

Sr

Sr1s[z_, r_] := 2 z^(3/2) Exp[-z r]

Sr2s[z_, r_] := 2 / Sqrt[3] z^(5/2) r Exp[-z r]

Sr3s[z_, r_] := 2^(3/2) / (3 Sqrt[5]) z^(7/2) r^2 Exp[-z r]

Sr4s[z_, r_] := 2 / (3 Sqrt[35]) z^(9/2) r^3 Exp[-z r]

Sr5s[z_, r_] := 2^(3/2) / (45 Sqrt[7]) z^(11/2) r^4 Exp[-z r]

Sr2p[z_, r_] := 2 / Sqrt[3] z^(5/2) r Exp[-z r]

General::spell1 : Possible spelling error: new symbol name "Sr2p" is similar to existing symbol "Sr2s".
More...

Sr3p[z_, r_] := 2^(3/2) / (3 Sqrt[5]) z^(7/2) r^2 Exp[-z r]

General::spell1 : Possible spelling error: new symbol name "Sr3p" is similar to existing symbol "Sr3s".
More...

Sr4p[z_, r_] := 2 / (3 Sqrt[35]) z^(9/2) r^3 Exp[-z r]

General::spell1 : Possible spelling error: new symbol name "Sr4p" is similar to existing symbol "Sr4s".
More...

Sr5p[z_, r_] := 2^(3/2) / (45 Sqrt[7]) z^(11/2) r^4 Exp[-z r]

General::spell1 : Possible spelling error: new symbol name "Sr5p" is similar to existing symbol "Sr5s".
More...

Sr3d[z_, r_] := 2^(3/2) / (3 Sqrt[5]) z^(7/2) r^2 Exp[-z r]

General::spell : Possible spelling error: new symbol name "Sr3d" is similar to existing symbols {Sr3p, Sr3s}. More...

Sr4d[z_, r_] := 2 / (3 Sqrt[35]) z^(9/2) r^3 Exp[-z r]

General::spell : Possible spelling error: new symbol name "Sr4d" is similar to existing symbols {Sr4p, Sr4s}. More...

Sk

Sk1s[z_, k_] := 1 / (2 Pi)^(3/2) 16 Pi z^(5/2) / (z^2 + k^2)^2

General::spell1 : Possible spelling error: new symbol name "Sk1s" is similar to existing symbol "Sr1s".
More...

Sk2s[z_, k_] := 1 / (2 Pi)^(3/2) 16 Pi z^(5/2) (3 z^2 - k^2) / (Sqrt[3] (z^2 + k^2)^3)

General::spell1 : Possible spelling error: new symbol name "Sk2s" is similar to existing symbol "Sr2s".
More...

Sk3s[z_, k_] := 1 / (2 Pi)^(3/2) 64 Sqrt[10] Pi z^(9/2) (z^2 - k^2) / (5 (z^2 + k^2)^4)

General::spell1 : Possible spelling error: new symbol name "Sk3s" is similar to existing symbol "Sr3s".
More...

Sk4s[z_, k_] :=

$$1 / (2 \text{ Pi})^{(3/2)} 64 \text{ Pi } z^{(9/2)} (5 z^4 - 10 z^2 k^2 + k^4) / (\text{Sqrt}[35] (z^2 + k^2)^5)$$

General::spell1 : Possible spelling error: new symbol name "Sk4s" is similar to existing symbol "Sr4s".
More...

Sk5s[z_, k_] := 1 / (2 Pi)^(3/2) 128 Sqrt[14]

$$\text{Pi } z^{(13/2)} (3 z^4 - 10 z^2 k^2 + 3 k^4) / (21 (z^2 + k^2)^6)$$

General::spell1 : Possible spelling error: new symbol name "Sk5s" is similar to existing symbol "Sr5s".
More...

Sk2p[z_, k_] := 1 / (2 Pi)^(3/2) 64 Pi k z^(7/2) / (Sqrt[3] (z^2 + k^2)^3)

General::spell : Possible spelling error: new symbol name "Sk2p" is similar to existing symbols {Sk2s, Sr2p}. More...

Sk3p[z_, k_] :=

$$1 / (2 \text{ Pi})^{(3/2)} 64 \text{ Sqrt}[10] \text{ Pi } k z^{(7/2)} (5 z^2 - k^2) / (15 (z^2 + k^2)^4)$$

General::spell : Possible spelling error: new symbol name "Sk3p" is similar to existing symbols {Sk3s, Sr3p}. More...

Sk4p[z_, k_] :=

$$1 / (2 \text{ Pi})^{(3/2)} 128 \text{ Pi } k z^{(11/2)} (5 z^2 - 3 k^2) / (\text{Sqrt}[35] (z^2 + k^2)^5)$$

General::spell : Possible spelling error: new symbol name "Sk4p" is similar to existing symbols {Sk4s, Sr4p}. More...

Sk5p[z_, k_] := 1 / (2 Pi)^(3/2) 128 Sqrt[14] Pi

$$k z^{(11/2)} (35 z^4 - 42 z^2 k^2 + 3 k^4) / (105 (z^2 + k^2)^6)$$

General::spell : Possible spelling error: new symbol name "Sk5p" is similar to existing symbols {Sk5s, Sr5p}. More...

Sk3d[z_, k_] := 1 / (2 Pi)^(3/2) 128 Sqrt[10] Pi k^2 z^(9/2) / (5 (z^2 + k^2)^4)

General::spell : Possible spelling error: new symbol name "Sk3d" is similar to existing symbols {Sk3p, Sk3s, Sr3d}. More...

Sk4d[z_, k_] :=

$$1 / (2 \text{ Pi})^{(3/2)} 128 \text{ Pi } k^2 z^{(9/2)} (7 z^2 - k^2) / (\text{Sqrt}[35] (z^2 + k^2)^5)$$

General::spell : Possible spelling error: new symbol name "Sk4d" is similar to existing symbols {Sk4p, Sk4s, Sr4d}. More...

R1s

$$\text{R1s} = 0.392290 \text{ Sr1s}[13.9074, r] + 0.425817 \text{ Sr1s}[8.2187, r] -$$

$$0.000702 \text{ Sr3s}[26.0325, r] + 0.217206 \text{ Sr2s}[11.9249, r] +$$

$$0.002300 \text{ Sr2s}[4.2635, r] + 0.000463 \text{ Sr2s}[2.8357, r] + 0.000147 \text{ Sr2s}[2.0715, r]$$

$$40.6917 e^{-13.9074 r} + 20.0659 e^{-8.2187 r} + 123.162 e^{-11.9249 r} r + 0.0996811 e^{-4.2635 r} r +$$

$$0.00723937 e^{-2.8357 r} r + 0.00104833 e^{-2.0715 r} r - 26.6429 e^{-26.0325 r} r^2$$

NIntegrate[R1s^2 r^2, {r, 0, Infinity}]

1.

R2s

$$\begin{aligned}
 R2s = & -0.053023 \text{ Sr1s}[13.9074, r] + 0.419502 \text{ Sr1s}[8.2187, r] - \\
 & 0.000263 \text{ Sr3s}[26.0325, r] - 0.055723 \text{ Sr2s}[11.9249, r] - \\
 & 0.349457 \text{ Sr2s}[4.2635, r] - 0.523070 \text{ Sr2s}[2.8357, r] - 0.246038 \text{ Sr2s}[2.0715, r] \\
 & -5.50001 e^{-13.9074 r} + 19.7683 e^{-8.2187 r} - 31.5966 e^{-11.9249 r} r - \\
 & 15.1453 e^{-4.2635 r} r - 8.17862 e^{-2.8357 r} r - 1.75462 e^{-2.0715 r} r - 9.9816 e^{-26.0325 r} r^2
 \end{aligned}$$

NIntegrate[R2s^2 r^2, {r, 0, Infinity}]

1.

R2p

$$\begin{aligned}
 R2p = & 0.004391 \text{ Sr2p}[12.3239, r] + 0.133955 \text{ Sr2p}[5.6525, r] + \\
 & 0.342978 \text{ Sr2p}[3.5570, r] + 0.395742 \text{ Sr2p}[2.2056, r] + 0.221831 \text{ Sr2p}[1.4948, r] \\
 & 2.70336 e^{-12.3239 r} r + 11.7498 e^{-5.6525 r} r + \\
 & 9.45029 e^{-3.557 r} r + 3.3014 e^{-2.2056 r} r + 0.69976 e^{-1.4948 r} r
 \end{aligned}$$

NIntegrate[R2p^2 r^2, {r, 0, Infinity}]

1.

pr

$$pr = 1 / (4 \text{ Pi } 10) (2 R1s^2 + 2 R2s^2 + 6 R2p^2)$$

$$\begin{aligned}
 & \frac{1}{40 \pi} \left(6 \left(2.70336 e^{-12.3239 r} r + 11.7498 e^{-5.6525 r} r + \right. \right. \\
 & \quad \left. \left. 9.45029 e^{-3.557 r} r + 3.3014 e^{-2.2056 r} r + 0.69976 e^{-1.4948 r} r \right)^2 + \right. \\
 & \quad \left. 2 \left(40.6917 e^{-13.9074 r} + 20.0659 e^{-8.2187 r} + 123.162 e^{-11.9249 r} r + 0.0996811 e^{-4.2635 r} r + \right. \right. \\
 & \quad \left. \left. 0.00723937 e^{-2.8357 r} r + 0.00104833 e^{-2.0715 r} r - 26.6429 e^{-26.0325 r} r^2 \right)^2 + \right. \\
 & \quad \left. 2 \left(-5.50001 e^{-13.9074 r} + 19.7683 e^{-8.2187 r} - 31.5966 e^{-11.9249 r} r - 15.1453 e^{-4.2635 r} r - \right. \right. \\
 & \quad \left. \left. 8.17862 e^{-2.8357 r} r - 1.75462 e^{-2.0715 r} r - 9.9816 e^{-26.0325 r} r^2 \right)^2 \right)
 \end{aligned}$$

4 Pi NIntegrate[pr r^2, {r, 0, Infinity}]

1.

SrNe = -4 Pi NIntegrate[pr Log[pr] r^2, {r, 0, Infinity}]

2.05514

K1s

$$\begin{aligned}
K1s = & 0.392290 \text{ Sk1s}[13.9074, k] + 0.425817 \text{ Sk1s}[8.2187, k] - \\
& 0.000702 \text{ Sk3s}[26.0325, k] + 0.217206 \text{ Sk2s}[11.9249, k] + \\
& 0.002300 \text{ Sk2s}[4.2635, k] + 0.000463 \text{ Sk2s}[2.8357, k] + 0.000147 \text{ Sk2s}[2.0715, k] \\
& \frac{0.0016729 (12.8733 - k^2)}{(4.29111 + k^2)^3} + \frac{0.0115524 (24.1236 - k^2)}{(8.04119 + k^2)^3} + \frac{0.159068 (54.5323 - k^2)}{(18.1774 + k^2)^3} + \\
& \frac{263.167}{(67.547 + k^2)^2} + \frac{196.539 (426.61 - k^2)}{(142.203 + k^2)^3} + \frac{903.072}{(193.416 + k^2)^2} - \frac{13281.5 (677.691 - k^2)}{(677.691 + k^2)^4}
\end{aligned}$$

NIntegrate[K1s^2 k^2, {k, 0, Infinity}]

1.

K2s

$$\begin{aligned}
K2s = & -0.053023 \text{ Sk1s}[13.9074, k] + 0.419502 \text{ Sk1s}[8.2187, k] - \\
& 0.000263 \text{ Sk3s}[26.0325, k] - 0.055723 \text{ Sk2s}[11.9249, k] - \\
& 0.349457 \text{ Sk2s}[4.2635, k] - 0.523070 \text{ Sk2s}[2.8357, k] - 0.246038 \text{ Sk2s}[2.0715, k] \\
& - \frac{2.79997 (12.8733 - k^2)}{(4.29111 + k^2)^3} - \frac{13.0512 (24.1236 - k^2)}{(8.04119 + k^2)^3} - \frac{24.1685 (54.5323 - k^2)}{(18.1774 + k^2)^3} + \\
& \frac{259.264}{(67.547 + k^2)^2} - \frac{50.4209 (426.61 - k^2)}{(142.203 + k^2)^3} - \frac{122.062}{(193.416 + k^2)^2} - \frac{4975.85 (677.691 - k^2)}{(677.691 + k^2)^4}
\end{aligned}$$

NIntegrate[K2s^2 k^2, {k, 0, Infinity}]

1.

K2p

$$\begin{aligned}
K2p = & 0.004391 \text{ Sk2p}[12.3239, k] + 0.133955 \text{ Sk2p}[5.6525, k] + \\
& 0.342978 \text{ Sk2p}[3.5570, k] + 0.395742 \text{ Sk2p}[2.2056, k] + 0.221831 \text{ Sk2p}[1.4948, k] \\
& \frac{6.67671 k}{(2.23443 + k^2)^3} + \frac{46.4788 k}{(4.86467 + k^2)^3} + \frac{214.565 k}{(12.6522 + k^2)^3} + \frac{423.936 k}{(31.9508 + k^2)^3} + \frac{212.658 k}{(151.879 + k^2)^3}
\end{aligned}$$

NIntegrate[K2p^2 k^2, {k, 0, Infinity}]

1.

nk

$$nk = 1 / (4 \text{ Pi } 10) (2 K1s^2 + 2 K2s^2 + 6 K2p^2)$$

$$\frac{1}{40 \pi}$$

$$\left(6 \left(\frac{6.67671 k}{(2.23443 + k^2)^3} + \frac{46.4788 k}{(4.86467 + k^2)^3} + \frac{214.565 k}{(12.6522 + k^2)^3} + \frac{423.936 k}{(31.9508 + k^2)^3} + \frac{212.658 k}{(151.879 + k^2)^3} \right)^2 + \right. \\ \left. 2 \left(\frac{0.0016729 (12.8733 - k^2)}{(4.29111 + k^2)^3} + \frac{0.0115524 (24.1236 - k^2)}{(8.04119 + k^2)^3} + \frac{0.159068 (54.5323 - k^2)}{(18.1774 + k^2)^3} + \right. \right. \\ \left. \frac{263.167}{(67.547 + k^2)^2} + \frac{196.539 (426.61 - k^2)}{(142.203 + k^2)^3} + \frac{903.072}{(193.416 + k^2)^2} - \frac{13281.5 (677.691 - k^2)}{(677.691 + k^2)^4} \right)^2 + \\ \left. 2 \left(-\frac{2.79997 (12.8733 - k^2)}{(4.29111 + k^2)^3} - \frac{13.0512 (24.1236 - k^2)}{(8.04119 + k^2)^3} - \frac{24.1685 (54.5323 - k^2)}{(18.1774 + k^2)^3} + \right. \right. \\ \left. \frac{259.264}{(67.547 + k^2)^2} - \frac{50.4209 (426.61 - k^2)}{(142.203 + k^2)^3} - \frac{122.062}{(193.416 + k^2)^2} - \frac{4975.85 (677.691 - k^2)}{(677.691 + k^2)^4} \right)^2 \Bigg)$$

$$4 \text{ Pi } \text{NIntegrate}[nk \, k^2, \{k, 0, \text{Infinity}\}]$$

1.

$$\text{SkNe} = -4 \text{ Pi } \text{NIntegrate}[nk \text{ Log}[nk] \, k^2, \{k, 0, \text{Infinity}\}]$$

General::spell1 : Possible spelling error: new symbol name "SkNe" is similar to existing symbol "SrNe".
More...

6.43707

$$\text{SrNe} + \text{SkNe}$$

8.49221

Smax

$$r2 = 4 \text{ Pi } \text{NIntegrate}[pr \, r^4, \{r, 0, \text{Infinity}\}]$$

0.937183

$$k2 = 4 \text{ Pi } \text{NIntegrate}[nk \, k^4, \{k, 0, \text{Infinity}\}]$$

25.7094

$$\text{Smax} = 3 (1 + \text{Log}[\text{Pi}]) + 3 / 2 \text{ Log}[4 / 9 \, r2 \, k2]$$

9.99077

$$w = 1 - (\text{SrNe} + \text{SkNe}) / \text{Smax}$$

0.149994

$$Sr_{\max} = \frac{3}{2} (1 + \log[\pi]) + \frac{3}{2} \log\left[\frac{2}{3} r^2\right]$$

General::spell1 : Possible spelling error: new symbol name "Srmax" is similar to existing symbol "Smax".
More...

2.51158

$$w_r = 1 - S_{rNe} / S_{r\max}$$

0.181736

$$Sk_{\max} = \frac{3}{2} (1 + \log[\pi]) + \frac{3}{2} \log\left[\frac{2}{3} k^2\right]$$

General::spell : Possible spelling error: new symbol name "Skmax" is similar to existing symbols
{Smax, Srmax}. More...

7.47918

$$w_k = 1 - S_{kNe} / S_{k\max}$$

0.139336

Oniscu

$$E_r = 4 \pi \text{NIntegrate}[pr^2 r^2, \{r, 0, \text{Infinity}\}]$$

1.70169

$$E_k = 4 \pi \text{NIntegrate}[nk^2 k^2, \{k, 0, \text{Infinity}\}]$$

0.00780986

$$o_n = 1 / (E_r E_k)$$

75.2447

ionization

$$i_p = 21.564 / 27.212$$

0.792445

$$p_2 = (2 i_p)^{3/2} / \pi \exp[-2 (2 i_p)^{1/2} r]$$

0.635109 $e^{-2.51785 r}$

$$4 \pi \text{NIntegrate}[p_2 r^2, \{r, 0, \text{Infinity}\}]$$

1.

$$k_{ul} = 4 \pi \text{NIntegrate}[pr \log[pr / p_2] r^2, \{r, 0, \text{Infinity}\}] + \\ 4 \pi \text{NIntegrate}[p_2 \log[p_2 / pr] r^2, \{r, 0, \text{Infinity}\}]$$

0.638092

```
jen = -4 Pi NIntegrate[(pr + p2) / 2 Log[(pr + p2) / 2] r^2, {r, 0, Infinity}] +
  1 / 2 4 Pi NIntegrate[pr Log[pr] r^2, {r, 0, Infinity}] +
  1 / 2 4 Pi NIntegrate[p2 Log[p2] r^2, {r, 0, Infinity}]
```

```
0.0662634
```

```
thomas fermi
```

```
Z = 10
```

```
10
```

```
p3 = 2^(3 / 2) Z^(3 / 2) 1 / r^(3 / 2)
  1 / (3 Pi^2) (1 + (r Z^(1 / 3) / 4.6405)^0.772)^(-5.829) ;
```

```
cc = 4 Pi NIntegrate[p3 r^2, {r, 0, Infinity}];
```

```
p4 = 1 / cc p3;
```

```
4 Pi NIntegrate[p4 r^2, {r, 0, Infinity}]
```

```
1.
```

```
ku12 = 4 Pi NIntegrate[pr Log[pr / p4] r^2, {r, 0, 10^4}] +
  4 Pi NIntegrate[p4 Log[p4 / pr] r^2, {r, 0, 10^4}]
```

```
NIntegrate::ncvb : NIntegrate failed to converge to prescribed accuracy after 7 recursive bisections in r
near r = 0.3343450673324588`. More...
```

```
NIntegrate::ncvb : NIntegrate failed to converge to prescribed accuracy after 7 recursive bisections in r
near r = 0.3343450673324588`. More...
```

```
1.23455
```

```
jen2 = -4 Pi NIntegrate[(pr + p4) / 2 Log[(pr + p4) / 2] r^2, {r, 0, Infinity}] +
  1 / 2 4 Pi NIntegrate[pr Log[pr] r^2, {r, 0, Infinity}] +
  1 / 2 4 Pi NIntegrate[p4 Log[p4] r^2, {r, 0, Infinity}]
```

```
0.0611295
```