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Ground state of a mass-3 boson system and Superfluid ^{3}He

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〈Abstract〉

Ground state energies of a mass-3 boson system are calculated at various densities by the mass-difference perturbation theory and Yim-Massey variational method for a binary boson system using the results of the corresponding liquid ^{4}He by Schiff and Verlet. These results agree fairly well with results of Massey, and Schiff and Verlet. The present correlation functions between two mass-3 bosons compared with those between two ^{4}He atoms are qualitatively in agreement with those in Massey theory. Also, we conclude there exist s-pairing states in the liquid ^{3}He from the present results.

한 질량-3 보존계의 기저 상태와 초유체 헤리윰—3

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〈요 약〉

한 질량-3 보존계의 기저상태 에너지들을 쉬프와 벨렛에 의한 대응되는 액체 헤리윰-4의 결과들을 사용하여 한 두개의 성분으로 된 보존계에 적용한 질량차 섭동 이론과 임—매시 변분 방법에 의하여 여러 밀도들에서 계산한다. 이 결과들은 매시에 의한 결과들과 쉬프와 벨렛에 의한 결과들과 상당히 잘 일치한다. 두 헤리윰-4 원자들 간의 상호 관계된 함수들과 비교된 계산된 두 질량-3 보존들 간의 상호 관계된 함수들은 매시 이론에서 비교된 것들과 정성적으로 일치한다. 또한, 계산된 결과들로 부터 액체 헤리윰-3에 애스-페어링 상태들이 존재한다는 것을 결론한다.

The ground state properties of a mass-3 boson system have received considerable attention, theoretically since these properties can be used for the input information of the liquid ^{3}He properties.[1,2] The properties for the mass-3 boson system can be calculated using a variety of variational method, [1-3] i.e., Integral equation,[1] Monte Carlo method[3] or Molecular dynamics.[2] The other interesting methods may be an application of the mass-perturbation theories[4] (MPT) and Yim-Massey[5] (YM) theory for the ^{3}He$-^4$He mixture to a mass-3 boson system and the liquid ^{3}He. As pointed by Feenberg,[6] YM[6] and Baym[6] the mass-difference perturbation calculations for a mass-3 boson system using the results of the liquid ^{4}He have been some interests among a few physicists. A few years ago Baym[6] remarked explicitly in his paper these interests in the first order MPT. Here, we calculate these properties using a MPT and YM variational method.[5] Before going into the details we briefly review the definitions and a common existing theory for boson systems.

A bulk boson system is defined by the Hamiltonian

$$H=\sum_{i=1}^{N}\frac{\vec{p}_i^{\,2}}{2m}+\sum_{i<j=1}^{N}V(r_{ij}), \qquad (1)$$

where $\vec{p}_i$, m and N are the momentum and the bare mass of a boson and the total number of particles of the system obeying Bose statistics; $V(r)$, the two-body potential, is usually taken the Lennard-Jones 6—12 potential. The ground state properties of boson systems, in particular for the liquid ^{4}He, are known to be fairly accurately described by a Bijil, Dingle and Jastrow-type wave function,

$$\phi^B{}_0(\vec{r}_1,\cdots,\vec{r}_N)=\exp\left(\frac{1}{2}\sum_{i<j=1}^{N}u(r_{ij})\right) \quad , \qquad (2)$$

where $u(r)$ measures the correlations between two bosons; these correlation functions satisfy the usual boundary conditions,

$$\lim_{r\to 0} u(r)=-\infty \quad ,$$

and

$$\lim_{r\to\infty} u(r)=0 \quad .$$

Now, the pair distribution function, $g(r_{ij})$, is defined by

$$g(r_{ij})=\frac{N(N-1)}{n^2}\frac{\int|\phi^B{}_0|^2\, d(\vec{r}_i,\vec{r}_j)}{\int|\phi^B{}_0|^2\, d\vec{r}_1\cdots d\vec{r}_N}, \qquad (3)$$

where n is the number density of this system and $d(\vec{r}_i, \vec{r}_j)$ denotes $d\vec{r}_1\cdots d\vec{r}_N$ with $d\vec{r}_i\ d\vec{r}_j$ omitted. Using the above equations the ground state energies, E, can be expressed

$$E(n)=Ne_0(n) \quad , \qquad (4)$$

where $e_0(n)$ is the ground state energy per a particle in the form

$$e_0(n)=-\frac{\hbar^2 n}{8m}\int g(r)\ \nabla^2 u(r)d\vec{r} + \frac{1}{2}n\int g(r)V(r)d\vec{r} \quad . \qquad (5)$$

For the numerical calculations $u(r)$ can be over the wide range chosen fairly accurately in the form[1-3]

$$u(r)=-\left(\frac{A}{r}\right)^y \quad , \qquad (6)$$

where A is a variational parameter and y is 5 by Schiff and Verlet[2] (SV) and 10 by Massey,[1] respectively. In the process of minimizing $e_0(n)$ $u(r)$ and $g(r)$ can be obtained.

The MPT for a N mass-3 boson system are defined by a Hamiltonian

$$H=H_0+H_1 \quad , \qquad (7)$$

where H_0 and H_1 are the Hamiltonian of the liquid ^{4}He and the mass-difference perturbation, respectively, given by

$$H_0=\sum_{i=1}^{N}\frac{\vec{p}_i^{\,2}}{2m_4}+\sum_{i<j=1}^{N}V(r_{ij}), \qquad (8)$$

and

$$H_1=\sum_{i=1}^{N}\left(\frac{1}{2m_3}-\frac{1}{2m_4}\right)\vec{p}_i^{\,2}=\frac{1}{3}\sum_{i=1}^{N}\frac{\vec{p}_i^{\,2}}{2m_4}\ . \qquad (9)$$

In the above equations m_3 and m_4 are the masses of a mass-3 boson and a ^{4}He-atom, respectively. To the second order perturbation theory using eigenfunctions of H_0 at density, n, the ground state energy of the mass-3 boson system, E_{30}, is expressed

$$E_{30}=E_{40}+\frac{1}{3}\sum_{i=1}^{N}\langle 0|\frac{\vec{p}_i^{\,2}}{2m_4}|0\rangle-\frac{1}{9}\sum_{s}\sum_{i,j=1}^{N}\frac{\langle 0|\vec{p}_i^{\,2}/(2m_4)|s\rangle\langle s|\vec{p}_j^{\,2}/(2m_4)|0\rangle}{E_{40}-E_{4s}} + \text{higher orders}, \qquad (10)$$

where E_{40} and E_{4s} are the ground state and the excitation energies of N ^{4}He atoms, respectively, and $|0\rangle$ and $|s\rangle$ are the ground state and the intermediate states of the liquid ^{4}He, respectively. YM[5] used the paired phonon analysis to calculate the partial remaining terms beyond the first order perturbation instead of calculating the third term in Eq. (10), while Baym[6] used an intelligent method for the ^{3}He—^{4}He mixture. (Aso refer to Ref. 7.) The results by MPT are

Table: The ground state energy of a mass-3 boson, $e_0(n)$. MPT and YM are the present results using the mass-difference perturbation theory and Yim-Massey variational method, respectively. In this calculation we use n_0=0.01962Å^{-3}.

n/n_0	$e_0(n)$ (°K)			
	Massey	SV	MPT	YM
0.722	−2.563	−2.92	−2.927	—
0.7778	−2.565	—	−2.921	—
0.814	—	—	—	−2.59
0.8333	−2.59	—	−2.685	—
0.889	−2.56	—	−2.608	—
0.944	−2.428	—	−2.471	—
1.	−2.248	—	−2.151	−2.155
1.0555	−2.00	—	−1.745	−1.798
1.1111	—	—	−1.208	−1.311

shown in Table and compared with the results of Massey,[1] SV[2] and YM variational method[5] to be given below.

In YM variational method for N mass-3 bosons the trial ground-state wave function of Eq. (7), H, is chosen as in a binary boson system[5] as follows,

$$\phi^B{}_{03}(\vec{r}_1,\cdots,\vec{r}_N)=\phi^B{}_{04}(\vec{r}_1,\cdots,\vec{r}_N)e^{\frac{1}{2}\sum_{i<j=1}^{N}t(r_{ij})}, \quad (11)$$

where $\phi^B{}_{03}$ and $\phi^B{}_{04}$ are the ground-state wave functions of N mass-3 bosons and N ^{4}He atoms at the number density, n, respectively, and $t(r)$ is the correlation-difference between (3,3) particle pairs and (4,4) particle pairs at the number density, n, in the form

$$t(r)=-\left(\frac{B}{r}\right)^5 .$$

As in the binary boson system due to YM[5] the mass-3 boson pair distribution function, $g_3(r)$, can be expressed in terms of $t(r)$ and the liquid ^{4}He-pair distribution function, $g_4(r)$, at the same number density as the mass-3 number density in the form

$$g_3(r)=g_4(r)e^{t(r)}\left(1+\frac{1}{(2\pi)^3 n}\int d\vec{k}e^{-i\vec{k}\cdot\vec{r}}(2(S_4(k)-1)T_{\vec{k}}+T_{\vec{k}}{}^2)+\Delta g_3(r)\right), \quad (12)$$

where $S_4(k)$ is the ^{4}He liquid structure function defined by

$$S_4(k)=1+n\int(g_4(r)-1)e^{i\vec{k}\cdot\vec{r}}\,d\vec{r},$$
$$T_k=n\int g_4(r)(e^{t(r)}-1)e^{i\vec{k}\cdot\vec{r}}\,d\vec{r}, \quad (13)$$

and the contribution of $\Delta g_3(r)$ to the ground state energy is negligible in the previous experience.[5] Using Eqs. (6), (12) and (13) in the process of minimizing $e_0(n)$ in Eq. (4) $e_0(n)$, $t(r)$ and $g_3(r)$ are calculated. The present results using $u(r)$ and $g_4(r)$ of SV[2] are shown in the same Table as the above. In the Table $e_0(n)$ in the results of Massey[1] are normalized such as $e_0(n_{eq})$ is equal to be -2.59 °K at $n_{eq}=0.0163$Å^{-3}, where n_{eq} is the equilibrium density of the mass-3 boson system. The present results by YM variational method[5] above $n=0.01597$Å^{-3} can be fitted using a function in the form

$$e_0(n/n_0)=A(P^2)(n/n_0)+B(P^2)(n/n_0)^2, \quad (14)$$

where P is the pressure of the mass-3 boson system, n_0 is the equilibrium density of the liquid ^{4}He and $A(P^2)$, $B(P^2)$ and $e_0(n_{eq})$ are given by

$$A(0)=-1.295\ \text{°K},$$
$$B(0)=-0.3567\ \text{°K},$$

and

$$e_0(n_{eq})+n_{eq}\frac{\partial e_0(n_{eq})}{\partial n_{eq}}\bigg|_P=-2.59\ \text{°K}$$
$$\text{at } n_{eq}=0.814n_0. \quad (15)$$

The present results are in good agreement with the previous results[1,3] above $n=0.0163$ Å^{-3} and also the correlation functions in the present calculation agree qualitatively with those of Massey[1] rather than SV[2] since $t(r)$ is a negative function. We believe these disagreements arise from the determinations of the liquid ^{4}He-pair distribution functions.[8] Also, from the present results by YM variational method[5] the long-wavelength effective interactions between two ^{3}He atoms up to 20 atm are negative(*e.g.*, -0.5807°K$/n_0$ at zero pressure) and indicate s-pairing states in the liquid ^{3}He.[9] (Refer to Refs. 4 and 5 for the detail procedures.)

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References

* Present Address:

1. W.E. Massey, Phys. **151**, 153(1966); W.E. Massey and C.-W. Woo, ibid. **164**, 256(1967).
2. D. Schiff and L. Verlet, Phys. Rev. **160**, 208

(1967).

3. W. L. Mcmillan, Phys. Rev. **160**, 208(1965).
4. J. Bardeen, G. Baym and D. Pines, Phys. Rev. **156**, 207(1967); W. F. Saam, Ann. Phys. **53**, 219 (1969) and Ph. D. thesis, published(University of Illinois, 1968).
5. M. Yim and W. E. Massey, Phys. Rev. B **19**, 3529(1979); M. Yim, Ph. D. thesis, published (Brown University, 1975).
6. E. Feenberg, See, for example, Theory of Quantum Fluids(Academic Press, New York, 1969); M. Yim and W. E. Massey(unpublished); G. Baym, J. Low Temp. Phys. **18**, 335(1975).
7. M. Yim and W. E. Massey, We obtained (5/9) of the results of Baym in considering the partial terms in the higher order perturbations (unpublished).
8. Eq. (12) combined with Eq. (7) instead of the massive computations can be used directly to calculate the pair distribution- and the correlation-functions of boson systems, $g(r)$ and $u(r)+w(r)$, using the first trial functions, $g_1(r)$, $u_1(r)$ and $w_1(r)$, where

$$g_1(r)=e^{u_1(r)} ,$$

$u_1(r)$ is chosen to be $g_1(r)$ normalized and $w_1(r)$ is the same form as $u_1(r)$.
9. For example, the effective interaction, $V(k)$, between two ^3He atoms in pure liquid ^3He at zero pressure is (2/3) $(n_{e3}/n_0)^2\, V_m(k)$, where $V_m(k)$ is the effective interaction between two ^3He quasiparticles in the mixture at zero pressure (to be published and ref. 5). For different pressures the same procedures as in Eqs. (14) and (15) are simply fairly accurately adopted. For the surface regions of this system the same procedures as in this text and outlined in ref. 8 can be accurately used. (Also, refer to papers by M. Yim and W.E. Massey (Phys. Rev. B. **19**, 4562 and submitted to Phys. Rev. B).)