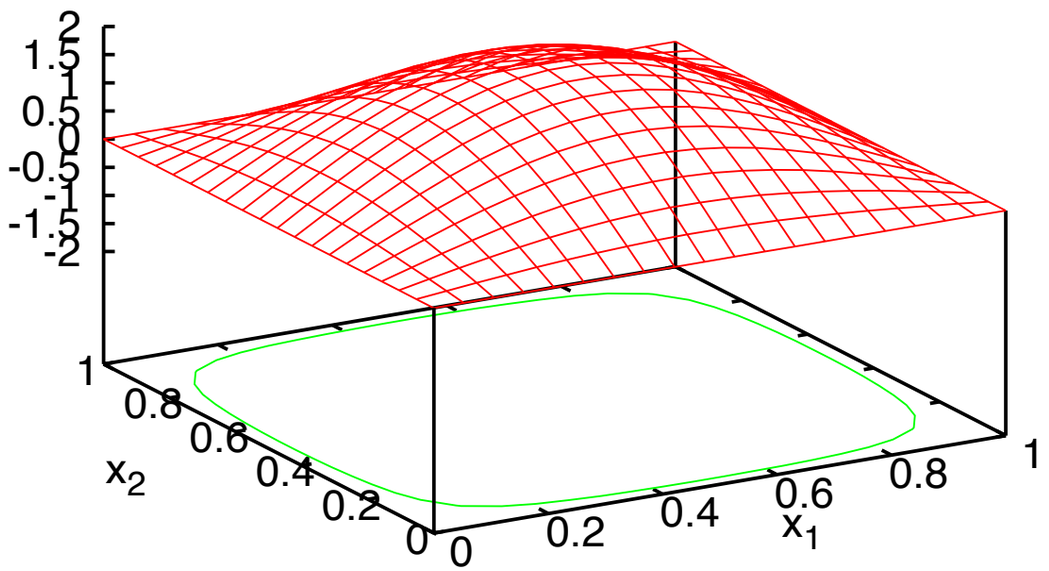
two particles in a box

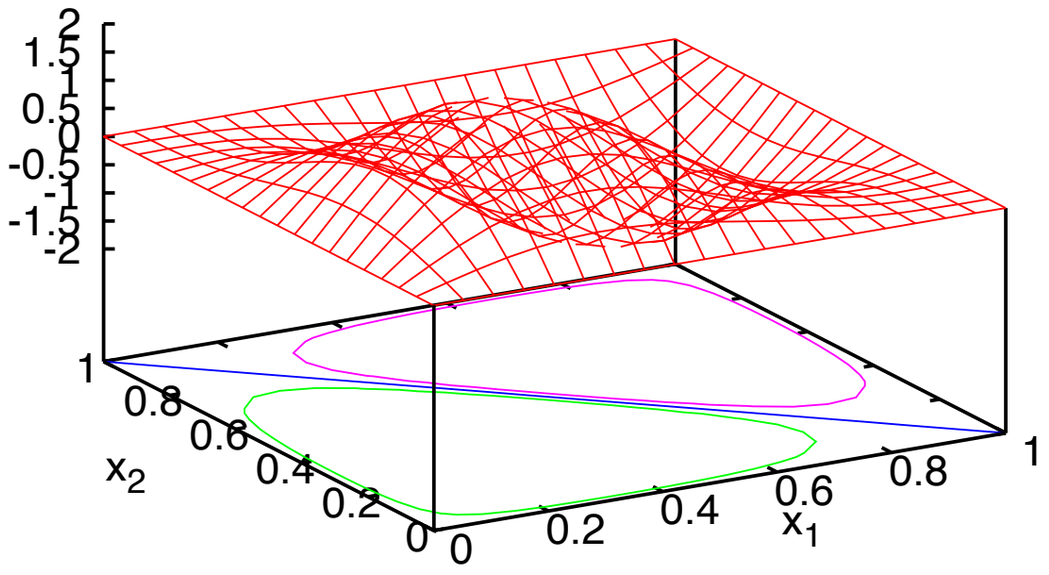
n=1,1 S=0



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

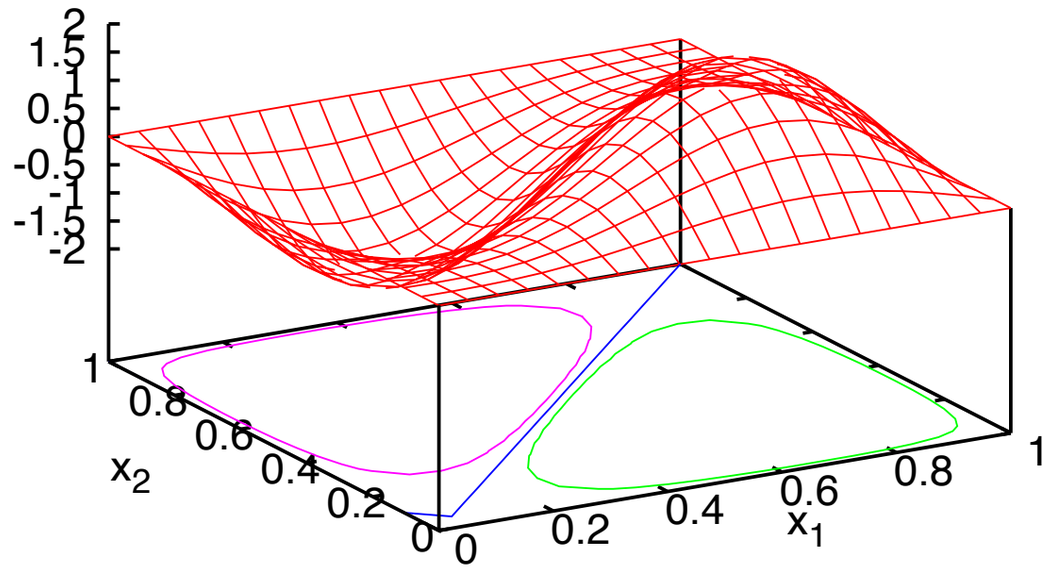
$$\Psi(r_1, r_2) = \frac{1}{\sqrt{2}} \left(\phi_a(r_1)\phi_b(r_2) + \phi_b(r_1)\phi_a(r_2)\right)$$

n=1,2 S=0

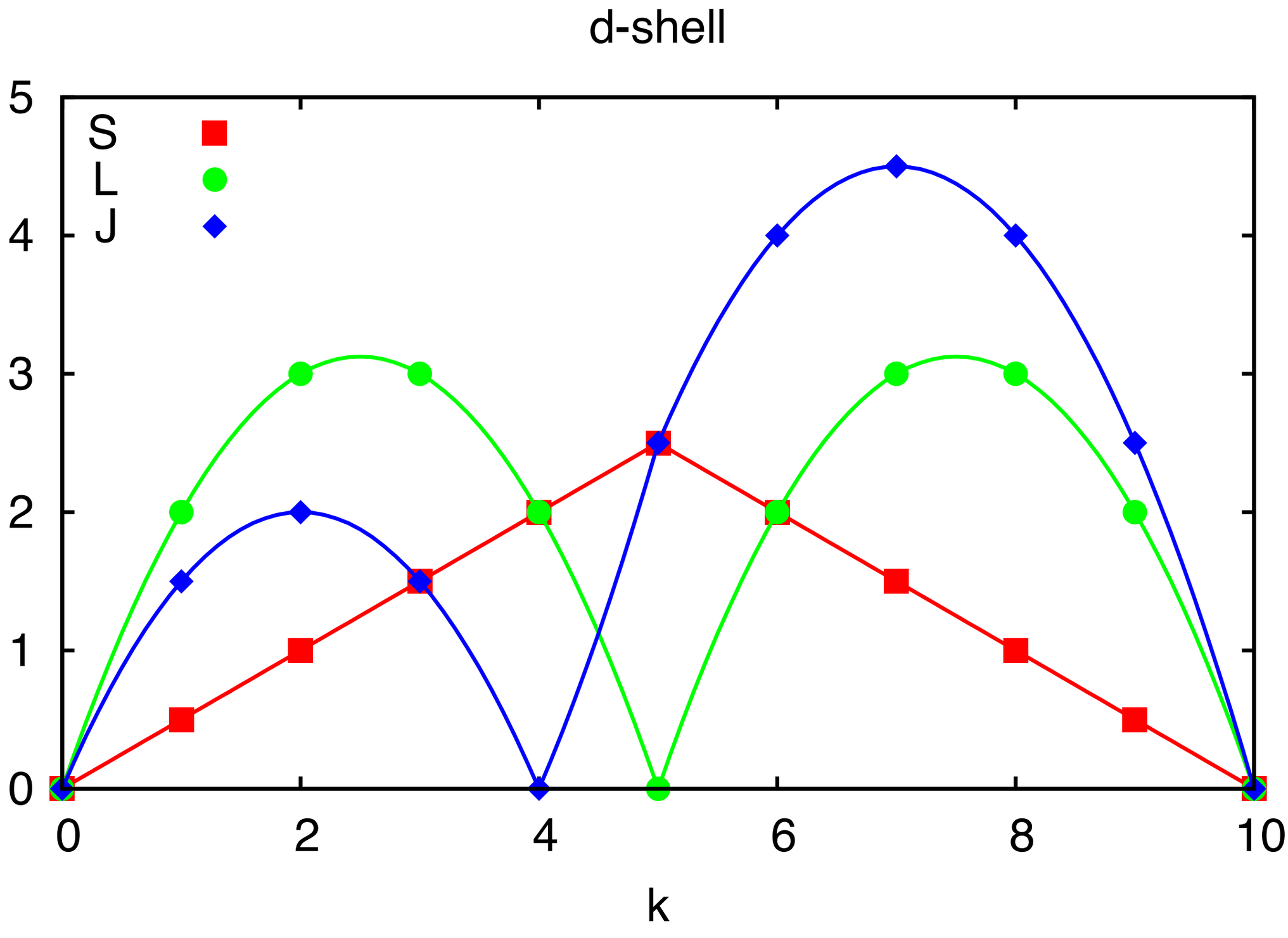


$$\Psi(r_1, r_2) = \frac{1}{\sqrt{2}} \left(\phi_a(r_1)\phi_b(r_2) - \phi_b(r_1)\phi_a(r_2)\right)$$

n=1,2 S=1



Hund's rules



possible multiplets for equivalent electrons

s														
p^1 or p^5														
p^2 or p^4														
p^3														
d^1 or d^9														
d^2 or d^8														
d^3 or d^7														
d^4 or d^6														
d^5														

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

closed shells: ^1S