Excitation energy spectrum in helium II

P. Lu and C. K. Chan
Department of Physics, Arizona State University, Tempe, Arizona 85281
(Received 5 March 1979)

We obtain the roton part of the excitation energy spectrum in He II qualitatively. We point out that the distinct difference between this calculation and that of Parry and Ter Haar is that we do not use the Born approximation in the evaluation of t-matrix elements. We found that in addition to the contribution due to the hard-core part, the attractive potential helps to form the roton dip.

It seems that the roton part of the excitation energy spectrum, namely, $E(k)$ vs k, of liquid He II has not been well explained yet. Brueckner and Sawada[1] applied the t-matrix method to a hard-sphere boson system with high density and gave the excitation spectrum $E(k)$ in terms of the t-matrix elements.

$$E(k)=[(N_0t_k+\hbar^2k^2/2m)^2 - N_0^2 t_{\vec{k}-\vec{k},00}t_{00,\vec{k}-\vec{k}}]^{1/2} \quad (1a)$$

with

$$t_k \equiv t_{0\vec{k},0\vec{k}}+t_{0\vec{k},\vec{k}0}-t_{00,00} \quad (1b)$$

Parry and Ter Haar used the Born approximation in the evaluation of these t matrices by including an outside attractive potential. Their conclusion is that this attractive potential gives a poorer agreement with experimental result than the hard core alone or that of the Brueckner and Sawada calculation.

We are going to see how the Parry and Ter Haar[2] formulas, namely, the Born approximation to the t-matrix elements, are reached. We know

$$t_{\vec{k}',\vec{k}}=\int d^3r\, \phi^*_{\vec{k}'}(\vec{r})v'(r)\psi_{\vec{k}}(\vec{r}) \quad (2a)$$

and

$$v'(r)\psi_k^{(l)}(r)=\gamma_k^{(l)}\delta(r-a)+v(r)\psi_k^{(l)}(r) \quad , \quad (2b)$$

where a is the hard-core size, and $\psi_k^{(l)}(r)$ is the lth partial wave and r-dependent component of $\psi_{\vec{k}}(\vec{r})$. $\phi_{\vec{k}}(\vec{r})$ is the plane-wave eigenfunction, while $\psi_{\vec{k}}(\vec{r})$ is the exact state wave function. If we know $\psi_{\vec{k}}(\vec{r})$, we can obtain $E(k)$ right away. Since $\psi_{\vec{k}}(\vec{r})$ [or its lth partial wave component $\psi_k^{(l)}(r)$] is not known, we substitute it by its free-wave counterpart $\phi_{\vec{k}}(\vec{r})$ [or its lth partial wave $(1/\sqrt{\Omega})j_l(kr)$], and get the result of Parry and Ter Haar, or the Born approximation result. Immediately we see that this substitution is not well justified, since, in general, $j_l(ka)\neq 0$ yet $\psi_k^{(l)}(a)=0$. What we do in our approximation is to set

$$\psi_k^{(l)}(r)=\frac{n_l(ka)j_l(k\gamma)-j_l(ka)n_l(kr)}{[n_l^2(ka)+j_l^2(ka)]^{1/2}} \quad . \quad (3)$$

This is different from the Born approximation, for we introduce $n_l(kr)$, which will play a very important role in giving us the roton part.

We are starting our calculation by accepting the Brueckner and Sawada hard-core results as the starting point. We set $t_{\vec{k}\vec{k}}=t^{(1)}_{\vec{k}\vec{k}}+t^{(2)}_{\vec{k}\vec{k}}$ with $t^{(1)}_{\vec{k}\vec{k}}$ indicating the hard-core part and

$$t^{(2)}_{\vec{k}\vec{k}}=\int d^3r\,\phi_{\vec{k}}(\vec{r})v(r)\psi_{\vec{k}}(\vec{r})$$

indicating the outside attractive potential part. We get

$$E(k)=[(\hbar^2k^2/2m+Y+N_0t_k^{(2)})^2 - (Y+N_0t^{(2)}_{00,\vec{k}-\vec{k}})(Y+N_0t^{(2)}_{k-k,00})]^{1/2} \quad , \quad (4a)$$

with

$$Y=\frac{X^2\hbar^2\sin ka}{2kma^3} \quad (4b)$$

as was given in Brueckner and Sawada; we will use $X^2=30$ as reported in Parry and Ter Haar. Note that in so doing, we are not fitting a parameter; here we merely follow the optimized process for hard-core potential as was done.

Khanna and Das[3] fitted the experimental curve with a potential

$$v(r)=\begin{cases}\infty, & \text{for } r<a \;, \\ 4\epsilon\left\{\exp\left[-\left(\dfrac{r-a}{\mu_R}\right)^2\right] - \exp\left[-\left(\dfrac{r-a}{\mu_A}\right)^2\right]\right\} & \text{for } r>a \;. \end{cases} \quad (5)$$

They use the following set of parameters:

$$\epsilon = 14.11 \times 10^{-16}\ \text{erg},\ \mu_R^2 = 0.1103\ \text{Å}^2\ ;$$

$$\mu_A^2 = 0.2206\ \text{Å}^2;\ a = 2.1\ \text{Å}\ .$$

In Khanna and Das, they used the approximation due to Brueckner and Sawada, for example,

$$t^{(1)}_{00,k\,-k} + t^{(2)}_{00,k\,-k} = [t^{(1)}_{00,00} + t^{(2)}_{00,00}]\,(\sin ka/ka)$$

and

$$t_k^{(1)} + t_k^{(2)} = -\frac{1}{G_0(a,a)}\frac{\sin ka}{ka}\ .$$

They found that they could find a quantitative agreement with the phonon part. And hence by using this very potential, Eq. (5), we can obtain everything, such as the sound velocity, etc., which characterizes the phonon parts.

We are going to approximate for $\psi_{\vec{k}}(\vec{r})$ in the following way. For $k \neq 0$,

$$\psi_{\vec{k}}(\vec{r}) = \frac{1}{\sqrt{\Omega}}\sum_{l=0} i^l(2l+1) \times \cos\delta_l[j_l(kr) - \tan\delta_l \eta_l(kr)]P_l(\cos\theta) \quad (6)$$

and it is subjected to the overall normalization, such that, $k \neq 0$

$$1 = \int_\Omega \psi^*_{\vec{k}}(\vec{r})\psi_{\vec{k}}(\vec{r})\,d^3r\ . \quad (7)$$

We will take the zero energy, zero momentum state as the ground state of He. This is, of course, an approximation (see Fig. 1). We have therefore

$$r\psi_{\text{ground}}(\vec{r}) = r\psi_{(E\to 0,l\to 0)}(r) = \begin{cases} C_1 r + C_2, & a' < r\ , \\ A_2 Ai(z) + B_2 Bi(z), & a < r < a'\ , \end{cases} \quad (8)$$

where

$$z = [2mV_0/\hbar^2(a-a')]^{1/3}(r-a)$$

and

$$1 = 4\pi\int_a^{R_{11}} dr\, r^2\psi^*_{(E\to 0,l\to 0)}(r)\psi_{(E\to 0,l\to 0)}(r)\ , \quad (9)$$

with C_1, C_2, A_2, and B_2 being determined by the normalization Eq. (9) and their continuities at boundaries. From experiment, we set $R_{11} = 4.36$ Å, or $\rho = 2.06 \times 10^{22}$ particle/cm^3.

It is seen that due to these approximations we have $\lim_{k\to 0}E(k) \neq 0$. Actually we ought to have $\lim_{k\to 0}E(k) = 0$; however here the roton part ($k > 1$), not the phonon part ($0 < k < 1$), is our main concern. Therefore we get

$$\begin{aligned} N_0 t_k(2) &= (t^{(2)}_{0k,0k} + t^{(2)}_{0k,k0} - t^{(2)}_{00,00})N_0 \\ &= 8\pi\rho\sum_{l\ \text{even}}(2l+1)\Big\{j_l(\tfrac{1}{2}ka)\int_a^\infty dr\, r^2 j_l(\tfrac{1}{2}kr)\eta_l(\tfrac{1}{2}kr)V(r) \\ &\qquad - \eta_l(\tfrac{1}{2}ka)\int_a^\infty dr\, r^2 j_l^2(\tfrac{1}{2}kr)v(r)\Big\}/[\eta_l^2(\tfrac{1}{2}ka) + j_l^2(\tfrac{1}{2}ka)]^{1/2} \\ &\quad - 4\pi\rho\Big\{\int_{a'}^{R_{11}} dr\, r(C_1 r + C_2)v(r) + \int_a^{a'} dr\, r[A_2\text{Ai}(z) + B_2\text{Bi}(z)]v(r)\Big\}\ , \end{aligned} \quad (10)$$

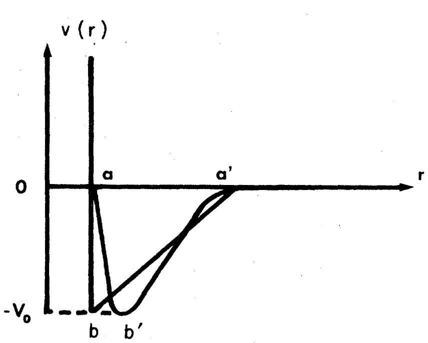

FIG. 1. We use the triangular part aba' as approximation in the ground-state wave function for the real potential $ab'a'$.

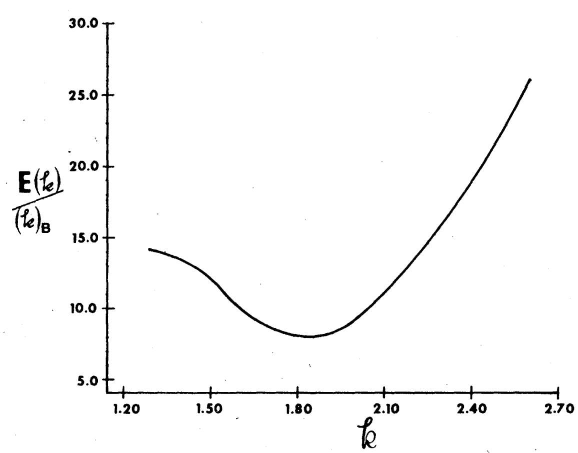

FIG. 2. E vs k curve, the roton part, from this calculation.

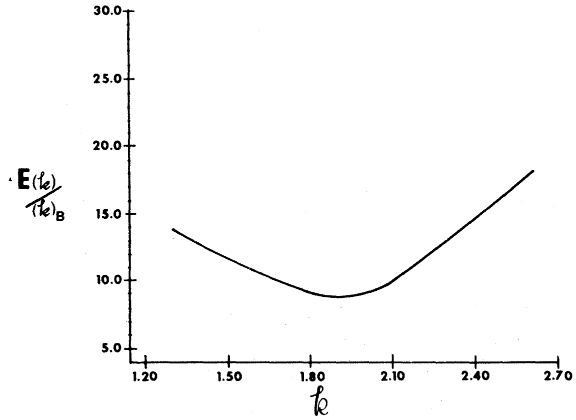

FIG. 3. E vs k curve, the roton part, from experiment.

TABLE I. Dispersion-curve values in ^4He given by our calculation compared with the experimental ones (see Ref. 4).

k	Expt. energy (eV)[a]	Theoretical result (eV)[a]
2.3	13.55	15.83
2.2	11.65	13.16
2.1	10.00	11.06
2.0	8.95	9.67
1.9	8.70	7.92
1.8	9.25	8.19
1.7	10.25	9.11
1.6	11.20	10.34
1.5	12.20	11.67
1.4	12.95	13.05

[a]eV is electron volt.

$$N_0 t^{(2)}_{00,k-k} = 4\pi\rho \int_a^{R_{11}} dr\, r^2 v(r)\, \psi_k^{(0)}(r) \tag{11}$$

and

$$N_0 t^{(2)}_{k-k,00} = 4\pi\rho \int_a^{R_{11}} dr\, r^2 j_0(kr) \times v(r)\, \psi_{(E\to 0,l\to 0)}(r) \; . \tag{12}$$

What we get then is a roton minimum, which is located at the same point on the curve as for the experiment (cf. Figs. 2 and 3 and Table I). However, we can not get the correct values at $k < 1$, as said above, and at $k > 2.8$, for then this must be due to some other mechanism.

Note here we do not use the Born approximation, instead we take care of hard core in Eqs. (6) and (8). We evaluate the matrix elements by very drastic approximation in wave functions. This is done mainly for convenience. In so doing, we think that, including the outside potential, we understand the roton minimum. There is an interesting paper[4] dealing with the same subject. They use a parameter to fit the experimental curve for hard-core potential only. Although their fit seems very satisfactory, however, this very parameter remains to be explained. What we are presenting here is a derivation with inclusion of the outside potential at the same time without the use of any parameter.

[1]K. A. Brueckner and K. Sawada, Phys. Rev. 106, 1128 (1957).
[2]W. E. Parry and D. Ter Haar, Ann. Phys. 19, 496 (1962).
[3]K. M. Khanna and B. K. Das, Physica (Utrecht) 69, 611 (1973).
[4]W. M. Alberico, M. W. Kirson, A. Molinari, and R. A. Broglia, Phys. Rev. B 13, 1080 (1976).