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THREE-BODY CORRELATION EFFECTS IN THE SPECTRUM OF ELEMENTARY EXCITATIONS IN LIQUID ^{4}He, II

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It was found that it is not possible to describe accurately the roton states in the spectrum of elementary excitations of liquid ^{4}He taking into account one and two-phonon functions. The effect of three-body correlations in this basis was found to be insignificant. It was also shown that the basic relation, obtained earlier, compared with the standard Brillouin-Winger perturbation procedure is not an improvement.

1. Introduction

In this paper we continued to investigate the effects of three-body correlations in the spectrum of elementary excitations in liquid ^{4}He. The first part of our investigations was published in Ref. 1 further on denoted by I.

Using the variational ansatz, in I we found a general relation

$$E = H_{mm} - \left\{ \sum_{\substack{n \\ (\neq m)}} \frac{|\langle m \mid H - E \mid n \rangle|^2}{E - H_{nn}} \right\}^2 \cdot$$

$$\cdot \left\{ \sum_{\substack{n\ n' \\ (\neq m)}} \sum \frac{\langle m \mid H - E \mid n \rangle \langle n \mid H - E \mid n' \rangle \langle n' \mid H - E \mid m \rangle}{(E - H_{nn})(E - H_{n'n'})} \right\}^{-1}, \qquad (1)$$

where H is the Hamiltonian of the system, E-energy, and $|m\rangle, |n\rangle, |n'\rangle$ are states of the system. Using this relation for the computation of energy of elementary excitations in liquid ^{4}He and taking for the basis one and two-phonon functions we obtained the expression

$$\varepsilon = \varepsilon_0 + \frac{\varepsilon_2}{1 - \frac{\varepsilon_3}{\varepsilon_2}}, \tag{2}$$

where

$$\varepsilon_0 = \frac{\hbar^2 k^2}{2m S_k}, \tag{3}$$

$$\varepsilon_2 = \frac{1}{2} \sum_{\vec{l}}{}' \frac{|\langle \vec{k} | W | \vec{k} - \vec{l}, \vec{l} \rangle|^2}{a_l}, \tag{4}$$

$$\varepsilon_3 = \frac{1}{4} \sum_{\vec{l}} \sum_{\vec{l}'} \frac{\langle \vec{k} | W | \vec{k} - \vec{l}, \vec{l} \rangle \langle \vec{k} - \vec{l}, \vec{l} | W | \vec{k} - \vec{l}', \vec{l}' \rangle \langle \vec{k} - \vec{l}', \vec{l}' | W | \vec{k} \rangle}{a_l a_{l'}}, \tag{5}$$

S_k — structure factor,
E_0 — ground state energy,

$$W = H - E_0 - \varepsilon_0, \tag{6}$$

$$a_l = \varepsilon - \varepsilon_0 (l) - \varepsilon_0 (|\vec{k} - \vec{l}|). \tag{7}$$

In paper I the computation was performed for the relation

$$\varepsilon = \varepsilon_0 + \varepsilon_2 \tag{8}$$

which follows from (2) if we do not take into account ε_3.

In this paper the complete expression (2) was computed numerically after the matrix elements had been analitically derived. Therein we used a three-body structure factor obtained in Refs. 2,3.

2. *Basic relation, numerical computation and discussion*

After introducing matrix elements the expressions ε_2 and ε_3 can be written in a form suitable for integration

$$\varepsilon_2 = \frac{1}{8\pi^2 \varrho} \int_0^\infty \mathrm{d}l\, l^2 \int_{-1}^{1} \mathrm{d}t \frac{1}{S_k S_l S_{k-l}} \frac{\{F(k, l, t)\}^2}{a_l}, \tag{9}$$

$$\varepsilon_3 = \frac{1}{4\,(2\pi)^6\,\varrho^2}\,\frac{1}{S_k}\int_0^\infty \mathrm{d}l \cdot l^2 \int_0^\infty \mathrm{d}l'\, l'^2 \int_{-1}^{1} \mathrm{d}t \int_{-1}^{1} \mathrm{d}t' \int_0^{2\pi} \mathrm{d}\varphi \int_0^{2\pi} \mathrm{d}\varphi' \, \frac{1}{S_{k-l}\,S_{k-l'}\,S_l\,S_{l'}} \cdot$$

$$\cdot \frac{F(k,l,t)}{a_l} \cdot \frac{F(k,l',t')}{a_{l'}} \cdot G(k,\vec{l},\vec{l'}), \tag{10}$$

where

$$F(k,l,t) = \frac{\hbar^2}{2m}\left[(k^2 - klt)\,S_l + klt\,S_{k-l} - \frac{k^2}{S_k}\,S_3(k,-k-l,l)\right], \tag{11}$$

$$G(k,\vec{l},\vec{l'}) = \frac{\hbar^2}{2m}\Big[l \cdot l'T \cdot S_3(k-l,-k+l',l-l') + (klt - ll'T)\,S_3(k-$$

$$-l,-l',-k+l+l') + (kl't' - ll'\,T)\,S_3(-k+l',l,k-l-l') + (k^2 -$$

$$- klt - kl't' + ll'\,T)\,S_3(l,-l',l'-l) - \frac{k^2}{S_k}\,S_4(k-l,l,-k-l',l')\Big], \tag{12}$$

$$T = t \cdot t' + \sqrt{(1-t^2)\,(1-t'^2)}\cos(\varphi - \varphi'). \tag{13}$$

S_3 and S_4 are three-body and four-body structure factors. Convolution approximation (CA) of these functions has the form of[1,4,5]

$$S_3^c(-k,l,k-l) = S_k \cdot S_l \cdot S_{k-l} \tag{14}$$

$$S_4^c(k-l,-k+l',l,-l') = S_{k-l}\,S_{k-l'}\,S_l\,S_{l'} \cdot \{-2 + S_k + S_{l-l'} + S_{k-l-l'}\}. \tag{15}$$

There are several more approximative relations for function S[6-9]. In this paper we used in addition to S^c the Feenberg's form of function S_3[2,3,10]

$$S_3^F(-k,l,k-l) = \frac{1}{\dfrac{k^2}{S_k} + \dfrac{l^2}{S_l} + \dfrac{|\vec{k}-\vec{l}|^2}{S_{k-l}}} \cdot \left\{\frac{1}{2}(k^2 + l^2 + |\vec{k}-\vec{l}|^2)\,S_3^c + \right.$$

$$\left. + \frac{1}{2}(|\vec{k}-\vec{l}|^2 - k^2 - l^2)\,(S_l + S_k - S_{k-l}) + l^2\,S_k + k^2\,S_l\right\}. \tag{16}$$

Relation (16) is transformed into a convolution relation (14) if we neglect three-body correlations in the ground-state wave function[2].

We used the iterative procedure to solve the integral equation (2) where ε is an unknown quantity. In this paper we achieved greater accuracy in calculating quantity ε_2. The integration region was divided into smaller areas and 32-point Gauss integration was applied to each area. Table presents the solution of equation

TABLE

k	Convolution approximation			Feenberg approximation		
	S_J	S	S_{exp}	S_J	S	S_{exp}
0.1	2.1371	2.2492	2.2164	2.1379	2.2501	2.2177
0.2	4.5667	4.8040	4.3361	4.5790	4.8216	4.3546
0.3	7.1504	7.6490	6.7182	7.2202	7.7530	6.8094
0.4	9.8493	10.495	8.8462	10.063	10.814	9.111
0.5	12.367	13.048	11.003	12.884	13.857	11.603
0.6	14.577	15.140	12.875	15.597	16.503	13.977
0.7	16.333	16.636	14.663	17.783	18.810	16.436
0.8	17.848	17.868	16.273	19.961	20.953	18.826
0.9	18.732	18.340	17.494	21.399	22.084	20.764
1.0	19.599	18.885	18.705	22.794	23.233	22.660
1.1	19.902	18.895	19.836	23.297	23.353	24.331
1.2	20.395	19.194	21.062	23.914	23.692	25.983
1.3	20.306	18.897	22.189	23.496	22.815	27.265
1.4	20.542	19.013	22.695	23.383	22.392	27.303
1.5	20.218	18.517	21.393	22.338	20.895	24.386
1.6	20.263	18.457	20.792	21.736	20.004	22.625
1.7	19.947	17.976	19.510	20.632	18.552	20.086
1.8	19.926	17.835	18.801	19.941	17.635	18.501
1.9	20.076	17.905	17.885	19.499	17.058	16.851
2.0	20.075	18.527	18.805	19.709	17.190	17.383
2.1	22.136	19.961	20.791	20.770	18.286	19.128
2.2	24.265	22.190	23.677	22.704	20.325	21.952
2.3	26.984	25.048	27.050	25.380	23.183	25.506
2.4	30.049	28.198	30.633	28.574	26.549	29.603
2.5	33.172	31.276	33.497	31.984	30.017	32.987
2.6	36.325	34.386	36.372	35.577	33.723	39.320
2.7	39.224	37.076	38.618	38.921	36.957	39.173

Energy spectrum of excitations in convolution and Feenberg approximation. Results are given in 10^{-23} J for density $\varrho = 2.185 \cdot 10^{28}\,\mathrm{m}^{-3}$ and k in $10^{10}\,\mathrm{m}^{-1}$.

(8) for the convolution and Feenberg approximation of three-body structure function S_3. For a two-body structure factor we used forms S_J and S from Ref. 11 and the experimental structure factor S_{exp} from Ref. 12. Functions S_J include the Jastrow correlation whereas S contains three-body correlations in addition to the Jastrow correlations.

In order to calculate the quantity ε_3 we used the number theoretic method[13] in which for 80.000 sub-integral points the relative error was 1—3%. We computed the complete expression only for the phonon and roton parts of the spectrum. We found that the effect of term ε_3 is insignificant both for the convolution and Feenberg approximation.

Considering the form of relation (2) it can be realized that it was derived from the Brillouin-Wigner (BW) perturbation formula for energy after collecting an infinite number of diagrams of the type drawn in Fig 1. The physical states described by these diagrams include only one and two-phonon functions. According to the results obtained, it can be concluded that one and two-phonon functions cannot describe roton states although three-body correlations were included.

The value of relation (1) in solving similar problems can be analysed extending the basis of states and using the in literature[8] already derived matrix elements.

If we also include into the calculation the states presented on the energy diagram, Figure 2, it can be found from relation (1) that the energy of elementary excitation in the roton part of the spectrum is $\varepsilon = 15.27 \cdot 10^{-23}$ J for $k = 1.99 \cdot 10^{10}$ m^{-1}.

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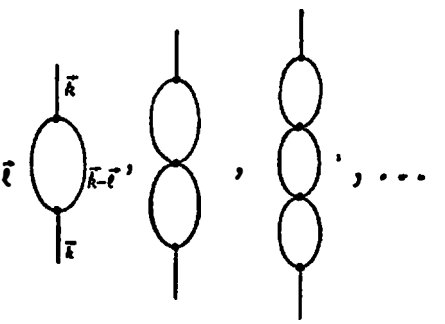

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Fig. 1. Energy diagrams which include one and two phonon states.

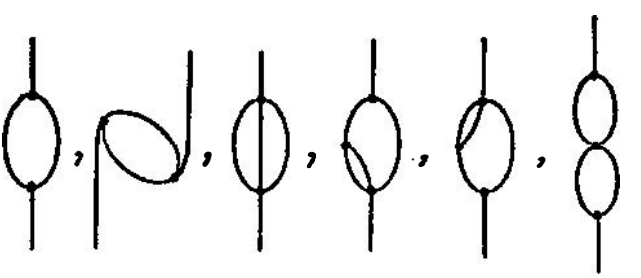

Fig. 2. Energy diagrams included in *BW* perturbation calculation.

As the result of the standard *BW* perturbation procedure in this case is $\varepsilon = 15.29 \cdot 10^{-23}$ J, it can be concluded that relation (1) is not more advantageous than the standard *BW* perturbation procedure. It should be noted that here many-body correlation of a certain form were also included into the computation of matrix elements[8].

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TROČESTIČNI KORELACIONI EFEKTI U SPEKTRU ELEMENTARNIH POBUĐENJA U TEKUĆEM ^{4}He, II

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Nađeno je da u okviru jedno-i dvo-fononskih funkcija nije moguće dobro opisati rotonska stanja u spektru elementarnih pobuđenja tekućeg ^{4}He. Nađeno je da je utjecaj tročestičnih korelacija u ovoj bazi zanemariv. Također je pokazano da osnovna relacija, izvedena u jednom ranijem radu, u ovoj problematici nema praktičnu prednost u odnosu na standardni Brillouin-Wignerov račun smetnje.