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On the Bose–Einstein condensation of exotic atoms

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Abstract
The scattering length for hydrogenic atoms with variable lepton mass, ranging from H to pμ, is calculated. The non-trivial sensitivity of the scattering length to non-adiabatic effects is investigated using the coupled-channel approach. The physical conditions for the Bose–Einstein condensation of exotic atoms are expressed in terms of this scattering length, which for the pμ atoms interacting via $^3\Sigma_u^+$ potentials, is calculated to be 1.13×10^{-2} au. The critical temperature for condensing the pμ atoms is estimated to be 0.5 K at a density of 2.2×10^{20} cm^{-3}. Under these conditions the phonon velocity in the condensate is 2.2 m s^{-1} and the coherence length is nearly 5 μm.

1. Introduction

More than ten years after the creation of dilute Bose–Einstein condensates (BEC) of alkali metal atoms in magneto-optical traps, the intense level of activity in ultracold atomic and molecular species continues unabated. Nearly all the alkali metal atoms have now been Bose condensed and degenerate Fermi gas and Bose condensation of molecules formed from the magnetically tunable interaction between Fermionic atoms have been spectacularly demonstrated [1, 2]. The demonstration of the reversible superfluid to Mott insulator phase transition in an optical lattice and the transition to the Bardeen–Cooper–Schrieffer regime are experiments [3, 4] in the condensed regime. More recently, the formation of a BEC of chromium atoms in an optical dipole trap is the first example of condensation with large anisotropic dipole–dipole interaction [5]. The prospect for condensation of light species, such as positronium atoms [6–9], raises tantalizing hopes for applications such as the γ-ray laser.

A great deal of knowledge about the collisional properties of atoms at ultracold temperatures has been gleaned from theoretical investigations of spin-polarized hydrogen collisions, aiming to understand the accuracy of hydrogen maser clocks [10] and Bose condensation of hydrogen [11]. Molecular hydrogen is unique in that it is the simplest of all neutral molecules and hence amenable to sophisticated quantum molecular theories which

can be applied to calculate accurate Born–Oppenheimer (BO) potential energy curves, non-adiabatic coupling interactions and properties characterizing H–H collisions such as cross sections and scattering lengths. Because the cold colliding atoms approach slowly and hence spend long times interacting with each other, they are susceptible to weak long-range forces. Substantial effort, in particular over the last decade, has been devoted to calculating long-range interaction forces between hydrogen, alkali-metal and group II atoms. In the case of hydrogen and alkali-metal atoms, considerable attention has been paid to the sensitivity of ultracold collisional properties—the s-wave scattering length in particular—to small changes in the BO potential energies, such as the inclusion of relativistic terms and diagonal interaction, the so-called adiabatic correction term, and other effects such as altering the reduced mass from nuclear to atomic mass [12, 13].

In this work, we calculate the scattering length for the hydrogen atom whose electron has been replaced by a negative lepton and study the influence of the adiabatic corrections and non-adiabatic molecular channel couplings. We concentrate on the muonic atom, an atomic complex of proton and muon and find that the ratio of the lepton mass to the hadron mass determines, to a large extent, the sensitivity of the scattering length to adiabatic corrections. Using the results, we explore new regimes of BEC and estimate the physical conditions for condensing light and strongly bound atoms such as pμ.

Collisions between muonic atoms are analogous to collisions between H atoms, except that the size of the pμ-atom is much smaller. Compared to hydrogen atoms, muonic atoms are more compact and more strongly bound by a factor $\eta = \mu_{\mathrm{p}\mu}/\mu_{\mathrm{pe}} \simeq 186$, where $\mu_{\mathrm{p}\mu}$ and μ_{pe} are the reduced masses of the proton–muon and proton–electron systems, respectively. In thermal collisions with hydrogen atoms or molecules, the pμ atom behaves like a spinless neutron. Muonic atoms penetrate the electronic shells of ordinary atoms without breaking them and collide with atomic nuclei (see [14]). Kinetics of collisions of muonic atoms has been extensively studied in connection with the catalysis of nuclear reactions [15–17]; here we discuss the quantal properties of the pμ gas.

2. Calculation and analysis of the scattering length for pμ atoms

The position of the minimum of the interaction potential for pμ atoms is reduced and the depth of the potential increased by a factor of $\eta \simeq 186$. The nuclear motion is described in the adiabatic approximation by the Schrödinger equation

$$\left(\hat{H}_i + C_{ii}^{\mu}(R)\right)\chi_i(R) = E\chi_i(R), \tag{1}$$

where $i = 0, 1, 2, \ldots$ refer to the ground and excited states of pμ–pμ of singlet or triplet symmetry, and

$$\hat{H}_i = -\frac{1}{2M}\frac{\mathrm{d}^2}{\mathrm{d}R^2} + \frac{1}{R} + V_i^{\mu}(R), \tag{2}$$

M is the reduced mass of two protons, E is the collision energy, $V_i^{\mu}(R) = \eta V_i^{e}(R\eta)$ is the ith muonic adiabatic potential obtained by scaling the electronic potential $V_i^{e}(R)$ for two hydrogen atoms, and atomic units have been used. In equation (1), $C_{ii}^{\mu}(R)$ is a diagonal adiabatic correction to the ith Born–Oppenheimer (BO) potential, arising from the coupling between the motion of the light and heavy particles. In the H_2 molecule, the correction $C_{ii}^{e}(R)$ is small, but since it involves second derivatives with respect to the coordinates it scales as $C_{ii}^{\mu}(R) = \eta^2 C_{ii}^{e}(R\eta)$, and hence its importance relative to the BO potential increases by a factor η.

The standard form of the diagonal adiabatic correction [18, 19] is

$$C_{ii}(R) = \langle \phi_i(\mathbf{r}_1, \mathbf{r}_2; R)| - \frac{1}{2M}\Delta_R - \frac{1}{8M}(\Delta_1 + \Delta_2) - \frac{1}{4M}\nabla_1 \cdot \nabla_2 |\phi_i(\mathbf{r}_1, \mathbf{r}_2; R)\rangle \tag{3}$$

where $\phi_i(\mathbf{r}_1, \mathbf{r}_2; R)$ is the leptonic BO wavefunction corresponding to the leptonic channel i, i.e. solution to the leptonic eigenvalue problem $\left[-\frac{1}{2m_l}(\Delta_1 + \Delta_2) + V\right]\phi_i(\mathbf{r}_1, \mathbf{r}_2; R) = V_i^l(R)\phi_i(\mathbf{r}_1, \mathbf{r}_2; R)$, with V being the potential energy of the proton–lepton interaction and m_l the lepton mass.

We use the leptonic Hamiltonian in which the muon mass is replaced by the reduced muon–proton mass. In changing the unit of energy from atomic units based on the muon mass to units based on the muon–proton *reduced* mass, an amount of the leptonic kinetic energy $\delta K = -1/(4M)(\Delta_1 + \Delta_2)$ is incorporated into the kinetic energy term of the BO Hamiltonian for the muons. Adding δK to the leptonic BO Hamiltonian $-1/(2m_l)(\Delta_1 + \Delta_2) + V$ changes it to $-1/(2\mu_{\rm pl})(\Delta_1 + \Delta_2) + V$, where $\mu_{\rm pl}$ is the reduced mass of the proton–lepton system, and subtracting δK from the term $-1/(8M)(\nabla_1 + \nabla_2)^2$ of the adiabatic correction changes it into $1/(8M)(\nabla_1 - \nabla_2)^2$. The adiabatic correction becomes

$$C_{ii}(R) = \langle \phi_i(\mathbf{r}_1, \mathbf{r}_2; R)| - \frac{1}{2M}\Delta_R + \frac{1}{8M}(\Delta_1 + \Delta_2) - \frac{1}{4M}\nabla_1 \cdot \nabla_2 |\phi_i(\mathbf{r}_1, \mathbf{r}_2; R)\rangle. \tag{4}$$

Hence the transformation leads to the leptonic BO Hamiltonian based on the reduced proton–muon mass and to the diagonal correction that vanishes asymptotically, providing the correct scattering limit [20].

We first calculate the scattering length of the $X^1\Sigma_{\rm g}^+$ ground-state potential, $a_{\rm s}$. We have used the interaction potential together with the diagonal (adiabatic), relativistic and radiative corrections from [13] and privately communicated data in the interval $R = 12$–20 au. The long-range part is described by the C_6, C_8 and C_{10} coefficients from [21] and the exchange correction from [22]. The phase shift, $\delta_0(k_i)$, where k_i is the asymptotic linear momentum in channel i, is obtained by numerically integrating equation (1) to a value of $R = 100$ mau, where mau are the modified muonic atomic units based on the reduced proton–muon mass. We have verified that the phase shift is converged by repeating the calculation to a BO distance of $R = 1000$ mau. Finally, we extract the scattering length in the limit, $a = -\lim_{k_i \to 0} \tan \delta_0(k_i)/k_i$.

Using in equation (1) the BO $X^1\Sigma_{\rm g}^+$ potential together with the appropriately scaled diagonal correction (4), we obtain the singlet scattering length $a_{\rm s} = 2.246\,{\rm mau} = 2.246\,{\rm au}/\eta = 1.208 \times 10^{-2}$ au. If the correction C_{00}^{μ} is omitted we obtain $a_{\rm s} = 2.323$ mau; the change induced by the diagonal adiabatic correction is -0.0764 mau or -3%. This is much less than the change of -27% reported in [23] for the H−H system. The insensitivity of the scattering length for pμ collisions is due to the absence of near threshold states of the pμ–pμ system. We calculated the vibrational energy levels for the ground state of pμ–pμ molecule and found that it has *only* one bound vibrational state with a binding of 354 eV.

We now consider the case of muonic atoms colliding with parallel spins, as is the case in a magnetic trap, when the nuclei interact through the muonic potential of triplet symmetry $^3\Sigma_{\rm u}^+$. This potential is almost entirely repulsive and has no bound states. The $^3\Sigma_{\rm u}^+$ scattering length calculated in the BO approximation is $a_{\rm t} = 2.281$ mau. Adding the diagonal adiabatic correction changes it by -8% to $a_{\rm t} = 2.107$ mau.

Thus far we have neglected the non-adiabatic radial coupling, which is much stronger for pμ–pμ compared to H–H and might significantly affect the cross sections. The energy of the nuclear vibrations in the muonic molecule is only moderately smaller than the energy of muonic transitions, corresponding to a non-adiabaticity parameter $E_{\rm vib}/\Delta E_{\mu} \simeq \sqrt{m_{\mu}/m_{\rm p}} \simeq 0.3$. However, the smallness of that ratio provides a sufficient rather than a necessary condition for the validity of the BO approximation [24].

In view of the unusually large non-adiabaticity parameter, we investigate the sensitivity of the triplet scattering length to the interaction between the adiabatic states.

With the inclusion of the non-adiabatic couplings $B_{01}(R)$ and $B_{10}(R)$ the resulting coupled equations have the form

$$(\hat{H}_0 - E)\chi_0(\mathbf{R}) = -\hat{B}_{01}(R)\chi_1(\mathbf{R}) \tag{5}$$

$$(\hat{H}_1 - E)\chi_1(\mathbf{R}) = -\hat{B}_{10}(R)\chi_0(\mathbf{R}) \tag{6}$$

where the indices refer to the two lowest $^3\Sigma_u^+$ states of pμ–pμ and the operators $\hat{H}_i$ are defined in equation (2). The above equations (5)–(6) are solved at an energy just above the lowest dissociation threshold to pμ(1s) + pμ(1s), at $E = -1 + \epsilon_i$ where ϵ_i is the relative kinetic energy of the colliding atoms. In the Hamiltonian $\hat{H}_0$, we used the appropriately scaled adiabatic potential $V_0^e(R)$ of the $b^3\Sigma_u^+$ state and the concomitant adiabatic correction from [25] up to $R = 8$ au and from [26] for 8 au $< R <$ 12 au. For larger R, we used the expansion from [21]. In the Hamiltonian $\hat{H}_1$ we used the $V_1^e(R)$ potential of the $e^3\Sigma_u^+$ state from [25] together with the long- and short-range data from [27]. The lowest state, which is almost entirely repulsive, correlates in the separated atom limit to the threshold energy $E_0 = E(\mathrm{H(1s)} + \mathrm{H(1s)}) = -1$ au. The next lowest state has a minimum $V_1^{\min} \simeq -0.68$ au at $R \simeq 2$ au and converges to the separated atom limit with energy $E_1 = E(\mathrm{H(1s)} + \mathrm{H(2s)}) = -0.625$ au. The coupling matrix elements B_{01} and B_{10} were obtained by fitting the graphical data from [28] to analytical functions. We adapted these couplings to the muonic situation by scaling them with a factor η according to $\hat{B}_{01}^{\mu}(R) = \eta B_{01}^{e}(\eta R)\partial/\partial R$.

The calculation of the triplet scattering length gave $a_t = 2.098$ mau $= 2.098$ au$/\eta = 1.128 \times 10^{-2}$ au. This is two orders of magnitude smaller than for hydrogen atoms: for spin-polarized hydrogen atoms interacting through the triplet $b^3\Sigma_u^+$ potential $a^{\mathrm{H}} = 1.216$ au [23]. We find that the inclusion of coupling to the first excited state (via B_{01}) results in a small change of the scattering length a_t. This effect is smaller than the effect of the adiabatic correction. The influence of coupling to the next excited state (via B_{02}) is also small and it is thus probable that couplings to more distant states will be at most comparable. The effects of non-adiabatic coupling are small because of the large energy gap between the muonic states and the ultralow kinetic energy of the colliding atoms. The numerical instabilities, encountered in calculations of the non-adiabatic scattering length for hydrogen [20], were not present in our calculation for pμ.

The mass scaling of the interaction potential provides us with an opportunity to study the dependence of the scattering length on the leptonic mass. In figure 1, we show our singlet and triplet scattering lengths, calculated by including the adiabatic correction in the BO Hamiltonian, as a function of the ratio of the light mass to heavy mass, m_l/m_h. The singularities in the singlet scattering length reflect the presence of bound states with zero binding energy. The triplet scattering length is smooth, indicating the absence of a bound state for $m_l/m_h \geqslant 0.169 \times 10^{-3}$. For $m_l/m_h \simeq 0.113$, corresponding to pμ, a_t attains a value which is coincidentally very close to a_s.

3. Conditions for condensation of pμ atoms

For an ideal Bose gas in three dimensions, the necessary condition for condensation takes the form [29, 30],

$$\rho\lambda_{\mathrm{dB}}^3 > 2.612 \tag{7}$$

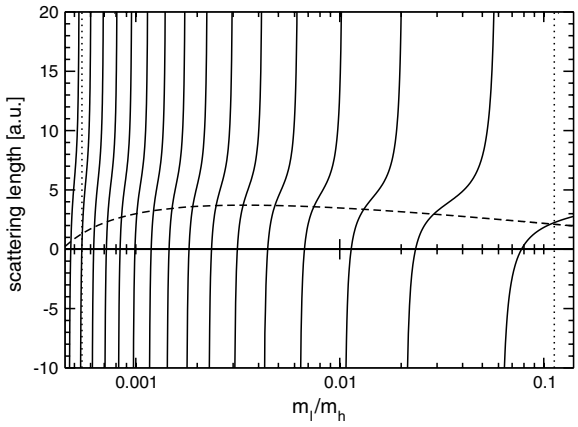

Figure 1. Singlet (a_s, solid line) and triplet (a_t, dashed line) scattering lengths for collisions of hydrogen-like atoms, given in mass-scaled atomic units, as a function of the mass ratio $\gamma = m_l/m_h$. The dotted line to the left corresponds to $\gamma = m_e/m_p \simeq 0.545 \times 10^{-3}$ for hydrogen, the dotted line to the right corresponds to $\gamma = m_\mu/m_p \simeq 0.113$ for pμ. The sensitivity of the scattering length to the change of the mass ratio is seen to be larger for hydrogen than for pμ. This effect would be seen even more clearly with a linear scale of the abscissa.

where ρ is the atom number density and λ_{dB} is the de Broglie wavelength, $\lambda_{dB} = \sqrt{2\pi\hbar^2/(mk_BT)}$, with m being the atomic mass, k_B Boltzmann's constant and T the absolute temperature. In a trap and in the presence of atomic interaction, a diluteness parameter, $D = a/\rho^{-1/3}$, may be introduced to describe how an interacting quantum gas approaches the ideal gas limit [29]. The almost ideal Bose gas is characterized by a small value of D [31] and in this situation the condition for condensation can be expressed as $\lambda_{dB}(T, m) \gg d \gg a$, where $d = \rho^{-1/3}$ is the average interparticle distance. For all the gaseous alkali-metal and hydrogen BECs, the diluteness parameter is small; $D \sim 10^{-2}$ for the alkali metals and $D \sim 10^{-4}$ for hydrogen, respectively [32]. We therefore assume that D will be small for the pμ condensate, thus $a^{p\mu}/d^{p\mu} \ll 1$, with $a^{p\mu}/d^{p\mu} = a^H/d^H = D^H$. The same diluteness does not mean the same density; the average distance between the pμ atoms is given by $d^{p\mu} = d^H a^{p\mu}/a^H$. Thus, if hydrogen condenses at the density $\rho^H = (d^H)^{-3}$ the corresponding density for pμ is

$$\rho_c^{p\mu} = \left(\frac{1}{d^{p\mu}}\right)^3 = \rho_c^H \left(\frac{a^H}{a^{p\mu}}\right)^3 = \rho_c^H \left(\frac{1.21}{0.0113}\right)^3 \sim 10^6 \rho_c^H. \tag{8}$$

The nearly ideal gas behaviour of the pμ atoms occurs therefore at densities six orders of magnitude higher than for the hydrogen gas.

Using $\lambda_{dB}^{p\mu} = \lambda_{dB}^H a^{p\mu}/a^H$ from condition (7) we obtain the critical temperature for condensation of the pμ atoms to be

$$T_c^{p\mu} = \frac{m^H}{m^{p\mu}} \left(\frac{a^H}{a^{p\mu}}\right)^2 T_c^H \sim 10^4 T_c^H. \tag{9}$$

Thus the condensation temperature $T_c^{p\mu}$ for the BEC of pμ atoms is four orders of magnitude higher than that necessary to condense hydrogen. Since hydrogen condenses at $T^H \simeq 50\ \mu$K [32] a modest $T^{p\mu} = 0.5$ K will be required to condense pμ. The hydrogen density at the transition point is $\rho^H = 1.8 \times 10^{14}$ cm^{-3} and the corresponding critical density of pμ is, according to equation (8), $\rho^{p\mu} \simeq 2.2 \times 10^{20}$ cm^{-3}.

A fascinating feature of the pμ BEC is its ultra high density, leading to condensed-matter type properties in the regime of weak interatomic interaction. We find that the phonon velocity in this condensate would be two orders of magnitude larger than in the hydrogen condensate. Indeed, for small collisional energies, the energy of the elementary collective excitations (the so-called Bogoliubov phonons corresponding to sound waves in the atomic gas) is a linear function of momentum, $\epsilon = v_s p$, where $v_s = \sqrt{4\pi\hbar^2 a\rho/m^2}$ is the sound velocity. Hence $v_s^{p\mu} = \frac{m_H}{m_{p\mu}}\sqrt{a^{p\mu}\rho^{p\mu}/(a^H\rho^H)} \simeq 96 v_s^H$ and the sound velocities may reach values of several m s^{-1}, creating favourable conditions for the propagation of the collective excitations and superfluidity.

The formation and confinement of large quantities of pμ atoms in the form of an atomic gas are challenging and unsolved experimental tasks, more difficult than for the case of Ps = [e$^+$e$^-$] atoms [9] although the annihilation rate of positronium is about the same as the decay rate of muons. Both types of atoms can in principle be formed by recombination. The formation of pμ atoms occurs spontaneously when muons are brought in contact with gaseous or liquid samples of hydrogen in atomic or molecular form. Muons replace electrons in ordinary atoms, forming muonic atoms under a wide range of physical conditions. The entire formation process, including slowing down of fast muons, capture of slow muons into the highly excited states of muonic atoms, and deexcitation cascade into the ground state takes on the order of 100 ps at liquid hydrogen density [14], a time much shorter than the natural lifetime of the muon, $\tau_\mu = 2.2$ μs. Large quantities of pμ atoms might be obtained in $\mu-H_2$ collisions by stopping a beam of muons in a sample of hydrogen. However, the available beam intensities are not sufficient for obtaining the critical density of pμ predicted in this work [33].

In conclusion, we have calculated the scattering length for a system consisting of two hydrogenic atoms with a variable lepton mass. The sensitivity of the scattering length to the non-adiabatic effects for pμ–pμ collisions was analysed using the coupled-channel approach. The results indicate that the pμ atoms interact very weakly, manifesting behaviour similar to that of an ideal gas, without extensive cooling or diluting. The pμ scattering length, $a^{p\mu} = 1.13 \times 10^{-2}$ au, is two orders of magnitude smaller than the corresponding scattering length for hydrogen and for ortho-positronium, and four orders of magnitude smaller than that for ^{87}Rb. Thus the pμ atoms are expected to form a BEC in conditions very different from those required for ordinary atoms, moving the BEC phenomenon into a completely new regime, yet permitting theoretical treatment without complications originating from the strong interatomic interactions. Our calculations show that the BEC of pμ would occur at the temperature of 0.5 K (four orders of magnitude higher than for BEC of hydrogen) and the density of 2.2×10^{20} cm^{-3} (six orders of magnitude denser than for BEC of hydrogen).

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