Eur. Phys. J. D **37**, 435–439 (2006)
DOI: 10.1140/epjd/e2006-00034-2

**THE EUROPEAN
PHYSICAL JOURNAL D**

Ultra-long-range states in excited ^{3}He$_2$

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Received 24 November 2005

Abstract. Long-range potentials have been calculated for ^{3}He$_2$ molecules dissociating to ^{3}He 2 ^{3}S + ^{3}He 2 ^{3}P, including the retarded dipole and the van der Waals interactions. Ultra-long-range wells with depths of up to about 2.4 GHz have been found in many of the adiabatic body-fixed potentials and rovibrational levels have been calculated for some of these wells, which have been found to support up to 4 rotationless vibrational levels.

PACS. 32.80.Pj Optical cooling of atoms; trapping – 31.50.Df Potential energy surfaces for excited electronic states – 33.20.Ea Infrared spectra

Highlight Paper

1 Introduction

Starting from a gas of cooled metastable ^{4}He atoms, He (1s 2s ^{3}S), He*, Léonard et al. [1,2] have observed ultra-long-range weakly-bound levels in ^{4}He$_2$, these levels dissociating to ^{4}He(1s 2s ^{3}S) + ^{4}He(1s 2p ^{3}P$_J$). The position of these levels is in excellent agreement with calculations based primarily on a knowledge of the fine-structure intervals in He(1s 2p ^{3}P$_J$) and the C_3 coefficient for the long-range resonance dipole interaction between He atoms in the (1s 2s ^{3}S) and (1s 2p ^{3}P) states [1–4]. Since ^{3}He(1s 2s ^{3}S) has been cooled and trapped [5] in a Magneto-Optical Trap (MOT) in the $f = 3/2, m_f = 3/2$ state with comparable densities and temperatures to ^{4}He*, we examine in this paper whether ultra-long-range states can also be expected for ^{3}He.

In ^{4}He(1s 2p ^{3}P$_J$) there is considerable cancellation between the different contributions to the fine-structure splittings [6] and the resulting splittings are small and far from satisfying the Landé interval rule. Since the fine-structure splittings are small, the usual clear separation of the fine and hyperfine structure does not occur: the fine structure in ^{4}He(1s 2p ^{3}P$_J$) spans ≈32 GHz while the corresponding fine and hyperfine levels in ^{3}He span 34 GHz. Hence some of the hyperfine levels have to be viewed as being in intermediate coupling. Also the hyperfine splitting in ^{3}He (1s 2s ^{3}S), 6.739701 GHz [7], is about three times the fine-structure splitting between the $J = 1$ and $J = 2$ levels of ^{4}He 2^{3}P$_J$.

Given the different separated-atom behaviour, a different pattern of long-range potentials from those in ^{4}He can be expected. Also, with more atomic levels involved, more potentials will be obtained. While the lighter ^{3}He atoms imply a zero-point energy about 15% larger than in ^{4}He for the same potential curvature, in that system up to six levels were obtained in one potential, so, given comparable well-depths and positions of minima, some bound vibrational levels should exist.

In this paper we derive the various potentials in a body-fixed description and solve for the vibrational levels in certain potentials displaying long-range wells and a repulsive dipole potential towards the short-range separations, where otherwise accurate ab initio calculations would be required. The use of single-channel calculations may allow a better assignation of the vibrational levels than the results from full close-coupled calculations. While a highly accurate treatment requires solution of the coupled equations, the work of Venturi et al. [3] for the long-range molecules in ^{4}He has shown that the effect of the Coriolis couplings on the position of the vibrational levels is relatively small. Similar success of a Body-Fixed approach has been noted by Williams et al. [8] for long-range states in Na$_2$. We recall that the dipole potentials of interest here behave as C_3/R^3, where R denotes the internuclear separation, while the neglected Coriolis interaction behaves as $\hbar^2/2\mu R^2$, μ being the reduced mass, so the two interactions become comparable at $R \approx 2\mu C/\hbar^2 \approx 35000a_0$ for this system. The most excited ^{4}He long-range state had an outer classical turning point of about 1150a$_0$ [1].

2 Theory

We consider first the calculation of the potential matrix where the ^{3}He(1s 2p ^{3}P$_J$) hyperfine levels can be labelled by J and f, where $\mathbf{f} = \mathbf{J} + \mathbf{i}$, $\mathbf{i}$ being the nuclear angular momentum, of magnitude ($\hbar$/2). Below we consider transforming the potential matrix to an intermediate coupling basis allowing for mixing of different J values with the same f value. Allowance must also be made for the

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inverted hyperfine levels of the metastable ^{3}He ($1s\ 2s\ ^3$S$_1$) level, separation 6.74 GHz [7].

The interactions to be considered are the resonance dipole interaction, including allowance for retardation [9,10], and the van der Waals dispersion interaction, where accurate values from Marinescu, as cited by [3], for the C_6 coefficient are known for Hund's case (a) Σ and Π potentials. We consider first the calculation of the interaction in an unsymmetrized basis and then examine the additional effects of symmetrization. Following [11] let $|[(L_1S_1)J_1\ i_1, f_1]_a\ [(L_2S_2)J_2\, i_2, f_2]_b; F\phi\rangle$ denote the body-fixed two-atom wavefunction with the z-axis along the internuclear axis, $[(L_1, S_1)J_1\, i_1, f_1]_a$ denoting the angular momenta of atom a, in the usual notation, and corresponding values with subscript 2 for atom b. To simplify the notation other quantum numbers needed to specify the levels completely are not indicated explicitly. Here $\mathbf{L}_x + \mathbf{S}_x = \mathbf{J}_x,\ \mathbf{J}_x + \mathbf{i}_x = \mathbf{f}_x,\ x = 1, 2,\ \mathbf{f}_1 + \mathbf{f}_2 = \mathbf{F}$, $\mathbf{i}_1 + \mathbf{i}_2 = \mathbf{I}$ and $\phi = \Lambda + \Sigma + \iota$ denotes the projection of the resultant angular momentum, $\mathbf{F}$, on the internuclear axis. Also for simplicity we shall on occasion use the shorthand notation $\alpha_x \equiv [(L_xS_x)J_x, i_x, f_x]$, $x = 1, 2$. A wavefunction for the complete system with total angular momentum T and space-fixed projection M_T can be written

$$|(\alpha_1)_a, (\alpha_2)_b, F, \phi; T, M_T\rangle = |(\alpha_1)_a, (\alpha_2)_b; F\phi\rangle$$
$$\times D^{T*}_{M_T\phi}(\varphi, \vartheta, 0)\ \mathcal{F}[(\alpha_1)_a, (\alpha_2)_b, ; F\phi; T, M_T](R), \quad (1)$$

where $D^{T*}_{M_T\phi}$ is the usual symmetric-top eigenfunction, ϑ and φ are the polar coordinates of the internuclear axis in the space-fixed system and $\mathcal{F}$ denotes the radial wavefunction. Gao [12] has formulated the space-fixed description of the scattering of two atoms, each with fine and hyperfine structure. The Body-Fixed wavefunction, equation (1), is closely related to the space-fixed wavefunction employed by Gao [12], who uses the relative angular momentum ℓ, $\mathbf{F} + \boldsymbol{\ell} = \mathbf{T}$:

$$|(\alpha_1)_a, (\alpha_2)_b, F, \ell; T, M_T, P_T\rangle = \sum_\phi [\ell]^{1/2}(-1)^{\ell - F - \phi}$$
$$\times \begin{pmatrix} T & F & \ell \\ -\phi & \phi & 0 \end{pmatrix} |(\alpha_1)_a, (\alpha_2)_b, F, \phi; T, M_T\rangle, \quad (2)$$

where P_T is the total parity of the space-fixed wavefunction, given by $P_1P_2(-1)^\ell$, where P_i is the parity of the state of atom i. Here $[k_1k_2\cdots]$ denotes $(2k_1 + 1)(2k_2 + 1)\cdots$ and $\begin{pmatrix} \cdots \\ \cdots \end{pmatrix}$ denotes a $3 - j$ symbol.

Given the level of angular momentum coupling required, the use of irreducible spherical tensors provides a convenient way of evaluating the necessary matrix elements. Following Zare [13] we introduce the bispherical harmonic

$$X(k, 0) = \sum_m [k]^{1/2} \begin{pmatrix} 1 & 1 & k \\ m & -m & 0 \end{pmatrix} Y_{1m}(\hat{\mathbf{r}}_a) Y_{1-m}(\hat{\mathbf{r}}_b),$$

where $Y_{\ell m}$ denotes the spherical harmonic and $\hat{\mathbf{r}}_x$ denotes the orientation of the p electron on atom $x, x = a, b$. Then the retarded dipole interaction, V_3, of Stephen [9] can be written:

$$V_3 = -\frac{4\pi}{3}\sqrt{6}\frac{q_aq_b}{R^3}\Big\{X(2, 0)[\cos y(1 - y^2/3) + y \sin y]$$
$$- \frac{\sqrt{2}}{3}X(0, 0)y^2 \cos y\Big\}, \quad (3)$$

where q_x is the magnitude of the transition dipole moment matrix element on atom x and $y = \kappa R, \kappa = 2\pi/\lambda$, is the magnitude of the wavevector of the 1089 nm photon for the He 2 ^{3}S – 2 ^{3}P transition. Since the wavefunctions for the relative motion do not affect the matrix elements of the interatomic interactions, for the dipole interaction we require "exchange" matrix elements of the form

$$\langle(\alpha_1)_a, (\alpha_2)_b, ; F\phi|X(0, 0)|\,(\alpha'_2)_a\,, (\alpha'_1)_b\,, ; F'\ \phi\rangle =$$
$$\frac{\delta_{FF'}}{4\pi\sqrt{3}}[f_1f'_1f_2f'_2J_2J'_2]^{1/2}(-1)^{f'_1+f_2+2f'_2+F}$$
$$\times \begin{Bmatrix} 1 & \frac{1}{2} & f_1 \\ f'_2 & 1 & J'_2 \end{Bmatrix} \begin{Bmatrix} 1 & \frac{1}{2} & f'_1 \\ f_2 & 1 & J_2 \end{Bmatrix} \begin{Bmatrix} f_1 & f_2 & F \\ f'_1 & f'_2 & 1 \end{Bmatrix}, \quad (4)$$

where $\begin{Bmatrix} \cdots \\ \cdots \end{Bmatrix}$ denotes a $6-j$ symbol and we have assumed $L_1 = L'_1 = 0, S_1 = S'_1 = J_1 = J'_1 = L_2 = S_2 = S'_2 = 1, i_1 = i_2 = 1/2$. Similarly

$$\langle(\alpha_1)_a, (\alpha_2)_b, ; F\phi|X(2, 0)|(\alpha'_2)_a, (\alpha'_1)_b, ; F'\phi\rangle =$$
$$\frac{\sqrt{5}}{4\pi}(-1)^{F+f'_1+f'_2-\phi+1}[FF'f_1f'_1f_2f'_2J_2J'_2]^{1/2} \begin{pmatrix} F & 2 & F' \\ -\phi & 0 & \phi \end{pmatrix}$$
$$\times \begin{Bmatrix} 1 & \frac{1}{2} & f_1 \\ f'_2 & 1 & J'_2 \end{Bmatrix} \begin{Bmatrix} 1 & \frac{1}{2} & f'_1 \\ f_2 & 1 & J_2 \end{Bmatrix} \begin{Bmatrix} f_1 & f'_2 & 1 \\ f_2 & f'_1 & 1 \\ F & F' & 2 \end{Bmatrix}, \quad (5)$$

where $\begin{Bmatrix} \cdots \\ \cdots \\ \cdots \end{Bmatrix}$ denotes a $9 - j$ symbol. For the dispersion interaction we introduce

$$\tilde{X}(2, 0) = \sqrt{5}\begin{pmatrix} 2 & 0 & 2 \\ 0 & 0 & 0 \end{pmatrix} Y_{00}(\hat{r}_a)Y_{20}(\hat{r}_b) \equiv \frac{\sqrt{5}}{4\pi}P_2(\cos\theta_b),$$

where $P_2(x)$ denotes the second Legendre polynomial and we need the matrix element of

$$V_6 = C_6^{(0)} + C_6^{(2)}\tilde{X}(2, 0). \quad (6)$$

Here

$$C_6^{(0)} = \left(C_6^\Sigma + 2C_6^\Pi\right)/3, \quad C_6^{(2)} = 5\left(C_6^\Sigma - C_6^\Pi\right)/3,$$

where C_6^Σ and C_6^Π are the case (a) van der Waals coefficients for Σ and Π symmetry, respectively. In this case only the ‘direct’ matrix element is non-vanishing:

$$\langle(\alpha_1)_a,(\alpha_2)_b,;F\phi|\tilde{X}(2,0)|(\alpha_1')_a,(\alpha_2')_b,;F'\phi\rangle =$$

$$\delta_{f_1 f_1'}\frac{\sqrt{6}}{4\pi}[FF'f_2f_2'J_2J_2']^{1/2}(-1)^{2f_2'-f_1+J_2+J_2'-\phi+1/2} \times \begin{pmatrix} F & 2 & F' \\ -\phi & 0 & \phi \end{pmatrix} \begin{Bmatrix} F' & F & 2 \\ f_2 & f_2' & f_1 \end{Bmatrix} \begin{Bmatrix} J_2 & \frac{1}{2} & f_2 \\ f_2' & 2 & J_2' \end{Bmatrix} \begin{Bmatrix} J_2 & J_2' & 2 \\ 1 & 1 & 1 \end{Bmatrix}, \quad (7)$$

with values assumed as in equation (4).

3 Symmetrization

The function $|(\alpha_1)_a,(\alpha_2)_b,F,\phi;T,M_T\rangle$ is not an eigenfunction of either the total parity operator, $\hat{P}_T$, or the exchange parity operator, $\hat{X}_n$, for exchange of the nuclei. Using the results from Gao [12] and the inverse of equation (2) it is straightforward to show that

$$\hat{P}_T|(\alpha_1)_a,(\alpha_2)_b,F,\phi;T,M_T\rangle = (-1)^{T+F}P_1P_2|(\alpha_1)_a,(\alpha_2)_b,F,-\phi;T,M_T\rangle, \quad (8)$$

consistent with the result of Launay [11], who did not consider hyperfine structure. Hence eigenfunctions of total parity, eigenvalue $(-1)^{P_T}$ where $P_T = 0, 1$, can be constructed as

$$|(\alpha_1)_a,(\alpha_2)_b,F,\bar{\phi};T,M_T,P_T\rangle = (|(\alpha_1)_a,(\alpha_2)_b,F,\bar{\phi};T,M_T\rangle + (-1)^{P_T+T+F}P_1P_2|(\alpha_1)_a,(\alpha_2)_b,F,-\bar{\phi};T,M_T\rangle) \times [2(1+\delta_{\bar{\phi},0})]^{-1/2}, \quad (9)$$

where $\bar{\phi} = |\phi|$.

Next it is necessary to ensure the wavefunctions employed are eigenfunctions of $\hat{X}_n$. Again following Gao [12] we find

$$\hat{X}_n|(\alpha_1)_a,(\alpha_2)_b,F,\bar{\phi};T,M_T,P_T\rangle = (-1)^{F+f_1+f_2+N_1N_2}P_1P_2|(\alpha_2)_a,(\alpha_1)_b,F,\bar{\phi};T,M_T,P_T\rangle, \quad (10)$$

where N_i is the number of electrons on atom i. Hence, for the case of interest here, $P_1P_2 = -1$, N_1N_2 even,

$$|\alpha_1,\alpha_2,F,\bar{\phi};T,M_T,P_T\rangle = \{|(\alpha_1)_a,(\alpha_2)_b,F,\bar{\phi};T,M_T,P_T\rangle + (-1)^{F+f_1+f_2+P_T}|(\alpha_2)_a,(\alpha_1)_b,F,\bar{\phi};T,M_T,P_T\rangle\}/2^{1/2}, \quad (11)$$

gives a fermion wavefunction.

Using this symmetrized wavefunction we find, since $\bar{\phi}, T, M_T$ and P_T are conserved for both direct and exchange operators:

$$\langle\alpha_1,\alpha_2,F,\bar{\phi};T,M_T,P_T|V_3|\alpha_1',\alpha_2',F',\bar{\phi};T,M_T,P_T\rangle = (-1)^{P_T+f_1'+f_2'+F'} \times \langle(\alpha_1)_a,(\alpha_2)_b,F,\bar{\phi}|V_3|(\alpha_2')_a,(\alpha_1')_b,F',\bar{\phi}\rangle, \quad (12)$$

$$\langle\alpha_1,\alpha_2,F,\bar{\phi};T,M_T,P_T|V_6|\alpha_1',\alpha_2',F',\bar{\phi};T,M_T,P_T\rangle = \langle(\alpha_1)_a,(\alpha_2)_b,F,\bar{\phi}|V_6|(\alpha_1')_a,(\alpha_2')_b,F',\bar{\phi}\rangle, \quad (13)$$

where the matrix elements on the right-hand sides can be obtained using equations (3–7). These results hold also for $\bar{\phi} = 0$, except that in that case, from equation (9), the choice of the total parity in effect selects the parity of F so that even and odd values of F are decoupled. For all values of $\bar{\phi}$, for each value of the total angular momentum, T, there are two possible solutions, depending on P_T, as for the space-fixed description. This symmetry is here associated with reflection in a plane through the nuclei, which is equivalent to inversion in a space-fixed system [14].

As a check, the potential matrix can also be calculated using a Hund’s case (a) basis, in which these long-range potentials are relatively simple, and then transformed. Denoting the case (a) energies by $\epsilon_{\Lambda S g}$ and $\epsilon_{\Lambda S u}$, again following Gao [12], we find

$$\langle\alpha_1,\alpha_2,F,\bar{\phi};T,M_T,P_T|H_{BO}|\alpha_1',\alpha_2',F',\bar{\phi};T,M_T,P_T\rangle = (-1)^{J_2+J_2'+1}[f_1f_1'f_2f_2'J_2J_2'FF']^{1/2} \times \sum_{JJ'IS\Lambda\iota}(-1)^{J+J'-I-\iota}[JJ'IS] \begin{Bmatrix} 1 & J_2 & J \\ \frac{1}{2} & \frac{1}{2} & I \\ f_1 & f_2 & F \end{Bmatrix} \begin{Bmatrix} 1 & J_2' & J' \\ \frac{1}{2} & \frac{1}{2} & I \\ f_1' & f_2' & F' \end{Bmatrix} \times \begin{Bmatrix} J & S & 1 \\ 1 & J_2 & 1 \end{Bmatrix} \begin{Bmatrix} J' & S & 1 \\ 1 & J_2' & 1 \end{Bmatrix} \begin{pmatrix} J & I & F \\ \bar{\phi}-\iota & \iota & -\bar{\phi} \end{pmatrix} \begin{pmatrix} J' & I & F' \\ \bar{\phi}-\iota & \iota & -\bar{\phi} \end{pmatrix} \times \begin{pmatrix} 1 & S & J \\ \Lambda & \bar{\phi}-\iota-\Lambda & \iota-\bar{\phi} \end{pmatrix} \begin{pmatrix} 1 & S & J' \\ \Lambda & \bar{\phi}-\iota-\Lambda & \iota-\bar{\phi} \end{pmatrix} \times\{\epsilon_{\Lambda S g}+\epsilon_{\Lambda S u}+\left[1+(-1)^{I-S+P_T-1}\right](\epsilon_{\Lambda S g}-\epsilon_{\Lambda S u})\}/2.$$

In this case H_{BO} is simply the sum of the retarded resonant dipole and the dispersion interactions.

As noted in the introduction, the levels of ^{3}He cannot be described in a pure $\{J, f\}$ basis. A careful description of the hyperfine structure in ^{3}He ($1s\ 2p\ ^3$P) has been provided by Hinds et al. [15], who included the interaction with the ($1s\ 2p\ ^1$P) level and were able to characterize the constants in their hyperfine Hamiltonian at the level of 20 kHz. Here, for the purposes of evaluating mixing in the intermediate basis, we have neglected some very small terms in their Hamiltonian and employed

$$H_{hfs} = C\mathbf{i}\cdot\mathbf{S} + D\mathbf{i}\cdot\mathbf{L}, \quad (14)$$

with $C = -4283.89$ MHz and $D = -28.13$ MHz. This Hamiltonian mixes states of the same f but different J. There is no mixing of the $\{J, f\} = \{2, 5/2\}$ level and the mixed $f = 3/2$ levels can be written

$$\{2,3/2\}' = \cos\theta_1\{2,3/2\} + \sin\theta_1\{1,3/2\}$$
$$\{1,3/2\}' = -\sin\theta_1\{2,3/2\} + \cos\theta_1\{1,3/2\},$$

where the primes denote the mixed levels and their J label now indicates the pure J state of larger overlap. For the $f = 1/2$ levels we have analogous relations with mixing angle θ_2. Using H_{hfs} from equation (14) and the pure-level

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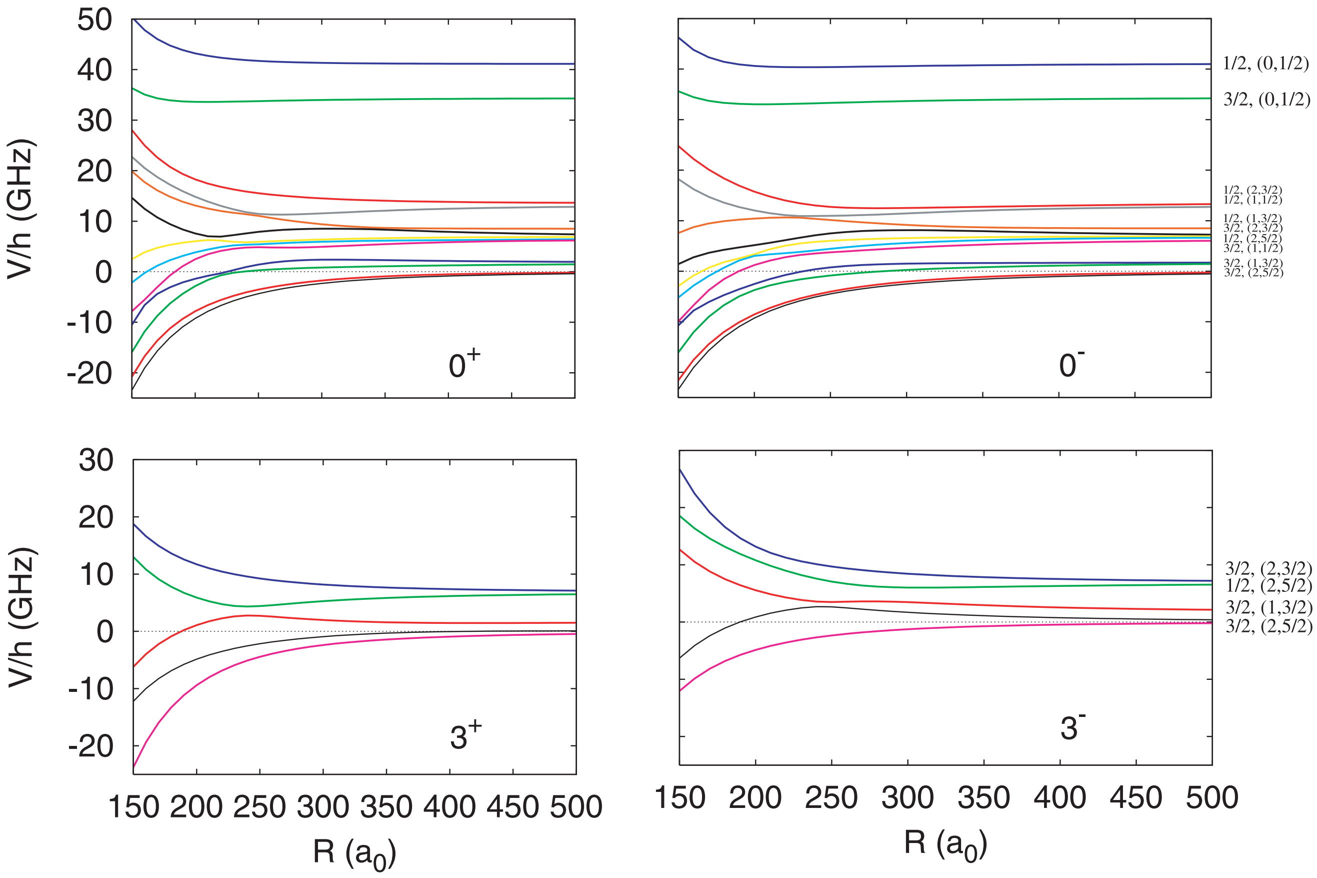

Fig. 1. The adiabatic potentials for ^{3}He 2 ^{3}S + 2 ^{3}P. Values of $\bar{\phi}$ and parity are indicated on each plot. The atomic limits are indicated as $f_1, (J, f_2)$, where f_1 and f_2 are the total angular momenta of the 2 ^{3}S and the 2 ^{3}P states, respectively, and J indicates the 2 ^{3}P pure J state of larger overlap - see text. A colour version of the figure is available online at `http://www.eurphysj.org`.

energies from Hinds et al. [15] we obtained $\theta_1 = 2.557$ and $\theta_2 = 0.108$. Almost identical values have been obtained by [16] with $D = 0$ in equation (14). The splitting of the $f = 3/2$ levels with this Hamiltonian is obtained as 5169 MHz, in satisfactory agreement with the best value of 5180.214 MHz [17]. Similarly the splitting for the $f = 1/2$ levels is obtained as 28 112 MHz, compared to the best value of 28 092.932 MHz [17]. Using these mixing angles the Hamiltonian has been transformed to the intermediate coupling basis. The 2 ^{3}P hyperfine energy spacings employed have been obtained from Zhao et al. [17].

4 Results

The appropriate energy splittings and the diagonal part of the $T = 0$ centrifugal potential, $(F(F+1) - 2\bar{\phi}^2)/2\mu R^2$, have been added to the potential matrix to obtain the body-fixed Hamiltonian matrix. The zero of energy has been taken as the $f_1 = 3/2, J_2 = 2, f_2 = 5/2$ level, where atoms 1 and 2 are in the 2 ^{3}S and 2 ^{3}P levels, respectively. This Hamiltonian has been diagonalized to yield the body-fixed adiabatic potentials. As there are ten sets of potential curves arising from two parities and five values of $\bar{\phi}$, we show in Figure 1 only those with promising ultra-long-range wells, $\bar{\phi} = 3^{\pm}$ and $0^{\pm}$. In the 0^+ and 0^- symmetries the twelfth state has a well of depth 0.74 GHz and 1.33 GHz, respectively, and these states are relatively isolated. The asymptote of both curves is the $f_1 = 3/2$, $J_2 = 0$, $f_2 = 1/2$ level. For the 3^+ and 3^- states, the fourth state has a well of 2.4 GHz and 0.74 GHz, respectively, due in this case to relatively distant avoided crossings. The asymptote for these states is the $f_1 = 1/2$, $J_2 = 2$, $f_2 = 5/2$ level. For the fourth 3^- state a Landau-Zener estimate suggests that the avoided crossing should be traversed adiabatically; however for the closer avoided crossing at generally higher speeds in the fourth 3^+ state the adiabatic approximation may be breaking down. Non-adiabatic effects appear unimportant for the twelfth $0^{\pm}$ states.

We have determined the rovibrational levels in these wells using the code LEVEL of LeRoy [18]. Some results are listed in Table 1, for $T \leq 4$ since the entrance channel for photoassociation at very low energies will have $T \leq 3$. We see from the table that indeed there are a number of rovibrational levels in the ultra-long range wells. The relatively isolated levels associated with the twelfth $0^{\pm}$ symmetry may offer the best chance of observation. While these levels are metastable, the predissociation widths of comparable levels in ^{4}He were of the order of, or smaller than, the natural linewidth [3].

Table 1. Rovibrational binding energies, relative to the dissociation limit, in units of MHz, for ^{3}He$_2$ close to the 2 ^{3}S + 2 ^{3}P asymptote.

State No.	Symmetry	$v \setminus T$	0	1	2	3	4
12	0^+	0	−365	−326	−251	−147	−28
		1	−58	−43	−17		
		2	−2				
12	0^-	0	−839	−794	−706	−578	−417
		1	−282	−256	−208	−141	−64
		2	−69	−58	−37	−13	
		3	−10	−7			
4	3^+	0				−1407	−1261
		1				−498	−403
		2				−111	−59
4	3^-	0				−306	−230
		1				−38	−3

5 Summary and conclusions

Various ultra-long range wells have been found for ^{3}He$_2$ dissociating to $1s\,2s\,^3\mathrm{S}_1 + 1s\,2p\,^3\mathrm{P}_J$. Several of these wells have been shown to support rovibrational levels. Calculations are in progress to refine these estimates by including the neglected non-adiabatic and Coriolis couplings. The new long-range potentials calculated here could also be combined with the recently determined [19] short range $^5\Sigma^+_{g/u}$, $^5\Pi_{g/u}$ potentials to obtain further near-dissociation rovibrational levels, particularly the lower levels for which predissociation is forbidden.

The same approach can readily be adapted to investigate long-range potentials dissociating to ^{3}He $2s\,^3\mathrm{S} + 3p\,^3\mathrm{P}$, though the convergence of the long-range expansion of the potential in the well regions might be open to question [20].

References

1. J. Léonard, M. Walhout, A.P. Mosk, T. Müller, M. Leduc, C. Cohen-Tannoudji, Phys. Rev. Lett. **91**, 073203 (2003)
2. J. Léonard, A.P. Mosk, M. Walhout, P. van der Straten, M. Leduc, C. Cohen-Tannoudji, Phys. Rev. A **69**, 032702 (2004)
3. V. Venturi, P.J. Leo, E. Tiesinga, C.J. Williams, I.B. Whittingham, Phys. Rev. A **68**, 022706 (2003)
4. J. Kim, U.D. Rapol, S. Moal, J. Léonard, M. Walhout, M. Leduc, Eur. Phys. J. D **31**, 227 (2004)
5. R.J.W. Stas, J.M. McNamara, W. Hogervorst, W. Vassen, Phys. Rev. Lett. **93**, 053001 (2004)
6. H.A. Bethe, E.E. Salpeter, Quantum mechanics of one- and two-electron systems, *Encyclopedia of Physics*, edited by S. Flugge (Springer-Verlag, Berlin, 1957), Vol. XXXV, p. 88
7. S.D. Rosner, F.M. Pipkin, Phys. Rev. A **1**, 571 (1970); Erratum, Phys. Rev. A **3**, 521 (1971)
8. C.J. Williams, E. Tiesinga, P.S. Julienne, Phys. Rev. A **53**, R1939 (1996)
9. M.J. Stephen, J. Chem. Phys. **40**, 669 (1964)
10. W.J. Meath, J. Chem. Phys. **48**, 227 (1968)
11. J.-M. Launay, J. Phys. B **10**, 3665 (1977)
12. B. Gao, Phys. Rev. A **54**, 2022 (1996)
13. R.N. Zare, *Angular Momentum: Understanding Spatial Aspects in Chemistry and Physics* (Wiley, New York, USA, 1988)
14. L.D. Landau, E.M. Lifschitz, *Quantum Mechanics* (Pergamon Press, London, 1959), p. 293
15. E.A. Hinds, J.D. Prestage, F.M.J. Pichanick, Phys. Rev. A **32**, 2615 (1985)
16. P.J. Nacher, M. Leduc, J. Phys. (France) **46**, 2057 (1985)
17. P. Zhao, J.R. Lawall, F.M. Pipkin, Phys. Rev. Lett. **66**, 592 (1991)
18. R.J. Le Roy, Technical Report CP-642R^3, University of Waterloo, 2001
19. A.S. Dickinson, F.X. Gadéa, T. Leininger, Europhys. Lett. **70**, 320 (2005)
20. J. Koelemeij, Ph.D. thesis, Free University of Amsterdam, 2004