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ON THE THEORY OF A GAP FOR A CLASS OF HAMILTONIANS

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1. INTRODUCTION

We shall consider a system of a large number, N, of particles in a large volume, V, with a Hamiltonian

$$H = \Sigma\, T(k)\, a^*_k a_k + \\ + \frac{1}{2V} \sum_{k,q} U(k_2 - k_1)\, \delta_{k_1 + q_1 - q_2 - k_2} \times \\ \times a^*_{k_2} a^*_{q_2} a_{q_1} a_{k_1} . \tag{1.1}$$

Here a, a^* are usual fermion annihilation and creation operators, $T(k)$ is kinetic energy of a particle with momentum k. Let us introduce, as usual, the Fermi momentum k_F. It is conventional to introduce new operators b_p and b_h of annihilation of particles and holes

$$a_k = \begin{cases} b_p & k = p, \quad |p| > k_F , \\ b^*_h & k = -h; \quad |h| < k_F . \end{cases} \tag{1.2}$$

Then Hamiltonian (1.1) transforms into the normal form:

$$H = H_0 + \{ \sum_p H_2(p)\, b^*_p b_p - \sum_h H_2(h)\, b^*_h b_h \} + \\ + (40) + (31) + (22) + (13) + (04). \tag{1.3}$$

Here $|p| > k_F > |h|$,

$$H_2(k) = T(k) + \frac{1}{V} \sum_h [U(0) - U(k-h)], \quad k = p, h, \tag{1.4}$$

$(40) = (pphh\,|\,0)$ is the part of interaction responsible for the simultaneous creation of two particles and two holes;

$$(31) = 2(pph|p) + 2(hhp|h), \tag{1.5}$$

here two twrms describe the process of one-particle annihilation with the creation of two particles and one hole, and the process of one-hole annihilation with the creation of two holes and one particle;

$$(22) = (pp|pp) + (hh|hh) + 4(ph|hp), \qquad (1.6)$$

where the last term, e.g. describes the annihilation of a state "particle + hole" and creation of an analogous state with other momenta;

$$(13) = (31)^*, \quad (04) = (40)^*. \qquad (1.7)$$

The quantity H_0 in eq. (1.3) is a constant.

1. We shall consider the following states:

a) a (supposed) ground state Ω_0, the state, which in the limit of weak interaction ($U \to 0$) tends to the Fermi-vacuum $|0_F>$, as defined by the condition

$$b_p|0_F> = b_h|0_F> = 0,$$

b) particle-hole scattering state Ω_{ph}, which tends to the state $b_p^* b_h^*|0>$ as $U \to 0$. We shall calculate the energies of states Ω_0 and Ω_{ph}, using the simplest perturbation theory formula[1]

$$E_n = E_n^0 - \sum_{\alpha \neq n} H_{n\alpha} H_{\alpha n} (E_\alpha^0 - E_n^0)^{-1} +$$
$$+ \sum_{\substack{\alpha, \beta \neq n \\ \alpha \neq \beta}} H_{n\alpha} H_{\alpha\beta} H_{\beta n} (E_\alpha^0 - E_n^0)^{-1} (E_\beta^0 - E_n^0)^{-1} - \dots . \qquad (1.8)$$

Let us denote the energy of the state Ω_0 by E_0 and the excitation energy of the state Ω_{ph} by Λ_{ph}. We shall take $E_n^0 \sim H_2(k)$ rather than $E_n^0 \sim T(k)$. We have

$$\Lambda_{ph} = \Lambda_p + \Lambda_h = H_2(p) - H_2(h) + \Sigma_2(p) +$$
$$+ \Sigma_2(h) + \Sigma_3(p) + \Sigma_3(h) + O(U^4). \qquad (1.9)$$

Here Σ_2 and Σ_3 are the second and third terms of eq. (1.8).

1.1. Equation (1.4) and the condition $T(p) > T(h)$, $|p| > k_F > |h|$ imply the quantity $H_2(p) - H_2(h)$ to be positive,

if $|p| > k_F > |h|$, and to be zero, if $|p| = k_F = |h|$ (interaction is supposed to be weak). Thus the perturbation corrections Σ_2 and Σ_3 may be significant only in a certain vicinity of the Fermi surface. We have shown (Sec. 2) that

$$\Sigma_2(p) + \Sigma_2(h) = 0 \qquad \text{if} \quad |p| = k_F = |h|.$$

But the third order contribution $\Sigma_3(p) + \Sigma_3(h)$ does not disappear on the Fermy surface. By virtue of the spherical symmetry, this contribution is constant on this surface.

1.2. If this constant is positive, there exists a gap between the excited-state energy spectrum, and the ground-state energy; our gap is an effect of the third-order perturbation theory.

1.3. If this constant is negative, the states Ω_{ph} with $|p| = k_F = |h|$ have lower energies than our (supposed) ground state. It seems to be of a considerable interest to construct an actual ground state in this case (Appendix A).

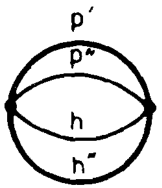
1.4. In a media with a crystal structure the quantity $\Sigma_3(p) + \Sigma_3(h)$ (item 1.1) is not a constant on the Fermi surface. This quantity may, e.g. change its sign on this surface. In this case one has to use the method of the Appendix A to construct the ground state and the gap will not exist. If, however, the lowest order correction is positive on the Fermi surface, the gap does exist.

II. THE PERTURBATION THEORY CALCULATIONS

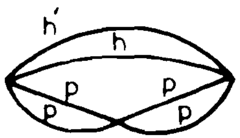
We shall start with the calculation of our ground state energy. Equations (1.3) and (1.8) give

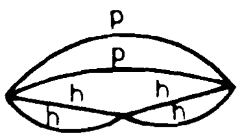
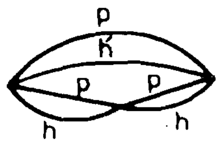
$$E_0 = H_0 - <0_F| \{(04)\frac{1}{H_2}(40) - (04)\frac{1}{H_2}(22)\frac{1}{H_2}(40)\} |0> +$$
$$+ H_0 + E_{20} + E_{30} + \dots . \qquad (2.1)$$

Here H_2 is the part of Hamiltonian (1.3) in brackets. The function $(p'p''h'h''|0) \sim (40)$ is antisymmetric in $(p'p'')$ and $(h'h'')$; thus

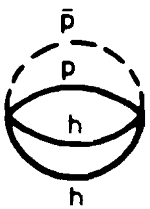
$$E_{20} = -4$$  (2.2)

One can prove, analogously,

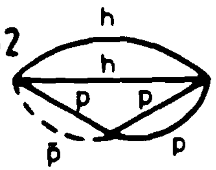
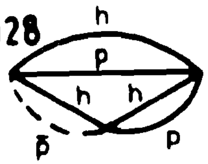
$$E_{30} = 8$$  (2.3)

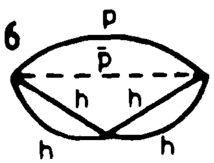
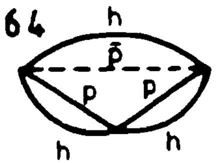
$+ 8$  $+ 64$ 

(see eq. (1.6)). If there is a particle of momentum $\bar{p}$, one has to eliminate values $p' = \bar{p}$ and $p'' = \bar{p}$ from the sum in eq. (2.2). Thus, eq. (2.2) gives the contribution

$\delta_1 \Sigma_2(\bar{p}) = 8$  (2.4)

to the quantity $\Sigma_2(\bar{p})$. Analogously, eq. (2.3) gives the contribution $\delta_1 \Sigma_3(\bar{p}) =$

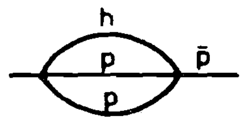
-32  -128  (2.5)

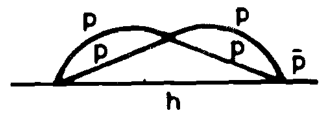
-16  -64 

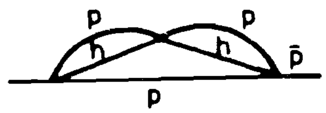
to the quantity $\Sigma_3(\bar{p})$. Another contribution to these quantities comes from the formula:

$$\delta_2 \Sigma_2(\bar{p}) + \delta_2 \Sigma_3(\bar{p}) =$$
$$= \langle 0_F | b_{\bar{p}} \{ -(13)(H_2 - H_2(\bar{p}))^{-1} (31) + \qquad (2.6)$$
$$+ (13)(H_2 - H_2(\bar{p}))^{-1} (22)(H_2 - H_2(\bar{p}))^{-1} (31) \} b^*_{\bar{p}} | 0_F \rangle .$$

Here $(31) \sim 2(pph|p)$, see eq. (1.5), $H_2(\bar{p})$ see eq. (1.4).
As a result, we have:

$\delta_2 \Sigma_2(\bar{p}) = -8$  (2.7)

$\delta_2 \Sigma_3(\bar{p}) = 16$  (2.8)

$+ 64$ 

These formulae and analogous formulae for the hole energies show the quantity $\Sigma_2(p) + \Sigma_2(h) = \sum_{i=1}^{2} [\delta_i \Sigma_2(p) + \delta_i \Sigma_2(h)]$ to disappear, and the quantity $\Sigma_3(p) + \Sigma_3(h) = \sum_{i=1}^{2} [\delta_i \Sigma_3(p) + \delta_i \Sigma_3(h)]$ not to dissappear on the Fermi surface $|p| = k_F = |h|$. We shall decipher our diagrams in Appendix B*.

ACKNOWLEDGEMENT

I am indebted to Professors V.K.Fedyanin, V.G.Makhankov, I.N.Mikhailov and V.G.Soloviev for discussions.

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* The consideration above is oversimplified beginning from eq. (1.6) which is to be substituted by eqs. (B2)-(B4). As a matter of fact, the quantity (2.8) cancels at $|\bar{p}| = |h'| = k_F$ the part of the quantity $\delta_1 \Sigma_3(h')$ which one can get by cutting off the lines h' on the diagrams (2.3). The remaining part of the quantity $\delta_1 \Sigma_3(h')$ and analogous part of the quantity $\delta_1 \Sigma_3(\bar{p})$ determine the non-zero value of $\Sigma_3(\bar{p}) + \Sigma_3(h')$ (at $|\bar{p}| = |h'| = k_F$).

APPENDIX A

Here we consider the problem of the ground-state when $\Lambda_{ph} < 0$ at $|p| = k_F = |h|$ (item 1.3). The state Ω_{ph} with an excitation energy Λ_{ph} and the analogously defined state $\Omega_{p_1h_1p_2h_2}$ with an excitation energy $\Lambda_{p_1h_1} + \Lambda_{p_2h_2}$ at

$$|p_1| = |p_2| = k_F = |h_1| = |h_2|$$

have energies lower than does the "ground state" Ω_0. Let us denote by G some region in the momentum space which is divided by the Fermi sphere $|k| = k_F$ into two equal parts. Let us denote by $\Omega(G)$ a state which in the limit $U \to 0$ tends to the state $(\prod_{p,h \in G} b_p^* b_h^*)|0_F>$; here momenta p, h cover all the region G (the volume V is finite, so is the number of states M(G)). We write down the energy E(G) of the state $\Omega(G)$ in the form

$$E(G) = H_0 + H_2(G) + \Sigma_2(G) + \Sigma_3(G) + \dots,$$

where

$$H_2(G) = \sum_{p \in G} H_2(p) - \sum_{h \in G} H_2(h)$$

and

$$\Sigma_n(G) = \delta_1 \Sigma_n(G) + \delta_2 \Sigma_n(G), \qquad n = 2, 3,$$

$$\delta_1 \Sigma_2(G) = E_{20}(G),$$

$$\delta_1 \Sigma_3(G) = E_{30}(G),$$

$$\delta_2 \Sigma_2(G) = \sum_{p \in G} \delta_2 \Sigma_2(p, G) + \sum_{h \in G} \delta_2 \Sigma_2(h, G),$$

$$\delta_2 \Sigma_3(G) = \sum_{p \in G} \delta_2 \Sigma_3(p, G) + \sum_{h \in G} \delta_2 \Sigma_3(h, G).$$

Here E_{20} and E_{30} are sums (2.2), (2.3), $E_{20}(G)$ and $E_{30}(G)$ are analogous sums, where the summation momenta do not belong to region G, quantities $\delta_2\Sigma_2(p, G), \dots \delta_2\Sigma_3(h, G)$ are defined as sums (2.7), (2.8), where the summation momenta do not belong to the region G. Having constructed the energy E(G), we can now minimise it via variation of the region G. Let the region $G = G_0$ give a minimal value to the energy E(G). The region seems to be something like $k_F < |p| < p_0$, $h_0 < |k| < k_F$. Thus for our case ($\Lambda_{ph} < 0$ at $|p| = |h| = k_F$) to the real ground state there corresponds not the totally filled Fermi sphere, but a certain filled sphere $|k| < h_0 < k_F$ and a filled spherical layer $k_F < |k| < p_0$ with an empty gap $h_0 < |k| < k_F$ between them. The width of the gap depends on U and tends to zero if $U \to 0$. There is no gap in the excitation energy spectrum in the considered case. Unpleasant feature of states Ω_0, $\Omega_{ph}, \dots$ is the fact that the norms of all these states tend to infinity as $V \to \infty$ (if $\Lambda_{ph} < 0$). The proof of this fact will be published separately.

APPENDIX B

Here we shall decipher the diagrams of Sec. 2. We shall start by drawing mentally a vertical line between every two subsequent vertices on all the diagrams.

Let us first consider the diagram of eq. (2.2). It contains the vertex function (40) $\sim (p'p''h''h'|0) =$

$$= [U(p'+h') - U(p''+h') - U(p'+h'') + U(p''+h'')]\,\delta_{p'+p''+h''+h'}/(2V) =$$

$$= A(p'p'')A(h'h'')U(p'+h')\,\delta_{p'+p''+h''+h'}/(2V), \tag{B1}$$

see eqs. (1.1), (1.2); here A(a,b) denotes the operator of antisymmetrization over arguments a and b. To the vertical line on the diagram (2.2) there corresponds the denominator $H_2(p') + H_2(p'') - H_2(h'') - H_2(h')$. There diagrams of eq.(2.3) contain three new vertices:

$$(2|2)_1 = (p_4p_3|p_2p_1) = A(p_3p_4)A(p_2p_1)U(p_4 - p_1)\,\delta_{p_4+p_3-p_2-p_1}/(2V), \tag{B2}$$

$$(2|2)_2 = (h_4h_3|h_2h_1) = A(h_4h_3)A(h_2h_1)U(h_1 - h_4)\,\delta_{h_1+h_2-h_3-h_4}/(2V), \tag{B3}$$

$$(2|2)_{12} = (p_2h_2|h_1p_1) = -A(-h_2, p_1)A(-h_1, p_2)U(p_2 - p_1)\,\delta_{p_2+h_2-h_1-p_1}/(2V). \tag{B4}$$

Vertical lines, e.g., on the first diagram (2.3) give the denominator

$$[H_2(p_3) + H_2(p_4) - H_2(h_2) - H_2(h_1)][H_2(p_2) + H_2(p_1) - H_2(h_2) - H_2(h_1)] .$$

The diagrams of eqs. (2.7), (2.8) contain new vertices

$$(3|1)_1 = (p_2 p_1 h|\bar{p}) = A(p_2 p_1) A(-h, \bar{p}) U(p_2 - \bar{p}) \delta_{p_2 + p_1 + h - \bar{p}} /(2V), \quad (B5)$$

$$(3|1)_2 = (h_2 h_1 p|\bar{h}) = A(-\bar{h}, p) A(h_1 h_2) U(h_2 - \bar{h}) \delta_{h_2 + h_1 + p - \bar{h}} /(2V). \quad (B6)$$

Vertical lines, e.g., on the second diagram of eq. (2.8) give the denominator

$$[H_2(p_2) - H_2(h_2) + H_2(p) - H_2(\bar{p})] [H_2(p_1) - H_2(h_1) + H_2(p) - H_2(\bar{p})]$$

(see the second term of eq. (2.6)). Here, the summation runs over $p_2 h_2 p_1 h_1 p$. Let us note also that the vertical lines of the fourth diagram of eq. (2.5) give the denominator

$$[H_2(\bar{p}) - H_2(h_2) + H_2(p) - H_2(h)] [H_2(p_1) - H_2(h_1) + H_2(\bar{p}) - H_2(h)] .$$

Here, the summation runs over $h p h_1 p_1 h_2$. In the diagram of eq.(2.4) the summation runs over $h_1 h_2 p$; one can get this diagram from that of eq. (2.2) by fixing $p' = \bar{p}$ and $p'' = \bar{p}$ of momenta p' , p'' . These values of summation momenta are forbidden in the presence of a particle with momentum $\bar{p}$.

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Note added in proof

Our problem is closely related to that of BCS Hamiltonian. Our method of consideration is valid also for the Hamiltonian

$$H = \Sigma\, \omega_k a_k^* a_k^* + \Sigma\, \Omega_q b_q^* b_q + \left(\frac{\lambda}{\sqrt{V}} \sum_{kq} a_k^* a_{k-q} b_q D_q + \text{c.c.} \right)$$

of the microscopic conductivity theory. A gap here is an effect of the fourth order (λ^4) perturbation theory.

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Заставенко Л.Г. E17-89-722

К теории щели для некоторого класса гамильтонианов

Рассматривается проблема щели между основным состоянием вторично-квантованного гамильтониана и спектром возбужденных состояний. Дан пример гамильтониана, для которого щель возникает при надлежащем выборе знака потенциала в третьем порядке теории возмущений. При противоположном знаке потенциала щели нет. Основному состоянию в этом последнем случае соответствует не полностью заполненная сфера Ферми, $|k| < k_F$, а некоторая заполненная сфера меньшего радиуса $|k| < h_0 < k_F$ плюс заполненный сферический слой $k_F < |k| < p_0$, в то время как слой $h_0 < |k| < k_F$ остается пустым. Итак: пусть первые n_0 поправки к энергии системы частица-дырка $\Sigma_n(p, h)$ с импульсами p, h, $n = 1, 2, \ldots, n_0$, равны нулю на поверхности Ферми $|p| = |h| = k_F$. Тогда, если величина $\Sigma_{n_0+1}(p, h)$ положительна на всей поверхности Ферми, то щель есть, если эта величина отрицательна на части поверхности Ферми, то щели нет.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

Препринт Объединенного института ядерных исследований. Дубна 1989

Zastavenko L.G. E17-89-722

On the Theory of a Gap for a Class of Hamiltonians

We study the problem of a gap between the ground state and the excited state spectrum of the second-quantized Hamiltonian. The class of Hamiltonians is found where the gap is an effect of the third-order perturbation theory. The gap exists if the sign of the potential is properly chosen. For the opposite sign of the potential there is no gap. In this case, to the ground state there corresponds not the totally filled Fermi sphere $|k| < k_F$, but a filled sphere of a smaller radius h_0, $|k| < h_0 < k_F$, plus a filled spherical layer $k_F < |k| < p_0$ with an empty gap $h_0 < |k| < k_F$ between them ($h_0, p_0 \to k_F$ as interaction tends to zero). Generally: suppose that the first n_0 perturbation-theory corrections $\Sigma_n(p, h)$, $n = 1, 2, \ldots n_0$, to the energy of a particle and a hole pair with momenta p, h are zero on the Fermi surface $|p| = |h| = k_F$. Suppose also that $\Sigma_{n_0+1}(p, h)$ is positive on the whole Fermi surface. Than, the gap exists. If quantity $\Sigma_{n_0+1}(p, h)$ is negative at some point of the Fermi surface, then there is no gap.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

Preprint of the Joint Institute for Nuclear Research. Dubna 1989