Mnemonic and Heuristic for Estimating Spin-only Magnetic Moments

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Abstract

A mnemonic and heuristic for estimating spin-only magnetic moments of free atoms and ions, and based on a continued fractions algorithm, are presented. Chemistry teachers and students might find these useful as problem-solving strategies for lectures and test sessions where calculators might not be permitted or available.

Keywords: mnemonic, heuristic, algorithm

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A mnemonic is a memory aid device designed to improve recall. For instance, a mnemonic may consist of words, letters, numbers, symbols, etc. By contrast, a heuristic is a problem-solving approach that yields an approximate or "good enough" solution. A heuristic can be an educated guess, a rule of thumb, or some guidelines based on tricks of the trade, observations, prior knowledge, common sense, experience, intuition, etc.

Mnemonics and heuristics can be implemented through algorithms. An algorithm is a sequence of well-defined instructions. Both mnemonics and heuristics may coexist, or one can be part of the other. Heuristics, however, do not have to have mnemonics (Johnson, 2012).

There are many strategies for designing mnemonics. For instance, we may look for trends and patterns in data sets. Another strategy consists in using graphs as mnemonics. The most effective are those that display patterns and shapes. The Rydberg Rule mnemonic is an example of this (Garcia, 2016). Mnemonics can even be generated from previous mnemonics.

In this article, we describe a mnemonic for estimating the spin-only magnetic moment, μ_s, of free atoms and ions. Traditionally, μ_s is computed as below.

$$\mu_s = \sqrt{n(n+2)} \quad (1)$$

In (1), n is the number of unpaired electrons, and μ_s is given in Bohr magneton units (B.M.), $1\ \text{B.M.} = \frac{eh}{4\pi mc}$, where e is the electronic charge, h is Planck's constant, m is the electron mass, and c is the speed of light. The ions with the largest n are Gd^{3+} and Cm^{3+} with seven, so it makes sense to report n values up to 7.

Proposed Mnemonic

Instead of computing μ_s with (1), we may estimate it with the mnemonic given below.

v	$\frac{3}{4}$	$\frac{5}{6}$	$\frac{7}{8}$	$\frac{9}{10}$	$\frac{11}{12}$	$\frac{13}{14}$	$\frac{15}{16}$
n	1	2	3	4	5	6	7
μ_s	$1\frac{3}{4}$	$2\frac{5}{6}$	$3\frac{7}{8}$	$4\frac{9}{10}$	$5\frac{11}{12}$	$6\frac{13}{14}$	$7\frac{15}{16}$

Figure 1. Mnemonic for estimating spin-only magnetic moments, μ_s.

In the figure, n values are added to the set of values $v = \frac{3}{4}, \frac{5}{6}, \frac{7}{8}, \frac{9}{10}, \frac{11}{12}, \frac{13}{14}, \frac{15}{16}$. The fractions listed are quite easy to memorize as these are constructed from the sequence {3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16}. The result is a set of mixed numbers representing μ_s estimates.

Heuristic

Figure 1 mnemonic was obtained by estimating μ_s with the heuristic given below

$$\mu_s \approx n + \frac{2n + 1}{2n + 2} \tag{2}$$

where (2) is valid for $n > 0$.

At the time of writing and to our knowledge, calculating μ_s with (2) has not been documented. Table 1 shows a comparative between (1) and (2) results. The deviations introduced by the heuristic are negligible.

Table 1.

Spin-only magnetic moments computed with (1) and (2)

n	μ_s (B.M.), (1)	μ_s (B.M.), (2)
1	1.73	$1\frac{3}{4} = 1.75$
2	2.83	$2\frac{5}{6} = 2.83$
3	3.87	$3\frac{7}{8} = 3.88$
4	4.90	$4\frac{9}{10} = 4.9$
5	5.92	$5\frac{11}{12} = 5.92$
6	6.93	$6\frac{13}{14} = 6.93$
7	7.94	$7\frac{15}{16} = 7.94$

Algorithm

The mnemonic and heuristic so far presented are the result of implementing the continued fractions algorithm, which we now discuss. Let N be the sum of two numbers, x^2 and y. Then

$$N = x^2 + y \tag{3}$$

$$N - x^2 = y \tag{4}$$

$$\left(\sqrt{N} + x\right)\left(\sqrt{N} - x\right) = y \tag{5}$$

$$\sqrt{N} = x + \frac{y}{x + \sqrt{N}} \tag{6}$$

Defining the ratio $r = \frac{y}{x}$, (3) and (6) become

$$\sqrt{N} = \sqrt{x(x + r)} \tag{7}$$

$$\sqrt{N} = x + \frac{rx}{x + \sqrt{N}} \tag{8}$$

We may now iterate (8) by replacing $\sqrt{N}$ in the denominator with the right side of (8). This can be done several times, until a desired precision is achieved. The result is a continued fraction expansion, hence the name of the algorithm.

The algorithm can be stopped at a given iteration step i, by truncating the fractional part, $\frac{rx}{x+\sqrt{N}}$, of the current iterate. Table 2 lists the results of implementing the first few iterates, from i = 1 to i = 3.

Table 2.

First three continued fractions of (6)

i	continued fractions	truncated iterates	rearranged iterates
1	$\sqrt{N} \approx x + \cfrac{rx}{2x + \cfrac{rx}{x + \sqrt{N}}}$	$\sqrt{N} \approx x + \frac{r}{2}$	$\sqrt{N} \approx \frac{2x + r}{2}$
2	$\sqrt{N} \approx x + \cfrac{rx}{2x + \cfrac{rx}{2x + \cfrac{rx}{x + \sqrt{N}}}}$	$\sqrt{N} \approx x + \cfrac{rx}{2x + \frac{r}{2}}$	$\sqrt{N} \approx x + \frac{2rx}{4x + r}$
3	$\sqrt{N} \approx x + \cfrac{rx}{2x + \cfrac{rx}{2x + \cfrac{rx}{2x + \cfrac{rx}{x + \sqrt{N}}}}}$	$\sqrt{N} \approx x + \cfrac{rx}{2x + \cfrac{rx}{2x + \frac{r}{2}}}$	$\sqrt{N} \approx x + \left(\frac{r}{2}\right)\frac{(4x + r)}{(4x + 2r)}$

For the sake of clarity, truncated iterates have been rearranged and listed in the last column of the table. Evidently, if N = 0, then x = 0, y = 0, and r is undetermined.

Because the precision of the results increases as i increases, we may ignore the first two iterations. From now on, let us focus on the results when i = 3 and examine the implications of setting r = 1 and r = 2. See Table 3.

Table 3.

First three continued fractions of (8) after setting r = 1 and r =2

i	continued fractions	r = 1	r = 2
1	$\sqrt{N} \approx x + \frac{r}{2}$	$\sqrt{N} \approx x + \frac{1}{2}$	$\sqrt{N} \approx x + 1$
2	$\sqrt{N} \approx x + \frac{2rx}{4x + r}$	$\sqrt{N} \approx x + \frac{2x}{4x + 1}$	$\sqrt{N} \approx x + \frac{2x}{2x + 1}$
3	$\sqrt{N} \approx x + \left(\frac{r}{2}\right)\frac{(4x + r)}{(4x + 2r)}$	$\sqrt{N} \approx x + \left(\frac{1}{2}\right)\frac{(4x + 1)}{(4x + 2)}$	$\sqrt{N} \approx x + \frac{2x + 1}{2x + 2}$

Implications of setting *r* = 1

Setting r = 1 and squaring (7) gives $N = x(x+1)$, which is an expression that is found in different contexts, in science and engineering disciplines. This expression, for instance, describes the area of a rectangle. Dividing it by 2 defines the area of a triangle and the Sum of Natural Numbers formula.

From Table 3, we can also see that, if i = 3 and r = 1, the square root of whatever is represented by N can be approximated as

$$\sqrt{N} = \sqrt{x(x+1)} \approx x + \left(\frac{1}{2}\right)\frac{(4x + 1)}{(4x + 2)} \tag{9}$$

where the fractional part of (9) is valid for $x > 0$.

Implications of setting r = 2

For $r = 2$, the following equivalency is evident.

$$\sqrt{N} = \sqrt{x(x+2)} \equiv u_s = \sqrt{n(n+2)} \tag{10}$$

Table 3 also shows, for $r = 2$ and $i = 3$, that

$$\sqrt{N} \approx x + \frac{2x + 1}{2x + 2} \equiv u_s \approx n + \frac{2n + 1}{2n + 2} \tag{11}$$

which was used to propose our mnemonic and heuristic.

Implementations

The maximum number of electrons in a subshell is $2(2l + 1)$, where l is the azimuthal quantum number. For l equals to 0, 1, 2, 3, and 4, the s, p, d, f, and g subshells have a maximum of 2, 6, 10, 14, and 18 electrons, respectively. Thus for free atoms from the first transition series, the 3d subshell holds k number of electrons out of a maximum of 10 electrons, distributed across five degenerated orbitals.

Because the first and second ionizations remove the 4s electrons, which are higher in energy than the 3d electrons (Clark, 2021), the electron configurations of free ions from the first transition series reduce to [Ar]3d^k, where [Ar] is the electron configuration of argon. This means that for $k = 0$ to $k = 5$, $n = k$, whereas for $k = 6$ to $k = 10$, $n = 10 - k$.

Therefore, the μ_s, n, and k terms are related and if one of them is known, the other two can be calculated. When ions from the first transition series form coordination compounds, however, determining μ_s, n, and k is not that easy because the 3d orbitals might no longer be degenerated but split into subsets due to the field strength of the ligands. In an upcoming article, we describe a mnemonic that addresses these cases.

In the meantime, teachers and students may find the proposed mnemonic and heuristic useful as a problem-solving strategy. As a mode of illustration, consider the following exercises.

Problem 1. M^+ and M^{2+} were formed during the first two ionizations of a free atom, M, from the first transition series, where μ_s = 0 B.M. for M^+ and μ_s = 1.73 B.M. for M^{2+}. Identify M, M^+, and M^{2+}.

Answer. Per Figure 1, n is the first digit of μ_s. Because μ_s = 1.73 B.M for M^{2+}, either $n = k = 1$, or $n = 10 - k = 1$ then $k = 9$. The former corresponds to Sc^{2+} with electron configuration [Ar]$3d^1$, whereas the latter corresponds to Cu^{2+} with electron configuration [Ar]$3d^9$. The electron configurations of the two possible atoms and their ions are:

Sc => [Ar]$3d^1 4s^2$ Sc^+ => [Ar]$3d^1 4s^1$ Sc^{2+} => [Ar]$3d^1$

Cu => [Ar]$3d^{10} 4s^1$ Cu^+ => [Ar]$3d^{10}$ Cu^{2+} => [Ar]$3d^9$

Because there are no unpaired electrons in M^+ (μ_s = 0 B.M.), which is true for Cu^+ but not for Sc^+, we may conclude that M is Cu, M^+ is Cu^+, and M^{2+} is Cu^{2+}.

Problem 2. M, a free atom from the first transition series, is ionized and becomes the M^{3+} ion. M^{3+} has only three electrons in its 3d orbitals and these are unpaired. Estimate μ_s for M^{3+} without using a calculator. Identify M^{3+} and M.

Answer. From the mnemonic given in Figure 1, or from the heuristic given in (2), if $n = 3$ then $\mu_s \approx 3 + \frac{2(3)+1}{2(3)+2} = 3\frac{7}{8}$. If after ionization three electrons remain in the 3d subshell, the configuration of M^{3+} and M must be $[Ar]3d^3$ and $[Ar]3d^5 4s^1$, respectively. Therefore, M^{3+} is Cr^{3+} and M is Cr.

Remarks

We presented a mnemonic and heuristic for estimating spin-only magnetic moments of free atoms and ions, based on a continued fractions algorithm. Teachers and students can use these for lecture or examination sessions where calculators might not be permitted or available. In theory, equations like (7), found in different contexts and disciplines, can be solved with the heuristic and algorithm herein discussed.

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