# Energy dependence in interatomic potentials—$He_2$†

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The energy dependence in interatomic potentials is shown to be expressible as angular momentum dependence of the potential. This means that a potential determined by scattering for a given partial wave can also be used to analyze the question of the existence of a bound state in the same partial wave. This procedure is not available for the problem of the existence of $He_2$ because of the lack of experimental data. However, it is shown that scattering experiments of He + He have been done at sufficiently low energy so that the extrapolation of the potential in energy necessitated by its energy dependence is too small to affect the existence of the bound state.

The fact that the existence of a bound state of $He_2$ is a problem stems from the extremely weak interaction of two ground-state He atoms. *Ab initio* calculations[1] of the adiabatic potential interaction give an attractive well depth of the order of only $10^{-3}$ eV and an either just-bound or just-unbound state of the atoms. The absolute accuracy of the calculations is well below that needed to conclude anything about the bound state but the shape of the potential is more accurately determined and this is what is used to discuss the existence of the bound state.

Recent accurate experiments[2] on the scattering of very-low-energy He by He have been analyzed to obtain the He-He potential with more accuracy than the calculations afford. The potential determined in this way can then be used to investigate the existence of the bound state. In using such a method an assumption concerning the energy dependence of the potential must be made and the one usually made is that it is energy independent.

In two earlier papers[3,4] the question of whether this is the case was investigated. The helium atom is a structure with internal degrees of freedom and the assumption that the interaction of two He atoms can be characterized by a local energy-independent potential must be substantiated. In the first paper[3] the nonlocal energy-dependent dispersive part of the potential was found to be negligible. In the second paper[4] another term, erroneously omitted in the first, was found which was energy dependent and not negligible. This arose from the inclusion of the Pauli principle for the electrons and the correct treatment of the boundary conditions. We shall show here that this energy dependence may be rigorously eliminated in some restricted cases.

The essential form of the scattering equation derived in Ref. 4 is

$$\left[E - W_0(\xi) + \frac{1}{2\mu}\left(1 + \frac{m}{\mu}\sigma(\xi)\right)\nabla^2 - \frac{m}{\mu}V(\xi)\right]F^{(+)} = 0, \tag{1}$$

where $m$ is the electron mass, $\mu$ is the reduced mass of the atoms, $W_0$ is the conventional interatomic potential obtained by molecular theorists, and $V(\xi)$ and $\sigma(\xi)$ are functions of the scattering coordinate whose details are not important here. Since Eq. (1) was obtained as a power series in $m/\mu$, it is equivalent to

$$\left(E - W_0 + \frac{1}{2\mu}\nabla^2 - \frac{m}{\mu}[V + (E - W_0)\sigma]\right)F^{+} = 0, \tag{2}$$

in which form the energy-dependent potential is evident. We see then that the effect can be interpreted as a position-dependent effective mass, or an energy-dependent potential.

If a given partial wave is selected from Eq. (1), the radial equation may be written

$$\left[E - W_0 + \frac{1}{2\mu}\left(1 + \frac{m}{\mu}\sigma\right)\left(\frac{d^2}{d\xi^2} - \frac{l(l+1)}{\xi^2}\right) - \frac{m}{\mu}V\right]u_l^{(+)} = 0. \tag{3}$$

Then the substitutions

$$\xi = r\left(1 + \frac{m}{\mu}\eta(r)\right) \tag{4}$$

and

$$u_l^{(+)}(\xi) = \left(1 + \frac{m}{2\mu}\sigma(r)\right)v_l^{(+)}(r), \tag{5}$$

with

$$(r\eta)' = \sigma(r), \tag{6}$$

convert Eq. (3) into (to order $m/\mu$)

$$\left[E - W_0(r) + \frac{1}{2\mu}\left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2}\right) - \frac{m}{\mu}\left(\frac{1}{4\mu}\sigma' + r\eta W_0' + V - \eta\frac{l(l+1)}{r^2}\right)\right]v_l^{(+)} = 0. \tag{7}$$

This is a conventional radial Schrödinger equation with a potential which, in order $m/\mu$, depends upon $l$. Now if the potential is determined experimentally from scattering for a given $l$, it is energy independent and may be used to analyze the bound-state problem for the *same* $l$.

In the experiments of Ref. 2 no angular-distribution measurements were made so it is not possible to isolate a given partial wave. Moreover, at the lowest energy used (0.3 meV) there are still about two partial waves participating in the scattering so that the $S$-wave scattering can not be isolated. Consequently, the analysis outlined above can not be performed.

If we return to Eq. (2) and consider the experimental analysis, the potential fit obtained to the data must represent

$$W_{\rm exp} = W_0 + (m/\mu)[V + (\bar{E} - W_0)\sigma], \tag{8}$$

where $\bar{E}$ is some average energy in the experiment. The determination of the potential in the region of the minimum is particularly sensitive to the low-energy scattering data, so we take $\bar{E} < 1$ meV. The potential relevant to the bound state (of energy $E_B$) is then

$$\begin{aligned} W_B &= W_0 + (m/\mu)[V + (E_B - W_0)\sigma] \\ &= W_{\rm exp} + (m/\mu)(E_B - \bar{E})\sigma . \end{aligned} \tag{9}$$

The last term represents an additional attractive potential of order $(m/\mu)(1\ \text{meV}) \simeq 0.3\times10^{-6}$ eV, since $\sigma$ is positive and of the order of unity or less in the region of interest. In Ref. 2 it is stated that an increase of the measured well depth of 1.4%, or about $10^{-5}$ eV, is necessary to produce binding. The energy-dependent term in Eq. (9) is too small to deepen the binding potential by this amount. Therefore the conclusion in Ref. 2 that there is no bound state need not be modified by the energy dependence of the potential.

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