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Guessing Harmonic Oscillator Wavefunctions using Maple

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I. SYNOPSIS

or, in atomic units

The guessing of eigenfunctions is not trivial at higher quantum numbers, no matter what the system being considered. Instead of guessing, one can employ a symbolic calculus program (Maple in this case) to aid in the reasoning process.

$$-\frac{1}{2} \frac{\partial^2}{\partial x^2} + \frac{1}{2} x^2$$

and an trial function

II.

$$\psi_{trial} = (x^4 + \beta x^2 + \gamma) e^{-\alpha x^2}$$

We assume a harmonic oscillator whose Hamiltonian is

$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{k}{2} x^2$$

where β and γ [1] are to be determined when making this an eigenfunction of the Hamiltonian.

```
> #temp ho n = 4 eigenfunctionality
> restart;
> psi := (x^4+beta*x^2+gamma_var)*exp(-alpha*x^2);
> H_psi_minus_E := expand(-(hbar^2/(2*m))*diff(psi,x$2)
+ (k/2)*x^2*psi - E*psi);
> term := collect(expand(exp(alpha*x^2)*H_psi_minus_E),x);
> t6 := coeff(term,x,6);
> result_alpha := solve(t6=0,alpha);#
> term := subs(alpha=result_alpha[1],term);
> H_psi_minus_E := subs(alpha=result_alpha[1],H_psi_minus_E);
> print('attempting the next term ');
> term := collect(expand(exp(result_alpha[1]*x^2)*H_psi_minus_E),x);
> t4 := coeff(term,x,4);
> result_E := solve(t4=0,E);#
> term := subs(E=result_E,term);
> H_psi_minus_E := subs(E=result_E,H_psi_minus_E);
> print('attempting the next term ');
> term := collect(expand(exp(result_alpha[1]*x^2)*H_psi_minus_E),x);
> t2 := coeff(term,x,2);
> result_beta := solve(t2=0,beta);#
> term := subs(beta=result_beta,term);
> print('final, gamma_var, term ');
> result_gamma_var :=
solve(term=0,gamma_var);
```

$$\psi := (x^4 + \beta x^2 + \text{gamma_var}) e^{(-\alpha x^2)}$$

This is a restatement of the wave function in more human readable form. Notice γ had to be re-written as `gamma_var`, since γ is an internal Maple defined quantity.

Next we apply the Hamiltonian, and in anticipation of the Schrödinger equation, we subtract $E\psi$, all in one fell

swoop. In symbolic terms, we form:

$$(H_{op} - E)\psi = 0$$

$$\begin{aligned}
H_psi_minus_E := & -\frac{6 \hbar^2 x^2}{m e^{(\alpha^- x^2)}} - \frac{\hbar^2 \beta}{m e^{(\alpha^- x^2)}} + \frac{9 \hbar^2 \alpha^- x^4}{m e^{(\alpha^- x^2)}} + \frac{5 \hbar^2 \alpha^- x^2 \beta}{m e^{(\alpha^- x^2)}} \\
& + \frac{\hbar^2 \alpha^- \text{gamma_var}}{2 \hbar^2 \alpha^{-2} x^6} - \frac{\hbar^2 \alpha^- \beta}{2 \hbar^2 \alpha^{-2} x^4} - \frac{\hbar^2 \alpha^- \text{gamma_var}}{2 \hbar^2 \alpha^{-2} x^2} \\
& - \frac{m e^{(\alpha^- x^2)}}{2 \hbar^2 \alpha^{-2} x^2 \text{gamma_var}} + \frac{1}{2} \frac{k x^6}{e^{(\alpha^- x^2)}} + \frac{1}{2} \frac{k x^4 \beta}{e^{(\alpha^- x^2)}} + \frac{1}{2} \frac{k x^2 \text{gamma_var}}{e^{(\alpha^- x^2)}} \\
& - \frac{E x^4}{e^{(\alpha^- x^2)}} - \frac{E \beta x^2}{e^{(\alpha^- x^2)}} - \frac{E \text{gamma_var}}{e^{(\alpha^- x^2)}}
\end{aligned}$$

Next, we remove the common exponential term.

We wish then to demonstrate that our result is a polynomial in x . To do this, we collect terms in de-

scending powers of x , purely for illustrative purposes. Since the l.h.s of this expression equals zero (making it a Schrödinger equation) we have:

$$\begin{aligned}
\text{term} := & \left(\frac{k}{2} - \frac{2 \hbar^2 \alpha^-}{m} \right) x^6 + \left(\frac{9 \hbar^2 \alpha^-}{m} + \frac{k \beta}{2} - \frac{2 \hbar^2 \alpha^- \beta}{m} - E \right) x^4 \\
& + \left(\frac{k \text{gamma_var}}{2} + \frac{5 \hbar^2 \alpha^- \beta}{m} - \frac{6 \hbar^2}{m} - \frac{2 \hbar^2 \alpha^- \text{gamma_var}}{m} - E \beta \right) x^2 \\
& - E \text{gamma_var} - \frac{\hbar^2 \beta}{m} + \frac{\hbar^2 \alpha^- \text{gamma_var}}{m}
\end{aligned}$$

We isolate the x^6 term's coefficient next, preparing to declare that this coefficient must be zero (as must the

coefficients of x^4 , x^2 and x^0):

$$t6 := \frac{k}{2} - \frac{2 \hbar^2 \alpha^-}{m}$$

Setting the coefficient of x^6 equal to zero and solving, we get two solutions. The first of these is positive def-

inite, and is the one corresponding to the eigenfunction assumptions made at the outset.

$$\begin{aligned}
\text{result_alpha} := & \frac{\sqrt{k m}}{2 \hbar}, -\frac{\sqrt{k m}}{2 \hbar} \\
\text{term} := & \left(\frac{9 \hbar \sqrt{k m}}{2 m} - E \right) x^4 + \left(\frac{5 \hbar \sqrt{k m} \beta}{2 m} - \frac{6 \hbar^2}{m} - E \beta \right) x^2 - E \text{gamma_var} \\
& - \frac{\hbar^2 \beta}{m} + \frac{\hbar \sqrt{k m} \text{gamma_var}}{2 m}
\end{aligned}$$

There are two roots here, we choose the positive definite one.

$$\begin{aligned}
H_psi_minus_E := & -\frac{6 \hbar^2 x^2}{m e^{(\frac{\sqrt{k m} x^2}{2 \hbar})}} - \frac{\hbar^2 \beta}{m e^{(\frac{\sqrt{k m} x^2}{2 \hbar})}} + \frac{9 \hbar \sqrt{k m} x^4}{2 m e^{(\frac{\sqrt{k m} x^2}{2 \hbar})}} + \frac{5 \hbar \sqrt{k m} x^2 \beta}{2 m e^{(\frac{\sqrt{k m} x^2}{2 \hbar})}} \\
& + \frac{1}{2} \frac{\hbar \sqrt{k m} \text{gamma_var}}{m e^{(\frac{\sqrt{k m} x^2}{2 \hbar})}} - \frac{E x^4}{e^{(\frac{\sqrt{k m} x^2}{2 \hbar})}} - \frac{E \beta x^2}{e^{(\frac{\sqrt{k m} x^2}{2 \hbar})}} - \frac{E \text{gamma_var}}{e^{(\frac{\sqrt{k m} x^2}{2 \hbar})}}
\end{aligned}$$

attempting the next term

$$term := \left(\frac{9 \hbar \sqrt{k m}}{2 m} - E \right) x^4 + \left(\frac{5 \hbar \sqrt{k m} \beta}{2 m} - \frac{6 \hbar^2}{m} - E \beta \right) x^2 - E \gamma_{var} - \frac{\hbar^2 \beta}{m} + \frac{\hbar \sqrt{k m} \gamma_{var}}{2 m}$$

Again, we remove the exponential. Then, we set the x^4 term's coefficient equal to zero, to obtain, as it turns out

$$t4 := \frac{9 \hbar \sqrt{k m}}{2 m} - E$$

$$result_E := \frac{9 \hbar \sqrt{k m}}{2 m}$$

$$E_n = \frac{9}{2} \hbar \sqrt{\frac{k}{m}} \quad \text{as expected, i.e., } 9 = 4 + \frac{1}{2}!$$

$$term := \left(-\frac{2 \hbar \sqrt{k m} \beta}{m} - \frac{6 \hbar^2}{m} \right) x^2 - \frac{4 \hbar \sqrt{k m} \gamma_{var}}{m} - \frac{\hbar^2 \beta}{m}$$

$$H_psi_minus_E := \frac{6 \hbar^2 x^2}{m e^{\left(\frac{\sqrt{k m} x^2}{2 \hbar}\right)}} - \frac{\hbar^2 \beta}{m e^{\left(\frac{\sqrt{k m} x^2}{2 \hbar}\right)}} - \frac{2 \hbar \sqrt{k m} x^2 \beta}{m e^{\left(\frac{\sqrt{k m} x^2}{2 \hbar}\right)}} - \frac{4 \hbar \sqrt{k m} \gamma_{var}}{m e^{\left(\frac{\sqrt{k m} x^2}{2 \hbar}\right)}}$$

attempting the next term

$$term := \left(-\frac{2 \hbar \sqrt{k m} \beta}{m} - \frac{6 \hbar^2}{m} \right) x^2 - \frac{4 \hbar \sqrt{k m} \gamma_{var}}{m} - \frac{\hbar^2 \beta}{m}$$

$$t2 := -\frac{2 \hbar \sqrt{k m} \beta}{m} - \frac{6 \hbar^2}{m}$$

$$result_beta := -\frac{3 \hbar}{\sqrt{k m}}$$

$$term := -\frac{4 \hbar \sqrt{k m} \gamma_{var}}{m} + \frac{3 \hbar^3}{m \sqrt{k m}}$$

final, γ_{var} , term

$$result_gamma_var := \frac{3 \hbar^2}{4 k m}$$

We now redo the computation in “atomic units” which allows us to see more clearly (for most of us) what’s going on. Thus, we set $\hbar \rightarrow 1$, $m = 1$, and $k = 1$.

```

> psi := (x^4+beta*x^2+gamma_var)*exp(-alpha*x^2);
> H_psi_minus_E := expand(-(1/2)*diff(psi,x$2)
+ (1/2)*x^2*psi - E*psi);
> term := collect(expand(exp(alpha*x^2)*H_psi_minus_E),x);
> t6 := coeff(term,x,6);
> result_alpha := solve(t6=0,alpha);#
> term := subs(alpha=result_alpha[2],term);
> H_psi_minus_E := subs(alpha=result_alpha[2],H_psi_minus_E);
> print('attempting the next term ');
> term := collect(expand(exp(result_alpha[2]*x^2)*H_psi_minus_E),x);
> t4 := coeff(term,x,4);
> result_E := solve(t4=0,E);#
> term := subs(E=result_E,term);
> H_psi_minus_E := subs(E=result_E,H_psi_minus_E);
> print('attempting the next term ');
> term := collect(expand(exp(result_alpha[2]*x^2)*H_psi_minus_E),x);
> t2 := coeff(term,x,2);
> result_beta := solve(t2=0,beta);#
> term := subs(beta=result_beta,term);
> print('final, gamma_var, term ');
> result_gamma_var :=
solve(term=0,gamma_var);
> psi := subs(alpha=result_alpha[2],E=result_E,beta
=
> result_beta,gamma_var=
result_gamma_var,psi);

```

$$\psi := (x^4 + \beta x^2 + \text{gamma_var}) e^{-\alpha x^2}$$

$$H_psi_minus_E := -\frac{6x^2}{e^{(\alpha x^2)}} - \frac{\beta}{e^{(\alpha x^2)}} + \frac{9\alpha x^4}{e^{(\alpha x^2)}} + \frac{5\alpha x^2\beta}{e^{(\alpha x^2)}} + \frac{\alpha \text{gamma_var}}{e^{(\alpha x^2)}} \\ - \frac{2\alpha^2 x^6}{e^{(\alpha x^2)}} - \frac{2\alpha^2 x^4\beta}{e^{(\alpha x^2)}} - \frac{2\alpha^2 x^2 \text{gamma_var}}{e^{(\alpha x^2)}} + \frac{1}{2} \frac{x^6}{e^{(\alpha x^2)}} + \frac{1}{2} \frac{x^4\beta}{e^{(\alpha x^2)}} \\ + \frac{1}{2} \frac{x^2 \text{gamma_var}}{e^{(\alpha x^2)}} - \frac{E x^4}{e^{(\alpha x^2)}} - \frac{E\beta x^2}{e^{(\alpha x^2)}} - \frac{E \text{gamma_var}}{e^{(\alpha x^2)}}$$

$$\text{term} := \left(\frac{1}{2} - 2\alpha^2\right) x^6 + \left(9\alpha + \frac{1}{2}\beta - 2\alpha^2\beta - E\right) x^4 \\ + \left(\frac{\text{gamma_var}}{2} + 5\alpha\beta - 6 - 2\alpha^2 \text{gamma_var} - E\beta\right) x^2 - E \text{gamma_var} - \beta \\ + \alpha \text{gamma_var}$$

$$t6 := \frac{1}{2} - 2\alpha^2$$

$$\text{result_alpha} := \frac{-1}{2}, \frac{1}{2}$$

$$\text{term} := \left(\frac{9}{2} - E\right) x^4 + \left(\frac{5}{2}\beta - 6 - E\beta\right) x^2 - E \text{gamma_var} - \beta + \frac{\text{gamma_var}}{2}$$

$$H_psi_minus_E := -\frac{6x^2}{e^{(\frac{x^2}{2})}} - \frac{\beta}{e^{(\frac{x^2}{2})}} + \frac{9}{2} \frac{x^4}{e^{(\frac{x^2}{2})}} + \frac{5}{2} \frac{x^2\beta}{e^{(\frac{x^2}{2})}} + \frac{1}{2} \frac{\text{gamma_var}}{e^{(\frac{x^2}{2})}} - \frac{E x^4}{e^{(\frac{x^2}{2})}} - \frac{E\beta x^2}{e^{(\frac{x^2}{2})}} \\ - \frac{E \text{gamma_var}}{e^{(\frac{x^2}{2})}}$$

attempting the next term

$$\text{term} := \left(\frac{9}{2} - E\right) x^4 + \left(\frac{5}{2}\beta - 6 - E\beta\right) x^2 - E \text{gamma_var} - \beta + \frac{\text{gamma_var}}{2}$$

$$t4 := \frac{9}{2} - E$$

$$\text{result_E} := \frac{9}{2}$$

$$\text{term} := (-2\beta - 6) x^2 - 4 \text{gamma_var} - \beta$$

$$H_psi_minus_E := -\frac{6x^2}{e^{(\frac{x^2}{2})}} - \frac{\beta}{e^{(\frac{x^2}{2})}} - \frac{2x^2\beta}{e^{(\frac{x^2}{2})}} - \frac{4 \text{gamma_var}}{e^{(\frac{x^2}{2})}}$$

Notice that we were forced to choose the second root here, rather than our previous first root choice. Symbollic

calculations sometimes have a mind of their own.

$$term := (-2\beta - 6)x^2 - 4\gamma - \beta$$

$$t2 := -2\beta - 6$$

$$result_beta := -3$$

$$term := 3 - 4\gamma$$

final, γ , term

$$result_gamma := \frac{3}{4}$$

$$\psi := (x^4 - 3x^2 + \frac{3}{4})e^{(-\frac{x^2}{2})}$$

This last result, the interpreted wave function with constants shown, is a variant on the textbook form, and shows that indeed the Hermite polynomial multiplied by

an appropriate exponential, is the desired eigenfunction.

All's well in the world.

[1] Sad to say, γ is a variable internal to Maple, so we need to define something which won't be handled improperly by

Maple.