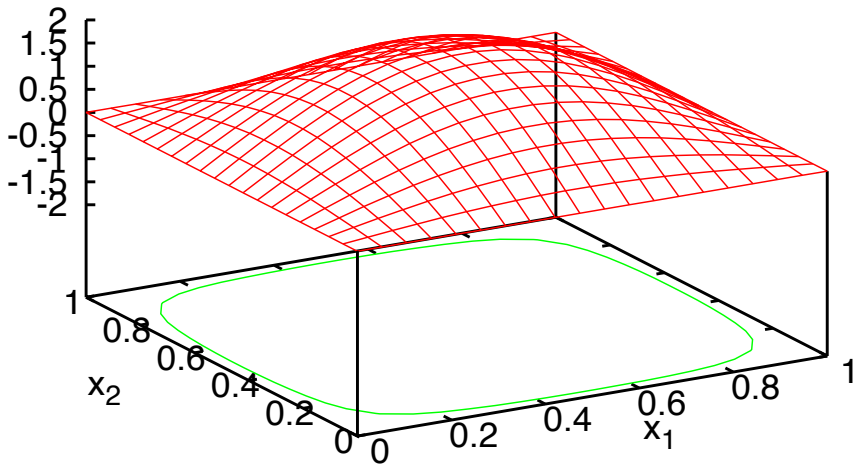
two particles in a box

n=1,1 S=0



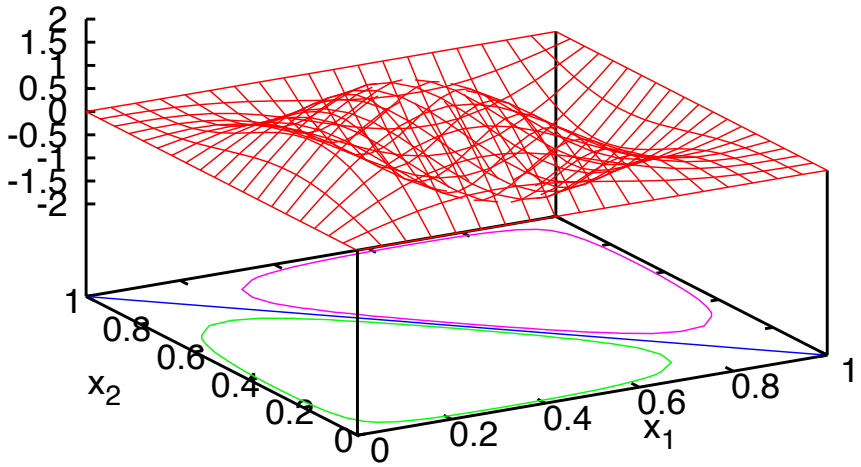
antisymmetric wave function:
small when electrons close
(diagonal $x_1=x_2$)

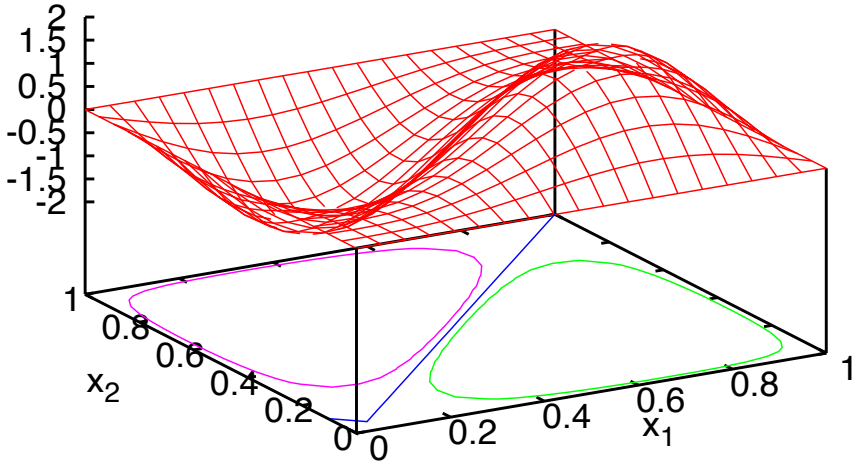
$$\Psi(r_1, r_2) = \frac{1}{\sqrt{2}} \left(\phi_a(r_1)\phi_b(r_2) + \phi_b(r_1)\phi_a(r_2)\right)$$

n=1,2 S=0

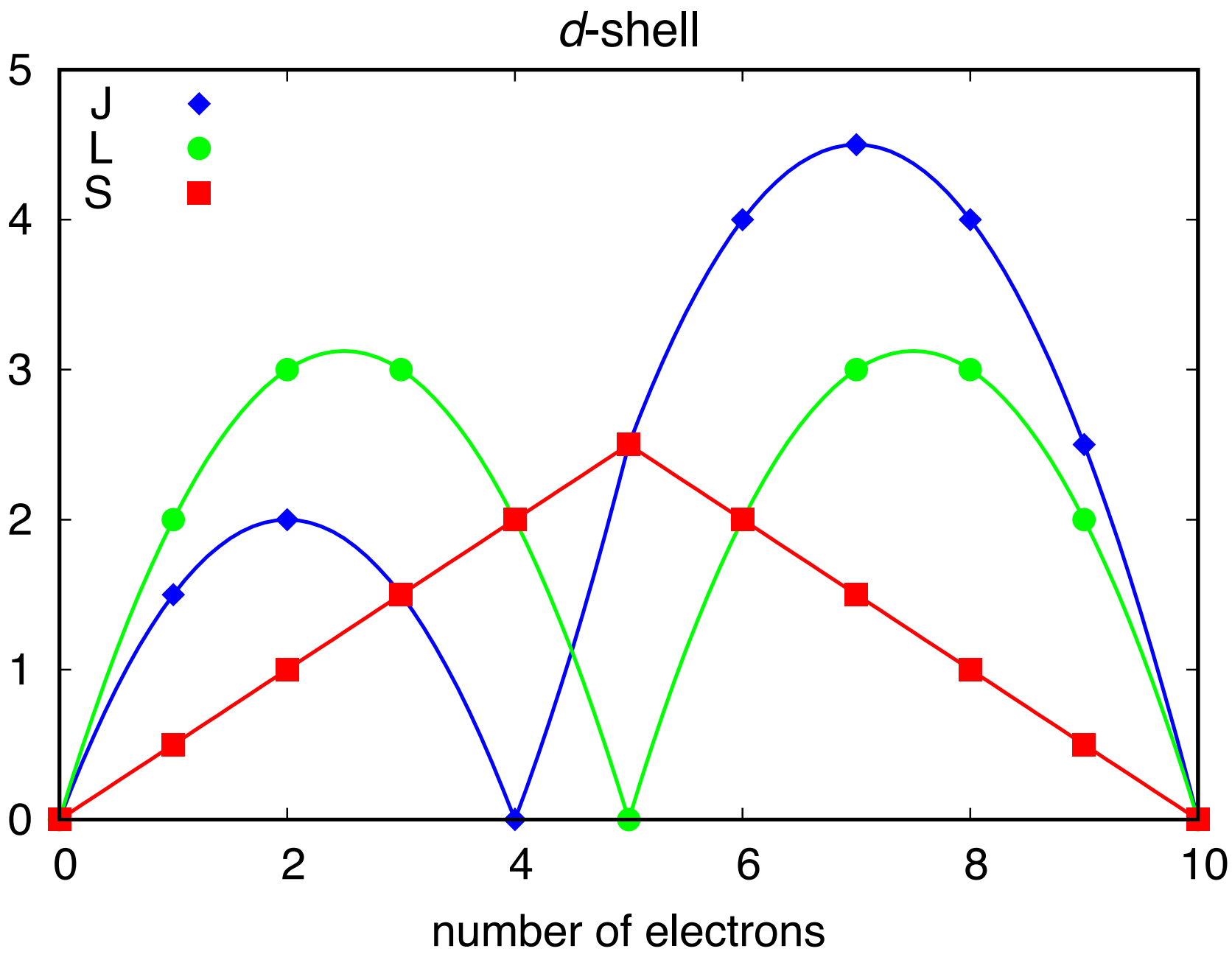
$$\Psi(r_1, r_2) = \frac{1}{\sqrt{2}} \left(\phi_a(r_1)\phi_b(r_2) - \phi_b(r_1)\phi_a(r_2)\right)$$

n=1,2 S=1





Hund's rules



possible multiplets for equivalent electrons

s			^{2}**S**		
p^1 or p^5			^{2}**P**		
p^2 or p^4	^1S ^1D			^{3}**P**	
p^3			^2P ^2D		^{4}**S**
d^1 or d^9			^{2}**D**		
d^2 or d^8	^1S ^1D ^1G			^3P ^{3}**F**	
d^3 or d^7			^2P ^2D ^2F ^2G ^2H		^4P ^{4}**F**
d^4 or d^6	^1S ^1D ^1F ^1G ^1I			^3P ^3D ^3F ^3G ^3H	^{5}**D**
d^5			^2S ^2P ^2D ^2F ^2G ^2H ^2I		^4P ^4D ^4F ^4G ^{6}**S**

Kramers pairs: $K_l^\dagger := \frac{1}{\sqrt{2l+1}} \sum_{m=-l}^{m} (-1)^m \, l_{m\uparrow}^\dagger l_{-m\downarrow}^\dagger$

add two electrons without changing *L, M, S, S_z*

need more operators for *f*-shell

d^4, d^6	2×^1S 2×^1D ^1F 2×^1G ^1I		2×^3P ^3D 2×^3F ^3G ^3H		^5D
d^5		^2S ^2P 3×^2D 2×^2F 2×^2G ^2H ^2I		^4P ^4D ^4F ^4G	
f^0, f^{14}	^1S				
f^1, f^{13}		^2F			
f^2, f^{12}	^1S ^1D ^1G ^1I		^3P ^3F ^3H		
f^3, f^{11}		^2P 2×?^2D 2×^2F 2×?^2G 2×?^2H ^2I ^2K ^2L		^4S ^4D ^4F ^4G ^4I	
f^4, f^{10}	2×^1S 4×^1D ^1F 4×^1G 2×^1H 3×^1I ^1K 2×?^1L ^1N		3×^3P 2×^3D 4×^3F 3×^3G 4×^3H 2×^3I 2×^3K ^3L ^3M		^5S ^5D ^5F ^5G ^5I
f^5, f^9		4×^2P 5×^2D 7×^2F 6×^2G 7×^2H 5×^2I 5×^2K 3×^2L 2×^2M ^2N ^2O		^4S 2×^4P 3×^4D 4×^4F 4×^4G 3×^4H 3×^4I 2×^4K ^4L ^4M	
f^6, f^8	4×^1S ^1P 6×^1D 4×^1F 8×^1G 4×^1H 7×^1I 3×^1K 4×^1L 2×^1M 2×^1N ^1Q		6×^3P 5×^3D 9×^3F 7×^3G 9×^3H 6×^3I 6×^3K 3×^3L 3×^3M ^3N ^3O		^5S ^5P 3×^5D 2×^5F 3×^5G
f^5		2×^2S 5×^2P 7×^2D 10×^2F 10×^2G 9×^2H 9×^2I 7×^2K 5×^2L 4×^2M 2×^2N ^2O ^2Q		2×^4S 2×^4P 6×^4D 5×^4F 7×^4G 5×^4H 5×^4I 3×^4K 3×^4L ^4M ^4N	

Because more than one multiplet of a given *L*, *S* may occur, some further differentiation of the multiplets is required. For this purpose we have followed consistently the classification scheme of Racah wherein additional quantum numbers, usually not of physical significance, are introduced by reference to the properties of certain mathematical groups. Specifically, the groups used are those denoted by R_5 in the case of the configuration d^n and by R_7 and G_2 for the configurations f^n. The so-called seniority quantum number is consistent with this scheme. Even with these additional quantum numbers, some duplications occur for f^n configurations, which were resolved arbitrarily by Racah in his work on the electrostatic energy of f^n configurations.

C.W. Nielson and G.F. Koster: Spectroscopic Coefficients for the p^n, d^n, and f^n Configurations (MIT Press, 1963)