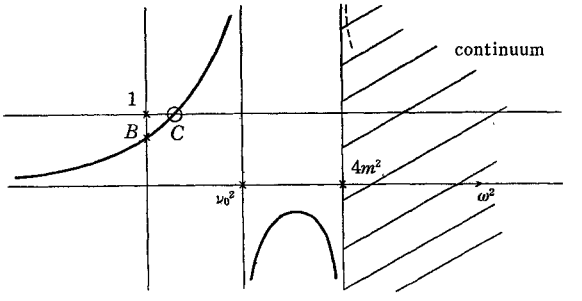

Fig. 2.

In the system which is described by the Hamiltonian Eq. (6·25), we can again construct (approximate) normal modes corresponding to Eq. (6·4), and the eigenvalue equation has a similar form to Eq. (6·6), the only difference being that w's and ε's are now replaced by ω's and λ's which satisfy Eq. (6·21), namely

$$\omega^2-\nu_k^2+2g_k^2\nu_k\sum_{\boldsymbol{p}ss'}\left\{\frac{|(w_{\boldsymbol{p}-}^{s*}\rho_2 w_{\boldsymbol{p}+-\boldsymbol{k}}^{s'})|^2}{\omega+|\lambda_p|+|\lambda_{p-k}|}+\frac{|(w_{\boldsymbol{p}+}^{s*}\rho_2 w_{\boldsymbol{p}--\boldsymbol{k}}^{s'})|^2}{-\omega+|\lambda_p|+|\lambda_{p-k}|}\right\}=0.$$

This leads to the eigenvalue equation (for $\boldsymbol{k}=0$)

$$1=-\frac{4g_0^2\nu_0}{\omega^2-\nu_0^2}\sum_p\frac{|\varepsilon_p|^2}{(|\lambda_p|^2-\omega^2/4)|\lambda_p|}.$$

The right hand side is an increasing function of ω^2 ranging from $-\infty$ to 0, and at $\omega^2=0$ we have

$$\text{right hand side}=\frac{4g_0^2}{\nu_0}\sum_p\frac{1}{|\lambda_p|}\frac{|\varepsilon_p|^2}{|\lambda_p|^2}<1,$$

owing to the eigenvalue equation for A_0, Eq. (6·24). One has therefore no imaginary solution for ω. There appears instead a solution for ω which lies between 0 and $Min(\nu_0, 2|\lambda_0|)$ and is to be connected with the solutions for $\boldsymbol{k}\neq 0$ to make a continuous spectrum.

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11) The last reference in (4).
12) Note that Eq. (6·24) is relativistically invariant, because $\sum_q 1/|\lambda_q|$ is scalar ($|\lambda_q|$ is the energy of the nucleon, see Eq. (6·25)) if one does not introduce the cutoff.