Int. J. Chem. Sci.: 9(1), 2011, 59-68
ISSN 0972-768X

A STUDY OF VARIOUS SEMI-EMPIRICAL POTENTIAL FOR THE BOGOLYUBOV QUASI PARTICLE SPECTRUM IN BOSE LIQUID

S. DIE[a], M. P JHA[b] and L. K. MISHRA[*]

Department of Physics, Magadh University, BODH-GAYA – 824 234 (Bihar) INDIA
[a]Department of Physics, Mahila College, Chaibasa, WEST SINGHBHUM – 833201 (Jharkhand) INDIA
[b]Department of Physics, Tata College, Chaibasa, WEST SINGHBHUM – 833201 (Jharkhand) INDIA

ABSTRACT

Using the theoretical model of E. A. Pashitskii et al., various semi-empirical potentials for interaction of helium atoms in real space have been studied. Theoretical evaluation of the Bogolyubov quasi particle spectrum in Bose liquid has been done and results were compared with inelastic neutron scattering experiments. Our theoretical results are in good match with the experimental data.

Key words: Semi-empirical potential, Quasi particle spectrum, Bose liquid, Inelastic neutron scattering experiments, Super fluid state.

INTRODUCTION

Although there are large numbers of calculations[1-6] for the spectrum of elementary excitation in the super fluid (SF) ^{4}He Bose liquid but there remains still some problem in this direction. There is an excellent agreement with experimental data in the region of the roton minimum obtained by Monte Carlo method making use of the shadow wave function[1] and by the correlation basis function[2]. These calculations also employed the modern inter atomic potentials[3-5] for ^{4}He. There are some calculation using microscopic perturbation theory[6-8] for long wave phonon part of the spectrum $E(p) = C_1p$, where C_1 is the speed of the first (hydrodynamic) sound in liquid ^{4}He. These calculations face some principal difficulties because the non-renormalized perturbation theory gives rise to infrared divergence and are non-analytical[9-12] at $p \rightarrow 0$ and $\varepsilon \rightarrow 0$. These difficulties have been removed by the application of combined variable techniques[13]. These variables reduces to hydrodynamic

[*]Author for correspondence; E-mail: muphysicslkm@gmail.com

variable of macroscopic quantum hydrodynamics[14] in the long-wavelength limit ($p \rightarrow 0$). On the other hand in the short wavelength domain, they correspond to the Bosonic quasi particle creation and annihilation operators.

Neutron inelastic data[15,16] and results in quantum evaporation of ^{4}He atoms[17] show that the maximal density ρ_0 of the single particle BEC (Bose-Einstein Condensate) at $T < T_\lambda$ does not exceed of the total density ρ of the liquid ^{4}He, whereas the density of the SF component $\rho_s \rightarrow \rho$ at $T \rightarrow 0$. This indicates that there is strong interaction between ^{4}He atoms and the quantum structure of the super fluid condensate in He-II carry an excess density $(\rho_s - \rho_0) >> \rho_0$. This requires much more investigations.

In this paper, we have studied various semi-empirical potentials to study helium-helium interaction. These potentials involve strong repulsion at small distances and weak Van der Waals attraction at large distances. We have also computed the Bogolyubov spectrum of a dilute quasi ideal Bose gas and compared our evaluated results with inelastic neutron scattering data. Our evaluated results are in good match with the experimental data.

Mathematical formula used in this study

In order to describe the interaction of He atoms in real space, one uses various semi-empirical potentials. These potentials involve strong repulsion at small distances and weak Van der Waals attraction at large distances. However, most of those potentials are characterized by strong divergence at $r \rightarrow 0$. For example, Lennard-Jones Potential[18] -

$$U_{LR}(r) = \in \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] \qquad r < r_c \qquad \ldots(1)$$

$\in$ and σ are potential parameters, if one takes the Fourier transform of the potentials.

$$V(p) = \int d^3r U(r)\, e^{ip.r}$$
$$= \frac{4\pi}{p}\int_0^\infty rU(r)\,\mathrm{Sin}(pr)\,dr \qquad \ldots(2)$$

One cannot use this potential for the description of pair interaction in momentum space as it is infinite, diverging as the lower limit.

The other potential, which is used for the calculation of inter atomic interaction and of possible bond state is Aziz potential[19].

$$U_A(r) = A\exp(-\alpha r - \beta r^2) - \exp[-((r_0/r) - 1)^2]\sum_{K=0}^{2} C_{2k+6}r^{-2k-6} \qquad r < r_0$$

$$= A\exp(-\alpha r - \beta r^2) - \sum_{K=0}^{2} C_{2k+6}r^{-2k-6} \qquad r \geq r_0 \qquad \ldots(3)$$

Where,

$A = 1.8443101 \times 10^5$ K

$\alpha = 10.43329537$ Å^{-1}

$\beta = 2.27965105$ Å^{-2}

$C_6 = 1.36745214$ K x Å^{-6}

$C_8 = 0.42123807$ K x Å^{-8}

$C_{10} = 0.17473318$ K x Å^{-10}

Such potentials remain finite at $r = 0$ due to the non-analytic exponential dependence on r, which suppresses any power divergence at $r \to 0$. The potential (3) is convenient for calculations in real space making use of Jastrow-like wave functions. But employing its Fourier component for solving nonlinear integral equations is technically difficult. The model potentials, which describes interaction of helium atoms in real space takes into account that the distance less than the quantum radius of the helium electron shell $r_0 = 1.22$ Å, the Coulomb repulsion between the nuclei sets in.

Piashitskij et al.[20] suggested a potential, which diverges as r^{-1} at $r \to 0$

$$U(r) = \frac{4e^2}{r}(1 + \mu r)\exp\left(-\frac{r}{\alpha}\right) \qquad r \leq r_c$$

$$= \in \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] \qquad r > r_c \qquad \ldots(4)$$

From the conditions of continuity of the potential U (r) and its first derivatives at $r = r_c$, one determines the value of the parameters $r_c = 2.38$ Å and $\mu = 229$ Å^{-1} for $\alpha = r_0/2 = 0.61$ Å, $\varepsilon = 10.8$ K and $\sigma = 2.642$ Å.

In many body problem, the quantum effects play an essential role and in that case, the two-body potential is irrelevant. For that, one should have a model potential with a simpler analytic expression. There is a model potential in the form of a Fermi type function in real space.

$$U_F\,(r) = U_0\left[\exp\left(\frac{r^2 - a^2}{b^2}\right) + 1\right]^{-1} \quad \ldots(5)$$

which at b = 0 degenerates into a state function at θ (a-r) with a finite height U_0 at r < a. This model corresponds to a model of 'soft' sphere. Its Fourier component is expressed in terms of first order spherical Bessel function.[21]

$$V\,(p) = V_0\,\frac{j_1\,(pa)}{pa},\ j_1\,(x) = \frac{\mathrm{Sin}\,(x) - x\mathrm{Cos}(x)}{x^2} \quad \ldots(6)$$

where $V_0 = 3V\,(0) = 4\pi\ U_0\ a^3$. It is an oscillating sign changing function of momentum transfer p. The same oscillating Fourier component is characteristics of smooth potential V (r) in the form of Linhardt type function[22] having an infinite negative derivatives at the inflection point r = a.

$$U_L\,(r) = \frac{U_0}{2}\left[1 + \frac{1-\frac{r^2}{a^2}}{\frac{2r}{a}}\,ln\left|\frac{a+r}{a-r}\right|\right] \quad \ldots(7)$$

Formally this problem is an inverse to one of periodic oscillations of spin density in real space of the exchange interacting spins of electrons in metal. This is popularly known as RKKY (Ruderman-Kittel-Kaisuya-Yosida) oscillation[23]. The same behavior is characteristics of the Fourier components of more realistic potentials diverging faster than r^{-1} at r = 0. It posses inflection points in the radial dependence at $r = r_c$. The amplitude of the oscillation of the Fourier component of the Fermi type potential (5) at b ≠ 0 is falling off exponentially with the increase of the parameter b due to the decreasing absolute value of the negative derivative at the inflection point.

If one substitutes the oscillating potential (6) into the Bogolyubov of a dilute quasi-ideal Bose-gas[24,25].

$$E_B\,(p) = \left\{\frac{p^2}{2m}\left[\frac{p^2}{2m} + 2nV\,(p)\right]\right\}^{1/2} \quad \ldots(8)$$

RESULTS AND DISCUSSION

In this paper, in order to describe the interaction of He atoms in real space, various empirical potentials are used, which involve strong repulsion at small distances and week Van der Waals attraction at large distances. Most of the potentials are characterized by a strong divergence at $r \to 0$. Among the various potential discussed, there is a repulsive potential in the frame work of 'soft spheres model'. The Fourier component v(p) is an oscillating sign-changing function of momentum transfer p. It appears that in a certain region of momentum space at $p \neq 0$, there is an effective attraction between Bosons $v(p) < 0$. This has nothing to do with Van der Waals forces and has a quantum mechanical diffraction nature. This attraction gets substantially enhanced due to the multi-particle effects of renormalization (screening) of the initial interaction[28-30].

We have theoretically compared the Bogolyubov quasi particle spectrum equation (8), with the oscillating Fourier component [$v(p) = V_0 \sin(pa)/pa$] and also with experimental spectrum[26,27]. The results are in close appearance with the hard sphere potential (equation 6). The results are shown in Table 5. In Table 1, we have shown the evaluated radial dependent of potential (4) and Aziz potential (5), in Table 2, the two forms of finite potential (5) has been shown in real space (r/a) keeping b = 0 [I-form] and b = 0.5a [II-form]. In Table 3, we have given the (Lindhardt function potential [$U_L(r) / Uo$] shown in equation (7) in real space (r/a). In Table 4, we have shown the momentum dependent of the Fourier component of the Fermi type potential (5) for b = 0 and potential (4).

From these studies, it looks that the soft sphere model repulsive potential, which gives very good agreement between the theoretical quasi particle spectrum $E_B(p)$ and the experimental spectrum of elementary excitation in quantum Bose liquid ^{4}He, is much smaller than the value of the Aziz-type potential at $r \to 0$. It is a result of strong quantum diffraction effects in Bose liquids, because the average distance between particles is equal or less than the de Broglie wavelength for Bosons.

Table 1: Evaluated results of radial dependence of potential (4) and Aziz potential (3)

r (Å)	Potential (4) U (r) (K)	Aziz Potential U_A (r) (K)
2.5	105.2	110.8
2.6	95.6	106.5
2.7	84.3	98.2
2.8	50.6	68.6
2.9	16.7	23.2
3.0	-12.2	-16.8

Cont…

r (Å)	Potential (4) U (r) (K)	Aziz Potential U_A (r) (K)
3.1	-14.6	-15.6
3.2	-10.4	-11.8
3.3	-8.6	-9.9
3.4	-6.5	-7.3
3.5	-5.6	-6.8
4.0	-4.32	-5.8
4.5	-4.00	-3.8
5.0	-0.08	-1.02

Table 2: Evaluated results of the finite potential model (5) in real space (r/a). [I–form for b = 0] and [II–form for b = 0.5a.]

r/a	$U_F(r) / U_0$ for b = 0	$U_F(r) / U_0$ for b = 0.5a
0.0	1.00	1.00
0.1	1.00	0.998
0.2	1.00	0.996
0.3	1.00	0.987
0.4	1.00	0.965
0.5	1.00	0.928
0.6	1.00	0.889
0.7	1.00	0.793
0.8	1.00	0.786
0.9	1.00	0.684
1.0	0.00	0.546
1.1	0.00	0.253
1.5	0.00	0.446
1.6	0.00	0.054

Table 3: Evaluated results of the Lindhart function potential $U_L(r) / U_0$ equation (7) in real space r/a

r/a	$U_L(r) / U_0$
0.0	1.00
0.1	0.984
0.2	0.975
0.3	0.952
0.4	0.886
0.5	0.825
0.6	0.795
0.7	0.705
0.8	0.659
0.9	0.613
1.0	0.526
1.1	0.508
1.2	0.432
1.3	0.326
1.4	0.286
1.5	0.239
1.6	0.187
1.8	0.144

Table 4: Evaluated results of the momentum dependence of the Fourier components of the Fermi type potential (5) for b = 0 and potential (4)

p ($Å^{-1}$)	V(p) / V(o)	
	Potential (5)	Potential (4)
0.0	1.0	1.0
0.2	0.869	0.986
0.4	0.792	0.924

Cont…

p (Å^{-1})	V(p) / V(o)	
	Potential (5)	Potential (4)
0.5	0.607	0.885
0.6	0.496	0.816
0.8	0.288	0.774
1.0	0.087	0.625
1.5	-0.156	0.463
2.0	-0.108	0.136
2.5	-0.088	-0.115
3.0	0.145	-0.056
3.5	0.208	0.069
4.0	0.125	0.145
4.5	0.086	0.186
5.0	-0.095	0.068

Table 5: Evaluated results of Bogolyobov quasi particle spectrum (equation 8) with the oscillating Fourier component of the hard sphere potential equation (6)

p (Å^{-1})	E_B(p), K	
	Hard sphere potential eq. (6)	Bogolyobov quasi particle Spectrum eq. (8)
0.0	0.052	0.046
0.25	3.628	4.554
0.50	6.836	7.397
0.75	10.957	11.412
1.00	14.254	15.350
1.25	12.868	13.145
1.50	10.296	11.254
1.75	8.144	9.266
2.00	9.686	10.052
2.25	11.234	12.645
2.50	16.286	17.128

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Revised : 02.09.2010 *Accepted : 04.09.2010*