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WAVE EQUATION OF THE PARTICLE DENSITY OPERATOR FOR CRYSTALS OF RARE GASES

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INTRODUCTION

The wave equation of the particle density oparator

$$\hat{\rho}(\vec{r},t) = \sum_i \delta(\vec{r}-\vec{r}_i(t)) \ , \tag{1}$$

$$\Delta\hat{\rho} - \frac{1}{v^2}\frac{\partial^2\hat{\rho}}{\partial t^2} = 0 \tag{2}$$

for large system of bosons has been derived in the paper [1] under the following assumptions:

(i) State wave functions have the form

$$\Psi = e^{\chi}\Phi_n \ , \tag{3}$$

where e^{χ} describes short-range correlative motion and Φ_n rest of the motion.

(ii) Specific contributions of the functions Φ_n in the matrix expression of the second derivative of $\hat{\rho}$ are negligible.

(iii) In the final expressions the sums over particles may be transformed into integrals,

$$\sum_i \rightarrow \frac{1}{\Omega_o}\int d\vec{r} \ , \quad \Omega_o = \textit{mean particle volume.} \tag{4}$$

Eq.(2) has been applied to the liquid He^4. The position probability of a particle was taken to be constant over the whole particle's volume. By this approximation the calculated

value of the sound velocity is 640 m/s. The experimental value is 240 m/s.

A better evaluation of the sums with correlative motions at small interatomic distances of first neighbors gives the value v = 355 m/s. The two-body interaction was asssumed to be [2] :

$$V(r) = A\, e^{-\alpha r} - \frac{b}{r^6} - \frac{c}{r^8} \quad . \tag{5}$$

According to [3] the wave function at small interatomic distances is

$$e^{-Be^{-\frac{\alpha}{2}r}} \quad , \quad B = \frac{2\sqrt{2mA}}{\alpha\hbar} \quad , \tag{6}$$

where m is the mass of an atom. The position probability of a particle is then

$$w(r_{12}) = \frac{\int e^{-B\sum'_{ij} e^{-\frac{\alpha}{2}r_{ij}}} \vec{dr}_3 \vec{dr}_4 \ldots \vec{dr}_N}{\int e^{-B\sum'_{ij} e^{-\frac{\alpha}{2}r_{ij}}} \vec{dr}_2 \vec{dr}_3 \ldots \vec{dr}_N} \tag{7}$$

With this probability the particle sums become

$$\sum_{i\neq j} f(r_{ij}) \;+\; (N-1)\int w(r) f(r) dr \tag{8}$$

and

$$\sum_{i\neq j} f(r_{ij}) + n_{s_1}\int^{3a/2} w(r) f(r) dr + \frac{1}{\Omega_0}\int_{non} (n_{s_1}+1)\Omega_0 f(r) dr \quad , \tag{9}$$

where only first neighbors are taken into account. n_{s_1} is the number of the first neighbors and a is radius of the mean particle volume.

CRYSTALS OF RARE GASES

In this paper we apply Eq.(2) to rare gas crystals. We assume also the Yntema-Schneider potentials [4,7] . Due to high localization of particle motions we make further simplifications in the approximation (8) :

$$\sum_{i \neq j} f(r_{ij}) \approx n_{s_1} \int_0^{3r_1/2} w(r) f(r) dr + n_{s_2} f(r_2) + \ldots \quad , \tag{10}$$

where n_{s_2} is the number of the second neighbors and r_1 is the crystal distance of the first neighbors, and so on. The motions of the first neighbors are then described by the asymptotic wave function at small interatomic distances. The sound velocity v is then given by

$$v^2 = \frac{\zeta}{m^2} + w_2 \quad , \tag{11}$$

where are

$$\begin{aligned} \zeta &= n_{s_1} \int_0^{3r_1/2} w(r) \zeta(r) dr + n_{s_2} \zeta(r_2) + \ldots \quad , \\ \zeta(r) &= - \frac{\hbar^2 \alpha B}{6} \left(\frac{2}{r} - \frac{\alpha}{2} \right) e^{-\frac{\alpha}{2} r} \quad , \end{aligned} \tag{12}$$

$$\begin{aligned} w_2 &= n_{s_1} \int_0^{3r_1/2} w(r) w_2(r) dr + n_{s_2} w_2(r_2) + \ldots \quad , \\ w_2(r) &= \frac{1}{3m} \left(A \alpha r \, e^{-\alpha r} - \frac{6b}{r^6} - \frac{8c}{r^8} \right) \quad . \end{aligned} \tag{13}$$

In Table I the sound velocities are given for uncorrelative (I) and correlative (II) motions of a particle in its volume. Various remarks are given in the last section.

Table I

Crystal	v_I (m/s)	v_{II}	v_{exp}
He	*1360*	*547*	*600*
Ne	*2500*	*401*	*1200*
Ar	*4200*	*719*	*1600*

CONCLUSIONS AND COMMENTS

From Table I we conclude that agreement with experimental values is satisfactory . A better evaluation of the sums (8) would give better theoretical values. Correct interaction potentials are also important, in particular at small interatomic distances. These potentials are not well established. They differ from author to author [4,5,6,7]. As we have mentioned we used here the Yntema-Schneider potentials.

The first column in Table I gives too large values for the sound velocities. This is due to the uncorrelated motion of a particle in its volume. The second column gives quite satisfactory result for He but the results for Ne and Ar are too small. We think that the reason for this lies in the potentials. A better knowledge of the potentials, especially at small interatomic distances, would give better results.

At the end we conclude that Eq.(2) is also useful in the studies of rare gas crystal properties.

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