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Effective mass of a ^{3}He quasiparticle near surfaces of liquid ^{4}He

Moo Bin Yim
Department of Applied Physics*

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〈Abstract〉

The effective mass of a ^{3}He atom near surfaces is calculated at zero bulk pressure and zero concentration using the model of Yim and Massey. The present is $1.32m_3$ in good agreement with the experimental result of Eckardt, Edwards, Fatouros, Gasparini and Shen.

액체 헤리움-4의 표면들 근처에 한 헤리움-3 유사입자의 유효질량

任 武 彬*
응 용 물 리 학 과

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〈요 약〉

표면들 근처에 한 헤리움-3 원자의 유효질량이 임과 메시의 모델을 사용하여 0체기압과 0용액량 하에서 계산되어진다. 계산된 결과는 에칼드, 에드왈즈, 체토로스, 가스파리니와 쉔의 실험결과와 잘 일치하는 $1.32m_3$이다.

A single ^{3}He quasiparticle near the surface may be defined by the excitation energy, $\epsilon(k_\rho)$, of the form

$$\epsilon(k_\rho)=\mu_{3s}+\frac{\hbar^2 k_\rho^2}{2m_s} \quad , \tag{1}$$

where the effective quasiparticle interaction is neglected and k_ρ, m_s and μ_{3s} are, respectively, the two-dimensional wave vector, the effective mass and the chemical potential of a ^{3}He quasiparticle near the surface of the mixture at zero concentration. Experimental result of m_s by Eckardt et al.[1] is $1.3m_3$ at zero bulk pressure, where m_3 is the bare mass of a ^{3}He atom. But no theoretical microscopic calculation of m_s has been published yet. In the previous paper[2] we briefly discussed the procedure for calculating the effective mass of a ^{3}He quasiparticle, m_s, in the surface region using the model of Yim and Massey[2] (YM). However, the wave function for the bulk phase was not explicitly taken into account. Here, the wave function for the bulk phase is explicitly taken into account.

A system considered here is composed of one ^{3}He atom in a ^{4}He-surface region, a surface region and the bulk phase of pure liquid ^{4}He. In **YM** model[2] the Hamiltonian, H^m, for this system is defined by

$$H^m=H_\rho{}^m+H_z{}^m+H_b, \tag{2}$$

with the appropriate boundary condition and symmetry (refer to Ref. 2), where

$$H_\rho{}^m=\frac{p_{\rho 1}{}^2}{2m_3}+\sum_{i=2}^{N_s}\frac{p_{\rho i}{}^2}{2m_4}+\sum_{i<j=1}^{N_s}V(\rho_{ij}), \tag{3}$$

$$H_z{}^m=\frac{p_{z1}{}^2}{2m_3}+\sum_{i=2}^{N_s}\frac{p_{zi}{}^2}{2m_4}+\frac{1}{2}\sum_{\substack{i\neq j=1\\ z_i\neq z_j}}^{N_s}V(r_{ij}), \tag{4}$$

and

$$H_b=\sum_{l=N_s+1}^{N}-\frac{p_l^2}{2m_4}+\sum_{l\le m=N_s+1}^{N}V(r_{lm}). \quad (5)$$

In the above m_4 is the mass of a ^{4}He atom, coordinates 1,2 through N_s and N_s+1 through N, respectively, denote a ^{3}He atom in the surface region, ^{4}He atoms in the surface region and ^{4}He atoms in the bulk, and $V(\rho)$ and $V(r)$ are two-and three-dimensional Lennard-Jones 6—12 potentials, respectively. $\vec{p}_\rho$, $\vec{p}_z$ and $\vec{p}$ are, respectively, the momentum operators of the $\vec{\rho}$-and z-components in the surface region and the momentum operators in the bulk where z is assumed to be positive coordinate. We assume the translational invariance for the bulk phase and the same symmetry and boundary condition as in Ref. 2 for the surface region. We assume

$$H^m\Psi_0{}^m=E_0{}^m\Psi_0{}^m, \quad (6)$$

where $E_0{}^m$ and $\Psi_0{}^m$ are the boson type ground state-energy and-wave function of H^m, respectively, and $\Psi_0{}^m$ is defined by[2]

$$\Psi_0{}^m(\vec{r}_1;\vec{r}_2,\cdots\cdots,\vec{r}_{N_s};\vec{r}_{N_s+1},\cdots\cdots,\vec{r}_N)=\zeta_0(z_1)\varphi_0(z_2)\times\cdots\cdots\varphi_0(z_{N_s})\Psi^m{}_{0\rho}(\vec{\rho}_1;\vec{\rho}_2,\cdots\cdots,\vec{\rho}_{N_s})\Psi_0{}^B(\vec{r}_{N_s+1},\cdots,\vec{r}_N), \quad (7)$$

and

$$\int|\zeta_0(z)|^2\,dz=\int|\varphi_0(z)|^2dz=\int|\Psi^m{}_{0\rho}|^2\,d\vec{\rho}_1\cdots d\vec{\rho}_{N_s}=\int|\Psi_0{}^B|^2\,d\vec{r}_{N_s+1}\cdots\cdots d\vec{r}_N=1. \quad (8)$$

In the above $\zeta_0(z)$ and $\varphi_0(z)$ are, respectively, ground state wave functions of a mass-3 boson and a ^{4}He atom in z-direction, and $\Psi^m{}_{0\rho}$ and $\Psi_0{}^B$, respectively, those of the two-dimensional boson mixture in the surface region and pure bulk ^{4}He.[2] In order to calculate m_3 we consider only no-, one- and two-ripplon states given by no-ripplon states:

$$|0;\vec{k}_1\sigma_1)=\Psi_0{}^m(\vec{r}_1;\vec{r}_2,\cdots\cdots,\vec{r}_{N_s};\vec{r}_{N_s+1},\cdots\cdots,\vec{r}_N)\times\frac{e^{i\vec{k}\vec{\rho}_1\cdot\vec{\rho}_1}\,e^{-k_{s1}z_1}\,\chi(\sigma_1)}{\left(\int|\zeta_0|^2e^{-2k_{s1}z_1}\,dz_1\right)^{1/2}},$$

one-ripplon states:

$$|Q;\vec{k}_1\sigma_1)=\frac{\rho_Q\Psi_0{}^m\,e^{i\vec{k}\vec{\rho}_1\cdot\vec{\rho}_1}\,e^{-k_{s1}z_1}\,\chi(\sigma_1)}{\left(N_{s_4}S^{(4,4)}(Q)\int|\zeta_0|^2e^{-2k_{s1}z_1}dz_1\right)^{1/2}},$$

and two-ripplon states:

$$|Q,\ H;\ \vec{k}_1\sigma_1)=\frac{\rho_Q\rho_H\Psi_0{}^m\,e^{i\vec{k}\rho_1\cdot\vec{\rho}_1z}-e^{\vec{k}_{s1}z_1}\,\chi(\sigma_1)}{\left(N_{s_4}{}^2\,S^{(4,4)}(Q)\,S^{(4,4)}(H)\int|\zeta_0|^2\,e^{-2k_{s1}z_1}dz_1\right)^{1/2}}, \quad (9)$$

where Q and N_{s_4} are, respectively, a set of $\vec{\rho}$- and z-components wave vectors of the surface region and the bulk wave vector(i.e., $\vec{q}_\rho$, iq_z and $\vec{q}$ $(q\equiv(q_\rho{}^2+q_z{}^2)^{1/2})$) and the number of ^{4}He atoms in the surface region. $\vec{k}_\rho$ and ik_z are $\vec{\rho}$- and z-components of $\vec{k}(k\equiv(k_\rho{}^2+k_z{}^2)^{1/2})$. $\chi(\sigma_1)$ is the spin function and ρ_Q is the density fluctuation operator of ^{4}He atoms[2] defined by

$$\rho_Q=\sum_{l=2}^{N_s}e^{i\vec{q}_\rho\cdot\vec{\rho}_l}e^{-q_zz_l}+\sum_{j=N_s+1}^{N}e^{i\vec{q}\cdot\vec{r}_j}, \quad (10)$$

and $S^{(4,4)}(Q)$ is defined by

$$S^{(4,4)}(Q)=\frac{1}{N_{s_4}}\int|\Psi_0{}^m|^2|\rho_Q|^2d\vec{r}_1\cdots d\vec{r}_N. \quad (11)$$

In the above q_z is a function of q_ρ and k_z a function of k_ρ. Under the Löwdin transformation the correlated basis functions, Eq. (9), can be transformed into orthogonalized basis functions. (Refer for details to Ref. 3.) Using the orthogonalized basis functions one renormalized-ripplon states can be represented as follow:

$$|\mathbf{Q};\vec{k}_1\sigma_1\}=|\mathbf{Q};\vec{k}_1\sigma_1\rangle+\frac{1}{2}\sum_{Q'\neq0}\frac{|\mathbf{Q}-\mathbf{Q}',\ Q';\ \vec{k}_1\sigma_1\rangle W_{QQ'}}{\omega(Q)-\omega_0(Q')-\omega_0(|Q-Q'|)}, \quad (12)$$

where the renormalized-ripplon spectrum, $\omega(\mathbf{Q})$ is assumed to be the ripplon spectrum, $\omega(q_\rho)$, calculated in Ref. 4, $\omega_0(Q)$ is one bare ripplon spectrum, $|\cdots\}$ and $|\cdots\rangle$ represent the renormalized and the orthogonalized states, respectively and $W_{QQ'}$ is defined by

$$W_{QQ'}=\langle Q-Q',\ Q';\vec{k}_1\sigma_1|W|Q\,;\,\vec{k}_1\sigma_1\rangle. \quad (13)$$

However, the explicit expression of W-vertex is not important, here. Now, the Hamiltonian, H^m, using the ground state and one renormalized-ripplon states reads

$$H^m=E_0+\sum_{\vec{k},\sigma}e_0(k)\ a_{\vec{k}\sigma}{}^+a_{\vec{k}\sigma}+\sum_{Q}\omega(Q)\beta_Q{}^+\beta_Q+\sum_{Q,\vec{k},\sigma}Y_Q\beta_Q{}^+a_{\vec{k}-Q\sigma}{}^+a_{\vec{k}\sigma}+H.C.+\cdots\cdots, \quad (14)$$

where when the negative sign operates on Q, it makes the sign of $\vec{q}_\rho$, only changed, $e_0(k)$ is

$$e_0(k)=\frac{\hbar^2k^2}{2m_3},$$

$$Y_Q=\frac{(1-S^{(4,3)}(Q))\ (e_0(Q)+\omega_0(Q))}{2(N_{s_3}S^{(4,4)}(Q))^{1/2}}+\cdots,$$

and

$$E_0=E_0^m+\frac{1}{4}\sum_Q(e_0(Q)+\omega_0(Q))(S^{(4,3)}(Q)-1)^2/S^{(4,4)}(Q)+\cdots\cdots\ , \quad (15)$$

In the above N_{s_3} is the number of ^{3}He atoms in the surface region and $S^{(4,3)}(Q)$ is defined by

$$S^{(4,3)}(Q)-1=(n_{s_3}n_{s_4})^{1/2}\int(g^{(4,3)}(\rho)-1)e^{iQ\cdot\vec{\rho}}\zeta_{q_z}\varphi_{q_z}\times d\vec{\rho}, \quad (16)$$

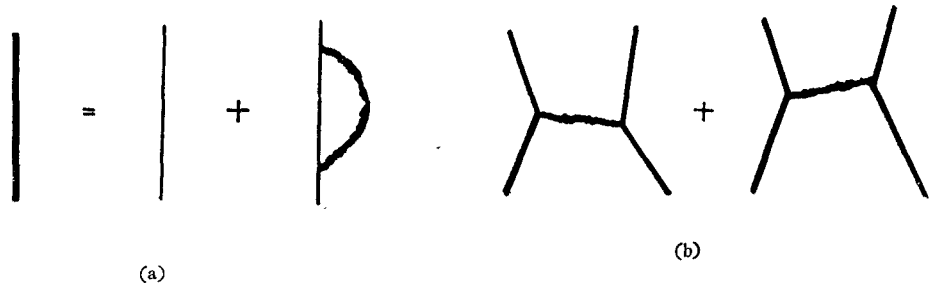
where n_{s_3} and n_{s_4} are number densities of ^{3}He atoms and ^{4}He atoms in the surface region and ζ_{q_z}, $\varphi_{q_z}$and $g^{(4,3)}(\rho)$ are defined by

$$\zeta_{q_z}=\int|\zeta_0(z)|^2\ e^{-q_z z}\ dz,$$

$$\varphi_{q_z}=\int|\varphi_0(z)|^2\ e^{-q_z z}\ dz,$$

and

$$n_{s_3}n_{s_4}g^{(4,3)}(\rho_{1N_s})=N_{s_3}N_{s_4}\int|\Psi_{0\rho}^m|^2 d\vec{\rho}_2\cdots\cdots d\vec{\rho}_{N_4-1}. \quad (17)$$



(a) (b)

Fig. (a). Self-energy of a ^{3}He induced by one-renormalized ripplon; (b). Effective interaction between two ^{3}He quasiparticles induced by one-renormalized ripplon.

Using the above Hamiltonian the effective mass, m_s, can be easily calculated by considering the self energy diagram shown in Figure (Here, we only consider ^{3}He-one renormalized-ripplon vertices as in the bulk mixture[3,5] and also shown is the effective interaction between two ^{3}He quasiparticles[3,5] induced by one renormalized-ripplon), i.e.,

$$e(k)=e_0(k)+\sum_Q\frac{|Y_Q|^2}{(e_0(k)-e_0(|\vec{k}-Q|)-\omega(Q))}, \quad (18)$$

where

$$e(k)=\frac{\hbar^2k^2}{2m_s}\ . \quad (19)$$

The leading term in Eq. (18) gives a constant contribution to $e(k)$ and the summation over $\vec{k}$ recovers E_0 to E_0^m. Since q_z is the function of q_ρ and k_z the function of k_ρ, keeping the term $O(k_\rho^2)$ of $e(k_\rho)$ gives the effective mass, m_s, as follows:

$$m_s/m_3=\Big(1-\frac{\hbar^2n_{s_4}}{24\pi}\int dq_\rho\ q_\rho^3\times\frac{(e_0(q_\rho)+\omega_0(q_\rho))^2\ (1-S^{(4,3)}(q_\rho))^2}{m_3n_{s_3}n_{s_4}S^{(4,4)}(q_\rho)(e_0(q_\rho)+\omega(q_\rho))^3}\Big)^{-1}, \quad (20)$$

where $n_{s\alpha}$ is the area number density of α-atoms and α can be either 3 or 4. The present result of m_s is $1.32m_3$ at zero bulk pressure and zero concentration using the results of YM[2,4] and pure ^{4}He liquid structure function, $S_0(q_\rho)$, in good agreement with the result of Eckardt et al.[1] (roton contribution to m_s in the present calculation is about 1%), where $S_0(q_\rho)$ is estimated from Ref. 4 by

$$S_0(q_\rho)=\frac{\hbar^2(q_\rho^2+q_z(q_\rho)^2)}{2m_4\omega(q_\rho)}\ . \quad (21)$$

The present effective interaction between two ^{3}He quasiparticles induced by one renormalized-ripplon, as q_ρ goes to zero, seems to be zero different from the bulk mixture.[6] We also note the long-wavelength effective interaction between two ^{3}He quasiparticles and the volume excess parameter near surfaces at constant pressure are approximately $0.8\ ^\circ K/n_s$ and 0.226 at zero bulk pressure and zero concentration, respectively, where $n_s=n_{s_3}+n_{s_4}$.

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