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Quantum Monte Carlo study of rovibrational states utilizing rotating wavefunctions: Application to H₂O

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We applied the procedure developed by Prudente *et al.* [Chem. Phys. Lett. **302**, 249 (1999)] to compute the rovibrational energy levels of the water molecule. The procedure utilizes rotating wavefunctions as the trial basis in the correlation-function quantum Monte Carlo method. The procedure originally tested for a rotating harmonic oscillator and rotating Morse potential, has been extended for triatomic systems, replacing the spherical harmonics by the Wigner functions. We computed the rovibrational levels of the water molecule and compared the results with the experiment, and they are shown to be accurate. © 1999 American Institute of Physics. [S0021-9606(99)00238-X]

I. INTRODUCTION

The study of the rovibrational levels of polyatomic molecules and clusters from a given potential energy surface (PES) is a topic of great importance in molecular physics. The most common method for the calculation of excited states are based in variational methods, where the wave functions are expanded in an appropriate basis set, and the required integrals are evaluated using quadrature or pointwise methods, and the resulting eigenvalue problem is solved in a subspace spanned by the basis set. The number of basis functions grows exponentially with the number of particles making the calculation of larger systems very time consuming. Only recently, calculations of rovibrational energy levels of tetratomic molecules have been reported,¹⁻⁵ but the extension to larger molecules is still doubtful.

An alternative approach is the use of quantum Monte Carlo techniques to compute the multidimensional integrals that appear in the time independent problems.⁶ These techniques have been employed with great success in the calculation of properties of ground state and finite temperature quantum systems. However, there are few studies of excited states. The use of the correlation function quantum Monte Carlo (CFQMC) method, developed by Bernu and co-workers,^{7,8} to calculate the excited vibrational states of triatomic⁸⁻¹⁰ and tetratomic^{8,9} molecules, the study of multidimensional tunneling motion in complexes using the rigid body diffusion Monte Carlo (RBDMC) method,^{11,12} the computation of the vibrational levels of Ar₁₃ cluster¹³ and the use of the projection operator imaginary time spectral evolution (POITSE)¹⁴ to calculate the rovibrational states of molecular systems¹⁵ are some examples of excited states study.

We have recently developed a novel procedure to calculate the excited rovibrational energy levels based in the CFQMC method.¹⁶ We have proposed the utilization of rotating functions as the trial basis functions in the CFQMC

method. The procedure was applied in the study of two low-dimensional systems: rotating harmonic oscillator and rotating Morse potential. The results were shown to be very accurate.¹⁶ In Ref. 17, a generalization to *N*-body molecular systems is proposed.

In this work we apply the procedure to compute the rovibrational levels, up to *J*=2, of the water molecule. The main difference from the diatomic cases, treated in Ref. 16, is the replacement of the spherical harmonics $Y_{lm}(\theta, \phi)$ by the Wigner functions $D_{MN}^L(\alpha, \beta, \gamma)$, where α , β , and γ are the Euler angles. Our calculations are performed using the Jacobi coordinates, and the matrix elements are computed using CFQMC. The current procedure can be applied to larger systems without major difficulties, as it is shown in Ref. 17 where the generalization of the *N*-particle systems is discussed.

This paper is organized as follows: in Sec. II we summarize the CFQMC method; in Sec. III we present the procedure to calculate rovibrational states of triatomic systems; in Sec. IV we present the results for the rovibrational levels of the water molecule; the last section is dedicated to concluding remarks.

II. CORRELATION FUNCTION QUANTUM MONTE CARLO

The rovibrational energy levels of a molecular system are obtained solving the following eigenvalue problem:

$$H\Phi_i(\mathbf{R}) = E_i\Phi_i(\mathbf{R}), \quad (1)$$

where the Hamiltonian associated with the relative motion of particles (excluding the kinetic energy of the center-of-mass)¹⁸ is given as

$$H = - \sum_{i=1}^{N-1} \frac{\hbar^2}{2\mu_i} \nabla_i^2 + V(\mathbf{R}). \quad (2)$$

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μ_i is the reduced mass, \mathbf{R} is the vector of $3(N-1)$ coordinates, $V(\mathbf{R})$ is the potential energy, usually a Born–Oppenheimer potential energy surface, and E_i and Φ_i are the eigenvalues and eigenvectors of H .

In this section we summarize the CFQMC method (at the variational level) used to solve Eq. (1). Let $\{f_\alpha(\mathbf{R})\}$ be a trial basis set of m known functions, we can define the overlap and Hamiltonian matrix elements as

$$N_{\alpha\beta} = \int d\mathbf{R} f_\alpha(\mathbf{R}) f_\beta(\mathbf{R}),$$

$$H_{\alpha\beta} = \int d\mathbf{R} H f_\alpha(\mathbf{R}) f_\beta(\mathbf{R}),$$
(3)

respectively. Associated to these matrices, we define the following generalized eigenvalue problem

$$\sum_{\beta=1}^m [H_{\alpha\beta} - \Lambda_k N_{\alpha\beta}] d_{k\beta} = 0, \quad (4)$$

with d_k being the k th eigenvector and Λ_k its associated eigenvalue.

The matrix elements defined in Eq. (3) are evaluated using Monte Carlo methods. The random walks are generated according to a given probability distribution, in our case $|\Psi(\mathbf{R})|^2$, where $\Psi(\mathbf{R})$ is a guide function chosen to integrate well all the states included in our calculation.

The matrix elements, after symmetrization, are evaluated as

$$n_{\alpha\beta} = \frac{1}{p} \sum_{i=1}^p F_\alpha(\mathbf{R}_i) F_\beta(\mathbf{R}_i),$$

$$h_{\alpha\beta} = \frac{1}{2p} \sum_{i=1}^p [F_\alpha(\mathbf{R}_i) F_\beta(\mathbf{R}_i) E_{L_\beta}(\mathbf{R}_i) + E_{L_\alpha}(\mathbf{R}_i) F_\alpha(\mathbf{R}_i) F_\beta(\mathbf{R}_i)],$$
(5)

where

$$F_\alpha(\mathbf{R}) = f_\alpha(\mathbf{R}) / \Psi(\mathbf{R}), \quad (6)$$

$$E_{L_\beta}(\mathbf{R}) = f_\beta^{-1}(\mathbf{R}) H f_\beta(\mathbf{R}), \quad (7)$$

where $E_{L_\beta}(\mathbf{R})$ is called the local energy associated with the f_β basis function.

The rovibrational spectrum is obtained solving the generalized eigenvalue problem.

III. ROTATING TRIAL FUNCTIONS

In Ref. 8, Bernu *et al.* presented a simple way to generate the trial functions $\{f_\alpha\}$ that are used to calculate the vibrational energy levels. In the method, the basis functions are directly expressed in terms of interatomic distances. Acioli and Soares Neto⁹ proposed a similar method, with a few differences in the excited state trial functions. In Ref. 16, we proposed the following procedure to generate rotating trial basis functions and applied it successfully to diatomic systems. First, start from a simple approximation to the excited vibrational state eigenfunctions $\{\tilde{f}_i\}$ (for example, the Acioli *et al.* trial basis). Second, using the variational Monte

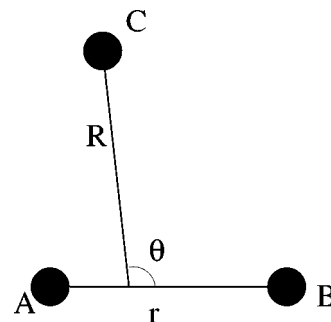


FIG. 1. Jacobi coordinate system for triatomic molecules. \mathbf{r} is the distance between atom A and atom B, \mathbf{R} is the distance between atom C and the center-of-mass of the AB diatom and θ is the angle between \mathbf{r} and \mathbf{R} .

Carlo (VMC) method, calculate a new orthonormal vibrational basis $\{f_i\}$. Then, the rotating trial basis set $\{f_\alpha\}$ is obtained as a combination of a $\{f_i\}$ function and the eigenfunctions of $\hat{\mathbf{J}}^2$ operator (e.g., spherical harmonics for spherical symmetrical potential and Wigner functions for general systems).¹⁹ The $\{f_\alpha\}$ basis functions are the trial basis set used in the CFQMC method. Here present and apply the procedure for triatomic molecules.

For triatomic molecules, the Hamiltonian in the Jacobi coordinate system, after removal of the motion of the center-of-mass, is

$$H = -\frac{\hbar^2}{2\mu_{AB}} \nabla_{\mathbf{r}}^2 - \frac{\hbar^2}{2\mu_{AB,C}} \nabla_{\mathbf{R}}^2 + V(r_{AB}, r_{BC}, r_{CA}), \quad (8)$$

where $\mu_{AB} = (m_A m_B) / (m_A + m_B)$, $\mu_{AB,C} = (m_A + m_B) m_C / (m_A + m_B + m_C)$, $\nabla_{\mathbf{r}}^2$ and $\nabla_{\mathbf{R}}^2$ are Laplacians in 3D Cartesian coordinates, and r_{AB} , r_{BC} and r_{CA} are the interatomic distances between atoms A and B, B and C, and C and A, respectively. The initial basis functions are given by¹⁰

$$\tilde{f}_{n_1, n_2, n_3} = \exp\left(\sum_{\nu, \mu} \Delta S_{\nu} A_{\nu, \mu} \Delta S_{\mu}\right) \prod_{\nu=1}^3 (\Delta S_{\nu})^{n_{\nu}}, \quad (9)$$

where $\Delta S_1 = r - r^0$, $\Delta S_2 = R - R^0$, and $\Delta S_3 = \cos \theta - \cos \theta^0$, r , r^0 , R , R^0 , θ and θ^0 are the distances and angles shown on Fig. 1 and their corresponding equilibrium values. The variational parameters $\{A_{\nu\eta}\}$ are optimized in order to minimize the variational energy of ground state [$n_{\nu}=0$ in Eq. (9)] or its variance.

Utilizing the VMC method, the new orthonormal vibrational basis set is

$$f_i(r, R, \cos \theta) = \sum_{n_1} \sum_{n_2} \sum_{n_3} c_i^{n_1 n_2 n_3} \tilde{f}_{n_1 n_2 n_3}(r, R, \cos \theta). \quad (10)$$

The rotating trial basis functions for triatomic molecules are given by

$$f_\alpha(R_x, R_y, R_z, r_x, r_y, r_z) \equiv f_i(r, R, \cos \theta) D_{MN}^J(\alpha, \beta, \gamma), \quad (11)$$

where D_{MN}^J is the Wigner function and α , β , and γ are the Euler angles. The local energy [Eq. (6)] associated with this basis function is given by:

TABLE I. Variational parameters $\{A_{\nu,\mu}\}$ for the ground state wave function of H_2O .

$A_{\nu,\mu}$	r	R	$\cos \theta$
r	-15.209 225	0.735 486	-0.100 498
R	0.735 486	-14.797 195	0.652 885
$\cos \theta$	-0.100 498	0.652 885	-11.943 161
	$r^0 = 1.823\,598$	$R^0 = 1.857\,711$	$\cos \theta^0 = 0.302\,035$

$$E_{L_\alpha} = f_\alpha^{-1} \left(-\frac{\hbar^2}{2\mu_{AB}} \nabla_{\mathbf{r}}^2 - \frac{\hbar^2}{2\mu_{AB,C}} \nabla_{\mathbf{R}}^2 \right) f_\alpha + V(r_{AB}, r_{BC}, r_{CA}). \quad (12)$$

In order to compute this local energy one needs the Laplacian and the gradient of f_α with respect to \mathbf{r} and \mathbf{R} , more specifically:

$$f_\alpha^{-1} \nabla^2 f_\alpha = \frac{\nabla^2 f_i}{f_i} + \frac{\nabla^2 D_{MN}^J}{D_{MN}^J} + \frac{\nabla f_i}{f_i} \cdot \frac{\nabla D_{MN}^J}{D_{MN}^J}. \quad (13)$$

Thus, in order to compute the kinetic energy part of the local energy one needs to write the Wigner functions, or the Euler angles, in terms of \mathbf{r} and \mathbf{R} . These relations are obtained solving the following system of equations:

$$\begin{pmatrix} R_x & r_x \\ R_y & r_y \\ R_z & r_z \end{pmatrix} = R^{-1}(\alpha, \beta, \gamma) \begin{pmatrix} 0 & r \sin \theta \\ 0 & 0 \\ R & r \cos \theta \end{pmatrix}. \quad (14)$$

Note that there is no problem with the Coriolis terms because our Hamiltonian is written in 6D Cartesian coordinates. Even working in other coordinate systems the coupling between states would not be a problem as they are numerically integrated using Monte Carlo techniques. Our choice of guiding function Ψ to generate the random walks is:

$$\Psi(\mathbf{r}, \mathbf{R}) = \left(\exp \left(\sum_{\nu, \mu} \Delta S_{\nu} A_{\nu, \mu} \Delta S_{\mu} \right) \right)^{1/n}, \quad (15)$$

where n is chosen in order to assure good integration of all states included in our calculation. Note that with the present procedure, we obtain several rotational states in one calculation.

IV. RESULTS

In this work we applied the CFQMC with rotating trial functions to compute the rovibrational levels, up to $J=2$, of H_2O . We have used the potential energy surface (PES) of Jensen²⁰ fitted from experimental data. To optimize our basis set we minimize the variance of the trial energy for the guiding function [Eq. (15) with $n=1$] with respect to the $\{A_{\nu,\mu}\}$ and $\{S_\nu^0\}$ parameters. The optimized parameters are displayed on Table I, and yield a zero-point-energy (ZPE) of 4663.4 cm^{-1} . For the vibrational basis set we have considered all states in which $2(n_1 + n_2) + n_3 \leq 12$, in a total of 140 basis functions. The results for the eight lowest excited states are displayed in Table II. The ZPE obtained after the diagonalization was 4628.2 cm^{-1} , showing that the guiding function, based on an harmonic type function, is a good guess for

TABLE II. Vibrational energy levels for the water molecule. Comparison between CFQMC, DVR^a and experiment.^b Energies are in cm^{-1} .

(ν_1, ν_2, ν_3)	CFQMC	DVR	EXP
0 1 0	1594.4	1594.3	1594.7
0 2 0	3151.4	3152.0	3151.6
1 0 0	3657.8	3656.5	3657.1
0 0 1	3756.6	3756.0	3755.9
0 3 0	4667.0	4667.7	4666.8
1 1 0	5236.6	5234.3	5235.0
0 1 1	5334.3	5332.1	5331.2
0 4 0	6135.5	6134.2	6134.0

^aReference 21.

^bReference 23.

the ground state of the system. After diagonalizing the vibrational part of the trial wave function we kept the lowest 14 states to construct our rotating basis set, which correspond to 42 and 70 states in the $J=1$ and $J=2$ calculations, respectively. The results for $J=1$ and $J=2$ for the lowest nine vibronic states are displayed in Tables III and IV. One can see that the agreement with the experimental results is very good, the average deviation was 1.73 cm^{-1} for $J=1$ and 4.89 cm^{-1} for $J=2$. We also compare our results with the results obtained by Fernley *et al.*²¹ with DVR calculation on the same PES, and the average deviations are 1.74 cm^{-1} for $J=1$ and 4.91 cm^{-1} for $J=2$. Other calculations on the same surface (e.g., the calculation of Yan *et al.*²²) have the same accuracy as the results obtained by Fernley *et al.* It should be pointed out that all the calculations presented in this work are at the variational level, the results should im-

TABLE III. Rovibrational energy levels ($J=1$) for H_2O molecule. Comparison between CFQMC, DVR,^a and experiment.^b Energies are in cm^{-1} .

(ν_1, ν_2, ν_3)		M=-1	M=0	M=1
0 0 0	CFQMC	22.25	36.04	41.61
	DVR	23.80	37.08	42.33
	exp	23.79	37.14	42.36
0 1 0	CFQMC	22.78	41.24	44.86
	DVR	23.82	40.18	45.72
	exp	23.81	40.22	45.76
0 2 0	CFQMC	22.52	47.08	52.24
	DVR	23.82	44.39	50.22
	exp	23.81	44.46	50.28
1 0 0	CFQMC	23.42	35.97	42.05
	DVR	23.43	36.24	41.45
	exp	23.40	36.24	41.43
0 0 1	CFQMC	23.64	39.31	42.64
	DVR	23.60	35.80	41.09
	exp	23.56	35.77	41.06
0 3 0	CFQMC	25.17	55.26	60.18
	DVR	23.82	50.53	56.63
	exp	23.77	50.66	56.74
1 1 0	CFQMC	24.80	40.67	45.80
	DVR	23.44	39.21	44.73
	exp	23.42	39.17	44.68
0 1 1	CFQMC	24.60	43.00	47.27
	DVR	23.63	38.57	44.17
	exp	23.63	38.52	44.13
0 4 0	CFQMC	24.65	63.67	69.68
	DVR	23.79	60.75	66.75
	exp	23.73		67.04

^aReference 21.

^bReference 23.

TABLE IV. Rovibrational energy levels ($J=2$) for H_2O molecule. Comparison between CFQMC, DVR^a and experiment.^b Energies are in cm^{-1} .

(ν_1, ν_2, ν_3)		M=-2	M=-1	M=0	M=1	M=2
0 0 0	CFQMC	71.40	79.45	99.51	135.81	137.13
	DVR	70.11	79.45	95.17	134.70	135.98
	exp	70.09	79.50	95.18	134.90	136.20
0 1 0	CFQMC	74.12	84.48	104.36	150.52	151.57
	DVR	70.23	82.27	98.88	147.39	148.57
	exp	70.22	82.32	98.90	147.56	148.74
0 2 0	CFQMC	72.52	89.68	99.82	170.16	175.84
	DVR	70.36	86.23	103.69	164.25	165.32
	exp	70.33	86.29	103.71	164.51	165.58
1 0 0	CFQMC	72.25	79.74	102.96	130.94	134.28
	DVR	68.97	77.89	93.50	131.63	132.92
	exp	68.89	77.84	93.41	131.64	132.92
0 0 1	CFQMC	71.86	78.48	98.74	133.46	137.94
	DVR	69.39	77.73	93.58	129.89	131.27
	exp	69.29	77.66	93.45	129.81	131.18
0 3 0	CFQMC	83.42	100.37	109.47	197.59	205.10
	DVR	70.48	92.12	110.36	187.95	188.87
	exp	70.40	92.21	110.39	188.49	189.41
1 1 0	CFQMC	72.80	86.19	100.15	148.19	149.60
	DVR	69.09	80.58	97.12	143.86	145.07
	exp	69.02	80.51	97.03	143.76	144.97
0 1 1	CFQMC	70.71	83.31	108.66	142.20	146.02
	DVR	69.55	80.26	97.03	141.36	142.66
	exp	69.49	80.17	96.93	141.11	142.42
0 4 0	CFQMC	69.29	117.18	126.18	225.23	245.77
	DVR	70.58	101.77	120.69	223.80	224.55
	exp	70.43	102.03			

^aReference 21.^bReference 23.

prove once we use the diffusion Monte Carlo method⁸ to project the excited states. These results are of the same accuracy as the variational methods to compute rovibrational levels of triatomic systems.

V. CONCLUSION

In this work, we reported the use of CFQMC method to obtain the rovibrational energy levels of triatomic molecules. We proposed a general procedure to generate rotating trial basis functions and have given their analytic forms for triatomic molecules. This is an extension of the work reported in Ref. 16. Note that the analytic forms are simple and easy to apply, the only difficulty is to write the Euler angles in terms of the Jacobi coordinates. We employed the present method to calculate the rovibrational energy levels of the water molecule. The procedure can be generalized to study rovibrational states of larger molecules following the basic steps shown in this work and of Refs. 16,17.

The results displayed in Tables III and IV have accuracy comparable with the traditional variational methods, and are in very good agreement with the experimental results. We conclude that the use of rotating trial basis sets to obtain the rovibrational excited energies employing CFQMC method is very efficient. The great advantage of the quantum Monte Carlo methods is that they do not grow exponentially with the number of degrees of freedom. The generalization to

larger systems is straightforward, as is discussed in more detail in Ref. 17. Currently, we are calculating the rovibrational energy levels for tetratomic molecules and are extending the present methodology to calculate the rovibrational energy levels for larger molecules.

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