Redetermination of hard-core square-well-potential parameters for helium using new constructive methods for the ground state of liquid ^{4}He

George A. Baker, Jr.,* Manuel de Llano, Justino Pineda, and William C. Stwalley†
Instituto de Física, Universidad de México, México 20, D.F., México
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It is shown how recent Padé-approximant schemes, in density and attractive two-body coupling strength, for the ground-state energy of liquid ^{4}He are not inconsistent with the present knowledge of two-body scattering data.

Recently a new procedure for describing the ground-state-energy equation of state for quantum fluids has been proposed.[1] However, the only example carried through in detail for comparison with experiment was liquid ^{4}He. In that case, agreement with experiment was poor, with the saturation density and binding energy each being approximately an order of magnitude too small. Part of the problem could have been the three-parameter interatomic potential model used, namely, the hard-core square-well (HCSW) model. Indeed we are now extending Ref. 1 to more realistic potentials, e.g., those proposed by Aziz *et al.*[2] However, we now believe the primary difficulty in Ref. 1 was in the HCSW potential parameters of Burkhardt[3] used there. The purpose of this report is to examine this question and present new potential parameters for the HCSW potential of $^4He_2$ determined by experimental bounds on the $^4He_2$ two-body scattering length[4] and the empirical saturation density and binding energy of liquid ^{4}He.

The starting point for constructing an equation of state for the ground state energy of boson fluids in Ref. 1 is the well-known,[5] low-density (non-power-series) expansion in $(\rho a^3)^{1/2}$, where ρ is the particle density and a is the S-wave scattering length of the two-body system. As it stands, the series is useless for two reasons: (a) only the first few coefficients are known, thus limiting its validity to very low densities and (b) the empirical value of a is often negative giving rise (since the leading term in the energy per particle is $2\pi\hbar^2\rho a/m$) to a negative pressure instability. The latter difficulty is circumvented by expanding the scattering length a in powers of the attractive strength parameter; one then has a power series in this parameter and a nonregular series in $(\rho c^3)^{1/2}$, where c is the diameter of the repulsive cores, which is then extrapolated to nonvanishing values by the use of different generalized Padé approximants,[6] as discussed in Ref. 1. One thus has a perturbation theory about the hard-sphere Bose system, in analogy with the highly successful schemes available for classical fluids,[7] except that for the quantum case perturbative corrections can be carried out to high orders with relative ease. In Ref. 1 this was done up to fourth order for liquid ^{4}He.

The two-body interatomic potential used was the HCSW potential defined by

$$v(r)=\begin{cases}+\infty & (r<c)\\ -v_0 & (c<r<R)\\ 0 & (r>R)\end{cases} \tag{1}$$

with the parameters given by Burkhardt as $v_0=1.42$ K, $R=5.5$ Å, and $C=1.685$ Å. For such a potential the S-wave scattering length is given in closed form by

$$a/c=1+\alpha(1-\tan\sqrt{\lambda}/\sqrt{\lambda})$$
$$\simeq 1+\alpha(-\tfrac{1}{3}\lambda-\tfrac{2}{15}\lambda^2-\cdots)\ , \tag{2}$$

where

$$\alpha\equiv(R-c)/c,\quad \lambda\equiv\frac{m v_0}{\hbar^2}(R-c)^2\ ,$$

where the power-series expansion diverges for $\lambda>\pi^2/4\simeq 2.467$. The parameters of Ref. 3 give $\lambda=1.719\,086$, $\alpha=2.264\,095$ and $a=-5.452\,89$ Å. This led in Ref. 1 both to a binding energy and a saturation density much too small for liquid ^{4}He.

However, existing low-energy experimental results on the two-body system imply that $|a|>20$ Å and in fact a recent study[8] shows the Aziz *et al.*[2] potential to have a very weakly bound state and $a=+122.252\,11$ Å.

Using Eq. (2) the energy/particle in Ref. 1 is, up to fourth order in λ,

$$E/N\equiv\epsilon(x,\lambda)=\sum_{i=0}\epsilon_i(x)\lambda^i+O(\lambda^5)\ , \tag{3}$$

where $x\equiv(\rho c^3)^{1/2}$. The hard-sphere energy $\epsilon_0(x)$ was found [Eq. (15) of Ref. 1] to fit the available Green's function Monte Carlo data points[9] and showed an "uncertainty-principle" divergence (random close packing) at $x=0.7082$. For $\epsilon_i(x)$, $i=1,2,3,4$, which contains four terms including a $\ln x$ one, the generalized Padé approximants denoted in

Ref. 1 by $H_1^{(1)}(x)$, $H_2^{(1)}(x)$, $F_3^{(1,1)}(x)$, and $F_4^{(1,1)}(x)$, respectively, were found adequate there to give a divergence-free representation in the region of physical densities. Finally, (regular) Padé approximants in λ were constructed but found to be unnecessary compared with the straightforward fourth-order perturbation series, denoted by [4/0], as the value of λ quoted above is apparently "small" compared with $\pi^2/4$.

We have reinvestigated the possibility of reducing the 90% error in both energy and density of Ref. 1 to essentially zero. This was done by first decreasing the hard-sphere diameter c to increase both the saturation density and binding. Once the correct density is obtained the value of c remains essentially fixed; we then change R accordingly so that α in Eq. (2) remains as before, otherwise unwanted poles develop in the x approximants as described in Ref. 1. This gave $c = 1.043$ Å and $R = 3.404$ Å, and Eq. (2) gives, for the empirical limit $|a| > 20$ Å, the limits $2.2614 < \lambda < 2.7439$. The intermediate value $\lambda = 2.527$ ($v_0 = 5.453$ K and $a = +82.17$ Å) gives the empirical binding with the best approximant, namely, the [3/1]. The energy/particle as function of density is shown in Fig. 1 for different λ Padé approximants. A 20% improvement in binding is seen as one goes from third- to fourth-order perturbation theory ([3/0] compared to [4/0]). A much larger improvement is noted in going from second to third order ([2/0] to [3/0]), as well as an abrupt increase in the saturation density.

We thus conclude that the constructive methods developed in Ref. 1 can claim not only to have found a proper "smallness parameter" (λ) for the description of boson liquids but also to give essentially the right binding and saturation density given the present empirical uncertainty in the two-body potential energy curve.

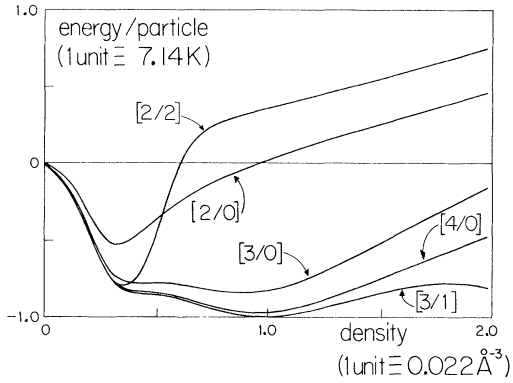

FIG. 1. Energy per particle in units of the empirical binding energy per particle of 7.14 K and the saturation density of 0.022 Å^{-3} of liquid ^{4}He, as obtained with several (regular) Padé approximants in λ, the attractive strength parameter of the HCSW potential used.

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*Permanent address: Theoretical Division, Los Alamos National Laboratory, University of California, Los Alamos, N.M. 87545.

†On leave from Departments of Chemistry and Physics, The University of Iowa, Iowa City, Iowa 52242.

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