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The entire code repository used to calculate the data for this report, and the `tex` file used to produce this `pdf` document, can be found at `https://github.com/dgsaf/acqm-workshop-3`.

Note that at this point section 2 has not yet been attempted - it may be at a later date, time permitting.

1   Quantum Harmonic Oscillator

Discussion of Theory

Discussion of Implementation

The vibrational wavefunctions were calculated using both the shooting-bisection and the Numerov-Cooley methods, on a grid $X_N = \{x_1, \ldots, x_N\}$. The grid X_N was constructed such that $x_1 = -5$, $x_N = 5$, with varying $N_k = 2^k$, and hence with correspondingly varying step size $(\delta x)_k = 10 \times 2^{-k}$, for $k = 10, \ldots 17$.

Wavefunctions

It was observed that the wavefunctions had converged indistinguishably close to the analytic functions by the first data point $k = 10$, corresponding to $N = 1024$ and $(\delta x) = 0.0097656$. Hence, we simply present the wavefunctions for one data point, $k = 15$.

The $n = 0, \ldots, 3$ wavefunctions, calculated using the shooting-bisection method with, are compared with the analytic wavefunctions in Figure 1.

The $n = 0, \ldots, 3$ wavefunctions, calculated using the Numerov-Cooley method, are compared with the analytic wavefunctions in Figure 2.

Energies

The $n = 0, \ldots, 3$ vibrational energies, calculated using the shooting-bisection method, are compared with the analytic energies in Table 1.

$k = 10$	$k = 11$	$k = 12$	$k = 13$	$k = 14$	$k = 15$	$k = 16$	$k = 17$	Analytic
0.50000	0.50000	0.50000	0.50000	0.50000	0.50000	0.50000	0.50000	0.50000
1.49998	1.50000	1.50000	1.50000	1.50000	1.50000	1.50000	1.50000	1.50000
2.49996	2.49999	2.50000	2.50000	2.50000	2.50000	2.50000	2.50000	2.50000
3.49993	3.49998	3.50000	3.50000	3.50000	3.50000	3.50000	3.50000	3.50000

Table 1: The $n = 0, \ldots, 3$ vibrational energies, calculated using the shooting-bisection method for $k = 10, \ldots, 17$, are presented and compared with the analytic energies, to 6 significant figures. It can be seen that they are already convergent to the analytic energies by $k = 12$ - perhaps smaller grid sizes should be investigated further.

The $n = 0, \ldots, 3$ vibrational energies, calculated using the Numerov-Cooley method, are compared with the analytic energies in Table 2.

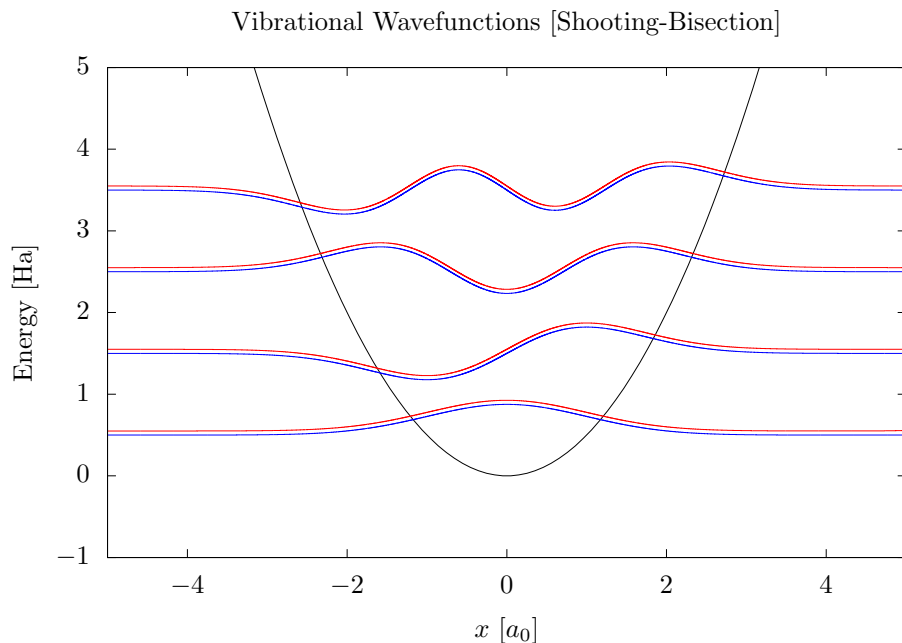Vibrational Wavefunctions [Shooting-Bisection]

Figure 1: The $n = 0, \ldots, 3$ vibrational wavefunctions, calculated using the shooting-bisection method for $k = 15$ (shown in blue), are compared with the analytic wavefunctions (shown in red). The potential is also presented for clarity (shown in black). Note that the calculated wavefunctions have been shifted and scaled to $\psi_i \rightarrow \frac{1}{2}\psi_i + E_i$, while the analytic wavefunctions have been shifted and scaled to $\psi_i \rightarrow \frac{1}{2}\psi_i + E_i + 0.05$.

Iterations

The number of iterations required to calculate the $n = 0, \ldots, 3$ vibrational energies and wavefunctions using the shooting-bisection method, for $k = 10, \ldots, 17$, is presented in Table 3.

The number of iterations required to calculate the $n = 0, \ldots, 3$ vibrational energies and wavefunctions using the Numerov-Cooley method, for $k = 10, \ldots, 17$, is presented in Table 4.
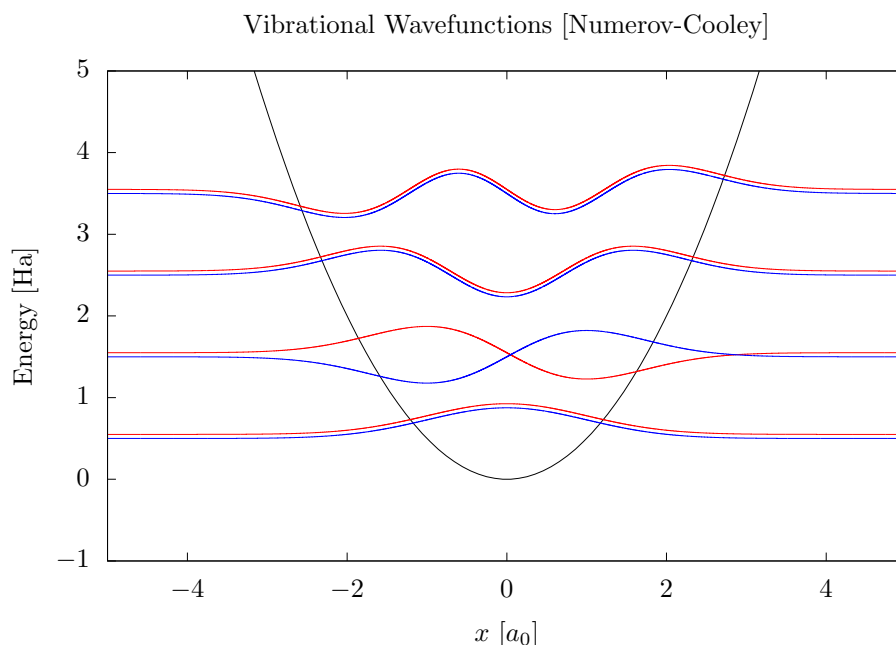
Vibrational Wavefunctions [Numerov-Cooley]

Figure 2: The $n = 0, \ldots, 3$ vibrational wavefunctions, calculated using the Numerov-Cooley method for $k = 15$ (shown in blue), are compared with the analytic wavefunctions (shown in red). The potential is also presented for clarity (shown in black). Note that the calculated wavefunctions have been shifted and scaled to $\psi_i \rightarrow \frac{1}{2}\psi_i + E_i$, while the analytic wavefunctions have been shifted and scaled to $\psi_i \rightarrow \frac{1}{2}\psi_i + E_i + 0.05$. Note also that $n = 1$ calculated wavefunction has a phase shift of -1, which is an arbitrary artifact of the calculation.

$k = 10$	$k = 11$	$k = 12$	$k = 13$	$k = 14$	$k = 15$	$k = 16$	$k = 17$	Analytic
0.50000	0.50000	0.50000	0.50000	0.50000	0.50000	0.50000	0.50000	0.50000
1.50000	1.50000	1.50000	1.50000	1.50000	1.50000	1.50000	1.50000	1.50000
2.50000	2.50000	2.50000	2.50000	2.50000	2.50000	2.50000	2.50000	2.50000
3.50000	3.50000	3.50000	3.50000	3.50000	3.50000	3.50000	3.50000	3.50000

Table 2: The $n = 0, \ldots, 3$ vibrational energies, calculated using the Numerov-Cooley method for $k = 10, \ldots, 17$, are presented and compared with the analytic energies, to 6 significant figures. It can be seen that they are already convergent to the analytic energies by $k = 10$ - perhaps smaller grid sizes should be investigated further.

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$k = 10$	$k = 11$	$k = 12$	$k = 13$	$k = 14$	$k = 15$	$k = 16$	$k = 17$
23	23	25	24	24	24	24	24
24	27	25	30	26	26	26	26
24	24	28	28	25	25	25	25
25	26	25	25	25	25	25	25

Table 3: *The number of iterations required to calculate the $n = 0, \ldots, 3$ vibrational energies and wavefunctions using the shooting-bisection method, for $k = 10, \ldots, 17$, are presented.*

$k = 10$	$k = 11$	$k = 12$	$k = 13$	$k = 14$	$k = 15$	$k = 16$	$k = 17$
6	6	6	6	6	6	6	6
6	6	6	6	6	6	6	6
6	6	6	6	6	6	6	6
6	6	6	6	6	6	6	6

Table 4: *The number of iterations required to calculate the $n = 0, \ldots, 3$ vibrational energies and wavefunctions using the Numerov-Cooley method, for $k = 10, \ldots, 17$, are presented.*

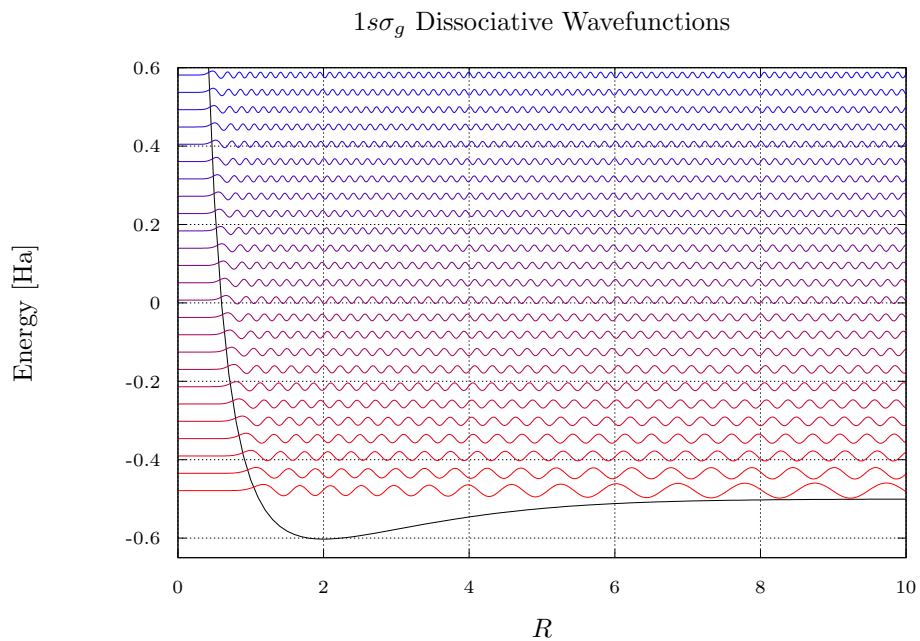# 2   Dissociative Wave Functions for H_2^+

Figure 3: A set of dissociative wavefunctions, for the $1s\sigma_g$ H_2^+ potential-energy-curve, (shown in red-to-blue) are presented across a range of inter-nuclear distances from $0\,a_0$ to $10\,a_0$.
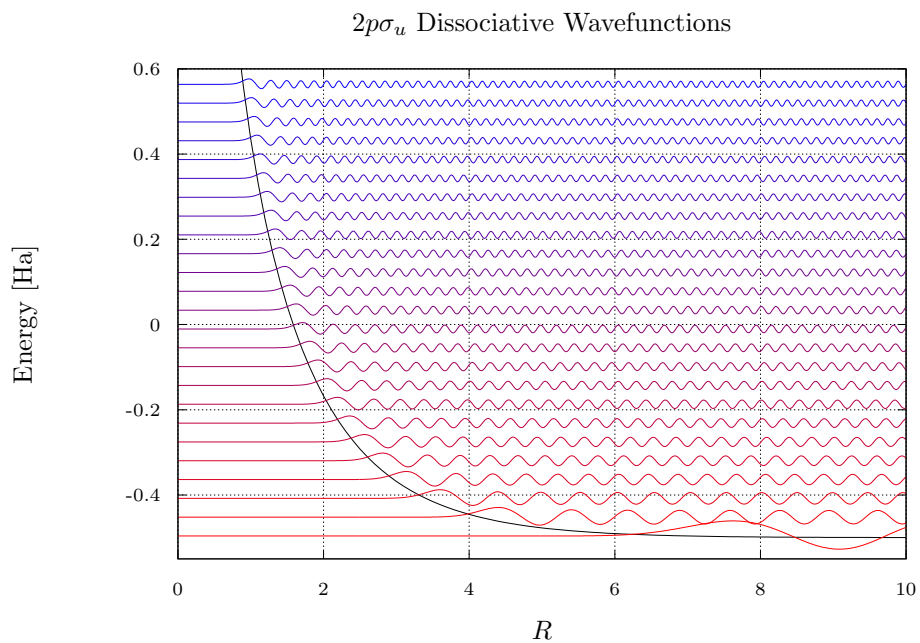
Figure 4: A set of dissociative wavefunctions, for the $2p\sigma_u$ H_2^+ potential-energy-curve, (shown in red-to-blue) are presented across a range of inter-nuclear distances from $0\,a_0$ to $10\,a_0$.
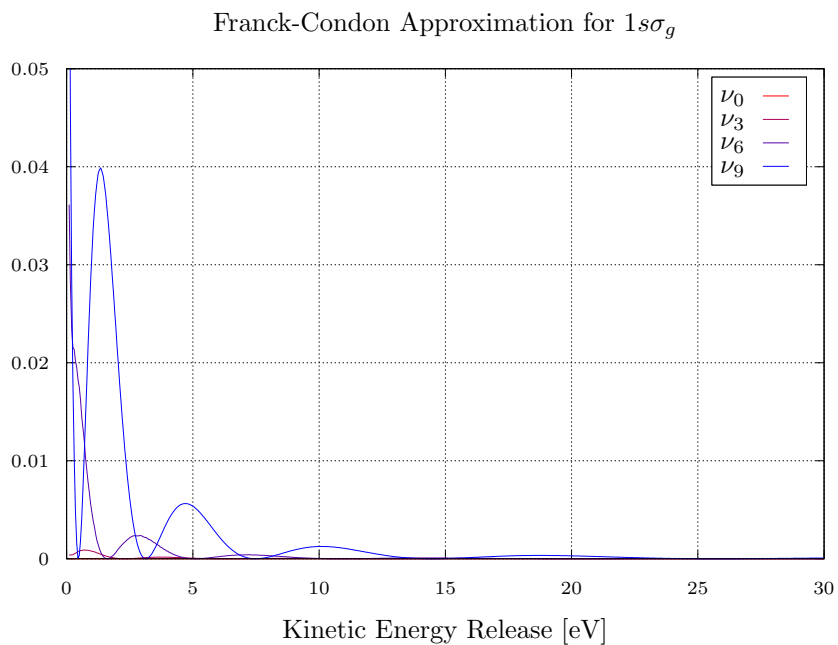
Figure 5: *The kinetic energy release distributions, for* $1s\sigma_g$, *calculated using the Franck-Condon approximation (shown in red-to-blue), are presented for the 0, 3, 6, 9 vibrational states of* $1s\sigma_g$ H_2^+, *across a range of kinetic energy release from* $0\,\mathrm{eV}$ *to* $30\,\mathrm{eV}$. *Note that the scaling is very funky due to the scaling of the dissociative wavefunctions.*