Diffusion Monte Carlo calculations of three-body systems*

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Abstract: The application of the diffusion Monte Carlo algorithm in three-body systems is studied. We develop a program and use it to calculate the property of various three-body systems. Regular Coulomb systems such as atoms, molecules, and ions are investigated. The calculation is then extended to exotic systems where electrons are replaced by muons. Some nuclei with neutron halos are also calculated as three-body systems consisting of a core and two external nucleons. Our results agree well with experiments and others' work.

Key words: diffusion Monte Carlo, three-body system, neutron-halo nuclei

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1 Introduction

The three-body problem plays an important role in atomic physics, molecular physics, and nuclear physics. The study of the Coulomb three-body systems in quantum physics dates back to the 1930s when physicists were trying to explain the helium spectrum. Many years have passed, but progress is still being made in this field. New systems such as exotic three-body atomic systems have aroused the great interest of physicists recently [1]. New wave functions are also being found [2]. The study of the three-body problem is also very common in nuclear physics [3, 4]. Tritium is a typical three-body system that was studied using Monte Carlo methods long ago [5]. Some exotic nuclei such as ^{6}He and ^{11}Li are also studied from a three-body perspective [6–11].

The fundamental difficulty in these fields is to solve the coupled three-body Schrödinger equation. The variational method with the trial wave function is one of the most common ways to solve this problem [12]. Some of these variational wave functions can be analytical and simple [2], while some of them are more sophisticated with a large number of variational parameters [13]. Another way is to solve the corresponding Faddeev equations, which is widely used both in scattering and bound problems [14, 15]. The diffusion Monte Carlo method is also very powerful in solving three-body problems such as Positronium-atom complexes [16], mesic molecules [17], light nuclei [18, 19], and medium nuclei [20].

We write a program to study three-body systems with diffusion Monte Carlo methods. We first study regular Coulomb systems such as a hydrogen molecular ion $p^+p^+e^-$, followed by the extension to muonic systems. Those calculations are carried out without Born-Oppenheimer approximation. We also apply the diffusion Monte Carlo method to nuclei which are considered as Yukawa three-body systems.

2 Theoretical framework

The Hamiltonian of a three-body system can be written as:

$$H = -\sum_i \frac{\hbar^2}{2m_i}\nabla_i^2 + \sum_{i<j} V_{ij} \ , \qquad (1)$$

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where m_i is the mass of each component and V_{ij} is the two-body potential. The exact wave function of the three-body system is written as $\psi(\boldsymbol{R},t)$, where $\boldsymbol{R}$ is the $3N$-dimensional configuration coordinate. Then a new wave function

$$f(\boldsymbol{R},t)=\psi(\boldsymbol{R},t)\psi_{\rm T}(\boldsymbol{R},t) \tag{2}$$

is introduced, where $\psi_{\rm T}(\boldsymbol{R},t)$ is a trial wave function which could be generated by variational Monte Carlo method. This function satisfies the equation [21],

$$\begin{aligned}-\frac{\partial}{\partial t}f(\boldsymbol{R},t) =& \sum_i -\frac{\hbar^2}{2m_i}\nabla_i^2 f(\boldsymbol{R},t)\\ &+\sum_i \frac{\hbar^2}{m_i}\nabla\cdot\left[\frac{\nabla_i\psi_{\rm T}(\boldsymbol{R})}{\psi_{\rm T}(\boldsymbol{R})}f(\boldsymbol{R},t)\right]\\ &+[E_{\rm L}(\boldsymbol{R})-E_{\rm T}(t)]\,f(\boldsymbol{R},t).\end{aligned} \tag{3}$$

Here $E_{\rm L}$ is the local energy given by

$$E_{\rm L}(\boldsymbol{R})=\frac{\hat{H}_{\rm L}\psi_{\rm T}(\boldsymbol{R})}{\psi_{\rm T}(\boldsymbol{R})}, \tag{4}$$

where

$$\hat{H}_{\rm L}=-\sum_i\frac{\hbar^2}{2m_i}\nabla_i^2+\sum_{i<j}V_{ij}. \tag{5}$$

$E_{\rm T}(t)$ is a shift energy which plays a role of normalization factor. Eq. (3) could be solved iteratively in an integral form,

$$f(\boldsymbol{R}',t+\tau)=\int {\rm d}\boldsymbol{R}\tilde{G}(\boldsymbol{R}',\boldsymbol{R},\tau)f(\boldsymbol{R},t), \tag{6}$$

where τ is the time step between iterations. In short-time approximation the Green's function $\tilde{G}(\boldsymbol{R}',\boldsymbol{R},\tau)$ has the form [21],

$$\begin{aligned}\tilde{G}(\boldsymbol{R}',\boldsymbol{R},\tau)=&\prod_i\frac{1}{(2\pi\sigma_i^2)^{3/2}}\exp\left[-\frac{(\boldsymbol{R}'-\mu_i(\boldsymbol{R}))^2}{2\sigma_i^2}\right]\\ &\times\exp[-\tau(E_{\rm L}(\boldsymbol{R}')+E_{\rm L}(\boldsymbol{R})-2E_{\rm T})/2],\end{aligned} \tag{7}$$

where

$$\sigma_i^2=\tau\hbar^2/m_i, \tag{8}$$

and

$$\mu_i(\boldsymbol{R})=\boldsymbol{R}+\sigma_i^2\nabla_i\ln|\psi_{\rm T}(\boldsymbol{R})|. \tag{9}$$

To simulate this short-time Green's function in the calculation, initial walkers will be generated according to the trial function $\psi_{\rm T}$ first. Then the walkers will diffuse and drift to new positions according to the Gaussian distribution

$$\frac{1}{(2\pi\sigma_i^2)^{3/2}}\exp\left[-\frac{(\boldsymbol{R}'-\mu_i(\boldsymbol{R}))^2}{2\sigma_i^2}\right]. \tag{10}$$

Then a branching technique is adopted to give the probability to kill or multiply the walkers at new configurations. The number of copies generated from each old walker is ${\rm INT}(p+\xi)$, where ξ is a random number between (0,1), and,

$$p=\exp[-\tau(E_{\rm L}(\boldsymbol{R}')+E_{\rm L}(\boldsymbol{R})-2E_{\rm T})/2]. \tag{11}$$

Iteration times are denoted by $\hat{t}=t/\tau$. At each iteration, the expectation value of energy is calculated by the mixed estimator, which is defined as [21],

$$E_{\rm mix}(T)=\frac{\sum_{\hat{t}=0}^{T}\Pi(\hat{t})\sum_{\alpha=1}^{N(\hat{t})}\frac{\hat{H}_{\rm L}\psi_{\rm T}(\boldsymbol{R}_\alpha(\hat{t}))}{\psi_{\rm T}(\boldsymbol{R}_\alpha(\hat{t}))}}{\sum_{\hat{t}=0}^{T}\Pi(\hat{t})N(\hat{t})}, \tag{12}$$

where

$$\Pi(\hat{t})=\prod_{m=0}^{\hat{t}}{\rm e}^{-\tau E_{\rm T}(\hat{t}-m)}. \tag{13}$$

To make the population of walkers stable, the $E_{\rm T}$ should be adjusted by

$$E_{\rm T}(\hat{t}+1)=E_{\rm mix}(\hat{t})-\log\frac{N(\hat{t})}{N_0}\ , \tag{14}$$

where $N(\hat{t})$ is the population at each iteration and N_0 is the initial one.

After many iterations, these walkers will distribute as $\psi_{\rm T}(\boldsymbol{R})\psi_0(\boldsymbol{R})$, where ψ_0 is the exact ground state of the system. $E_{\rm mix}(t)$ will also equal the exact ground state energy. To avoid time-step error, the results of different τ should be calculated and then extrapolated to $\tau=0$.

3 Numerical results and analyses

We calculate different systems of atoms, molecules, ions, and nuclei with the diffusion Monte Carlo method. In these calculations, except for nuclei, the trial wave functions have variational form:

$$\psi_{\rm T}=\prod_{i<j}{\rm e}^{\alpha_l r_{ij}}. \tag{15}$$

For nuclei, the trial wave functions are taken as:

$$\psi_{\rm T}=\prod_{i<j}{\rm e}^{\alpha_l r_{ij}}+\gamma\prod_{i<j}{\rm e}^{\beta_l r_{ij}}. \tag{16}$$

The parameters $\{\alpha_l\}$, $\{\beta_l\}$ and γ are optimized by a variational Monte Carlo program. The number of initial walkers is taken to be 2000. Each system is calculated with eight different τ. For each τ, the iteration continues until the error bar of energy, taken from the average of last 10000 mixed estimators, is

smaller than expected. The final result is then constructed by extrapolation from the results of different τ to $\tau = 0$.

3.1 Atoms, molecules and ions

We make diffusion Monte Carlo calculations of some regular Coulomb three-body systems such as atoms, molecules and ions. Our calculations are performed without Born-Oppenheimer approximation. The introduction of nuclear degrees of freedom will increase running time, but it is acceptable for few-body systems.

The calculation results are listed in Table 1. The results from experiments or accurate variational calculations are also listed for comparison. For systems with only one heavy core, such as a helium atom, variational calculation results are already very close to the experimental values. But for systems with two heavy cores, such as hydrogen molecular ion $p^+p^+e^-$, variational results are much higher than the experimental value. This is not surprising because we only use a quite simple trial wave function. However, this simple wave function is good enough to be a diffusion Monte Carlo program input.

Table 1. Results of regular Coulomb systems. $E_{\rm VMC}$ is the variational Monte Carlo result of ground state energy from optimizing the trial wave function. $E_{\rm DMC}$ is the ground state energy result from the diffusion Monte Carlo calculation. The compared results from others' work or experiments are also listed. All values are in atomic units.

system	$E_{\rm VMC}$	$E_{\rm DMC}$	results in Refs.	
$e^+e^-e^-$	−0.2372	−0.2614	−0.2620	Frolov [22]
$p^+e^-e^-$	−0.5061	−0.5273	−0.5274	Frolov [23]
$p^+p^+e^-$	−0.4759	−0.5938	−0.5974	Exp. [24]
$^4He^{2+}e^-e^-$	−2.886	−2.902	−2.902	Exp. [25]
$^7Li^{3+}e^-e^-$	−7.253	−7.275	−7.279	Ancarani [1]

Most of these diffusion Monte Carlo results agree with experiment very well with an error of only 0.05%. This proves that our program is accurate enough to calculate three-body system combined by Coulomb interaction. The result of a hydrogen molecular ion has a larger error of about 0.6%. This larger error may be due to the fact that it has two heavy cores and the trial wave function with the form of Eq. (15) is not a good description of the system.

3.2 Muonic systems

We also calculate some muonic three-body systems. Unlike regular three-body systems, the Born-Oppenheimer approximation will cause serious error when the electrons are replaced by muons. In these systems, the motion of nuclei cannot be omitted, since the mass of a muon is comparable to a proton or light nuclei. Therefore our diffusion Monte Carlo calculations of muonic systems are performed without Born-Oppenheimer approximation. The calculation results are listed in Table 2. Results for comparison are also listed.

Table 2. Results of muonic systems. $E_{\rm VMC}$ is the variational Monte Carlo result of ground state energy from optimizing the trial wave function. $E_{\rm DMC}$ is the ground state energy result from the diffusion Monte Carlo calculation. The compared results from others' work or experiments are also listed. All values are in atomic units.

system	$E_{\rm VMC}$	$E_{\rm DMC}$	results in Refs.	
$\mu^+e^-e^-$	−0.5023	−0.5228	−0.5251	Frolov [23]
$\mu^+\mu^+e^-$	−0.4685	−0.5832	—	—
$\mu^+\mu^-\mu^-$	−49.21	−54.07	—	—
$p^+\mu^-\mu^-$	−92.71	−96.97	−97.57	Frolov [26]
$p^+p^+\mu^-$	−87.78	−101.8	−96.86	Bailey [27]
$He^{2+}\mu^-\mu^-$	−579.1	−582.3	−582.4	Ancarani [1]

Some of the muonic systems in our calculations have been rarely studied before such as $\mu^+\mu^+e^-$. So only diffusion Monte Carlo results are given. Some of these systems have been calculated with accurate variational methods in others' work. Our results of these systems agree very well with them. A bigger difference can be found in the calculation of system $p^+p^+\mu^-$, and our result is lower than the result in Ref. [27]. Considering that our diffusion Monte Carlo results are always a little bit higher than the accurate values, this difference is very strange and should be confirmed by more theoretical work or experiments.

3.3 Nuclei

In a three-body model, a nucleus can be treated as a system composed of a core and two external nucleons [28]. This is particularly useful in the study of exotic nuclei with neutron halos. Three typical halo nuclei, ^{11}Li, ^{14}Be and ^{17}B, were studied by equivalent two-body methods and Faddeev equations before [9–11]. We investigate these nuclei with the diffusion Monte Carlo method. The two-body Yukawa potential is taken from Ref. [10]. The calculation results and various compared values are listed in Table 3.

Our results of ground state energy are lower than the equivalent two-body methods, but agree with the Faddeev equation well. Considering that the equivalent two-body methods are variational methods, our

Table 3. Results of some exotic nuclei. E is the ground state energy. $R_{\rm m}$ is the matter root-mean-square radius. The lines denoted by (F&R) are the results from equivalent two-body methods [9]. The lines denoted by (Faddeev) are the results from Faddeev equations [11].

system		E/MeV	$R_{\rm m}$/fm
^{11}Li	(DMC)	-0.59	2.83
	(Faddeev)	-0.54	2.95
	(F&R)	-0.35	3.18
	(exp.)	$-0.35(\pm0.05)$	$3.10(\pm0.17)$
^{14}Be	(DMC)	-1.18	2.78
	(Faddeev)	-1.07	2.85
	(F&R)	-1.12	2.90
	(exp.)	$-1.12(\pm0.20)$	$3.10(\pm0.30)$
^{17}B	(DMC)	-1.09	2.73
	(Faddeev)	-1.01	2.76
	(F&R)	-0.84	2.81
	(exp.)	$-1.49(\pm0.20)$	$3.00(\pm0.40)$

results and Faddeev results are better. These results show that the diffusion Monte Carlo method can be as precise as Faddeev equations in the calculations of three-body systems. However, the diffusion Monte Carlo method can be also used to calculate many-body systems, which is difficult for Faddeev equations.

4 Conclusion

In this paper, diffusion Monte Carlo algorithm with importance sampling technique is formulated for systems consisting of components with different masses. A mixed estimator is used to obtain the average of physical quantities. We write a program and study various systems with this method. We calculate the ground state energy of regular and exotic three-body systems. These calculations are all performed without Born-Oppenheimer approximation. Our results agree very well with experiments and with other high precision variational methods. We also produce the properties of some three-body systems which are rarely studied before. Halo nuclei are investigated as three-body systems. The results are better than the equivalent two-body method but almost the same as that from the Faddeev equations. All these results have proven the accuracy of our program and the power of diffusion Monte Carlo method in studying three-body systems.

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