

Nodes of wavefunctions

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We give a simple argument to show that, in one dimensional quantum mechanics, the n -th wave-function has $n - 1$ nodes, and show that if $n_1 < n_2$, then between two consecutive zeros of ψ_{n_1} there is a zero of ψ_{n_2} .

I. THE n -TH WAVE-FUNCTION HAS $n - 1$ NODES.

The Schroedinger equation in one dimension is a simple, linear, second-order differential equation, which in units where $\hbar^2/2m = 1$, reads

$$-\psi'' + V\psi = E\psi \quad (1)$$

All the physical properties of the wave-function are encoded in this simple equation, and, among the many questions we would like to answer, we would like to know what can be said about the zeros of its eigenfunctions, that is, how many nodes the wave-function ψ_n , which corresponds to the n -th energy level, has. There are some arguments based on the variational principle^{1,2} that show that the ground state wave-function has no nodes, but that do not say much about the higher energy levels. This is, in general, considered a technical question^{3,4}, and one is referred to the more mathematical literature, such as⁵⁻⁷.

The question of how many zeros a solution of a linear, second-order, differential equation has, and how are these zeros distributed, is the subject of the Sturm-Liouville (SL) theory⁶. Two of the main theorems in the SL theory are the separation and the comparison theorems. In the case of the Schroedinger equation, the separation theorem states that the zeros of two linearly independent solutions of (1) alternate, and the comparison theorem states that if $n_1 < n_2$, then between two consecutive zeros of ψ_{n_1} there is a zero of ψ_{n_2} . There are stronger results that show that the solution corresponding to the n -th eigenvalue has precisely $n - 1$ zeros, and, if the potential goes to infinity as $|x| \rightarrow \infty$, the eigenvalues form a discrete unbounded sequence.

These theorems are very important in quantum mechanics, but they are usually left out from quantum mechanics textbooks, and one is referred to the mathematical literature for their proof. The purpose of this note is to provide a simple, intuitive, argument for some of these results. We show that ψ_n has $n - 1$ nodes⁸, and that, if $n_2 > n_1$, then between two zeros of ψ_{n_1} , there is a zero of ψ_{n_2} . The second result is simpler to prove, and we include it here for completeness. The first result is usually harder to prove, and it is the main contribution of this paper.

We should stress that proving that the ground state function has no nodes is not just an academic exercise: it was one of the ingredients Feynman used in his theory of liquid Helium¹. In the following we assume that the normalizable solutions of (1) exist, and that they are real, which is always true for the time-independent Schroedinger equation in one dimension. Let us proceed with our argument.

We are given a potential $V(x)$. Construct a new family of potentials $V_a(x)$, such that $V_a(x) = V(x)$ for $-a < x < a$, and $V(x) = \infty$ for $|x| > a$. For $a = \epsilon$ small enough we have, essentially, an infinite potential well, and the wave functions are well-known: $\psi_k^{(o)}(x; \epsilon) \propto \sin(k\pi x/\epsilon)$, $k = 1, 2, \dots$, and $\psi_k^{(e)}(x; \epsilon) \propto \cos((2k + 1)\pi x/2\epsilon)$, $k = 0, 1, 2, \dots$, where the superscripts (e) and (o) refer to the even/odd parity of the wavefunctions. Clearly, $\psi_n(x; \epsilon)$ has $n - 1$ nodes between $-\epsilon$ and ϵ , where it vanishes. Let us focus on the ground state wave function for the time being, which we may assume to be positive, by multiplying by -1 , if necessary. This means that $\psi_1'(-\epsilon; \epsilon) > 0$ and $\psi_1'(\epsilon; \epsilon) < 0$.

Imagine now that we separate the “walls” by increasing a . The wave-function $\psi_1(x; a)$ will become a better and better approximation to the true ground-state wave function, starting from a wave-function without any nodes. Can this wave-function develop a node between $\pm a$, for some a ? If this is the case, then there are two possibilities: either, 1) at least one of the derivatives at $\pm a$ must change sign; or, 2) the derivatives at $\pm a$ do not change sign, but the wave-function develops two zeros through its deepening at some point between $-a$ and a . In both cases there will be a critical value of a such that the wave-function and its first derivative vanish at the same point. In case 1) this happens at one of the points at the boundary, and in case 2), there must be a value of a such that the wave-function touches the real axis just before the wave-function dips down and develops two zeros, and therefore has zero value and zero slope there. But since the Schroedinger equation is a linear, second-order, ordinary differential equation, it has a unique solution, given the value of the function and its derivative at the same point. But if the solution and its first derivative are zero at the same point, one concludes that the wave-function must be identically zero. Since we are assuming that there is always a non-trivial solution of the Schroedinger equation for any value of a , we conclude that in both cases the ground-state function can develop no nodes.

The same reasoning shows that, since the n -th wave-function starts with $n - 1$ nodes, their number can not increase nor decrease, since in order to develop a new zero, or ‘lose’ a zero, the wave-function must go through one of the stages described in 1) and 2), as a increases.

There are cases, of course, where the potential can support only a finite number of bound-states, say N . What happens to the wave functions with $n > N$? As we separate the walls, some of the wave functions go to zero, through the spreading apart of the zeros as $a \rightarrow \infty$, and the positive energy states become the continuum spectrum. This can be seen clearly in the case of the potential well with two walls, as discussed in problems 25 and 26 of Flügge’s book⁹.

Finally we should mention that it is quite straightforward to show that between two consecutive zeros of the n_1 -th wave-function there is a zero of the n_2 -th wave-function, for any $n_2 > n_1$. This can be proved as follows: from the Schrodinger equation for ψ_{n_1} and ψ_{n_2} , one readily sees that $(\psi'_{n_1}\psi_{n_2} - \psi'_{n_2}\psi_{n_1})' = (E_{n_2} - E_{n_1})\psi_{n_1}\psi_{n_2}$. If ψ_{n_1} has two consecutive zeros at x_1 and x_2 , we may assume that ψ_{n_1} is positive in this interval. If ψ_{n_2} does not vanish in this interval, we may also assume it is positive. Integrating from x_1 to x_2 , and noting that $\psi'_{n_1}(x_1) > 0$ and $\psi'_{n_1}(x_2) < 0$ we arrive at a contradiction. Therefore ψ_{n_2} has a zero between two consecutive zeros of ψ_{n_1} . Since we have shown that ψ_n has $n - 1$ zeros, if we take ψ_n and ψ_{n+1} , this result shows that the zeros of the wavefunctions are simple. This, together with the previous results, gives a fairly good description of the node structure of wavefunctions.

As a last remark we should remark that the method presented can also be applied to establish that the ground-state wave-function has no nodes in dimensions higher than one. All one has to do is to consider an infinite potential well around the origin, similarly to what we have done here, and separate the walls. Since the ground-state wave-function starts with no node, it can develop no nodal lines, for reasons similar to what we have just discussed.

II. ACKNOWLEDGEMENTS

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- ⁷ Géza Makay, “A Simple Proof for Sturm’s Separation Theorem”, *Amer. Math. Monthly* **99** (1992), 218–219.
- ⁸ We will call the ground state function ψ_1 , instead of the more common ψ_0 .
- ⁹ S. Flügge, *Practical Quantum Mechanics*, Springer, New York, 1998.