Comparison of Analysis for H_2^+

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The H_2^+ Problem

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  - Wavelength: 790 nm
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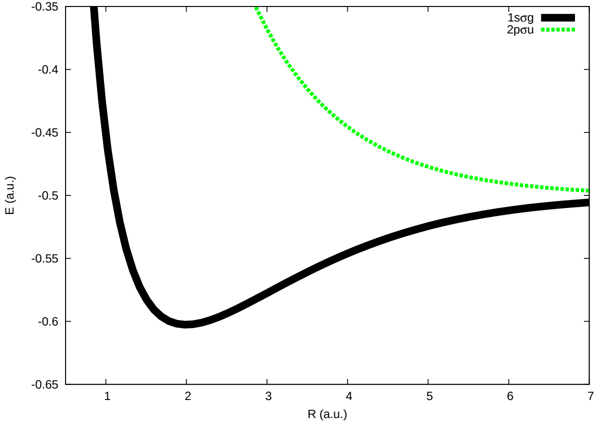
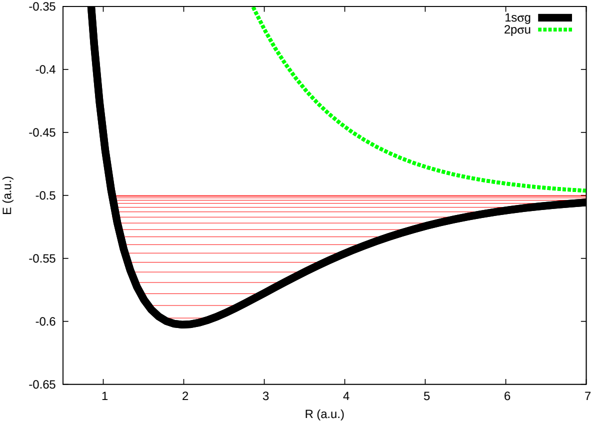
  - Intensity: 10^{14} W/cm^2
- First 19 vibrational states

Potentials



Vibrational States



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- Integrate KER spectrum for P_A, P_B

Analysis of Continuum States-Theory

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$$\Psi_c(R,t) = \Psi(R,t) - \sum_n < \Psi_{b_n}(R)|\Psi(R,t) > \Psi_{b_n}(R)$$

Analysis of Continuum States-Cont.

$$\Psi^c_M(R,r,t) = F^c_g(R,t)\Phi_g(R;r) + F^c_u(R,t)\Phi_u(R;r)$$

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- $R \to \infty$

$$\Phi_{g,u}(R \to \infty; r) = \frac{\Phi_A(r) \pm \Phi_B(r)}{\sqrt{2}}$$

$$\Psi^c_M(R, r, t) = F^c_g(R, t)\left[\frac{\Phi_A(r) + \Phi_B(r)}{\sqrt{2}}\right] + F^c_u(R, t)\left[\frac{\Phi_A(r) - \Phi_B(r)}{\sqrt{2}}\right]$$

$$\Longrightarrow \; F_{A,B} = \frac{1}{\sqrt{2}}(F^c_g \pm F^c_u)$$

Fourier Transform

$$\tilde{\Psi}^{A,B}(k) = \frac{1}{\sqrt{2\pi}} \int \Psi_A(R) e^{-ikR} dR$$

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$$\tilde{\Psi}^{A,B}(E) = \sqrt{\frac{\mu}{k}} \tilde{\Psi}^{A,B}(k)$$

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$$\tilde{\Psi}^{A,B}(E) = \sqrt{\frac{\mu}{k}} \tilde{\Psi}^{A,B}(k)$$

$$P_{A,B} = \int \tilde{\Psi}^{A,B*}(E) \tilde{\Psi}^{A,B}(E) dE$$

Quanities

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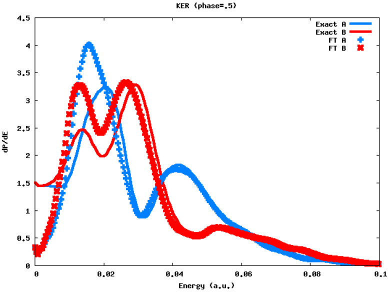
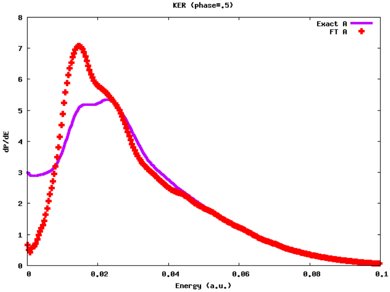
- Dissociation (What percent is breaking apart?)
- KER (At what energies does it break apart?)
- Asymmetry (Does the electron tend to go in one direction?)
- $A = \frac{P_A - P_B}{P_A + P_B}$

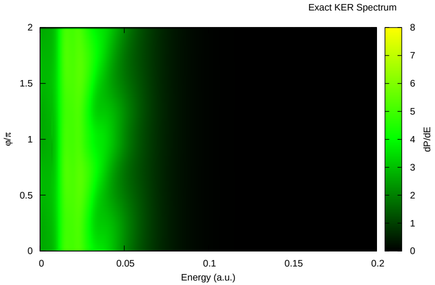
Dissociation Data					
Method	φ/π	P_A	P_B	Total_D	Total_A
$\int \frac{dP_{A,B}}{dE} dE$	0.00	0.10916	0.22367	0.33283	-0.34406
	0.25	**0.10788**	**0.21953**	**0.32742**	**-0.34100**
	0.50	0.10964	0.21930	0.32894	-0.33336
	0.75	0.11388	0.22366	0.33755	-0.32523
	1.00	0.11451	0.22367	0.33819	-0.32278
$\int \left\lvert \frac{F_g^c \pm F_u^c}{\sqrt{2}} \right\rvert^2 dR$	0.00	0.10889	0.22395	0.33284	-0.34568
	0.25	**0.10793**	**0.21981**	**0.32774**	**-0.34137**
	0.50	0.11018	0.21959	0.32977	-0.33178
	0.75	0.11457	0.22396	0.33852	-0.32314
	1.00	0.11506	0.22395	0.33900	-0.32121
$\int \left\lvert FT\left[\frac{F_g^c \pm F_u^c}{\sqrt{2}}\right] \right\rvert^2 dE$	0.00	0.10862	0.22340	0.33202	-0.34571
	0.25	**0.10765**	**0.21925**	**0.32690**	**-0.34139**
	0.50	0.10988	0.21899	0.32887	-0.33177
	0.75	0.11427	0.22337	0.33764	-0.32311
	1.00	0.11478	0.22340	0.33819	-0.32118

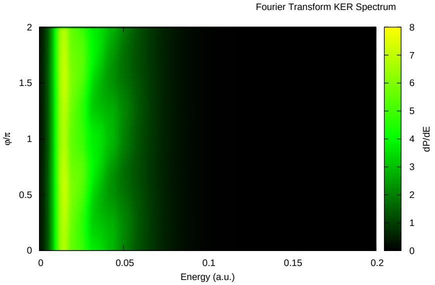
KER


KER (phase=.5)
Exact A
Exact B
FT A
FT B
dP/dE
Energy (a.u.)
4.5
4
3.5
3
2.5
2
1.5
1
0.5
0
0.02
0.04
0.06
0.08
0.1

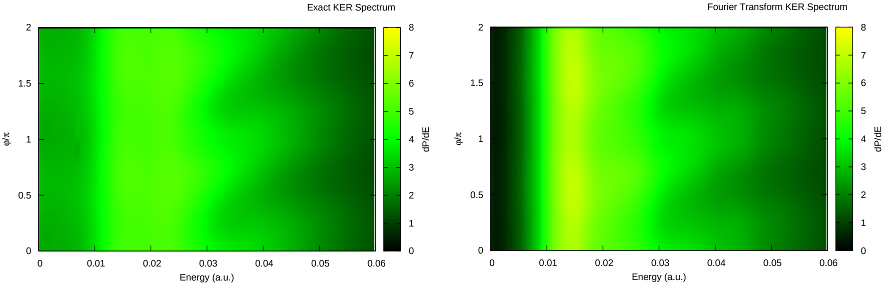

KER (phase=.5)
Exact A
FT A
dP/dE
Energy (a.u.)
8
7
6
5
4
3
2
1
0
0.02
0.04
0.06
0.08
0.1

KER


Exact KER Spectrum
φ/π
Energy (a.u.)
dP/dE
0
0.5
1
1.5
2
0.05
0.1
0.15
0.2
3
4
5
6
7
8


Fourier Transform KER Spectrum
φ/π
Energy (a.u.)
dP/dE
0
0.5
1
1.5
2
0.05
0.1
0.15
0.2
3
4
5
6
7
8

KER-Zoomed


Exact KER Spectrum
φ/π
Energy (a.u.)
dP/dE
0
0.5
1
1.5
2
0.01
0.02
0.03
0.04
0.05
0.06
3
4
5
6
7
8
Fourier Transform KER Spectrum
φ/π
Energy (a.u.)
dP/dE

Percent Difference KER

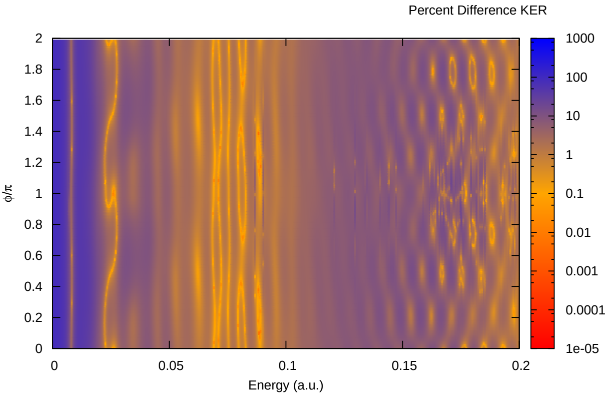


Figure: $\%_D = \frac{\text{Exact}-\text{FT}}{\text{Exact}} * 100$

Percent Difference KER - Zoomed

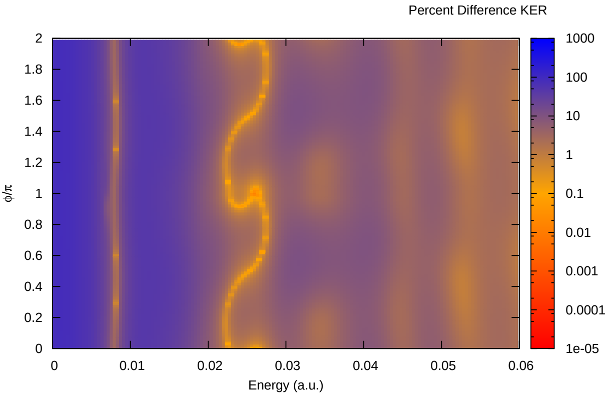
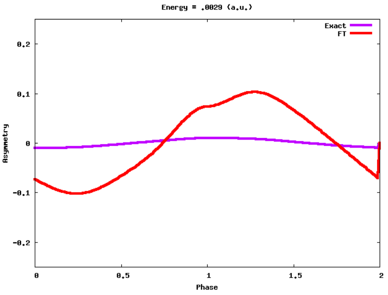
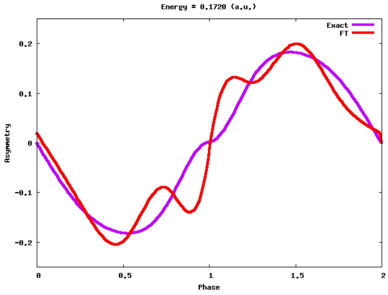


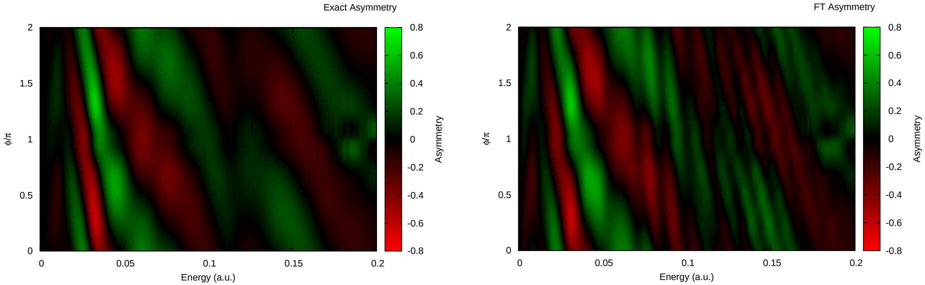
Figure: $\%_D = \frac{\text{Exact} - \text{FT}}{\text{Exact}} * 100$

Asymmetry


Energy = .0029 (a.u.)
Exact
FT
0.2
0.1
0
-0.1
-0.2
Asymmetry
0
0.5
1
1.5
2
Phase


Energy = 0.1720 (a.u.)
Exact
FT
0.2
0.1
0
-0.1
-0.2
Asymmetry
0
0.5
1
1.5
2
Phase

Asymmetry


Exact Asymmetry
FT Asymmetry
φ/π
Energy (a.u.)
Asymmetry
0
0.05
0.1
0.15
0.2
0.5
1
1.5
2
0.8
0.6
0.4
0.2
-0.2
-0.4
-0.6
-0.8

Percent Difference Asymmetry

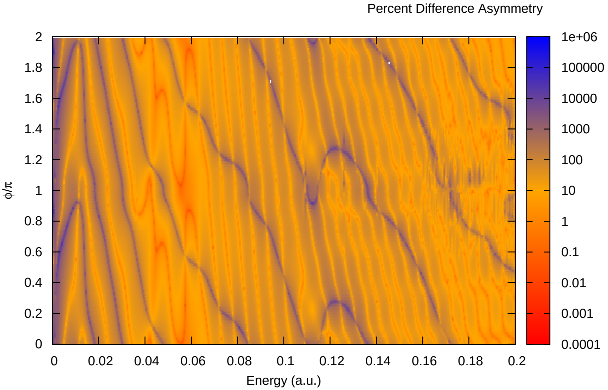


Figure: $\%_D = \frac{\text{Exact} - \text{FT}}{\text{Exact}} * 100$

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