A guide to the literature of the finite rectangular well

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A guide to the literature of the finite rectangular well

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The finite rectangular well (FRW) has been a staple of quantum mechanics texts and classes for decades and is the subject of a rich literature. Despite being a problem about which there would apparently be not much more to be said, the FRW continues to serve as a system for introducing students to various analytic techniques and has numerous connections to current technology and research. This paper gives a survey of past and recent FRW literature, with an emphasis on pedagogical contributions directed at graphical and analytic solutions for energy eigenvalues.
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I. INTRODUCTION

The one-dimensional quantum finite rectangular well (FRW) potential, also known as the finite square well, has been a feature of modern physics and quantum mechanics texts and classes for decades, from at least the late 1940s–early 1950s to the present day.[1–3] For generations of students, the finite well has usually followed on the heels of the analytically easier but less-realistic infinite well, and serves as their first exposure to applying wavefunction continuity conditions, examining parity effects, quantifying barrier penetration, appreciating the value of developing a dimensionless parameter to characterize a problem, and exploring techniques for determining energy eigenvalues by graphical or approximate analytic techniques when the corresponding equations cannot be solved exactly. Quantum wells are now also a staple of simulation programs and a subject of physics education research.[4,5] Even the infinite potential well with embedded attractive delta functions has been the subject of a lengthy review paper.[6]

For current students, the pervasiveness of fast personal computers makes the problem of solving for eigenvalues something that can be knocked off in a few minutes with a symbolic manipulator or spreadsheet. While this is convenient, it is also somewhat unfortunate in that the older graphical techniques often incorporated real artistry and ingenuity. But progress will not be denied, and one might consequently expect that discussions of the FRW would have essentially vanished from the literature after about the early 1990s. However, this is not at all the case: The FRW continues to maintain a strong presence in both pedagogical and higher-level research papers, with some of the latter published in journals as prestigious as *Physical Review*.[7] The literature on potential wells is so extensive that an online search keyed on the phrase "finite rectangular well" will yield millions of hits. Even restricting a search to journals and texts that instructors and students of physics are likely to consult, a quick and certainly incomplete survey will yield dozens of potentially interesting references, and it can be difficult to know where to start. On examining these, however, it becomes clear that while the FRW is often involved with forefront research, it has also been prone to frequent cases of re-discovery and modifications of existing treatments. In view of this, I thought it worthwhile to summarize some of the history and current status of this workhorse problem. My intent is not to exhaustively review the literature or to dissect the merits of various techniques in detail, but rather to provide some orientation for instructors and students. To this end, while it is not typical to quote publication years in citations in AJP papers, I do so to help keep a sense of the chronology involved.

The structure of this paper is as follows. In Sec. II, I summarize the traditional textbook solution for the eigenvalues of the FRW and some of the early attempts at finding simplified approaches. (Most of the references cited in this paper also summarize the wavefunctions for the FRW; the emphasis here is on the energy eigenvalues.) Given the pre-calculator era in which they were developed, these techniques were naturally of a graphical nature, and this approach remains active today. In the early 1990s, however, another trend began to emerge, that of more sophisticated analytic investigations aimed at developing very accurate approximate expressions for energy eigenvalues. These developments are surveyed in Sec. III, and a few techniques are compared for a specific numerical example. The distinction between Secs. II and III is not entirely clear-cut, as some papers do involve both graphical and analytic techniques. While the complexity of some of these techniques might seem superfluous in an age of rapid computation, they often involve analytic and modeling strategies with which all students should become familiar. Finally, technological developments in the 1990s began to turn potential wells from textbook abstractions into physical devices, while analytic work turned to exploring the behavior of time-dependent wave packets and use of the FRW as a testbed for applying advanced mathematical techniques to a long-established problem. These treatments are likely to lie beyond the curricula of most undergraduate-level classes, but I touch on them in Sec. IV for the benefit of readers who may wish to delve into them. Section V offers a few closing thoughts.

Before plunging in, it is important to alert readers that there is no universal convention for how authors construct rectangular wells. Some place the top of the well at a potential energy of zero and the bottom at energy $-V_o$, while most put the bottom at zero energy and the top at $+V_o$. Some put the left edge at $x=0$ and the right edge at (say) $x=L$, while other prefer a symmetric arrangement with a full width of L or $2L$ about $x=0$. The convention adopted in this paper is sketched in Fig. 1: A well of width $2L$ symmetric about $x=0$ with its bottom at zero energy.

II. SUMMARY OF ESSENTIAL RESULTS AND THE GRAPHICAL ERA

The traditional textbook approach to the FRW is to establish separate equations of constraint for the even and odd-parity solutions and then explore graphical procedures for isolating the energy (E) eigenvalues. For a particle of mass m trapped in a FRW as sketched in Fig. 1, the even and odd-parity solutions are given, respectively, by

$$\xi \tan \xi = \eta, \tag{1}$$

and

$$\xi \cot \xi = -\eta, \tag{2}$$

where ξ and η are dimensionless variables given by

$$\xi^2 = 2mEL^2/\hbar^2 \tag{3}$$

and

$$\eta^2 = (2mL^2/\hbar^2)(V_o - E). \tag{4}$$

The even solution applies in the first, third, fifth… quadrants and the odd one in the second, fourth, sixth… quadrants. ξ and η are not independent of each other; the sum of their squares forms a dimensionless strength parameter K for the well:

$$\xi^2 + \eta^2 = 2mV_oL^2/\hbar^2 = K^2. \tag{5}$$

K dictates the number of bound energy states N according as

$$N(K) = 1 + [2K/\pi], \tag{6}$$

where the square brackets designate the truncated integer value of the enclosed argument. In comparing various approximation methods, I will work with the dimensionless energy ξ.

Solutions usually proceed by plotting the left and right sides of Eqs. (1) and (2) with the help of Eq. (5) and isolating appropriate intersections. As might be imagined, this is a tedious procedure which in pre-calculator days begged for simplification. The seminal contribution to this end appears to be that of Pitkanen, who in a paper published in this journal in 1955 used standard trigonometric identities to cast the equations into a form where the even-parity solutions involved cosines and the odd-parity ones sines.[8] In the above notation, these take the form

$$K \cos \xi = \pm \xi \tag{7}$$

and

$$K \sin \xi = \pm \xi. \tag{8}$$

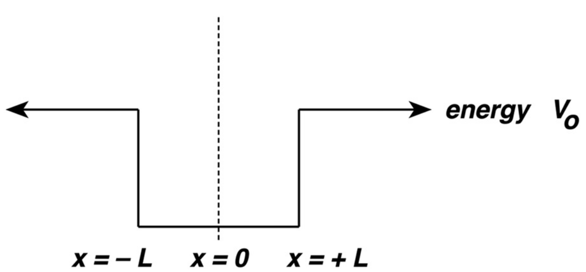

Fig. 1. Geometry of the finite rectangular well.

The sign ambiguities arise from the need to take square roots upon invoking identities such as $1 + \tan^2 \xi = \sec^2 \xi$, and, as discussed by Pitkanen, lead to restrictions on which quadrants contain valid solutions. His graphical constructions involved seeking the intersections of straight lines with sine and cosine curves; he showed how all solutions could be combined into a single graph.

Cantrell rediscovered and elaborated on Pitkanen's method in a paper published in early 1971, giving a reference to Landau and Lifshitz's classic text (where the solution is treated as a problem in small type), but not to Pitkanen; he also applied the method to the case of a semi-infinite well.[9] Subsequently, Murphy pointed out that Cantrell had reproduced Pitkanen's method (which had also been referenced in an electronics text), lamenting that such occurrences were becoming more and more common with the growth of published material(!); Cantrell replied that his purpose had been to bring the method to the attention of teachers and students who might not be familiar with older literature.[10,11] At about the same time, Elmore developed an ingenious polar-form graphical solution involving intersections of semicircles with an Archimedes spiral, a scheme that could be constructed so as to eliminate spurious roots.[12]

Between the times of Murphy's criticism and Cantrell's reply, Guest developed an adaptation of Cantrell's approach that involved functions of the form $KL/|\sin KL|$ and $KL/|\cos KL|$, and which was notable for apparently being the first case where a calculator-plotter (a Hewlett-Packard 9125) was used to render the graphs, although the even and odd solutions still had to be handled separately.[13] This was about the time that pocket calculators were becoming affordable, and Murphy & Phillips (a different Murphy from that above) described a calculator-oriented iterative method of finding the eigenvalues that was subsequently put in terms of the familiar Newton-Raphson technique of calculus classes in a paper by Memory; again, however, the even and odd states still had to be handled separately.[14,15]

The Pitkanen/Cantrell/Guest graphical solution can be compactly summarized as follows, as described in a recent paper by Lima.[16] First, express Eqs. (1) and (2) in terms of sines and cosines. Square both and invoke the identity $\cos^2 \xi + \sin^2 \xi = 1$. The equations of constraint then become

$$|\cos \xi| = \frac{\xi}{K} \tag{9}$$

and

$$|\sin \xi| = \frac{\xi}{K} \tag{10}$$

for the even and odd solutions, respectively, with the even solution still applying in the first and third quadrants and the odd one in the second and fourth. To determine solutions, now define $y = \xi/K$; the eigenvalues are determined by the intersection of a plot of the straight line y vs. the sine and cosine curves of Eqs. (9) and (10). This is illustrated in Fig. 2 for the case $K = 7\pi/4$, which in Eq. (6) has $N = 4$ eigenvalues. The descending curves are the quadrant-relevant sine and cosine curves. The straight line for $y = \xi/K$ cannot exceed a value of unity as we must have $\xi \le K$. Lima gives a detailed discussion of the behavior of such plots as a function of K.

At least three authors subsequently elaborated on Cantrell's method, developing "universal" graphical

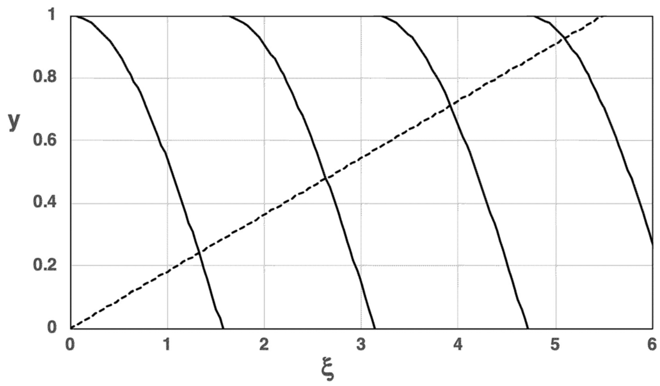

Fig. 2. Pitkanen-type graphical solution for $K = 7\pi/4$. The descending curves are the sine and cosine functions of Eqs. (9) and (10), and the dashed straight line corresponds to $y = \xi/K$.

solutions involving plots of normalized potentials versus energies. The first of these (1972) was Cottey, although he did not reference Cantrell.[17] A more extensive analysis which referenced both Cantrell and Cottey was published by Burge in 1985, who extended the analysis to consider probability densities.[18] The same method was rediscovered more recently by Chiani, who referenced Cantrell but neither Burge nor Cottey.[19] In 1996, Mallow offered yet another variant of the Guest/Cantrell approach which involved plots of squares of sine and cosine functions whose arguments involved energy versus energy itself; the solutions are given by intersections of straight lines with such curves. Again, however, spurious roots still appear.[20]

In 1990, this author developed an equation of condition which includes both the even and odd-parity solutions and which is free of any discontinuities or spurious roots by treating the fundamental boundary conditions of the system as four equations in four "unknowns," namely, the amplitude factors in the wavefunctions.[21] The amplitudes all cancel out, leaving an eigenvalue constraint of the form

$$f(K,\xi) = (K^2 - 2\xi^2)\sin(2\xi) + 2\xi\sqrt{K^2-\xi^2}\cos(2\xi) = 0 \quad (\xi \le K). \tag{11}$$

Figure 3 shows this solution, with $y = f/K$ and setting $K = 7\pi/4$; here the eigenvalues are given by the intersections of the sine-like curve with the ξ-axis, occurring at $\xi \sim 1.32$, 2.64, 3.92, and 5.12.

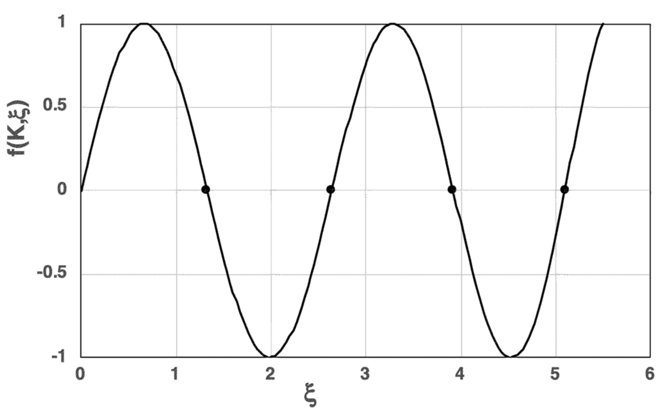

Fig. 3. Reed graphical solution for $K = 7\pi/4$. The dots along the f-axis designate the roots of Eq. (11).

So far as graphical solutions go, it is really a matter of taste as to whether one prefers the quadrant approach of Fig. 2 or the single-curve method of Fig. 3, although this author admits to a preference for the latter.

III. ANALYTIC DEVELOPMENTS

In parallel with the largely graphical methods of eigenvalue determination cited above, several approximate numerical and analytic approaches also came to be developed; these have tended to increase in mathematical and conceptual complexity over time, a feature that makes them appropriate for a range of student preparations.

The first such method was published by Garrett (1979), a scheme designed to be convenient for use with the first generation of programmable calculators.[22] This method involved using the characteristic exponential penetration length of the wavefunction into the sides of the well as a correction to be applied to the width of the well in the standard expression for the eigenvalues of an *infinite* well; the scheme could be iterated as desired, with the caution of not applying it to an infinite-well eigenfunction whose energy exceeded the depth of the finite well being investigated. While this approach has a pedagogically appealing physical foundation and simplicity, it has no obvious path to convergence to the correct answers because the actual eigenvalue equations of the finite well are never invoked. Garrett did not address this point; his example utilized only two iterations.

In a paper that has received several citations, Barker *et al.* (1991) developed a reasonably accurate approximation for the energy eigenvalues based on a Taylor-series expansion of Cantrell's sine and cosine formulations about their approximate roots. This approach would be appropriate for students who have been exposed to some advanced calculus, and gives energies accurate typically to within a few percent, even for weakly bound states near the top of the well.[23] This has the form

$$\xi_n \sim \frac{K}{K+1}\left[\frac{n\pi}{2} - \frac{1}{6(K+1)^3}\left(\frac{n\pi}{2}\right)^3\right], \tag{12}$$

with $n \le N$ as dictated in Eq. (6). Reminiscent of Garrett's approach, Barker *et al.* also showed that the energy levels of a finite well of full width $2L$ and strength K can be approximated as the first n levels of an infinite well of full width $2L(1+1/K)$, and that the eigenfunctions of these states can be approximated as the eigenfunctions of such an infinite well. Soon thereafter, Sprung *et al.* (1992), in a paper that was received between the time of acceptance and publication of Barker *et al.*'s, developed an easier way of deriving Eq. (11).[24] This was based on multiplying Eqs. (1) and (2), and led to a form featuring an explicit quantum number n, namely,

$$\xi + \arcsin(\xi/K) = n\pi/2. \tag{13}$$

For $K \to \infty$, this corresponds to an infinite well of width $2L$.

Based on this formulation, Sprung *et al.* developed an approximation for the eigenvalues, a more complicated one than Barker *et al.*'s in that it included terms up to seventh order in n; this was done by a combination of considering the energy ranges of various bound states and using series solutions:

$$\xi_n \sim \zeta K\left[1-\frac{\zeta^2}{6(K+1)}\left(1+\zeta^2\frac{(9K-1)}{20(K+1)}+\zeta^4\frac{(4K^2-K+(K+1)^2/56)}{15(K+1)^2}\right)\right], \tag{14}$$

where

$$\zeta = \frac{n\pi}{2(K+1)}. \tag{15}$$

The two leading terms of this expression are identical to Barker *et al.*'s result. Many years later (2015), Barsan rederived the leading term Barker *et al.*'s expression and the prefactor in Sprung *et al.*'s as a binomial expansion of its leading term[25]

$$\xi_n = \frac{n\pi}{2}\left(1-1/K+1/K^2\right). \tag{16}$$

Barsan's approach utilized a de Broglie wavelength argument that avoids introducing Schrödinger's equation. He claimed that this development should be accessible to gifted high-school students; if this is the case in his native Romania, the rest of us have some serious catching-up to do.

Aronstein and Stroud (2000) developed an expression for the ξ_n to a higher order than did Barker *et al.* via a series expansion by reversion of Eq. (13); truncated by one term, this is[26]

$$\xi_n \sim K\sqrt{r^2+\left[\frac{2rx}{1+Kx}\right]\eta+\left[\frac{x^2(1+Kx)-r^2}{(1+Kx)^3}\right]\eta^2}, \tag{17}$$

where

$$r = \frac{(\pi/2)}{K+\pi/2}, \tag{18}$$

$$\eta = n\pi/2-\arcsin(r)-Kr, \tag{19}$$

and

$$x = \sqrt{1-r^2}. \tag{20}$$

As described below, this is certainly the most accurate of the expressions given here; their paper actually includes an additional η^3 term.

About a year after Aronstein and Stroud's paper appeared, Bloch and Ignatovich (2001) offered a quite different tack on the FRW problem, determining the eigenvalue condition by demanding that the wavefunctions representing successive reflections of the particle from the well walls be consistent in the sense of being stationary; they also arrived at Eq. (13), but were apparently unaware of the work of Sprung *et al.*[27] They also applied their method to an asymmetric well, a generalization of the Bohr-Sommerfeld quantization rule, and reflections from a step potential and a rectangular barrier.

Also apparently unaware of the work of Sprung *et al.* (but referencing Barker *et al.*), de Alcantara Bonfim and Griffiths developed a parametric representation of FRW eigenvalues based on an approximation to the cosine function and offered yet another approximation for the energies[28]

$$\xi_n \sim \frac{\pi}{8K}\left[4K(n-1)-\pi+\sqrt{(4K+\pi)^2-8\pi Kn}\right]. \tag{21}$$

They also applied their technique to the cases of a semi-infinite well, a delta-function inside an infinite square well, and a double delta-function potential.

Most recently, Lima (2020) reduced the graphical solution for the FRW to having n parallel straight lines intersecting a single cosine curve over the range 0 to $\pi/2$ rad. The exact energy eigenvalues are then approximated using a three-point (parabolic) interpolation, which leads to the approximate expression[16]

$$\xi_n \sim \frac{\pi}{2}[2z_n+n-1], \tag{22}$$

where

$$2z_n = -b+\sqrt{b^2-\frac{2\pi(n-1)}{3K}+\frac{4}{3}} \tag{23}$$

and

$$b = \frac{1}{6}+\frac{\pi}{3K}. \tag{24}$$

This set of expressions could be programmed into a pocket calculator, a useful feature for in-class and test use.

The accuracies of all of these methods (except Barsan's) are compared in Table I, which lists exact ξ-values for the ten states that can be supported by a well with $K=15$, along with the percentage errors for each state for each method; a positive error means that the method overestimates the energy, and a negative error that it underestimates the energy. Errors in the expressions of Barker *et al.*, Sprung *et al.*, and Aronstein and Stroud all increase with n, although those associated with Aronstein and Stroud's expression remain miniscule. In contrast, the error in Bonfim and Griffiths' expression decreases with n, as does that of Lima, which goes from positive to negative at the half-way point. For practical purposes, any of these methods will provide sensible seed values for solving Eq. (13) exactly.

A worthwhile class exercise might be to assign students, depending on their level of expertise, to research one of the graphical or analytic methods described here and present their understanding to their peers; perhaps they might develop variants of their own.

IV. A FEW REMARKS ON RELATED RESEARCH

Beyond the analyses described above, various authors have explored more advanced aspects of the finite well. Siewert derived exact expressions for the energy eigenvalues by an analysis involving complex variables, but his resulting integrals are by no means solvable analytically.[29] Baltin developed the exact Green's function for the FRW.[30] Sprung *et al.* followed up their 1992 paper with an analysis of how the finite well can be used to illustrate concepts of poles of the scattering matrix and resonances, linking their discussion

Table I. Percentage errors for the ten states of a finite well of strength $K = 15$. Positive values indicate overestimates. The exact values in the second column were determined by solving Eq. (13).

n	ξ_n	Barker *et al*. (1991)	Sprung *et al*. (1992)	Aronstein and Stroud (2000)	Bonfim and Griffiths (2006)	Lima (2020)
1	1.47247	<0.001	<0.001	<0.001	1.238	0.510
2	2.94404	0.001	<0.001	<0.001	1.123	0.382
3	4.41372	0.003	<0.001	<0.001	1.013	0.257
4	5.88035	0.011	<0.001	<0.001	0.906	0.135
5	7.34247	0.029	0.001	<0.001	0.800	0.013
6	8.79801	0.066	0.003	<0.001	0.694	-0.109
7	10.24382	0.135	0.011	<0.001	0.585	-0.234
8	11.67443	0.264	0.040	<0.001	0.468	-0.362
9	13.07815	0.517	0.132	0.001	0.336	-0.487
10	14.41691	1.120	0.485	0.002	0.164	-0.549

back to Pitkanen's 1955 paper.[31] Paul and Nkemzi (2000) analyzed the FRW from the perspective of Cauchy integrals and developed their own expression for the energy eigenvalues, which was pointed out to be in error by Aronstein and Stroud; Paul and Nkemzi had actually recreated the leading term of Barker *et al*.'s expression.[32,33] A variant of the standard FRW problem that allows for different particle masses inside and outside of the well relates to semiconductor heterostructures, an issue that has been explored by Singh *et al*.[34]

Perhaps the most striking development is that technological progress has enabled finite wells to move from being textbook abstractions to real-life devices: Advances in semiconductor fabrication and atomic force microscopy have facilitated the construction of particle-confining quantum "corrals," albeit in two dimensions.[35–37]

Most textbook treatments of the FRW are time-independent; moving to time-dependent behavior opens up some fascinating physics. Wavefunctions can experience so-called revivals, fractional revivals and super-revivals. A revival occurs when a wavefunction evolves in time to a state closely resembling its initial form and, as described by Aronstein and Stroud, a fractional revival occurs when a wavefunction evolves to a state describable as a collection of spatially distributed sub-wavefunctions, each of which closely reproduces the shape of the initial wavefunction; such behavior has been observed in, among other systems, micromaser cavities, Rydberg electron packets, and molecules.[7] While the shapes of fractional revivals go on to decay in time, they can eventually re-form over very long timescales to shapes very close to that of the initial packet; the timescale is dictated by the derivatives of the energy spectrum with respect to quantum number in the vicinity of the wave packets' mean quantum number. The relative simplicity of infinite and finite quantum wells facilitates calculations of such effects, and both have been studied by theorists seeking deeper insights into these exotic behaviors.[7,38]

V. CONCLUSIONS

The contributions summarized in this paper were made over several decades by researchers located in a dozen countries, a testimony to the ubiquity of the finite well in physics curricula. The variety of techniques involved make the various methods accessible to students of a broad range of preparations.

As we approach the centennial of the development of modern quantum mechanics, it is encouraging to see that the finite well remains a vibrant element of physics pedagogy while also being involved in current research. Like various problems of Newtonian physics, it will likely remain in the canon of quantum physics for years to come.

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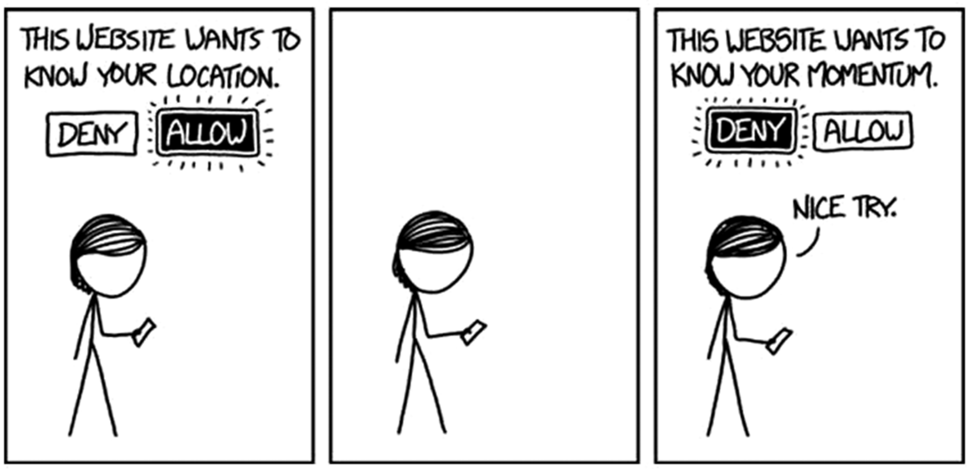

Location Sharing

Our phones must have great angular momentum sensors because their compasses really suck. (Source: https://m.xkcd.com/1473/)