

Ground state of liquid helium-3: off-shell effects due to non-local potentials

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Abstract. It is shown that by incorporating the off-shell effects through the introduction of phase equivalent nonlocal potentials, (that are essentially equivalent so far as two-body properties are concerned) one could obtain a much better agreement regarding the important properties of the ground state of liquid helium-3, in lowest order Brueckner-Goldstone theory. The binding energy, equilibrium density and the convergence character of Brueckner-Goldstone series improve drastically.

Keywords. Liquid helium-3; off-shell effects; non-local potentials.

1. Introduction

Attempts to understand the ground state of normal phase of liquid helium-3 starting from the basic atom-atom interaction, have been undertaken by several workers (Brueckner and Gammel 1958, Ostgaard 1968), Burkhardt 1968, Ghassib *et al* 1974, Rama Rao and Rao 1975). The last two references will be hereafter referred to as GII and RR respectively. However none of these calculations seems to yield satisfactory results. The binding energy and saturation density come out to be too low and the higher order corrections are expected to be fairly large. The present authors are engaged in serious attempts to study the various assumptions and approximations made in earlier calculations and to try new and unorthodox approaches to study liquid helium-3.

In our recent paper we presented a thorough calculation of liquid helium-3, in the first order Brueckner theory with as few assumptions and approximations as possible. Our calculation was free from *ad hoc* parameters. Although the results are more reliable than any previously published result, they are just as unsatisfactory. Just like previous workers, we also obtain too little binding and too low density.

In the present work, we investigate one particular aspect of the problem that has not been investigated so far in the literature. This concerns the uncertainty in the off-shell extension of the two-body interaction. For any conventionally accepted two-body interaction (potential) the actual observables are the hypothetical phase shifts in the scattering of one He³ atom by another, there being no two-body bound state. It is well known that for a given set of phase shifts, the potential is not unique and a whole class of non-local potentials (that give the same phase shifts) can be constructed.

All these potentials that give the same phase shifts are essentially equivalent so long as we deal with two-body phenomena like scattering. Their mutual differences show up only when we use them to study three body systems and many body systems. But then we have to deal with three body forces and three body correlations and other complications. There does not seem to be a simple way to separate all these effects. In this sense, there is a possibility that a choice of proper off-shell behaviour of the interaction may somehow take into account some of these effects. Thus these different phase equivalent potentials may yield widely varying results in the study of many body systems and may give us a clue as to the convenient choice of the off-shell behaviour of the interaction.

Previous work on nuclear matter and finite nuclei (Haftel and Tabakin 1971, Haftel *et al* 1972; also for a good review see Srivastava and Sprung 1975) has shown that properties of a many body system do vary drastically when different off-shell behaviours are considered. One particular feature is very striking. Softer potentials give higher binding energy and higher saturation density. Also for such potentials Brueckner-Goldstone series may be expected to have better convergence properties. All these shifts are in the right direction and may improve the results of Brueckner theory and bring them closer to the observed values. In this paper we show that with the introduction of off-shell effects through a proper choice of phase equivalent potential, we can come very close to the observed properties of liquid helium-3.

The outline of the paper is as follows: In section 2, we outline the results of some calculations in nuclear physics using phase equivalent potentials so as to prepare the ground for their use in the present problem. In Section 3, we describe our method of generating phase equivalent potentials suitable for the study of liquid helium-3. Section 4 discusses the trends in the reaction matrix elements for phase equivalent potentials. In section 5, we present a simplified calculation of the lowest order binding energy and lastly, section 6 contains a discussion of our results. Unless explicitly mentioned otherwise, we measure momenta in A^{-1} and energies in A^{-2} , the conversion factor being $\hbar^2/M = 16.36 \text{ }^\circ\text{KA}^2$.

2. Results in nuclear matter and finite nuclei

We now sketch briefly the results obtained in nuclear physics to guide us how to proceed and what type of results to expect. With the realistic Reid potential (Reid 1967), (which has a repulsive core at about 0.5 fermi compared to the range of nuclear force $r_0 = 1.2$ fermi), typically one obtains a binding energy of 11 to 12 MeV per particle at a saturation density corresponding to fermi momentum $k_f = 1.2$ fermi $^{-1}$. These results are to be compared with the corresponding values from the semiempirical formula: 15 MeV and 1.36 fermi $^{-1}$ respectively. Due to the smallness of the value c/r_0 , the contribution to the binding energy from three body clusters, etc., is expected to be small (Bethe 1971). Within the uncertainties in the nuclear interaction, these results are supposed to be fairly satisfactory.

In the calculations with phase equivalent potentials (Haftel and Tabakin 1971), it was found that the two numbers B.E. (binding energy) and k_f , the fermi momentum could change significantly. However in almost all cases the binding energy is

less than the value corresponding to the Reid potential. This is mostly due to the fact that the Reid potential is already very soft. Similarly Haftel *et al* (1972) obtain widely different results for the B.E. of O^{16} for various phase equivalent potentials. Here also Reid potential yields most binding.

In both these cases, they have an interesting observation to make: there is an approximate linear relation between the B.E. and the 'hardness' of the repulsive core as measured by the norm of the defect function, *i.e.*, the so called wound integral (Brandow 1967). They give a formal proof of this linear relation based on modified Moskowsky-Scott separation distance method. With smaller wound integrals, the B.E. and the saturation density increase. In fact, from their calculations, it appears that for a super soft potential with a very small wound, there is a striking agreement for the B.E. of nuclear matter and O^{16} .

These improvements in nuclear physics were considered to be just marginal as there is already enough binding. However, for liquid helium-3, the results with local potentials are not quite so satisfactory. The best numbers to date are $k = 0.52 \text{ \AA}^{-1}$ and B.E. = 0.2°K per particle, as compared to the observed values of 0.79 \AA^{-1} and 2.5°K respectively. Clearly a drastic shift is needed to get any agreement with experiment.

In contrast to nuclear systems, we notice that, with a local potential [like say Frost-Musulin (1954) potential] repulsive core radius c ($= 2.65 \text{ \AA}$) and the mean interparticle distance r_0 ($= 2.55 \text{ \AA}$) are of the same order. Consequently we expect strong short range two-body correlations and hence very large defect functions and large wound integrals. Hence even a simplistic attempt to replace the repulsive (local) core by a nonlocal repulsion through the phase equivalent potentials is bound to decrease the wound integral and increase B.E. and k , significantly.

To this end, in the next section we focus our attention on how to construct phase equivalent potentials keeping all the desirable properties unchanged.

3. Phase equivalent potentials for $\text{He}^3 - \text{He}^3$

In the conventional calculations the starting point is the basic two-body local potential. This potential is believed to have a long range behaviour of van der Waals type (C/r^6) and the potential is known to have no bound state. If we assume that the potential is local, it is also known that it should have a minimum of about $10-13^\circ\text{K}$, at about $r = 2.8-3.0 \text{ \AA}$ distance and it has a strong repulsive core at about $2.6-2.7 \text{ \AA}$. The repulsion should probably be of the order of a few electron volts. However the potential is very difficult to measure directly or to derive from a more fundamental theory. The only measurable consequences of the potential are the two-body phase shifts at various energies for different partial waves. The detailed behaviour of the wavefunction at short distances is (probably) strictly not an observable but its asymptotic behaviour is. Formally, the phaseshifts exist up to energies of the order of a few electron volts, before inelastic processes due to the excitation of the He atom set in.

Since we are not really interested in the electron-volt range, we may assume that the phaseshifts are known for all energies these being calculated from a conventional local potential, say the Frost-Musulin potential (Frost and Musulin 1954). Now we ask the question if the phaseshifts are the only data available,

what can we say about the interaction? Of course, if we assume that the potential is local, by Gel'fand-Leviton theorem (Gel'fand and Leviton 1951) we ought to get back our original potential. However, if we admit nonlocal potentials the answer is not unique any more. We can generate a class of the so-called phase equivalent potentials (PEP) that give exactly the same phase shifts. Any two members of this set cannot be distinguished from each other solely by the study of two-body phenomena. Thus they are equivalent so far as two-body problems are concerned. Their mutual differences show up when we investigate problems involving several particles.

Physically in the generation of such PEP, we are replacing the local strong repulsive core by a somewhat weaker momentum dependent repulsion. Consequently the reaction matrix elements become more attractive and the wound integrals decrease. This makes the contributions from three and higher body correlations less important as compared to the corresponding local potential.

However in generating these potentials we should follow a few guidelines. We should keep the non locality restricted to reasonably short range say, $r < 4A$, as for larger distances there seem to be good reasons to believe that the potential is local. Similarly, we should not completely annihilate the repulsive core, for in such a case the saturation density may turn out to be too high.

In literature, we have a number of methods of generating phase equivalent potentials (See for example Srivastava and Sprung 1975). It is known that the PEP form a one parameter family (Preston and Bhaduri 1964). We have chosen a simple method of generating the PEPs, through the use of rank one unitary transformation (Haftel and Tabakin 1971, Coester *et al* 1970, Baker 1962, Ekstein 1960). In the following we restrict our attention to s -waves only as they are the only ones that are promising.

If the local potential is $V(r)$, the radial Schrödinger equation gives us:

$$(T + V)\psi = E\psi \quad (3.1)$$

Now we introduce a short range unitary operator U through

$$\psi \rightarrow \psi' = U\psi \quad \text{and} \quad H \rightarrow UHU^{-1} \quad (3.2)$$

so that, $\psi'(r) \rightarrow \psi(r)$ for large r , and the phase shifts remain unchanged. Also we choose U to be unitary so that the spectrum of the Hamiltonian is preserved. We introduce U through a short range projection operator A as follows:

$$U = 1 - 2A. \quad (3.3)$$

The fact that U is unitary implies that

$$A^2 = A = A^+. \quad (3.4)$$

Equation 3.2 implies that A should be a short range operator and we use a simple rank one separable approximation for A through:

$$\langle r|l m | A | r' l' m' \rangle = \delta_{ll'} \delta_{mm'} \delta_{l0} f(r) f(r'). \quad (3.5)$$

Equation (3.4) implies that

$$\int_0^\infty r^2 dr |f(r)|^2 = 1. \quad (3.6)$$

Since we want a short range modification, we choose a simple analytical representation for $f(r)$:

$$f(r) = Ae^{-ar} (1 - \beta r) \quad (3.7)$$

where a, β are parameters and A is fixed by the normalisation condition (3.6). We choose $a > 1.5 \text{ \AA}^{-1}$ so that the radial wave function ψ' is modified at short range only and approaches ψ very well by about $r = 4 \text{ \AA}$. Under such a choice for A , the S-wave radial wave function $R(r)$ will be modified to $R'(r)$ as given below.

$$R(r) \rightarrow R'(r) = R(r) - 2cf(r),$$

where

$$c = \int dr r^2 f(r) R(r) \quad (3.7)$$

Equations 3.2 and 3.3 imply that

$$H \rightarrow H' = T + V' = (1 - 2A)(T + V)(1 - 2A) \quad (3.8)$$

or

$$V' = V + 4ATA - 2AT - 2TA + 4AV A - 2AV - 2VA. \quad (3.9)$$

Thus we have shown that the potential V' gives the same phase-shifts as the potential V .

The functional form for $f(r)$ is chosen so that the momentum space matrix elements for the potential V' can be obtained analytically in a simple manner. With the help of these matrix elements and using the methods outlined in our earlier work (RR), we can solve Bethe-Goldstone equation by direct matrix inversion in momentum space to obtain the reaction matrix elements.

4. Reaction matrix elements for $\text{He}^3 - \text{He}^3$ problem

Due to the centrifugal barrier, the repulsive core does not play as important role in higher partial waves as in the s waves. Hence we expect the off-shell effects to be important in s waves and to a lesser extent in the p waves. We now present the Bethe-Goldstone equation in the operator language in a formal way. Explicit representation in partial waves with practical details can be seen in GII, RR or Haftel and Tabakin (1970, 1971). The equation giving the reaction matrix g is:

$$g = V - V \frac{Q}{T - \omega} g \quad (4.1)$$

where V is the two-body interaction Q the angle averaged Pauli operator, T the kinetic energy operator, the intermediate state (particle) potentials being kept zero and ω is the starting energy. The corresponding correlated wave function ψ and the defect wave function χ are related to the uncorrelated free particle wave function ϕ through:

$$g\phi = V\psi \quad \text{and} \quad \chi = \phi - \psi = \frac{QV}{T - \omega} \psi. \quad (4.2)$$

The norm of the defect function $\langle \chi | \chi \rangle$ measures the short range correlation introduced in the correlated wavefunction due to the repulsive core. The wound integral κ , is given by (Ostgaard 1968 *a*, eq. 3.25)

$$\kappa = \rho \langle \chi | \chi \rangle. \quad (4.3)$$

It is also related to the derivative of the g -matrix with respect to the starting energy ω through (Haftel and Tabakin 1970):

$$\kappa = -\frac{\pi^2}{4} \rho \frac{\partial g}{\partial \omega}, \quad (4.4)$$

where ρ is the density.

The wound integral κ has great significance in that it determines the convergence of the compact cluster expansion (Brandow 1965)

The equation (4.1) is to be solved by separating it into partial waves. We solve this equation by matrix inversion in momentum space with usual approximations. We use the angle averaged Pauli operator and reference spectrum approximations.

We represent the occupied state single particle energies by the usual quadratic function

$$\mathcal{E}(k) = \frac{k^2}{m^*} - \Delta k_f^2. \quad (4.5)$$

Here Δ measures the overall attractive interaction and m^* gives an idea as to behaviour of single particle energies as function of momentum. Our criteria of Brueckner convergence is that Δ and m^* should both agree selfconsistently. (So far in literature, only Δ is determined selfconsistently and m^* is fixed arbitrarily).

We perform the calculations for the g -matrix elements for various phase equivalent potentials obtained by choosing different values for α and β . Since the correlated wavefunction vanishes for distances smaller than $2A$ (due to repulsive core), from the structure of the equation (3.7a), we see that for large value of α , $f(r)$ is a short range function and the integral $\int f(r) R(r) r^2 dr$ will be very small and hence ψ' will be very close to ψ . This limiting choice of large α thus corresponds to an identity transformation for our practical purposes (contrary to the statement in Haftel and Tabakin 1970, that there is no way of generating identity transformation through a continuous change of parameters α and β). For some ranges of values of α and β , the reaction matrix elements are more attractive than the reaction matrix elements of the local potential. Some typical g -matrix elements are given in table 1. As we decrease α , for suitable choice of β , we get considerably more attractive g -matrices. However, we cannot decrease α indefinitely, as we want only short range modifications. It can also be seen that as g -matrix elements become more attractive, the derivatives of g -matrix elements with starting energy also decrease in magnitude, and so do the wound integrals. Just as was seen in nuclear matter, here also we see a linear relation between the g -matrix elements and the wound integrals. This can be seen from figure 1 and also table 2. Under a rank one unitary transformation with two parameters adopted by us, we can reduce the wound integral almost by half. With a more sophisticated procedure we should be able to make the g -matrix more attractive and the wound integral smaller. If we extrapolate the linear dependence to a super soft potential with $\kappa = 0$, the g -matrix elements are highly attractive. These extrapolated values are quite reliable (to within 5°KA^3) at least in the least square sense. These enormous shifts compared to the local potential (see table 3) could shift the binding energy and saturation density considerably.

Table 1. Reaction matrix elements (in $^{\circ}\text{KA}^3$) for various phase equivalent potentials ($k_f = 0.80 \text{ \AA}^{-1}$, $\mathbf{K} = 0.5 k_f$ and $\omega = 1.0 \text{ \AA}^{-2}$).

α	β	$k/k_f = 0.1$	0.5	1.0
local	..	128.3	180.1	147.3
2.50	0.55	122.4	175.2	144.9
2.00	0.50	109.1	164.4	140.8
2.00	0.45	112.3	167.8	143.2
1.75	0.50	94.7	151.3	135.5
1.75	0.45	95.1	154.6	139.4
1.50	0.50	91.6	137.2	127.7
1.50	0.45	69.4	131.6	133.4
1.50	0.40	73.1	142.0	142.1
extrapolated to $\kappa = 0.0$		-47.4	11.4	53.8

Table 2. Reaction matrix elements (in $^{\circ}\text{KA}^3$), wound integrals $\langle \chi | \chi \rangle$ (in A^3), and Brandow convergence parameter κ for various phase equivalent potentials represented by α, β . ($k_f = 0.8 \text{ \AA}^{-1}$; $\mathbf{K} = 0.5 k_f$; $k = 0.1 k_f$; $\omega = 1.0 \text{ \AA}^{-2}$).

α	β	g	wound integral	κ
30.0	1.0	128.3	6.78	0.278
2.50	0.55	122.4	6.51	0.267
2.00	0.50	109.1	5.92	0.242
2.00	0.45	112.3	6.13	0.251
1.75	0.50	94.6	5.27	0.216
1.75	0.45	95.1	5.23	0.214
1.50	0.45	69.4	4.46	0.183
1.50	0.40	73.1	4.69	0.192

Table 3. Extrapolated values of reaction matrix elements (in $^{\circ}\text{KA}^3$) for wound integral $\kappa = 0.0$ ($k_f = 0.8 \text{ \AA}^{-1}$), $\mathbf{K} = 0.5 k_f$; $\omega = 1.0 \text{ \AA}^{-2}$).

k/k_f	g (extrapolated)	g (local)
0.2	-38.9	141.7
0.4	-8.3	170.9
0.6	28.1	183.9
0.8	47.8	174.8
1.0	53.8	147.3

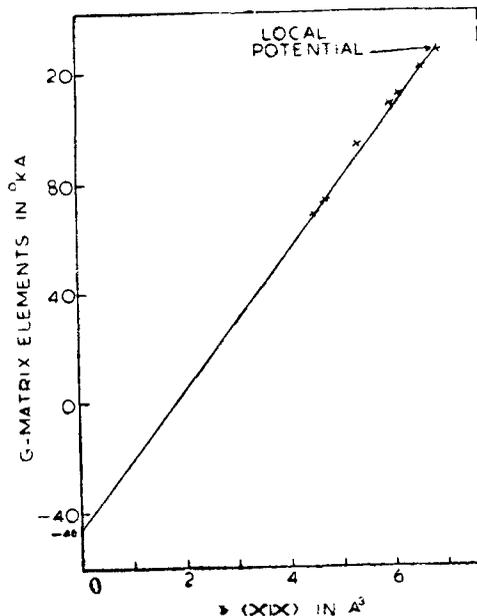


Figure 1. Dependence of reaction matrix element (in $^{\circ}\text{KA}^3$) on wound integral $\langle \chi | \chi \rangle$ (in \AA^3) (Parameters are the same as in those of table 2).

5. Calculation of the binding energy

In the present work, we have not seriously attempted to obtain a phase equivalent potential that actually gives highly attractive g -matrix elements. We assumed that this could, in principle, be done by a more complicated procedure (may be by using higher rank unitary transformations with more parameters) without altering the long range local behaviour. We also assumed that when this is done the linearity referred to above is still obeyed at least approximately. Thus we generate g -matrix elements for smaller κ by just interpolating or extrapolating the linear behaviour (like the one in figure 1) obtained for the phase equivalent potentials for ten conveniently chosen sets of α and β . We repeat similar calculations for three different values of starting energy. As expected, the extrapolated values of g -matrix elements (for small values of κ) are fairly independent of the starting energy. This is to be expected as for smaller κ , the ω -dependence is to be weak (see eq. 4.4).

In calculating the two-body interaction energy, we adopted the procedures same as in RR and GII. We fix the centre of mass momentum $K = 0.5 k_f$. For the single particle potential we use:

$$\begin{aligned}
 U(k) = & \frac{4}{\pi^2} \int_0^{\frac{1}{2}(k_f-k)} dk_0 k_0^2 \langle k_0 | g | k_0 \rangle \\
 & + \frac{2}{\pi^2} \int_{\frac{1}{2}(k_f-k)}^{\frac{1}{2}(k_f+k)} dk_0 k_0^2 \langle k_0 | g | k_0 \rangle \left[1 + \frac{k_f^2 - k^2 - 4k_0^2}{4k_0 k} \right] \quad (5.1)
 \end{aligned}$$

and the average interaction energy per particle is given by:

$$W_2 = \frac{2}{3k_f^3} \int_0^{k_f} dk k^2 U(k). \quad (5.2)$$

We obtain the energy per particle in the lowest order Brueckner theory through

$$E_2 = \frac{3}{10} k_f^2 + W_2. \quad (5.3)$$

Table 4 gives the energy per particle for three values of k_f for various choices for the values of the wound integral. It is to be noticed that for the local potential (*i.e.*, $\kappa/\kappa_L \approx 1$), the energy per particle is positive. This is to be compared with the value of -0.12°K at the saturation density corresponding to $k_f = 0.60$ for the local potential (*RR*). As the repulsion is made softer and softer, and as the wound integral decreases, the saturation shifts to higher densities and energy per particle decreases. At about $\kappa/\kappa_L = 0.23$, we get for saturation, $k_f = 0.79 \text{ \AA}^{-1}$ and for energy about -1.69°K . For a still softer potential, the density and absolute value of energy keep on increasing.

These results for the phase equivalent potential with $\kappa/\kappa_L = 0.23$ represent sizable shift from the results of the local potential. However the binding energy still differs considerably from the experimentally observed -2.5°K .

6. Discussion

The results obtained above for phase equivalent potentials are encouraging and promising. These potentials reproduce the two-body scattering phaseshifts and

Table 4. Energy per particle (in $^\circ\text{K}$) for three different values of Fermi momentum k_f (in \AA^{-1}), for potentials with different wound integrals κ . κ_L is the wound integral for the local potential.

κ/κ_L	$k_f = 0.76$	0.80	0.84
0.00	-2.93	-3.62	-4.59
0.05	-2.55	-3.06	-3.68
0.10	-2.21	-2.56	-2.93
0.15	-1.90	-2.12	-2.29
0.20	-1.62	-1.73	-1.74
0.22	-1.51	-1.59	-1.54
0.25	-1.36	-1.38	-1.26
0.30	-1.12	-1.07	-0.85
0.40	-0.70	-0.52	-0.30
0.60	-0.12	+0.33	+0.86
0.80	0.51	0.96	1.55
1.00 (local)	0.93	1.44	1.95

thus are in some sense equivalent so far as two-body systems are concerned. We have shown that by generating the phase equivalent potentials, we can generate potentials that explain not only two-body data but many body data also simultaneously. To achieve better understanding it is necessary to actually construct a potential that is soft and also to estimate the three-body clusters (Bethe and Rajaraman 1967). It is expected that these clusters might give a little more attraction of the order of 0.5 to 1.0 °K without changing the saturation density appreciably (Coester *et al* 1970). Calculations on these lines are in progress.

Similarly, one cannot judge the interaction just by the binding energy and saturation density alone. One should probably calculate other properties *e.g.*, correlation function in liquid state, effective mass parameters, effective interactions. Similarly one should see what might happen if this interaction is used for He⁴ — He⁴ atomic systems.

At a more fundamental level, one should investigate if the basic atom-atom potential might have some nonlocality from an *ab initio* calculational point of view. On the other hand, one should also investigate if by a suitable choice of off-shell continuation, one is actually taking (somehow) the three body interaction into account.

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