Zeeman effect
Masatsugu Sei Suzuki
Department of Physics, SUNY at Binghamton
(Date: March 16, 2014)

We discuss the exact solution for the Zeeman effect using the Kronecker product

The Hamiltonian is given by

$$H = \frac{\xi\hbar^2}{2}\frac{1}{\hbar^2}(L_x \otimes S_x + L_y \otimes S_y + L_z \otimes S_z) + \mu_B B \frac{1}{\hbar}(L_z \otimes I_2 + 2I_3 \otimes S_z)$$

where

$$S_x = \frac{\hbar}{2}\sigma_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad S_y = \frac{\hbar}{2}\sigma_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad S_z = \frac{\hbar}{2}\sigma_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

$$L_x = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \qquad L_y = \frac{i\hbar}{\sqrt{2}}\begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, \qquad L_z = \hbar\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

The magnitude of the spin-orbit coupling and the Zeeman energy for atom with Z

$$A_{SO} = \frac{\xi\hbar^2}{2} = \frac{Ze^2\hbar^2}{4m_e c^2}\left\langle r^{-3}\right\rangle_{av}$$

$$A_Z = \mu_B B = \frac{e\hbar B}{2m_e c}$$

where

$$\left\langle r^{-3}\right\rangle = \frac{Z^3}{n^3 a_B{}^3 l(l+1/2)(l+1)}$$

$$
\begin{aligned}
A_{so} &= \frac{\xi\hbar^2}{2} = \frac{Ze^2\hbar^2}{4m_e c^2}\left\langle r^{-3}\right\rangle \\
&= \frac{Ze^2\hbar^2}{4m_e c^2}\frac{Z^3}{n^3 a_B{}^3 l(l+1/2)(l+1)} \\
&= \frac{Z^4 e^2\hbar^2}{4m_e c^2 a_B{}^3}\frac{1}{n^3 l(l+1/2)(l+1)} \\
&= \frac{m_e c^2}{4}\alpha^4 \frac{Z^4}{n^3 l(l+1/2)(l+1)}
\end{aligned}
$$

where

$$
a_B = \frac{\hbar^2}{m_e e^2}\,, \qquad \alpha = \frac{e^2}{\hbar c}
$$

The ratio is given by

$$
\begin{aligned}
k &= \frac{A_Z}{A_{SO}} \\
&= \frac{\dfrac{e\hbar}{2m_e c}}{\dfrac{1}{4}m_e c^2\alpha^4}\frac{n^3 l(l+1/2)(l+1)B(Oe)}{Z^4} \\
&= 1.59784\times 10^{-5}\,\frac{n^3 l(l+1/2)(l+1)B(Oe)}{Z^4}
\end{aligned}
$$

where

$$
\frac{1}{4}m_e c^2\alpha^4 = 5.8041\times 10^{-16} \qquad \text{[erg]}
$$

$$
\mu_B = \frac{e\hbar}{2m_e c} = 9.27403\times 10^{-21} \quad \text{[emu=erg/Oe]}, \qquad\qquad 1\text{T} = 10^4 \text{ Oe.}
$$

We have the ratio k as

$$\begin{aligned} k &= \frac{A_Z}{A_{SO}} \\ &= \frac{1.59784\times 10^{-5}}{Z^4} n^3 l(l+1/2)(l+1)B(Oe) \\ &= \frac{1.59784\times 10^{-1}}{Z^4} n^3 l(l+1/2)(l+1)B(T) \end{aligned}$$

Note that

$$k = 1$$

at the characteristic field,

$$B = B_0 = 6.25845\frac{Z^4}{n^3 l(l+1/2)(l+1)} \text{ [T]}$$

For Na (Z = 11, n = 3, l = 1)

$$B_0 = 1131.23 \text{ T.}$$

((**Examnple-2**))

For H (Z = 1. l = 1, n = 2),

$$k = 3.83482\ B[\mathrm{T}]$$

For Na (Z = 11. l = 1, n = 3),

$$k = 8.83991\times 10^{-4} B(T)$$

We use the matrices

$$S_x = \frac{\hbar}{2}\sigma_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad S_y = \frac{\hbar}{2}\sigma_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad S_z = \frac{\hbar}{2}\sigma_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

$$L_x = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \qquad L_y = \frac{i\hbar}{\sqrt{2}}\begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, \qquad L_z = \hbar\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

For simplicity we use the unit of $\hbar = 1$. The the Hamiltonian is obtained as

$$H = \begin{pmatrix} \frac{a}{2} + 2b & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{a}{2} & \frac{a}{\sqrt{2}} & 0 & 0 & 0 \\ 0 & \frac{a}{\sqrt{2}} & b & 0 & 0 & 0 \\ 0 & 0 & 0 & -b & \frac{a}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & \frac{a}{\sqrt{2}} & -\frac{a}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{a}{2} - 2b \end{pmatrix}$$

where

$a = A_{SO}$, $\qquad b = A_Z$

Eigenvalues	Eigen vectors:
$\frac{1}{2}(a - 4b)$,	$\{0,0,0,0,0,1\}$
$\frac{1}{2}(a + 4b)$	$\{1,0,0,0,0,0\}$
$\frac{1}{4}(-a - 2b - \sqrt{9a^2 - 4ab + 4b^2})$	$\{0,0,0,\frac{a - 2b - \sqrt{9a^2 - 4ab + 4b^2}}{2\sqrt{2}a},1,0\}$
$\frac{1}{4}(-a - 2b + \sqrt{9a^2 - 4ab + 4b^2})$	$\{0,0,0,\frac{a - 2b + \sqrt{9a^2 - 4ab + 4b^2}}{2\sqrt{2}a},1,0\}$
$\frac{1}{4}(-a + 2b - \sqrt{9a^2 + 4ab + 4b^2})$	$\{0,\frac{-a - 2b - \sqrt{9a^2 + 4ab + 4b^2}}{2\sqrt{2}a},1,0,0,0\}$

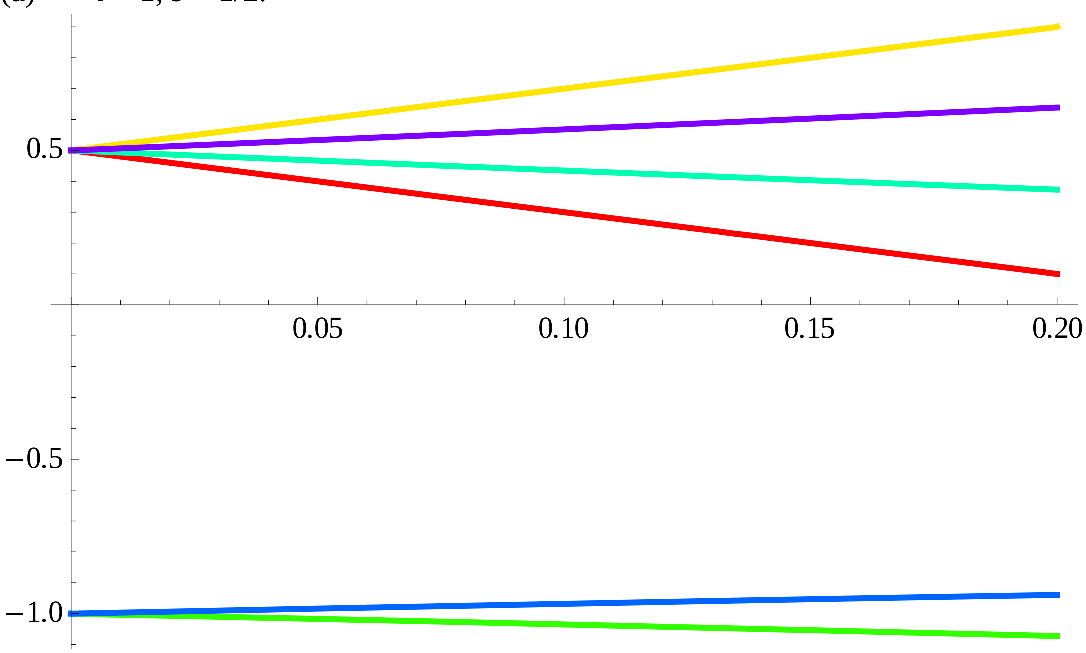
$$\frac{1}{4}(-a+2b+\sqrt{9a^2+4ab+4b^2}) \qquad \{0,\frac{-a-2b+\sqrt{9a^2+4ab+4b^2}}{2\sqrt{2}a},1,0,0,0\}$$

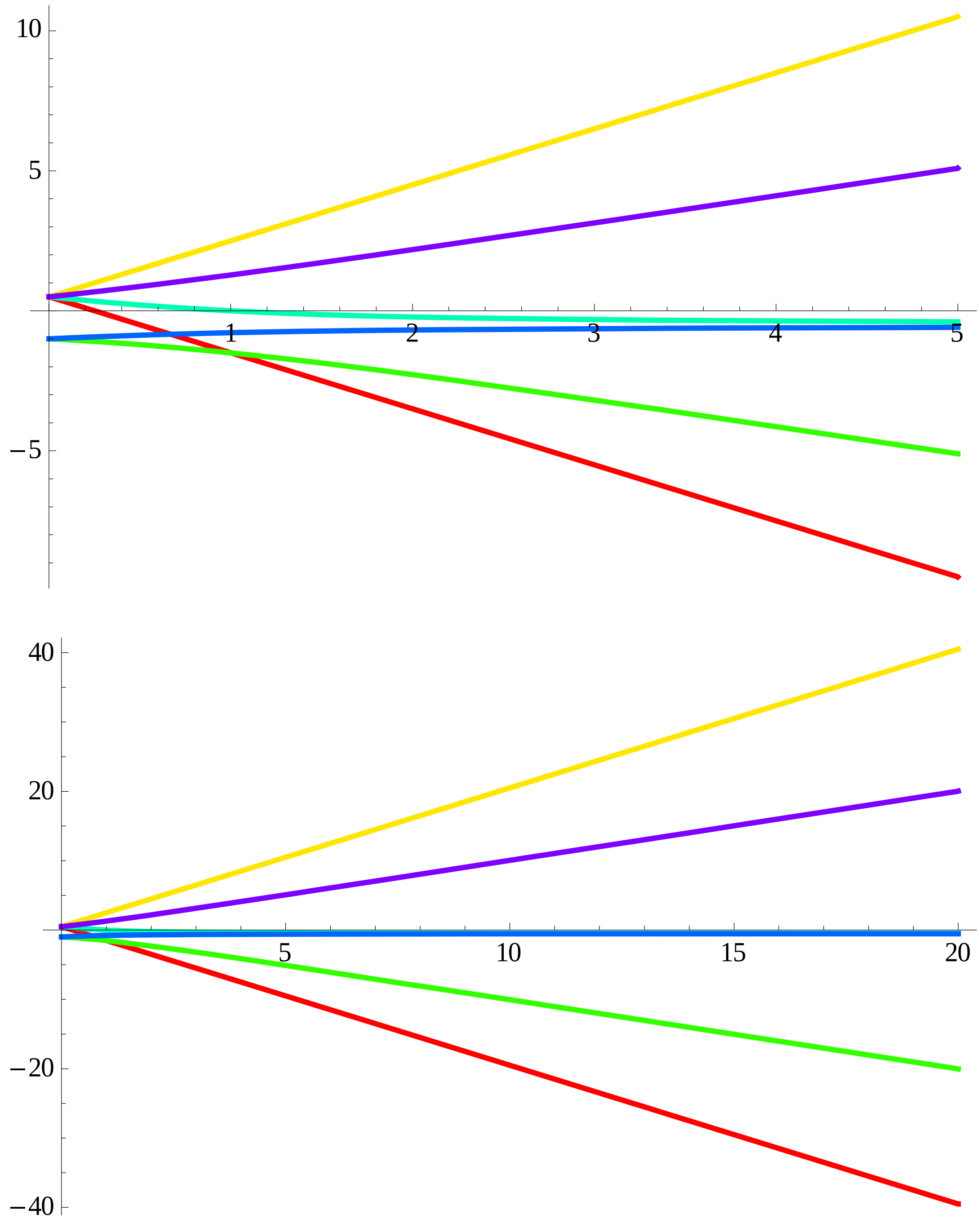
Suppose that

$$\frac{H}{\frac{A_{SO}}{\hbar^2}}=(L_x\otimes S_x+L_y\otimes S_y+L_z\otimes S_z)+k(L_z\otimes I_2+I_3\otimes S_z)$$

We make a plot of the eigenvalue as a function of *k*, where k is proportional to the magnetic field.

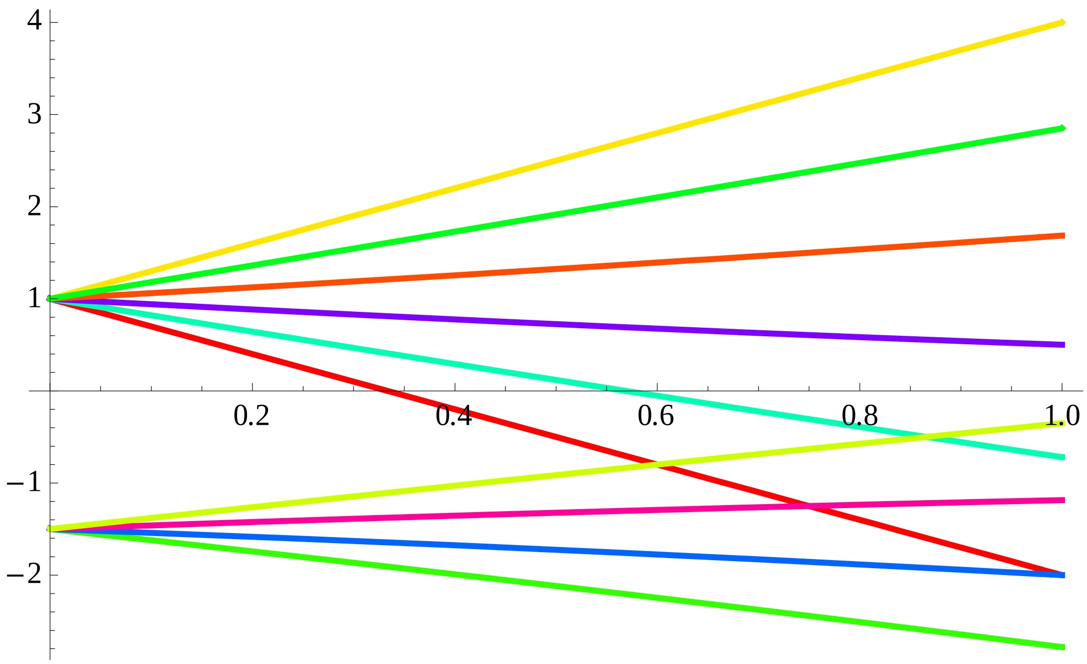
(a) $l = 1$, $s = 1/2$.





(b) $l = 2, s = 1/2$

Out[47]=



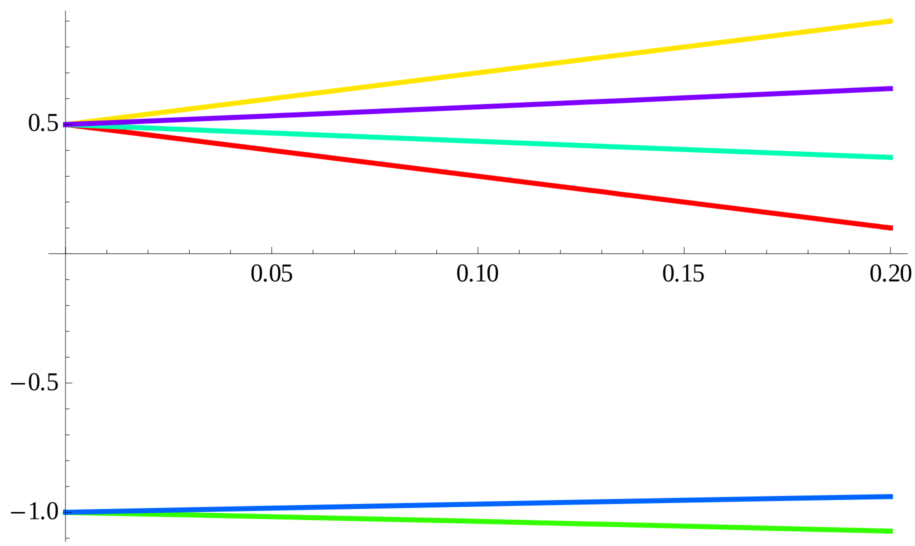
((**Mathematica**))

```
Clear["Global`*"]; L = 1; ℏ = 1; S = 1 / 2;
exp_* := exp /. {Complex[re_, im_] ⧴ Complex[re, -im]}; ψ1 = {{1}, {0}};
ψ2 = {{0}, {1}}; ϕ1 = {{1}, {0}, {0}}; ϕ2 = {{0}, {1}, {0}}; ϕ3 = {{0}, {0}, {1}}; I3 = IdentityMatrix[3];
I2 = IdentityMatrix[2]; j = 1;
Jx[j_, n_, m_] := ℏ/2 Sqrt[(j - m) (j + m + 1)] KroneckerDelta[n, m + 1] +
   ℏ/2 Sqrt[(j + m) (j - m + 1)] KroneckerDelta[n, m - 1];
Jy[j_, n_, m_] := -ℏ/2 ⅈ Sqrt[(j - m) (j + m + 1)] KroneckerDelta[n, m + 1] +
   ℏ/2 ⅈ Sqrt[(j + m) (j - m + 1)] KroneckerDelta[n, m - 1];
Jz[j_, n_, m_] := ℏ m KroneckerDelta[n, m];
Lx = Table[Jx[j, n, m], {n, j, -j, -1}, {m, j, -j, -1}];
Ly = Table[Jy[j, n, m], {n, j, -j, -1}, {m, j, -j, -1}];
Lz = Table[Jz[j, n, m], {n, j, -j, -1}, {m, j, -j, -1}];
Sx = ℏ/2 PauliMatrix[1]; Sy = ℏ/2 PauliMatrix[2];
Sz = ℏ/2 PauliMatrix[3];
```

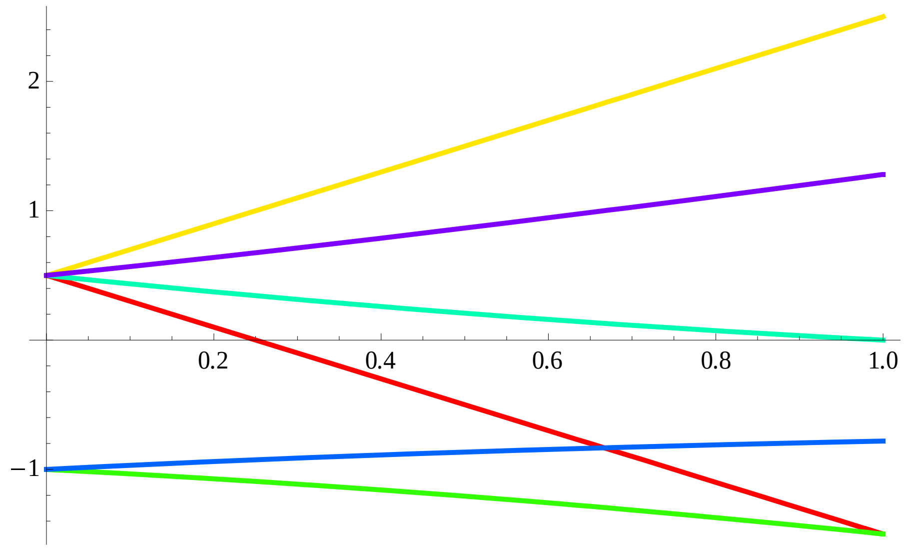
```
ES[α_, β_] := Module[{α1, β1, A1, eq1}, α1 = α; β1 = β;
   A1 = α1 (KroneckerProduct[Lx, Sx] + KroneckerProduct[Ly, Sy] +
        +KroneckerProduct[Lz, Sz]) +
     β 1 (KroneckerProduct[Lz, I2] + 2 KroneckerProduct[I3, Sz]);
   eq1 = Eigensystem[A1] // Simplify; s1 = eq1[[1]]];

p1 = ES[1, k];

p1
```

$$\left\{\frac{1}{2} - 2\,k,\ \frac{1}{2} + 2\,k,\ \frac{1}{4}\left(-1 - 2\,k - \sqrt{9 - 4\,k + 4\,k^2}\right),\ \frac{1}{4}\left(-1 - 2\,k + \sqrt{9 - 4\,k + 4\,k^2}\right),\ \frac{1}{4}\left(-1 + 2\,k - \sqrt{9 + 4\,k + 4\,k^2}\right),\ \frac{1}{4}\left(-1 + 2\,k + \sqrt{9 + 4\,k + 4\,k^2}\right)\right\}$$

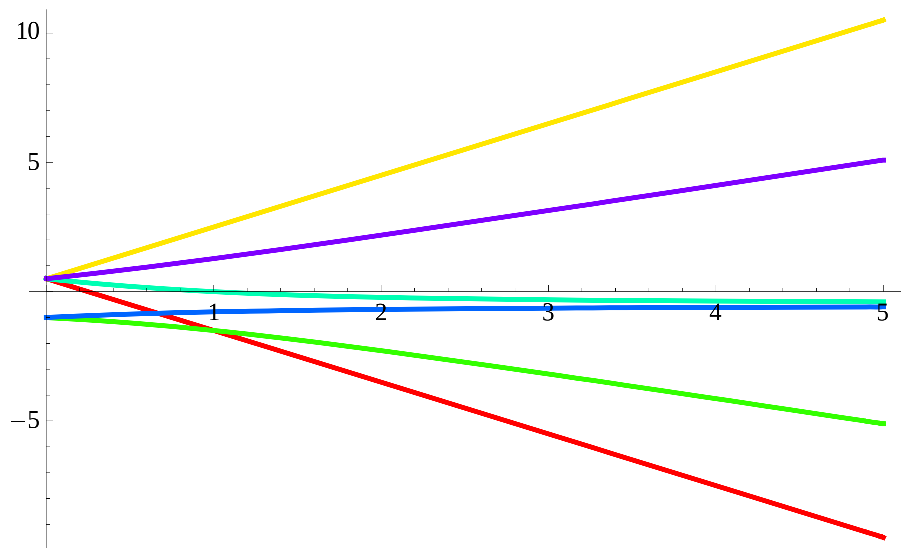
```
Plot[p1, {k, 0, 0.2},
 PlotStyle → Table[{Hue[0.15 i], Thick}, {i, 0, 10}]]
```



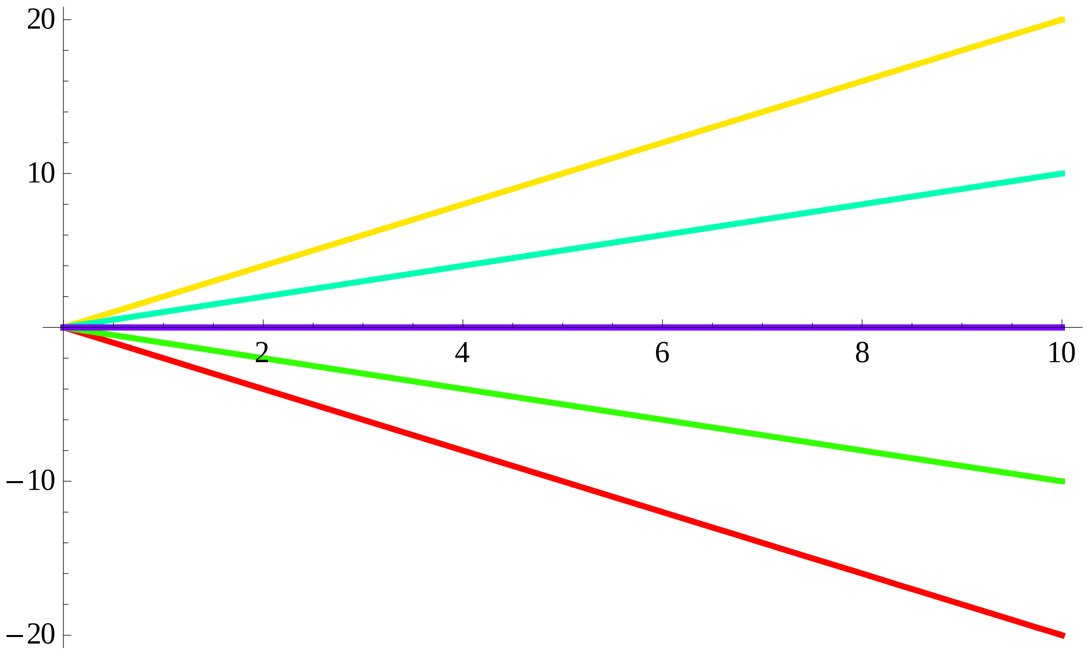
```
Plot[p1, {k, 0, 1}, PlotStyle → Table[{Hue[0.15 i], Thick}, {i, 0, 10}]]
```




```
Plot[p1, {k, 0, 5}, PlotStyle → Table[{Hue[0.15 i], Thick}, {i, 0, 10}]]
```



```
p2 = ES[0, k];
Plot[p2, {k, 0, 10},
 PlotStyle → Table[{Hue[0.15 i], Thick}, {i, 0, 10}]]
```




```
KroneckerProduct[ϕ1, ψ1] // MatrixForm
```

$$\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

---

k = 0.65

$$\left|\frac{3}{2},\frac{3}{2}\right\rangle$$

$$0.975 \left|\frac{1}{2},-\frac{1}{2}\right\rangle + 0.224 \left|\frac{3}{2},-\frac{1}{2}\right\rangle$$

$$-0.224 \left|\frac{1}{2},-\frac{1}{2}\right\rangle + 0.975 \left|\frac{3}{2},-\frac{1}{2}\right\rangle$$

$$0.985 \left|\frac{1}{2},\frac{1}{2}\right\rangle + 0.173 \left|\frac{3}{2},\frac{1}{2}\right\rangle$$

$$-0.173 \left|\frac{1}{2},\frac{1}{2}\right\rangle + 0.985 \left|\frac{3}{2},\frac{1}{2}\right\rangle$$

$$\left|\frac{3}{2},-\frac{3}{2}\right\rangle$$