# Faddeev calculation of the $dt\mu^-$ mesic molecule

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(Received 1 June 1992)

An improved version of our previously developed method [C.-Y. Hu, A. A. Kvitsinsky, and S. P. Merkuriev, Phys. Rev. A **45**, 2723 (1992)] of solving the Faddeev equations in the total angular momentum representation is applied to calculate the $dt\mu^-$ ground and excited $S$-state energies with an accuracy of $10^{-6}$.

PACS number(s): 11.80.Jy, 31.20.−d, 36.10.−k

Recently [1,2] we developed a method of solving the three-dimensional Faddeev equations in the total angular momentum representation [3,4] for the three-body Coulomb bound-state problem. The numerical part of the method is based on the triquintic spline expansion of the Faddeev components. Previous applications of the method to the ground states of the $e^-e^-e^+$ and $pp\mu^-$ systems [1,2] demonstrated that it performs very efficiently and allows one to get high-accuracy results at a relatively low cost.

In this Brief Report, we apply an improved version of the method to calculate the $S$ states of the $dt\mu^-$ mesic molecule. Being composed of particles of very different masses, this system provides one of the most difficult tests of the efficiency of the Faddeev approach.

A full survey of our method and comparison with other approaches is given in Ref. [2]. That is why we omit many details and mostly restrict ourselves with modifications made in the present work and the final results.

The equations to be solved are the Faddeev equations at zero total angular momentum in the three-dimensional internal space parametrized via the hyperradius $\rho$ and hyperangles $\theta_\alpha,\chi_\alpha$ [1–3],

$$(H_0+V_\alpha-E)\Psi_\alpha(\rho,\chi_\alpha,\theta_\alpha)=-V_\alpha\sum_{\beta(\neq\alpha)}\Psi_\beta(\rho,\chi_\beta,\theta_\beta)\ , \tag{1}$$

where the index $\alpha=1,2,3$ labels pairs of the particles; $V_\alpha$ is the Coulomb potential in the pair $\alpha$ and $H_0$ denotes a second-order partial differential operator. We introduce renormalized Faddeev components

$$\Phi_\alpha=\rho^{5/2}\sin(\chi_\alpha)\sin(\theta_\alpha)\Psi_\alpha \tag{2}$$

and rewrite Eq. (1) for $\Phi_\alpha$ using a mapping of the hyperradius $\rho\in[0,\infty)\to r\in[0,1)$ proposed initially in Ref. [4],

$$r=1-e^{-\lambda\rho}\ , \tag{3}$$

with a parameter $\lambda$ to be optimized in calculations.

Next, the components $\Phi_\alpha$ as functions of $r,\chi_\alpha,\theta_\alpha$ are expanded in a spline basis,

$$\Phi_\alpha(r,\chi,\theta)=\sum_{l=1}^{L}\sum_{m=1}^{M}\sum_{n=1}^{N}f_{\alpha lmn}s_l(\theta)s_m(r)s_n(\chi)\ , \tag{4}$$

where $s_i$ are the quintic Hermite polynomial splines (piecewise polynomials of fifth degree) that have continuous first and second derivatives. Upon using the expansion (4) and a collocation procedure, the Faddeev equations are reduced to a matrix-eigenvalue problem.

If the domain of a variable is divided on $K$ intervals, the total cardinal basis of the quintic splines consists of $3K+3$ functions. In our previous calculations [1,2], we exploited the orthogonal collocation procedure with two-point Gauss quadrature points per interval, which yields only $2K$ equations. Thus one must drop a set of $K+1$ splines out of the total basis to match the number of unknowns and equations (two more splines can be excluded due to zero boundary conditions at the end points [2]). By doing so, one breaks the continuity of the second derivative within the interior region. Apparently, this deteriorates the convergence of the spline expansion and

TABLE I. $dt\mu^-$ ground-state calculations. The modified atomic units (m.a.u.) are used: $\hbar=m_\mu=e^2=1$.

| | $M\times N\times L$ | | | | |
|---|---|---|---|---|---|
| Quantity | 12×12×12 | 15×15×15 | 18×15×15 | 18×15×18 | Ref. [7] |
| $-E$ (m.a.u.) | 0.499 279 | 0.538 595 7 | 0.538 594 2 | 0.538 594 7 | 0.538 594 8 |
| $\lambda$ | 0.115 | 0.130 56 | 0.135 26 | 0.135 259 | |
| $\Lambda$-1 | $-8\times10^{-7}$ | $2\times10^{-7}$ | $-2\times10^{-7}$ | $-1\times10^{-7}$ | |

 

TABLE II. $dt\mu^-$ excited $S$-state calculations. The modified atomic units (m.a.u.) are used: $\hbar = m_\mu = e^2 = 1$.

| | $M \times N \times L$ | | | | |
|---|---|---|---|---|---|
| Quantity | $12\times9\times9$ | $12\times12\times12$ | $15\times15\times15$ | $18\times15\times15$ | Ref. [6] |
| $-E$ (m.a.u.) | 0.386 711 | 0.454 526 | 0.488 063 | 0.488 067 0 | 0.488 065 1 |
| $\lambda$ | 0.117 | 0.081 5 | 0.137 44 | 0.143 21 | |
| $\Lambda-1$ | $-2\times10^{-7}$ | $-1\times10^{-7}$ | $-1\times10^{-7}$ | $1\times10^{-7}$ | |

is somewhat unstable for systems with unequal masses.

That is why in the present work we propose to give up the orthogonal collocation procedure. Instead, for the collocation points we take the three-point Gauss quadrature points on each interval. This collocation procedure yields $3K$ equations. To incorporate boundary conditions, we exclude three splines (out of $3K+3$) that are nonzero either for their values or first derivatives in the end points. In this way, the numbers of equation and unknowns are matched and one preserves continuity of first and second derivatives within interior. The number of splines involved in the resulting expansion (4) is three times that of intervals in each variable.

The above collocation procedure reduces the Faddeev equations to an algebraic eigenvalue problem,

$$(A+EB)f = Cf \ , \tag{5}$$

where $A$, $B$, and $C$ are matrices of the rank $3LMN$ with elements given in Refs. [1,2]. Equation (5) is solved as described in Ref. [2], by means of the Lanczos algorithm [5] dealing with a generalized eigenvalue problem,

$$(A+E_0B)f = \Lambda Cf \ , \tag{6}$$

where one fits trial energy $E_0$ to get the eigenvalue $\Lambda=1$. As before, we use the so-called tensor method [4,2] to invert explicitly the matrix $A+E_0B$ to do the Lanczos iteration procedure.

In our $dt\mu^-$ $S$-state calculations we use uniform grids of natural knots in all three variables. For a given grid, the mapping parameter $\lambda$ of Eq. (3) and the trial energy $E_0$ are adjusted until the eigenvalue $\Lambda=1$ of Eq. (6) is reproduced with an accuracy $10^{-6}$. The results are given in Tables I and II for the ground and excited $S$ states, respectively. References [6,7] are high-accuracy variational calculations.

Compared to our previous calculations [1,2], the improved version of the triquintic spline expansion performs much better for unequal masses. For instance, four right digits of the $pp\mu^-$ binding energy were obtained in Ref. [2] with $20\times20\times18$ spline expansion, whereas for the more complicated case of $dt\mu^-$ we get five correct digits already with $15\times15\times15$ expansion.

Clearly, the method converges amazingly fast and enables one to reach easily an accuracy of $10^{-6}$ that is far beyond what one is accustomed to expect from a Faddeev calculation. We believe our numerical procedure brings the Faddeev approach up to a level where it is quite competitive even with variational calculations, especially since it can provide very high local accuracy of wave functions.

A. A. K. is grateful to S. P. Merkuriev for stimulating support. C.-Y. H. wishes to thank J. Cohen for helpful discussions. This work is made possible by a NSF Grant No. PHY-9013072, and by a generous allocation of computer time from the San Diego Supercomputer Center.

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