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Hypergeometric Function $_3F_2$ Applied to Morse Potential

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Abstract: We obtain an identity for the hypergeometric function $_3F_2$ which allows to show the equivalence of two formulas for the matrix elements of the Morse potential.

Key words: Hypergeometric function · Morse interaction · Diatomic molecules

INTRODUCTION

The Morse potential [1, 2]:

$$V(r) = D(e^{-2au} - 2e^{-au}), \quad u = r - r_0, \tag{1}$$

where D is the well-depth, r_0 is the equilibrium position, and a is a range parameter, and its matrix elements:

$$< m \,|\, e^{-\beta au} \,|\, n >= \int_0^\infty \psi_m^* \, e^{-\beta au} \, \psi_n \, du, \quad \beta = 0,1,2,... \tag{2}$$

are important in quantum mechanics.

Rosen [3] and Vasan- Cross [4] evaluated directly the integral (2) to obtain the following hypergeometric expression [5]:

$$< m \,|\, e^{-\beta au} \,|\, n >= \frac{(-1)^{n+m}}{k^\beta} \frac{\Gamma(\beta+n)\Gamma(k-n-1+\beta)}{m!\Gamma(k-m)\Gamma(\beta)} \sqrt{\frac{b_1 b_2 m!\Gamma(k-m)}{n!\Gamma(k-n)}} \; x \tag{3}$$

$$x \; {}_3F_2\,(-m,\, 1-\beta,\, 1-k+m;\, 1-n-\beta,\, 2-k+n-\beta;\, 1),\ n \geq m$$

where $b_1 = k - 2n - 1$, $b_2 = k - 2m - 1$ and $k = \frac{2}{a}\sqrt{2D}$.

On the other hand, Berrondo *et al.* [6] used the relationship between (1) and the two-dimensional harmonic oscillator, to deduce the formula [5]:

$$< m \,|\, e^{-\beta au} \,|\, n >= \frac{(-1)^{n+m}}{k^\beta} \frac{n!\Gamma(\beta+n-m)\Gamma(k-n-1+\beta)}{m!\Gamma(k-m)\Gamma(\beta)(n-m)!} \sqrt{\frac{b_1 b_2 m!\Gamma(k-m)}{n!\Gamma(k-n)}} \; x \tag{4}$$

$$x \; {}_3F_2\,(-m,\, 1-\beta,\, 1-\beta+n-m;\, 1+n+m,\, 2-k+n-\beta;\, 1),\ n \geq m.$$

In Sec. 2 we employ a result of Melvin-Swamy [7] to prove an identity verified by the generalized hypergeometric function $_3F_2$, which shows that (3) is completely equivalent to (4).

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An Identity for $_3F_2$: We can demonstrate the equivalence of (3) and (4) if we establish the relation:

$$ {}_3F_2(-m,1-\beta,1-k+m;\ 1-n-\beta,\ 2-k+n-\beta;1)=\frac{n!\Gamma(n-m+\beta)}{(n-m)!\Gamma(n+\beta)}x \tag{5}$$

$x\ {}_3F_2\,(-m,\ 1-\beta,\ 1\ -\ \beta+n-m;\ 1+n+m,\ 2-k+n-\beta;\ 1).$

Now in the interesting expression of Melvin-Swamy [7]:

$$ {}_3F_2(\alpha_1,\alpha_2,\alpha_3;\lambda_1,\lambda_2;1)=\frac{\Gamma(\lambda_1)\Gamma(\lambda_1-a_1-a_2)}{\Gamma(\lambda_1-a_1)\Gamma(\lambda_1-a_2)}\ {}_3F_2(\alpha_1,\alpha_2,\lambda_2-\alpha_3;\alpha_1+\alpha_2-\lambda_1+1,\lambda_2;1), \tag{6}$$

we employ the values:

$$\alpha_1=-m,\ \alpha_2=1-\beta,\ \alpha_3=1-k+m,\ \lambda_1=1-n-\beta,\ \lambda_2=2-k+n-\beta, \tag{7}$$

then (5) is immediate because the properties of the gamma function [8] allow to show that:

$$\frac{\Gamma(1-n-\beta)\Gamma(-n+m)}{\Gamma(1-n-\beta+m)\Gamma(-n)}=\frac{n!\Gamma(n-m+\beta)}{(n-m)!\Gamma(n+\beta)},\quad n\geq m. \tag{8}$$

Hence the formula of Rosen –(Vasan-Cross) [3-4] is equivalent to the relation of Berrondo *et al.* [6] for the matrix elements of the Morse potential.

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