Are there locally precise three-body wave functions?

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Abstract

This paper concentrates on two topics. First it presents cases which show that even in atomic physics, contrary to expectations, variational methods have problems on the 4-5th digits in expectation values which depend on the values of Ψ at the cusps, as opposed to the energy. Second, we compare the results of the direct method, CFHHM (Correlation function hyperspherical harmonic method), in atomic ionization calculations of the single and double ionization of the Helium atom and the Helium isoelectronic sequence for Z up to 10 and excited states up to $n = 5$. We calculate more n, Z dependencies than before; make predictions on corrections due to quasi-free mechanism using a new formula (several new light sources are becoming available).

Sophisticated variational methods nowadays try to overcome the fact that mathematically there is no reason to assume that a variational method would give accuracy for the expectation values comparable to that of the energy E. The motivations in this section is to show several examples where such variational calculation indeed break down.

CFHHM [1] is a direct solution of the Schrödinger equation by the separation of Ψ into the singular part (caused by the Coulomb interaction; this is specific to the atomic physics) and the smooth part, $\Psi = e^f \phi$. The Schrödinger equation is converted into the equation for $\chi = \rho^2 \phi$ expanded into the hyperspherical harmonic basis (index ν; μ is connected with the global angular momentum):

$$\chi''_{\mu\nu} + \frac{1}{\rho}\chi'_{\mu\nu} + \left[2E - \frac{(2\mu+2)^2}{\rho^2}\right]\chi_{\mu\nu} = 2\sum_{\mu'\nu'} \overline{W}_{\mu\nu,\mu'\nu'}\chi_{\mu'\nu'}, \tag{1}$$

where ρ is the hyperradius (a permutation-invariant measure of system size, given by a weighted sum of squares of the Jacobi coordinates), and W is the velocity-dependent potential, $\overline{W} = V - (\nabla f, \nabla) - \frac{1}{2}\nabla^2 f - \frac{1}{2}(\nabla f)^2 + \frac{2}{\rho^2}\frac{\partial f}{\partial \rho}$. The essential physical input to CFHHM is the correlation function which in general is nonlinear

$$f = \sum_{k=1}^{3}\left[a_k + (b_k - a_k)\exp\left(\frac{r_k}{n_k\langle r_k\rangle}\right)\right] r_k, \quad a_k = Z_i Z_j \frac{m_i m_j}{m_i + m_j},$$

where $\{i, j, k\}$ are a permutation of $\{1, 2, 3\}$, and Z_i and m_i are charges and masses of the particles. f but can be used in its linear form ($b_k = a_k$) for Helium and its isoelectronic sequence except H^-. Mathematically this function is an accelerator of the convergence

but it also lowers the minimum μ where convergence starts; it reduces the number of HH required for a given precision by orders of magnitude; in addition, it can at the same time incorporate some asymptotic (clustering) properties. For example, the nonlinear correlation function for the positronium negative ion (Ps-) reduces the error of observables by two orders of magnitude while making the calculation even less time consuming.

The sticking probabilities (Table 1) in the muon-catalyzed fusion process are an example of CFHHM giving much smaller error margins than even the discrepancies between different variational calculations.

Table 1: Sticking probabilities ω_{nl} ($Q = 5.844$).

Method	$K_{\rm m}$	1s	2s	4s	2p
CFHHM		0.6819(1)	0.0978	0.0126	0.0238
HCM (Abramov)	15	0.829 (?)			
	21	0.906 (?)			
	21	0.7001	0.1004	0.0130	0.0245[1)]
Var. (Hu)		0.6932	0.0992	0.0128	0.0241
Var. (Haywood)		0.6846			
Var. (Hu)		0.6817			
Kamimura		0.6842			
Var. (Hu)		0.6802	0.0975	0.0126	0.0237
Var. (recent)		0.6802-			
		0.8422			

[1)] $Q = 5.846$.

In $e\mu^4$He we have a case where CFHHM has resolved high precision discrepancies. Even E converged faster than in a variational method (SVM), but the "local" expectation values definitely are better than the differences between two high-precision calculations by the same author:

$10^8\langle\delta(\mathbf{r}_{\mu\rm He})\rangle$	0.207 001 3**5**4 2(6)	CFHHM
	0.207 001 373 **6**10	Smith-Frolov 1995
	0.207 001 373 **4**3	Frolov 2000
$\langle\delta(\mathbf{r}_{e\mu})\rangle$	0.313 76**2** 07(7)	
	0.313 76**3** 0	
	0.313 76**0** 812	
$\langle\delta(\mathbf{r}_{e\rm He})\rangle$	0.320 63**3** 27(6)	
	0.320 62**6** 88	
	0.320 63**1** 162	

Bartlett (in 1935) suggested comparing the local energy, $D = H\Psi/E\Psi - 1$. Fig. 1 shows the comparison of SVM (Varga, Kukulin) and CFHHM for Ps- from Ref. [2]. While CFHHM is clearly better especially around the repulsive cusp which SVM avoids because it contributes little to E, CFHHM turns out to be "much worse" than SVM for almost all expectation values. However the δ operators are much better:

$\langle H\rangle$	0.262 005 069 5	CFHHM
	0.262 005 070 226	SVM
	0.262 005 070 232 965	EVE

$\langle r_{ee} \rangle$	8.548 5(2)
	8.548 580 655 061
	8.548 580 655 12
$\langle \delta(\mathbf{r}_{ep}) \rangle$	0.020 733 14(6)*
	0.020 731 048 976
	0.020 733 198 0
$\langle \delta(\mathbf{r}_{ee}) \rangle$	0.170 997(2)[-3]
	0.171 112 600 741[-3]
	0.170 996 99[-3]

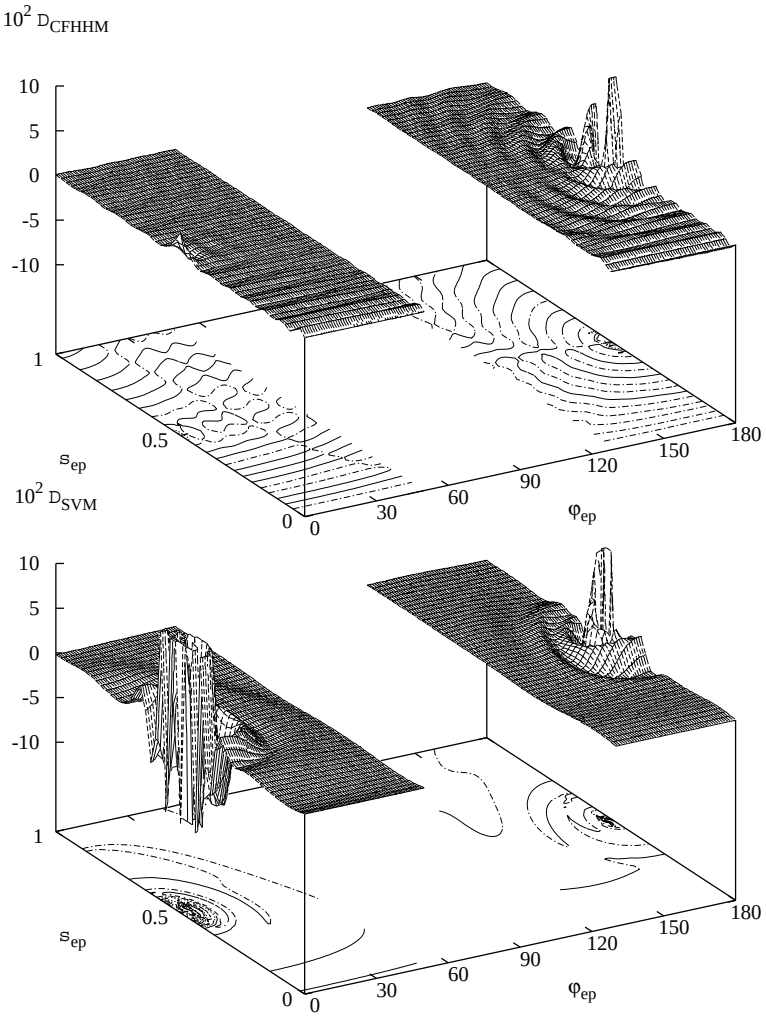

Figure 1: $D = H\Psi/E\Psi - 1$ for Ps-.

The motivations of ionization calculations is to test CFHHM against systematic variational calculations by Forrey [3].

Experimentally it turns out that one electron takes away almost all energy (shake-off mechanism). Very soon (Byron et al.) it was also realized that in the early calculations the shake-off mechanism underestimates $\sigma^{++}(\omega)$ by a factor of 2, which indicates the importance of correlations in this three-body system; indeed, Helium is very strongly correlated. We shall calculate ratios of cross sections because they are independent of the photon energy at high (but nonrelativistic) photon energies (this just gets rid of the $\omega^{-7/2}$ factor). For precise calculations the dipole approximation (golden rule) is good but good initial three-body wave function is needed. This leads to the expressions for the double

ionization cross section,

$$\sigma^{++}(\omega) \approx \frac{\mathbf{32\sqrt{2}Z^2\pi^2}}{\mathbf{3c\omega^{7/2}}}\left\{\int\left|\mathbf{\Psi(0,s)}\right|^{\mathbf{2}}\mathbf{ds}-\sum_{\nu\mathbf{lm}}\left|\int\mathbf{\Psi(0,s)}\psi_{\nu\mathbf{lm}}\mathbf{(s)ds}\right|^{\mathbf{2}}\right\} \tag{2}$$

where $\psi_{\nu lm}(\mathbf{s})$ describes the unperturbed second electron in the field of the nucleus. (The cross section $\sigma^{+}(\omega)$ contains only the lowest integral, and $\sigma^{+*}(\omega)$ contains only the excitation integrals.) We start out with Ψ corresponding to reasonable E which need not be very precise (in CFHHM), but also should not be too imprecise (Table 2). Nevertheless, we end up with differences at $3^{\rm rd}$ – $4^{\rm th}$ digit (Table 3).

Table 2: Helium binding energy and R values: various methods.

Work	**Basis**	E	R
Present/	121	**2.9037243643**	**.01644**
CFHHM	441	**2.9037243765**	**.01644**
[3]		**2.903724377034**	**.01644**
Kheifets	7/MCHF	2.90181	.0167
Dalgarno	20	2.9037179	.0168

Table 3: $R = \sigma^{++}(\omega)/(\sigma^{+}(\omega)+\sigma^{+*}(\omega))|_{\omega\to\infty}$ values for the n^1S states in the Helium isoelectronic sequence (in percent), and the differences with Ref. [3].

n / Z	1	2	3	4	5
1	1.602				
2	**1.644**	0.903	0.369	0.169	0.088
3	0.85**5**	1.204	0.830	0.546	0.360
4	0.508	0.99**4**	0.849	0.677	0.530
5	0.334	0.768	0.728	0.643	0.553
6	0.23**5**	0.595	0.599	0.561	0.512
7	0.175	0.469	0.491	0.479	0.453
8	0.135	0.37**7**	0.406	0.406	0.395
9	0.107	0.309	0.339	0.346	0.344
10	0.087	0.258	0.287	0.297	0.299

We anticipate several works with relevant data for experiments. For example, we obtain a 35 % quasi-free correction at 100 keV [4]. Rather small computational demands have been placed on CFHHM, but state-of-the-art results were improved. This calculation for the first time separates the three-body input from approximations like the dipole approximation. Higher excited states and QF corrections were calculated for the first time. We plan to extend this work to triplet states and Compton scattering.

References

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