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Ripplon spectrum of liquid ^{4}He

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〈**Abstract**〉

Ripplon spectrum using the model of Yim and Massey is calculated for entire wave vectors, variationally, at zero bulk pressure. For small wave vectors less than 0.1565Å^{-1} it is also obtained using a hydrodynamics. The present result is in good agreement with the result of Edwards. Eckardt and Gasparini.

액체 헤리움-4의 리플론 스펙트럼

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〈**요 약**〉

임과 매시의 모델을 사용한 리플론 스펙트럼이 변분적으로 전 파벡터들에 대하여 계산되어 진다. 0.1565Å^{-1} 보다 적은 작은 파벡터들에대하여 0체기압에서 역시 유체동역학을 사용하여 구해진다. 계산된 결과는 에드왈즈, 에칼트와 가스파리니의 결과와 잘 일치한다.

There has been quite interest over the past two decades, both theoretically and experimentally, in the ripplon spectrum of liquid ^{4}He with free surfaces after papers of Atkins.[1] A few years ago Edwards et al.[2] obtained the ripplon spectrum for entire wave vectors by hydrodynamics. However, there is still lacking in the microscopic consideration.[3] Here, the ripplon spectrum is calculated for entire wave vectors, variationally. Yim and Massey[4] (YM) gave a simple model for surface regions of liquid ^{4}He in calculating surface properties of liquid ^{4}He and properties of the surface state of ^{3}He atoms near surfaces of liquid ^{4}He. The system considered here is composed of a surface region and the bulk phase. In YM model[4] the Hamiltonian, H, of this system is defined by(Assume the translational invariance for the bulk phase)

$$H=H_s+H_b \quad , \tag{1}$$

where H_s is the Hamiltonian for a surface region given by

$$H_s=\sum_{i=1}^{N_s}\frac{p_{\rho i}^2}{2m_4}+\frac{1}{2}\sum_{i\neq j=1}^{N_s}V(\rho_{ij})+\sum_{i=1}^{N_s}\frac{p_{zi}^2}{2m_4}+\frac{1}{2}\sum_{\substack{i\neq j=1\\ z_i\neq z_j}}^{N_s}V(r_{ij}), \tag{2}$$

and H_b is the Hamiltonian for the bulk phase given by

$$H_b=\sum_{l=N_s+1}^{N}\frac{p_l^2}{2m_4}+\sum_{l<m=N_s+1}^{N}V(r_{lm}) \quad . \tag{3}$$

m_4, N, N_s, z_i, $\vec{\rho}_i$, $\vec{p}_{\rho_i}$, $\vec{p}_{z_i}$, and $\vec{p}_l$ in the above are, respectively, the mass of a ^{4}He atom, the total number of ^{4}He atoms of this system, the number of ^{4}He atoms, the positive vertical and two-dimensional positional coordinates of ith

particle, momentum operators of $\vec{\rho}_i$- and z_i-components of ith particle in the surface region and the momentum operator of lth particle in the bulk. $V(\rho)$ and $V(r)$ are the two-and three-dimensional Lennard-Jones 6-12 potentials, respectively, given by

$$V(\rho)=4e_0\left(\left(\frac{\sigma}{\rho}\right)^{12}-\left(\frac{\sigma}{\rho}\right)^{6}\right), \tag{4}$$

and

$$V(r)=4e_0\left(\left(\frac{\sigma}{r}\right)^{12}-\left(\frac{\sigma}{r}\right)^{6}\right). \tag{5}$$

with $e_0=10.22\ ^\circ K$ and $\sigma=2.556$Å, and $r_n^2=\rho_n^2+z_n^2$.

One-ripplon states are chosen as

$$\Psi_K=\rho_K\Psi_s(\vec{r}_1,\cdots\cdots,\vec{r}_{N_s})\Psi_b(\vec{r}_{N_s+1},\cdots\cdots,\vec{r}_N)\times(NS(K))^{-1/2}, \tag{6}$$

where K denotes a set of two-dimensional and z-directional wave vectors of the surface region and the bulk wave vector(*i.e.*, k_ρ, ik_z and k). Ψ_s and Ψ_b are the ground state wave functions of H_s and H_b given by

$$H_s\Psi_s=E_s\Psi_s,$$

and

$$H_b\Psi_b=E_b\Psi_b, \tag{7}$$

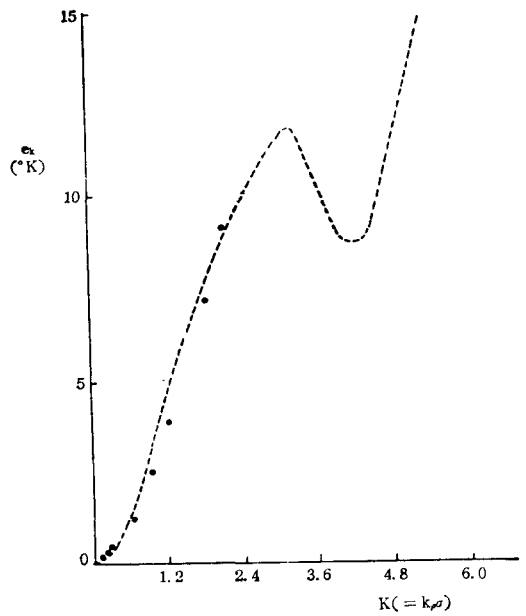

Fig. ···and--- are the classical capillary wave and the present result at zero bulk pressure respectively.

ρ_K is the density fluctuation operator defined by

$$\rho_K=\sum_{j=1}^{N_s} e^{i\vec{k}_\rho\cdot\vec{\rho}_j}e^{-k_z z_j}+\sum_{l=N_s+1}^{N} e^{i\vec{k}\cdot\vec{r}_l}, \tag{8}$$

and $S(K)$ is the liquid structure function of this system. Then the elementary excitation spectrum of liquid ^{4}He with free surfaces, *i.e.*, ripplon spectrum, e_K,[5] is given by

$$e_K\leq(N_s\hbar^2(k_\rho^2+k_z^2)\varphi_{2k_z}+(N-N_s)\hbar^2k^2)/(2m_4\times(N_s(\varphi_{2k_z}+\varphi_{k_z}^2(S_s(k_\rho)-1))+(N-N_s)S_b(k))), \tag{9}$$

where $S_s(k_\rho)$ and $S_b(k)$ are the two-dimensional[4] and bulk liquid structure functions, respectively, and φ_{mk_z} is Laplace transform of the ground state wave function in z-direction, $\varphi_0(z)$, obtained in Ref. 4 given by

$$\varphi_{mk_z}=\int_0^\infty|\varphi_0(z)|^2e^{-mk_z z}\,dz. \tag{10}$$

In order to minimize e_K for given wave vectors, K, the following procedures are chosen: (a) e_K is minimized with respect to k_z and k for given wave vectors, k_ρ. (b) e_K is minimized with respect to k_ρ and k_z for given wave vectors, k. The upper bound of e_K at zero bulk pressure presently calculated by the above procedures is shown and compared with the classical capillary wave, $e_{k_\rho}=\left(\frac{\hbar^2\alpha_0}{n_bm_4}\right)^{1/2}k_\rho^{3/2}$, 1(refer also to Appendix *A*) in Figure, and it is in good agreement with the result of Edwards et al.[2] at zero bulk pressure where n_b and α_0 are the number density of the bulk and the surface tension, respectively. In this calculation we take, for k larger than 1.58Å^{-1}, e_k as the exact elementary excitation spectrum of the bulk, where

$$e_k=\frac{\hbar^2k^2}{2m_4S_b(k)}. \tag{11}$$

The present ripplon spectrum, e_{k_ρ}, is not reliable for wave vectors, k_ρ, less than 0.1565 Å^{-1} since the long-range correlation seems not to be included in calculating $\varphi_0(z)$. Therefore for this limit we obtain e_{k_ρ} by hydrodynamics as shown in Figure, where we use the experimental result[6] $\alpha_0=0.27$°K/Å^2 at zero bulk pressure instead of using the theoretical calculation in YM model[4] $\alpha_0=0.264\ ^\circ K/$Å^2 at zero

bulk pressure. (Refer to Appendices *A* and *B*.) Also, it is noted using the results in YM model[4] the experimental result of the roton minimum, Δ, by Baliber et al.[7] can be explained such as the roton minimum, Δ, by them reduces to Δ in the bulk ^{4}He as in Figure and a good explanation[8] for a mechanism of a phonon-liquid ^{4}He with free surfaces[9] can be also qualitatively given.

Appendix *A*: Ripplon spectrum, e_{k_ρ}, and ground state wave function, Ψ_0, for small $k_\rho(k_\rho<0.1565\ \AA^{-1})$(Refer also to Ref. 10)

The system considered is defined as follows: a surface region for $0<z<d$, the surface at $z=0$ and the bulk for $z<0$. In order to obtain e_{k_ρ} to $0(k_\rho^{3/2})$ we only consider the Hamiltonian, H, for the small displacement, u, of the surface, A, and the small bulk number density fluctuation, δn_b, where

$$H=\frac{n_b m_4}{2}\int_\Omega \nabla\phi\cdot\nabla\phi d\Omega+\frac{\alpha_0}{2}\int_A \nabla_\rho u\cdot\nabla_\rho u\, dA + \frac{m_4 c^2}{2n_b}\int_\Omega \delta n_b^2 d\Omega. \quad (A1)$$

In the above Ω, ϕ and c are the volume of the bulk, the velocity potential and the sound speed, respectively, and $u=u(\vec{\rho},t)$. From Green's theorem the Hamiltonian, H, can be seperated into two parts, i.e.,

$$H=H_s+H_b, \quad (A2)$$

where

$$H_s=\frac{n_b m_4}{2}\int_A \phi\nabla\phi\cdot\vec{l}\,dA+\frac{\alpha_0}{2}\int_A \nabla_\rho u\cdot\nabla_\rho u\, dA, \quad (A3)$$

and

$$H_b=-\frac{n_b m_4}{2}\int_\Omega \phi\nabla^2\phi d\Omega+\frac{m_4 c^2}{2n_b}\int_\Omega \delta n_b^2 d\Omega, \quad (A4)$$

where $\vec{l}$ is the unit vector of the surface. The above Hamiltonian is subjected by the following two equations, *i.e.*, one is the Euler's equation for the bulk and the other is the boundary condition assumed the particle velocity to be equal to the velocity of the surface displacement, u, at the surface

$$-n_b\dot{\phi}=\frac{c^2}{n_b^2}\delta n_b, \quad (A5)$$

and

$$\nabla\phi\cdot\vec{l}=\dot{u}, \quad (A6)$$

where $\dot{\phi}$ and $\dot{u}$ represent the derivatives of ϕ and u with respect to the time t. Substituting Eqs. (A5) and (A6) into H results in

$$H_s=\frac{n_b m_4}{2}\int_A \phi\dot{u}dA+\frac{\alpha_0}{2}\int_A \nabla_\rho u\cdot\nabla_\rho u dA, \quad (A7)$$

and

$$H_b=-\frac{n_b m_4}{2}\int_\Omega \phi\nabla^2\phi+\frac{m_4^2 n_b^4}{2c^2}\int_\Omega \dot{\phi}^2 d\Omega. \quad (A8)$$

The representation of Eq. (A6) in the momentum space gives

$$\dot{u}_{k\rho}=k_z\dot{\phi}_{k_\rho}, \quad (A9)$$

where k_z is assumed an even function of $\vec{k}\rho$,

$$\phi=\frac{1}{A}\sum_{k_\rho}\phi_{\vec{k}_\rho}e^{i\vec{k}_\rho\cdot\vec{\rho}}e^{k_z z}\ ,\quad (z\leq 0)$$

and

$$u=\frac{1}{A}\sum_{k_\rho}u_{k_\rho}e^{i\vec{k}_\rho\cdot\vec{\rho}}e^{k_z z},\quad (z\leqslant 0) \quad (A10)$$

Using Eqs. (A9) and (A10) H_s is as follows:

$$H_s=\frac{n_b m_4}{2A}\sum_{k_\rho}\frac{|\dot{u}_{k\rho}|^2}{k_z}+\frac{\alpha_0}{2A}\sum_{k_\rho}k_\rho^2|u_{k_\rho}|^2, \quad (A11)$$

Using the real amplitudes Q_{k_ρ}, H_s in the Q_{k_ρ}-space becomes

$$H_s=\frac{\sigma^6 n_b m_4}{2A}\sum_{k\rho}\frac{\dot{Q}_{\vec{k}_\rho}^2}{k_z}+\frac{\sigma^6\alpha_0}{2A}\sum_{k_\rho}k_\rho^2 Q_{k_\rho}^2,$$

and

$$H_s=\frac{A}{2n_b m_4\sigma^6}\sum_{k_\rho}k_z P_{k_\rho}^2+\frac{\alpha_0\sigma^6}{2A}\sum_{k_\rho}k_\rho^2 Q_{\vec{k}_\rho}^2, \quad (A12)$$

where

$$Q_{k_\rho}=\frac{1}{2^{1/2}\sigma^3}(u_{k_\rho}+u_{-k_\rho}),$$

for $k_x>0$; $k_x=0$, $k_y>0$; $k_x=k_y=0$ with $k_z\geq 0$;

$$Q_{k_\rho}=\frac{i}{2^{1/2}\sigma^3}(u_{k_\rho}-u_{-k_\rho}),$$

for $k_x<0$; $k_x=0$, $k_y>0$; $k_x=k_y=0$ with $k_z\geq 0$

and

$$P_{k_\rho}=\frac{\sigma^6 n_b m_4}{Ak_z}\dot{Q}_{k_\rho}.$$

From Eq. (A12) we obtain

$$\frac{n_b m_4}{k_z}\ddot{Q}_{k_\rho}+\alpha_0 k_\rho^2 Q_{k_\rho}=0. \quad \text{(A13)}$$

In the process of solving Eq. (A13) we obtain the ripplon spectrum, e_{k_ρ}, as the below:

$$e_{k_\rho}^2=\frac{\hbar^2\alpha_0}{n_b m_4}k_\rho^2 k_z. \quad \text{(A14)}$$

We also obtain e_{k_ρ} for the bulk in the same procedures as the above:

$$e_{k_\rho}^2=\hbar^2c^2(k_\rho^2-k_z^2). \quad \text{(A15)}$$

From the above result k_z should be equal to k_ρ for the small k_z in order that the bulk is not disturbed by the surface excitation. Combining the above argument with Eq. (A14) renders e_{k_ρ} for the small k_ρ the following:

$$e_{k_\rho}=\left(\frac{\hbar^2\alpha_0}{n_b m_4}\right)^{1/2}k_\rho^{3/2}. \quad \text{(A16)}$$

Now, we give the ground state wave function, Ψ_0, for the small k_ρ, where $z\leq 0$ and for the completeness this type of wave function may be included in the bulk part. (However, it should yield negligible effects on the bulk.) From Eqs. (A12) and (A16) Ψ_0 for the small k_ρ is

$$\Psi_0=\text{Const}\ \exp\left(-\frac{(n_b m_4\alpha_0\sigma^{12})^{1/2}}{2A\hbar}\times\sum_{k_c}k_\rho^{1/2}e^{-k_\rho/k_c}|\rho_{\vec{k}}|^2\right), \quad \text{(A17)}$$

where Const and k_c are the normalization constant and the cutoff, respectively, $\rho_{\vec{k}}$ is the density fluctuation operator defined by

$$\rho_{\vec{k}}=\sum_{j=1}^{N}e^{i\vec{k}_\rho\cdot\vec{r}_j}e^{ik_z z_j}. \quad \text{(A18)}$$

In the above N is the total number of particles of the surface, A, and the bulk. Using Eqs. (A17) and (A18) we obtain

$$\Psi_0=\text{Const}\ \exp\left(-\frac{1}{2}\left(\sum_{i=1}^{N}t(z_i)+\sum_{i<j=1}^{N}u(\vec{r}_i,\vec{r}_j)\right)\right), \quad \text{(A19)}$$

where

$$t(z_i)=\frac{\Gamma(5/2)(n_b m_4\alpha_0\sigma^{12})^{1/2}}{2\pi\hbar((1/k_c)-2z_i)^{5/2}},$$

and

$$u(\vec{r}_i,\vec{r}_j)=\Gamma(1.5)\sin(1.5\sin^{-1}(\rho_{ij}(((\frac{1}{k_c})-z_i-z_j)^2+\rho_{ij}^2)^{-1/2}))/(2\pi\hbar\times(n_b m_4\alpha_0\sigma^{12})^{-1/2}(((1/k_c)-z_i-z_j)^2+\rho_{ij}^2)^{3/4}\rho_{ij}). \quad \text{(A20)}$$

Appendix *B*: Theoretical calculation of the surface tension, α_0

The system considered is given in Appendix *A*. The surface tension, α_0, can be calculated by the following equation:

$$\alpha_0=\int_0^d(P_b-P(z))dz, \quad \text{(B1)}$$

where d is the positive value to render $\varphi_0(z)$ zero calculated in Ref. 4. P_b and $P(z)$ are the bulk pressure and the local pressure of the surface region. We may define the average pressure of a surface region, $\bar{P}$, as follow:

$$\bar{P}d=\int_0^d P(z)dz,$$

and

$$\bar{P}=\left(\frac{n_s}{\tau}\right)^2\frac{\partial\varepsilon_s(n_s)}{\partial(n_s/\tau)}, \quad \text{(B2)}$$

where n_s, τ and ε_s are the area number density, the surface thickness, and the ground state energy per a ^{4}He atom of the surface region. Using the results of d, τ and ε_s by YM,[4] α_0 is 0.264°K/Å^2 at zero bulk pressure.

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