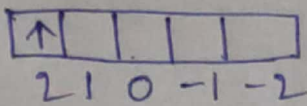
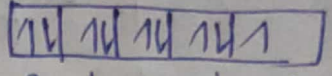
correlation and spin-orbit coupling in Free ions for First Series of Transition Metal :—

1. Sc^{2+} and Cu^{2+} (d^1, d^9)

d^1 — 

d^9 — 

Both have one unpaired electron.

d^1 - No. of microstates $= \binom{n}{r} = \frac{n!}{r!(n-r)!}$

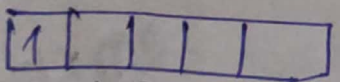
$n = 10, r = 1$ $= \binom{10}{1} = \frac{10!}{1!(10-1)!}$

$= \frac{10(9\times8\times7\times6\times5\times4\times3\times2\times1)}{1(9\times8\times7\times6\times5\times4\times3\times2\times1)}$

$= \frac{10}{1} = 10$

d^9 - No. of microstates $= 10$

Term symbol for d^1 —

d^1 — 

$^{2S+1}L_J$

$S = \frac{1}{2}$

$L = 2$

Term - D

spin multiplicity $= 2S+1 = 2\times\frac{1}{2}+1 = 2$

Possible term symbol.

$J = L+S = 2+\frac{1}{2} = \frac{5}{2}$ $\quad {}^2D_{5/2}$

$L+S-1 = \frac{5}{2}-1 = \frac{3}{2}$ $\quad {}^2D_{3/2}$

d^9 - ↑↓ ↑↓ ↑↓ ↑↓ ↑

2 1 0 -1 -2

$S = \frac{1}{2}$

$L = 4+2+0-2-2$

$= 6-4 = 2$

$^{2S+1}L_J$

Term = D

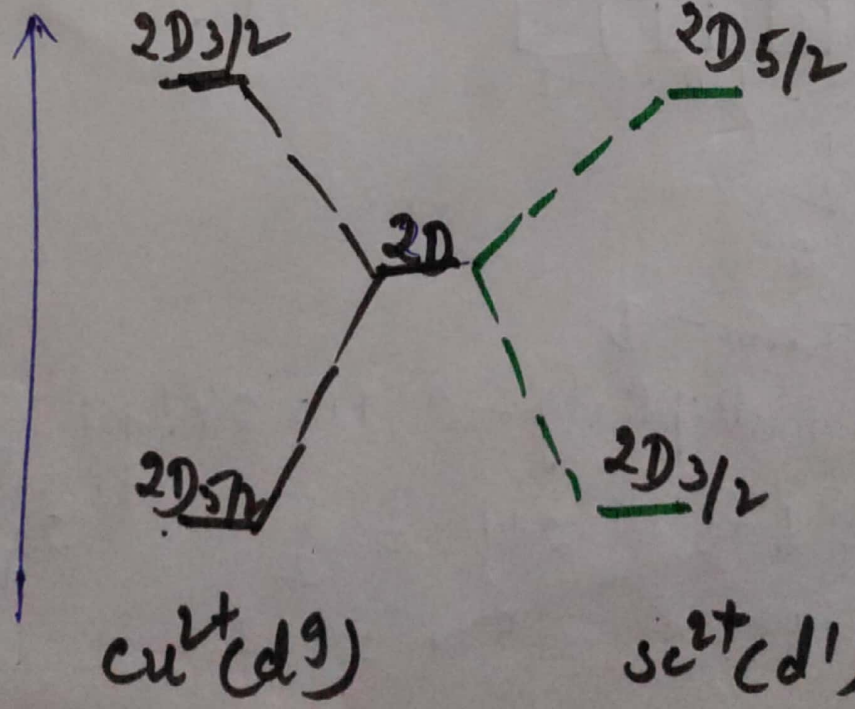
spin multiplicity $2S+1 = 2 \times \frac{1}{2} + 1 = 2$

$J = L+S = 2+\frac{1}{2} = 5/2$

$L+S-1 = 3/2$

Possible term symbol = $^2D_{5/2}$, $^2D_{3/2}$.

Both ion have same microstate and Term Symbol 2D which split into $^2D_{5/2}$ & $^2D_{3/2}$ but ground state term symbol for d^1 system - $^2D_{3/2}$ & for d^9 system is $^2D_{5/2}$.



correlation and spin-orbital coupling of free ion term of Sc^{2+} and Cu^{2+}