Size

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Size

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Dedication

This book is dedicated to the large and small.

"*The miracle of the appropriateness of the language of mathematics for the formulation of the laws of physics is a wonderful gift which we neither understand nor deserve*," – Eugene Wigner

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Preface

This tiny book is based on a manuscript that I wrote on the topic of size, which had trouble finding a good home. The work is not new science, but rather a description of a very basic quantity in physics that we have come to know as length. It's a topic that might have been discussed by early physicists; but perhaps not since length is derived from the more general concept of coordinates. I have done my due diligence in trying to find references to the quantum description of length, but my searches are overwhelmed by more searched-for quantities such as the Planck Length, the units for measuring length, and pornography.

After obsessing over my manuscript for 3 years, making it longer, then cutting it back to the barest of bones, then expanding it again in several cycles, I decided with some trepidation that it was time to submit it to American Journal of Physics. My reasoning was that AJP publishes pedagogical papers that dive deeply into topics that on the surface seem to have been fully understood by physicists. I felt that my paper was of this sort, but the editor disagreed, asserting that my exposition was more appropriate for a specialized journal. I see nothing specialized about the topic and believe it to be of the broadest interest to physicists. But I relented without complaint, then decided to turn the manuscript into a book for self publication. Perhaps in the end, this format will get greater exposure than a physics journal.

I am concerned that this un-refereed book has errors, but I convinced myself that the topic is of enough interest for me to be forgiven for inaccuracies. If you find errors or have suggestions, please email me at `mgk.wsu@gmail.com` or start a public discussion on my blog at `http://unknownphysicist.blogspot.com/`. I intend to continue toying with length in my very small bursts of spare time, and to release future editions that both have more for the general audience and the expert alike. For example, the fascinating history of counting and measurement can easily be expanded. For the expert, I might extend the book to talk about metrics, which I have totally ignored. Hopefully, the deficiencies of this book will be outweighed solely by the merits of the topic without the need for polished embellishment by an author.

The gist of the book is as follows:

The size of an object is quantified by its characteristic dimensions, which are determined from a set of length measurements. Such measurements implicitly assume that objects are spatially confined and that one-to-one correspondence connects each part of the object to be measured with an interval on a ruler. We should question such macroscopic reasoning when in the quantum realm.

Since size is typically considered a classical quantity, its quantum definition is not commonly discussed, but essential in understanding the basis of measurement. Here, the reader is led through the obvious definition of length as the spread of the probability density, which we evaluate in the noninteracting many-body approximation to solve textbook examples. In the asymptotic limit of many electrons in an infinite well potential, the result converges to sharp boundaries and uniform density as we would expect of a classical system.

Bosons, however, are shown to behave in a counterintuitive way. We spend our lives interacting with electrons, so it's not surprising that being unfettered from the shackles of Pauli Exclusion, bosons are far less constrained and can do as they please.

In addition to the ground state, the length of excited states and coherent states are discussed to glean the meaning of length of systems that cannot be characterized without invoking quantum principles, yet can be interpreted classically.

A quantum ruler may appear to misbehave unless we carefully rethink the meaning of a length measurement; the act of making finer markings leads to systematic error that must be taken into account. If left uncorrected, ever finer rulings lead to more accuracy until the onset of quantum effects, resulting in an optimum parsing for making the most precise ruler. Furthermore, greater accuracy as a result of making finer rulings costs energy.

The effects of entanglement between the object and the ruler are also analyzed. Under certain circumstances, the act of measurement causes electrons to be exchanged between the two, changing the length of both the object and the ruler. In the most extreme case, the ruler evaporates as a result of a measurement.

A consequence of the quantum definition of length is that quantum principles can be used to set an upper bound of the object's length in terms of the ground to first excited state energy difference, independent of the system's Hamiltonian. In the classical limit, the energy spectrum becomes continuous, thus allowing for arbitrarily long length – a property that meets with our classical expectations.

Pedagogically, this line of reasoning shows that interesting physics lurks behind the simplest concepts, which reveals subtleties about measurement and illustrates how the many-particle limit converges to the classical result.

I hope that my narrative is instructive, fun and leads to a better understanding of many-particle quantum mechanics. The classical limit is often associated with systems that are large or in high-energy eigenstates. Here we will see situations where size does not matter as much as the number of particles.

Enjoy!

`Mark G. Kuzyk`
`Pullman, WA`
`July 2017`

Chapter 1

Introduction

Shepherds set out a stone for each sheep they let out to pasture and removed it from the pile when they returned to make sure that none of their flock went missing. Such simple counting systems undoubtedly were used in many aspects of life. The shepherd's stones system is an example of one-to-one correspondence – a stone for each sheep. Counting with fingers and stones progressed to counting boards and then the abacus, where beads on wires provided a bridge to more sophisticated systems of counting and computation.[1] More abstract representations, such as numbers that are expressed in various bases, are also rooted in one-to-one correspondence.[2] Arguably, one-to-one correspondence is the foundation of science since it is the basis for quantification.[3]

The fact that items can be counted is a critical assumption that is not obvious and deserves further thought. The premise is that physical objects have distinct boundaries. In everyday life, this assumption appears to apply to what we think of as discrete objects.

Length is a construct that is based on one-to-one correspondence for continuous things that are not easily separable but in principle divisible. Several identical objects can build a ruler, where they are laid end-to-end along the thing to be measured, the number of them straddling it being the length; i.e. there is a one-to-one correspondence between the ruler and the imaginary slices of the thing if it were made of discrete units. Rather than using discrete rulers end-to-end, one can use markings on a ruler to represent the end-to-end objects. Alternatively, one can use the same ruler segment over and over, moving it sequentially by one length and counting the number of repetitions required to span the object. Indeed, this was a method of choice since earliest recorded times, and is the basis of the cubit, defined by the distance between the tip of the middle finger and the elbow. The ancient builder thus had a convenient portable ruler.[4]

One-to-one correspondence defines the process of addition, where the number of objects is represented by tick marks on a counting stick or knots in a counting rope, which can then be more compactly expressed by symbols. Multiplication is then defined by counting the numbers of groups of numbers of objects, and so on. The more abstract concept of volume is also in one-to-one correspondence with the number of objects that fit inside it, connects with multiplication and leads to integral calculus. The number of oscillations of a periodic system quantifies the passage of time; the time slices being analogous to sections of a ruler with the "object" being the time between events.

This connection between seemingly disparate things by their numbers is not obvious. The Thimshian language of a tribal people of British Columbia have seven sets of distinct words for numbers that apply to different kinds of objects.[5] There are number words for flat objects and animals and others for round objets and time. Number words for men are distinct from those that enumerate long objects and trees. Counting canoes and measures also carry a distinct set of number words. This redundancy implies a perceived underlying difference between two sets with the same number of elements but of a different kind.

The one-to-one correspondence between length and time is based on the observation that an object can move so many intervals of distance over this many clicks of a clock. Velocity quantifies the correspondence between the two. Though the same set of number words describes both time intervals and lengths, our language separates time and space by assigning them different units, implying they are distinct things – a vestige of humanity's pre-Einstein understanding of space-time. This one-to-one correspondence between ever-more abstract quantities forms our more sophisticated present-day understanding of the universe.

A measurement of length requires a correspondence between the numbers of markings on a ruler and parts of the object, with the implicit assumption that additivity of the units of each forms the whole. Now imagine making finer subdivisions. Our knowledge of quantum mechanics teaches us that sharp boundaries disappear on smaller scales, where wave functions take over as the descriptions of stuff. The concept of separate units comes into question in the quantum realm, where wave functions of identical particles are required to be entangled, and lose all essence of individuality. The most universal theories that are formulated using human intuition often spit back at us an accurate description of nature that rejects the intuitive assumptions that went into formulating those theories. We are thus compelled to accept this strange behavior, and use it to develop a more abstract and nuanced intuition. So too is the concept of length, which is well defined in the macroscopic world, which when extrapolated into the quantum realm takes on a different meaning.

This book focuses on length and seeks to define a rigorous method for computing it in the quantum limit using the classical everyday description as a guide. A rigourous quantum definition of length can be evaluated in the classical limit as a pedagogical tool to understanding how quantum effects fade away when many particles are involved; and, perhaps more interestingly, quantum mechanics sets constraints that must carry over into the classical world. For example, there is a deep connection between length and energy spectrum. This connection is made apparent with quantum-mechanical identities called sum rules, which set an upper limit for length in terms of the energy difference between the two lowest-energy states and the number of particles – typically electrons – that make up the system. Length seemingly becomes boundless when energy separations become small, as it does in the classical world.

Going by the classical definition, the only one known at the time, the French National Assembly recognized in 1791 the importance of a standard of length, and defined the standard meter to be one ten-millionth the distance from the north pole to the equator on the meridian passing through Paris. In 1799, a platinum bar was made in France and placed in the National Archives, and later, duplicates were made to be used as a standard in the United States and elsewhere. In 1960, a more precise definition was established in terms of the the number of wavelengths of light, then in 1983 in terms of the distance traveled by light in vacuum in a tiny fraction of a second. Ironically, all these definitions assume a classical length that is known to break down for small objects. This book takes us into the quantum realm where these assumptions are scrutinized.

Chapter 2 starts with an intuitive argument for how we perceive length, and these perceptions are used to define a more rigourous definition of length that applies to the quantum realm. Chapter 3 then uses the length definition for a single particle in a quantum well. Chapter 4 takes a small detour to define a convention of many-particle state vectors and operators that is amenable to straightforwardly evaluating many-particle quantities. Chapter 5 shows how the spread of the wave function of a single particle of a many-particle state vector determines the length. With the quantum theory of length established, Chapter 6 shows how the Thomas-Reich-Kuhn sum rules,[6, 7, 8] purely quantum relationships between the position matrix elements and the energies, set an upper bound on length as a function of the number of electrons in the material and the energy difference between the two lowest-energy states. Appendix A derives the sum rules to provide the reader with a self-contained document.

Chapter 7 applies the theories to many particles in a box and in a harmonic potential. For each system, the fundamental limit is calculated and verified by comparing it with calculations of the actual length. The classical limit is then studied by extrapolating the quantum expressions to many electrons, and the particle density in the box is shown to approach the classical limit – having sharp boundaries and uniform density. Then the length of a system of Bosons is analyzed in Chapter 8 showing that the upper bound of the ground state length of an infinite well energy spectrum grows substantially beyond the walls as bosons are added and no sharp boundaries are ever observed. Also studied are the energies required to subdivide the ruler into smaller sections and the accuracy of such rulers is analyzed. Chapter 9 shows that the length of a coherent state is the width of the wave packet rather than the approximate distance between classical turning points, as are the energy eigenstates. Chapter 10 completes the discussion by focusing on the meaning of measurement; and, how a ruler will introduce systematic errors in the measured length. Also discussed is the necessary entanglement of the measuring device and the object and how it affects the measurement process. An extreme case can be constructed in which the ruler evaporates in the process of making a measurement. Chapter 11 summarizes it all and offers points for further thought.

Chapter 2

Classical Length

A classical measurement of a length requires a comparison between a standard, such as a ruler, and the extreme ends of the object. In the small size limit, where quantum effects dominate, the measurement is intrinsically fuzzy because an edge cannot be represented by a single point. When such fuzziness becomes extreme, the classical concept of length is nonsensical. Here we seek to define size in a way that can be applied to the quantum realm and asymptotes to the "correct" classical result for large familiar objects.

Classical systems are characterized by objects with uniform density and sharp boundaries whereas quantum system are described by wavefunctions that oscillate. The quantum object is characterized by the expectation value of the position, which gives its location; and, the variance, which quantifies the spread of the wavefunction. This spread is the uncertainty in the position of the particle(s) that define the system. These concepts are quantified below.

Consider a classical rod of length L as shown in Figure 2.1a. If it is uniform, in the spirit of quantum mechanics, we can define a linear density amplitude

$$\psi(x) = \frac{1}{\sqrt{L}}, \tag{2.1}$$

which is normalized, so $\int_0^L |\psi(x)|^2 \, dx = 1$. Equation 2.1 can be used to get the expectation of the position, a fancy name for its average

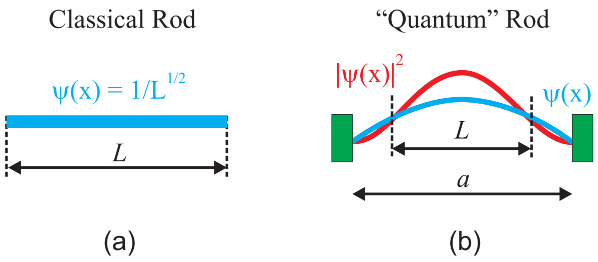


Figure 2.1: (a) A classical rod can be represented by a uniform density with sharp edges. (b) The ground state wavefunction of an electron in a box has a probability density that is proportional to the square of the wave fucntion.

position or midpoint, which yields

$$\langle x \rangle = \int_0^L dx\, x\, |\psi(x)|^2 = \frac{L}{2}, \tag{2.2}$$

a result that we expect; and, $\langle x^2 \rangle$ is given by

$$\langle x^2 \rangle = \int_0^L dx\, x^2\, |\psi(x)|^2 = \frac{L^2}{3}. \tag{2.3}$$

We apply the quantum approach to determine the uncertainty in the position of the classical rod, which with the help of Equations 2.2 and 2.3 gives

$$\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = \frac{L}{\sqrt{12}}. \tag{2.4}$$

We postulate that the quantum length is proportional to the uncertainty, so to make it match the classical length, we define it to be of the form

$$L = \sqrt{12}\Delta x = \sqrt{12\left(\langle x^2 \rangle - \langle x \rangle^2\right)}. \tag{2.5}$$

We can test this definition by checking if the length of a quantum system asymptotes to the expected length in the classical limit when the number of particles becomes large.

The length along x in agnostic form,

$$\boxed{L = \sqrt{12 \int \rho(\mathbf{r})\,(x^2 - \bar{x}^2)\,d^3\mathbf{r}},} \tag{2.6}$$

works equally well for the classical and quantum case. $\rho(\mathbf{r})$ is the dimensionless density with $\int d^3\mathbf{r}\,\rho(\mathbf{r}) = 1$ and $\bar{x}$ is the x coordinate of the "center" of the object. The integral is over all space. In this form, $\rho(\mathbf{r})$ can be the classical dimensionless density or the quantum probability density $\psi^*(\mathbf{r})\psi(\mathbf{r})$. The length in any direction can be calculated by rotating the object so that the coordinate x-axis is along the desired dimension of measurement. This is no different than laying a ruler across an object along the desired direction. Equation 2.6 is the central definition that is the subject of the investigations that follow.

Aside from having an abrupt edge, a second criteria for a classical length to be well-defined is a sufficiently uniform material; if enough material is missing from an object, it is reasonable to consider it to be multiple separate objects. Classically, distinct objects are simple to identify. From the quantum perspective, wave functions can partially overlap, making it unclear where one object begins and the other one ends. We will not provide a rigourous definition for the uniformity of an object, nor when one object becomes two. Instead, we will apply our definition to simple systems and investigate its consequences.

Chapter 3

Single-Particle Length

We begin the discussion with one particle in a box, as shown in Figure 2.1b, to gain a foothold before delving into the more complex many-particle case. The ground state wave function, given by

$$\psi(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{\pi x}{a}\right), \tag{3.1}$$

is plotted in blue (light curve in grayscale) in Figure 2.1b. The square of the wave function is shown in red (darker curve). Is the size of the box the size of the system? If so, half the wavelength of the ground state wavefunction defines the size, which is given by a.

To see why this is not so, consider the fact that contact forces between objects are what allow the dimensions of a wood block to be measured with a vernier calliper; and, these forces originate in the electrons. The nuclei provide the scaffolding for the electrons and the electrons in one object interact with the electrons in the another one. So when we touch a table, the electrons in our finger repel the electrons in the table. Thus, we assume that the particle in the box is an electron and the box provides the confinement potential as do nucleons in atoms and molecules. When we "touch" the box, we are in fact touching the electron cloud. The walls of the box merely provide the forces that keep the electrons confined and are not physical objects that we can directly sense no more than we can sense the nucleons in everyday interactions with our environment.

The quantum size of the system, we argue, is determined from the breadth of the electron density, which is given by the square of the wavefunction as shown in red (darker curve) in Figure 2.1. The uncertainty in the position of the ground state wavefunction is given by

$$\Delta x = a\sqrt{\frac{1}{12} - \frac{1}{2\pi^2}}. \tag{3.2}$$

Substituting Equation 3.2 into Equation 2.5 yields the length of a quantum particle in a box, or

$$L = a\sqrt{1 - \frac{6}{\pi^2}} \approx 0.63a. \tag{3.3}$$

The length given by Equation 3.3 defines an interval over which the probability density remains above about 30% of its peak value. This picture is a fully quantum one that offends our common sense that objects have well-defined boundaries.

Chapter 4

Many-Particle Systems

4.1 Wave Functions

This Chapter introduces a precise notation that both reduces confusion and simplifies taking expectation values of operators. The highlighted text below describes the notation for two and three particles for illustration. The reader who is interested in the general results can skip the highlighted sections.

Using two particles for illustration, their joint state vector is expressed as

$$|n, m\rangle = \frac{1}{\sqrt{2}}\Big(|n\rangle\,|m\rangle \pm |m\rangle\,|n\rangle \Big), \tag{4.1}$$

where the plus and minus signs are for bosons and fermions. We understand $|n\rangle\,|m\rangle$ to mean "Particle #1 is in state n and Particle #2 is in state m." Thus, when kets are written side-by-side, from left to right, they represent Particle #1, Particle #2, and so on. Even though the particles are indistinguishable, they are not treated as such at this point.

The ket $|n, m\rangle$ is expressed in agnostic form, and represents two particles that occupy states n and m without distinguishing which one is in which state. If we exchange the two particles we find that $|n, m\rangle \to \pm\,|m, n\rangle$. Since state vectors are unique up to a phase, both of them represent the same state, so we chose to express the arguments in ascending order of their numerical values, i.e. $m > n$.

We have used classical concepts to build a quantum-mechanical object that no longer has these classical properties. We start by treating the particles as distinguishable, write an expression with built-in indistinguishability, then get a purely quantum object. Our goal is to formulate the theory in a way that is fully quantum in nature.

It follows that for a three-particle system, the wave function is given by

$$\begin{aligned} |n, m, \ell\rangle &= \frac{1}{\sqrt{6}}\Big(|n\rangle\,|m\rangle\,|\ell\rangle \pm |n\rangle\,|\ell\rangle\,|m\rangle + |\ell\rangle\,|n\rangle\,|m\rangle \\ &\pm |l\rangle\,|m\rangle\,|n\rangle + |m\rangle\,|\ell\rangle\,|n\rangle \pm |m\rangle\,|n\rangle\,|\ell\rangle \Big). \end{aligned} \tag{4.2}$$

We can express Equation 4.2 in a form that singles-out the state vector of Particle #1

$$|n, m, \ell\rangle = \frac{1}{\sqrt{3}}\Big(|n\rangle\,|\bar{n}\rangle + |m\rangle\,|\bar{m}\rangle + |\ell\rangle\,|\bar{\ell}\rangle \Big), \tag{4.3}$$

where

$$|\bar{n}\rangle = \frac{1}{\sqrt{2}}\Big(|m\rangle\,|\ell\rangle \pm |\ell\rangle\,|m\rangle \Big), \tag{4.4}$$

and where the other barred operators can be determined by comparing Equations 4.3 and 4.2. Thus, we can view $|\bar{n}\rangle$ as the state that remains when Particle #1 is removed from state $|n\rangle$. Note that Equation 4.3 shows all plus signs because the signs can be absorbed into the barred states. It is straightforward to verify that the barred states are orthonormal, or

$$\langle \bar{n} \,|\, \bar{n}' \rangle = \delta_{n,n'}. \tag{4.5}$$

The contracted form given by Equation 4.3 is useful in situations where the property of Particle #1 is to be calculated.

For example, the probability density of Particle #1 is given by

$$\begin{aligned} \rho(x_1) &= \left|\langle x_1 \,|\, n, n, \ell\rangle\right|^2 \\ &= \left|\frac{1}{\sqrt{3}}\Big(\langle x_1 \,|\, n\rangle \,|\bar{n}\rangle + \langle x_1 \,|\, m\rangle \,|\bar{m}\rangle + \langle x_1 \,|\, \ell\rangle \,|\bar{\ell}\rangle \Big)\right|^2 . \end{aligned} \tag{4.6}$$

Orthonormality of the barred states collapses Equation 4.6, yielding

$$\rho(x_1) = \frac{1}{3}\Big(\rho_n(x_1) + \rho_m(x_1) + \rho_\ell(x_1)\Big), \tag{4.7}$$

where $\rho_i(x_1) = |\langle x_1|i\rangle|^2$ is the probability density of finding Particle #1 at coordinate x_1 when in state $|i\rangle$. Note that the sign of the barred state is irrelevant when calculating $\rho(x_1)$ because the barred states always appear in pairs of the form $\langle \bar{n} \,|\, \bar{n}\rangle$. Since the particles are indistinguishable, the result can be no different if we had done the calculation for any other particle. Thus, Equation 4.7 is the probability density for the system of three particles as a whole. As such, the density can be expressed simply as $\rho(x_1) \to \rho(x)$.

All of the above concepts apply to many-particle states. As is evident from the antisymmetric nature of the fermion wave functions, if two particles occupy the same state, the wave function vanishes, as required by the Pauli exclusion principle. As such, the ground state $|G\rangle$ of the N-particle fermionic system can be expressed as the determinant

$$|G\rangle = \frac{1}{\sqrt{N!}} \begin{vmatrix} |1\rangle & |2\rangle & \dots & |N\rangle \\ |1\rangle & |2\rangle & \dots & |N\rangle \\ \vdots & \vdots & \ddots & \vdots \\ |1\rangle & |2\rangle & \dots & |N\rangle \end{vmatrix}, \tag{4.8}$$

where we label the single-particle ground state $|1\rangle$. Similarly, any state of noninteracting particles can be represented by

$$|n_1, n_2, \dots, n_N\rangle = \frac{1}{\sqrt{N!}} \begin{vmatrix} |n_1\rangle & |n_2\rangle & \dots & |N\rangle \\ |n_1\rangle & |n_2\rangle & \dots & |N\rangle \\ \vdots & \vdots & \ddots & \vdots \\ |n_1\rangle & |n_2\rangle & \dots & |N\rangle \end{vmatrix}. \tag{4.9}$$

The contracted form given by Equation 4.3 is made clear by recognizing that the barred state vector $|\bar{n}\rangle$ is just the determinant of the $(N-1) \times (N-1)$ sub-matrix formed by excluding the n^{th} row and n^{th} column of the matrix.

Note that it is simpler to write Equation 4.8 than Equation 4.9, so in the derivations that follow, we can express state vectors in the form of Equation 4.8 and get the more general result by making the substitution $|i\rangle \to |n_i\rangle$. Note that if any two indices are the same, i.e. $n_i = n_j$, two of the columns will be the same and the determinant vanishes. This enforces the Pauli exclusion principle – the state vector vanishes if *any* pair of fermions are in the same state. In the calculations that follow for fermions, Pauli exclusion is obeyed by constructing states vectors in which all occupied single-particle states are different.

4.2 Many-Particle Matrix Elements

Again, we start with two- and three-particle examples to introduce the student to how many-particle operators act on state vectors. The shaded example can be skipped by the reader who wants to move on to the general results.

It is straightforward to show that the expectation of the operator A_1, which acts only on Particle #1 reduces to

$$\begin{aligned}\langle n, m, \ell \,|\, A_1 \,|\, n, m, \ell\rangle &= \frac{1}{3}\Big(\langle n \,|\, A_1 \,|\, n\rangle \\ + \quad \langle m \,|\, A_1 \,|\, m\rangle &+ \langle \ell \,|\, A_1 \,|\, \ell\rangle \Big), \end{aligned} \tag{4.10}$$

where orthonormality of the barred states forces only the diagonal components to contribute.

Using this convention, the multi-particle operations can be generalized as follows:

Equation 4.3 becomes

$$|1, 2, \ldots, N\rangle = \frac{1}{\sqrt{N}} \sum_{n=1}^{N} |n\rangle \, |\bar{n}\rangle \,. \tag{4.11}$$

Equation 4.7 becomes

$$\rho(x) = \frac{1}{N}\sum_{n=1}^{N}\rho_n(x), \tag{4.12}$$

where we drop the subscript because the particles are indistinguishable so that Equation 4.12 gives the probability density of *any* particle.

Equation 4.10 becomes

$$\langle 1,2,\ldots,N \,|\, A_1 \,|\, 1,2,\ldots,N\rangle = \frac{1}{N}\sum_{n=1}^{N}\langle n \,|\, A_1 \,|\, n\rangle\,. \tag{4.13}$$

The notation used above is a bit sloppy. The operator A_i, which acts on Particle #i, should more rigourously be expressed as

$$A_i \to \prod_{j\neq i}\mathbb{1}_j A_i, \tag{4.14}$$

where $\mathbb{1}_j$ is the identity operator in the Hilbert space of particle j. Similarly, we can define the many-particle position operator in terms of the single particle operators using

$$X = \sum_{i=1}^{N}\prod_{j\neq i}\mathbb{1}_j x_i. \tag{4.15}$$

Equation 4.15 will be imprecisely written as

$$X = \sum_{i=1}^{N} x_i, \tag{4.16}$$

where the identity operators are implicitly understood. We will be imprecise in this way to avoid the proliferation of symbols.

Calculations must include the spin, and account for the Pauli exclusion principle to fill the single-particle states. The ground state vector of a spin-up electron we assign to $|1\rangle$ and a spin down-electron is $|2\rangle$; the first excited statevector of a spin-up electron and spin-down electron are designated $|3\rangle$ and $|4\rangle$; and so on. Thus, an odd integer

n represents a spin-up electron in state $\left|\frac{n+1}{2},+\right\rangle$ and an even integer n represents a spin-down electron in state $\left|\frac{n}{2},-\right\rangle$. In this latter representation, the first argument of the ket labels the single particle energy eigenstate and the second argument labels the spin. We use the former notation with only one index because of its simplicity, especially when sums are involved, but move to the latter notation when evaluating sums over occupied states.

Chapter 5

Quantum Length

This Chapter calculates the length using the observation that each electron in a material is spread over the whole material. Since all electrons are identical, the one-particle density is representative of the whole material so its spread is the length.

We choose to get the length from Particle #1, which has a spread

$$\Delta x_1^2 = \left\langle G \,\middle|\, x_1^2 \,\middle|\, G \right\rangle - \langle G \,|\, x_1 \,|\, G \rangle^2 . \tag{5.1}$$

Using Equation 4.13, Equation 5.1 takes the form

$$\Delta x_1^2 = \frac{1}{N} \sum_{n=1}^{N} \Big(\langle n \,|\, x^2 \,|\, n \rangle - \langle n \,|\, x \,|\, n \rangle^2 \Big), \tag{5.2}$$

where we have dropped the subscript identifying Particle #1 since this result holds for any particle. Using Equation 2.5, the length is then given by

$$\boxed{\begin{array}{l} L = \sqrt{\dfrac{12}{N} \displaystyle\sum_{n=1}^{N} \Big(\langle n \,|\, x^2 \,|\, n \rangle - \langle n \,|\, x \,|\, n \rangle^2 \Big)}. \\ \text{Single-Particle Length} \\ \text{Many-Particle Wavefunction} \end{array}} \tag{5.3}$$

When the potential is centrosymmetric about position $x = 0$, the single-particle energy eigenfunctions have a definite parity, i.e.

$$\psi_n(-x_i) = \pm \psi_n(x_i), \tag{5.4}$$

so Equation 5.4 yields

$$\langle n \,|\, x_i \,|\, n \rangle = \int dx_i \, \psi^*(x_i) x_i \psi(x_i) = 0. \tag{5.5}$$

If the zero of the coordinate system is shifted to $x = c$,

$$\begin{aligned} \langle n \,|\, x_i \,|\, n \rangle &= \int dx_i \, \psi^*(x_i - c) x_i \psi(x_i - c) \\ &= \int dx_i \, \psi^*(x_i)(x_i + c)\psi(x_i) = c. \end{aligned} \tag{5.6}$$

If the coordinate system of a centrosymmetric system is chosen so that the symmetry axis is at $x = c$, Equation 5.6 can be substituted into Equation 5.3, yielding

$$\boxed{\begin{array}{l} L = 2\sqrt{3}\left(\dfrac{1}{N}\displaystyle\sum_{n=1}^{N} \langle n|\, x_i^2 \,|n\rangle - c^2\right)^{1/2}. \\ \text{Single-Particle Length} \\ \text{Many-Particle Wavefunction} \\ \text{Centrosymmetric Potential} \end{array}} \tag{5.7}$$

Equation 5.7 is convenient because all quantities are calculated from single-particle states and operators.

Chapter 6

Upper Bound of Length

Quantum constraints must be obeyed even in the classical limit. One consequence of such constraints is an upper bound of length, which depends on the energy spacing. The fact that the energy scale is the important quantity makes intuitive sense for the particle in a box since half the de Broglie wavelength defines the size of the box, and the particles' spatial spread must be smaller than the box.

All systems must obey the sum rules even when all electrons interact with each other. The sum rules are derived in Appendix A and used in this chapter. Let's start with the simple single particle case, whose sum rules are given by Equation A.4. Since all of the terms in the sum are positive definite, replacing $E_{n1} \equiv E_n - E_1$ with E_{21} makes each term smaller, thus yielding the inequality

$$\sum_{n \neq 1}^{\infty} \langle 1| x |n\rangle \langle n| x |1\rangle E_{21} \leq \frac{\hbar^2}{2m}. \tag{6.1}$$

The sum rules exclude the ground state. Adding the ground state to the sum, then subtracting it yields

$$\sum_{n=1}^{\infty} \langle 1| x |n\rangle \langle n| x |1\rangle - \langle 1 \,|\, x \,|\, 1\rangle^2 \leq \frac{\hbar^2}{2mE_{21}}, \tag{6.2}$$

where we have divided both sides by the constant E_{21}. Using closure, defined by

$$\mathbb{1} = \sum_n |n\rangle \langle n| , \tag{6.3}$$

we get from Equation 6.2

$$\left\langle 1 \left| x^2 \right| 1 \right\rangle - \langle 1 \,|\, x \,|\, 1 \rangle^2 \leq \frac{\hbar^2}{2mE_{21}}. \tag{6.4}$$

The lefthanded side of Equation 6.4 is simply Δx^2, so gives the length limit

$$\boxed{L_{max} = \sqrt{\frac{6\hbar^2}{mE_{21}}}. \quad \text{One Electron Length Limit}} \tag{6.5}$$

For an object with N electrons, the ground-state sum rule is given by

$$\sum_{M=1}^{\infty} \langle G| \, X \, |M\rangle \, \langle M| \, X \, |G\rangle \, E_{MG} = \frac{\hbar^2 N}{2m}, \tag{6.6}$$

where we define $E_{MG} = E_M - E_G$ as the energy difference between the many-particle excited state M and the many-particle ground state, G. $\langle M| \, X \, |Q\rangle$ is the matrix element of the position operator between the many-electron energy eigenstates labelled by M and Q. Here X is given by

$$X \equiv \sum_{i=1}^{N} x_i, \tag{6.7}$$

where x_i is the coordinate of the i^{th} electron

We might be tempted to replace X, the many-particle operator, with x_1 as we did in calculating the length. However, this trick will not work since it misses cross terms of the form $\langle G| \, x_1 \, |M\rangle \, \langle M| \, x_2 \, |G\rangle$. This trick works in general when calculating the length – even when the electrons interact – because each electron is delocalized over the the whole system. No such physical argument applies to the sum rules.

We calculate the many-particle length limit along the same lines as we did for the single-particle case, but instead will get an upper bound for ΔX^2. Given Equation 6.7, it is not difficult to show that $\Delta x_1 \leq \Delta X$.

Since E_{MG} is positive definite, if we replace it with the smallest energy difference E_{FG} in the sum on the left-hand side of Equation

6.6, where F is the many-particle first excited state, we get

$$\sum_{M=1}^{\infty} \langle G|\, X \,|M\rangle \, \langle M|\, X \,|G\rangle \, E_{FG} \leq \frac{\hbar^2 N}{2m}. \tag{6.8}$$

E_{FG} is a constant, so dividing both sides of Equation 6.8 by E_{FG} yields

$$\begin{aligned} &\sum_{M=G}^{\infty} \big(\langle G|\, X \,|M\rangle \, \langle M|\, X \,|G\rangle \\ &- \langle G|\, X \,|G\rangle \, \langle G|\, X \,|G\rangle \big) \leq \frac{\hbar^2 N}{2mE_{FG}}, \end{aligned} \tag{6.9}$$

where the sum starts with $M = G$, and the extra term that results is explicitly subtracted.

The left-hand side of Equation 6.9 defines ΔX^2. Calculating the length with ΔX yields

$$\boxed{L_{max} = \sqrt{\frac{6\hbar^2 N}{mE_{FG}}}. \quad \text{General Length Limit}} \tag{6.10}$$

Equation 6.10, while an overestimate, is nevertheless an upper bound. We will see that in certain special cases, the calculated length will be close to the calculated upper bound – making it a useful computational tool.

Equation 6.10 is a fundamental relationship that gives the upper bound of length in terms of the quantum energy scale E_{FG}, the lowest possible energy above the ground state. In the classical limit, where objects are large, the bound state energy differences approach a continuum, permitting an arbitrarily-large length.

The length of a quantum system in its excited state Q is also well defined. Consider the sum rule

$$\sum_{M=G}^{\infty} \langle Q|\, X \,|M\rangle \, \langle M|\, X \,|Q\rangle \, E_{MQ} = \frac{\hbar^2 N}{2m}, \tag{6.11}$$

where terms with $M < Q$ have a non-potive energy difference ($E_{MQ} \leq 0$). Moving these terms to the righthand side of Equation 6.11 yields an expression where all the terms are non-negative, or

$$\begin{aligned}\sum_{M=Q+1}^{\infty} \langle Q| X |M\rangle \langle M| X |Q\rangle E_{MQ} = \frac{\hbar^2 N}{2m} \\ + \sum_{M=G}^{Q-1} \langle Q| X |M\rangle \langle M| X |Q\rangle E_{MQ}.\end{aligned} \tag{6.12}$$

Since $E_{M,Q} \geq E_{Q+1,Q}$ for $M > Q$,

$$\begin{aligned}\sum_{M=Q+1}^{\infty} \langle Q| X |M\rangle \langle M| X |Q\rangle E_{MQ} \geq E_{Q+1,Q} \Bigg[\\ \sum_{M=G}^{\infty} \langle Q| X |M\rangle \langle M| X |Q\rangle \\ - \sum_{M=G}^{Q} \langle Q| X |M\rangle \langle M| X |Q\rangle \Bigg].\end{aligned} \tag{6.13}$$

Being a constant, $E_{Q+1,Q}$ can be moved outside the sum. Applying closure so that $\sum_{M=G}^{\infty} \langle Q| X |M\rangle \langle M| X |Q\rangle = \left\langle Q \,\middle|\, X^2 \,\middle|\, Q\right\rangle$, Equation 6.13 can be used to re-express Equation 6.12 to get the length of a system in excited state Q, L_Q:

$$\boxed{\begin{aligned}L_Q^{\max} = 2\sqrt{3}\Delta X_Q = \Bigg(\frac{6\hbar^2 N}{m E_{Q+1,Q}} \\ + 12 \sum_{M=G}^{Q-1} \langle Q| X |M\rangle \langle M| X |Q\rangle \frac{E_{Q+1,M}}{E_{Q+1,Q}} \Bigg)^{1/2}. \\ \text{Many Particle Excited State Length Limit}\end{aligned}} \tag{6.14}$$

Equation 6.14 is not as elegant as Equation 6.10 because it depends on the energy spectrum of the system below state Q. Itmn is of interest, however, because the excited state length can be much larger than the ground state length, implying that the length is not an immutable material property.

Chapter 7

Applications

This Chapter applies the above formalism to particles in a box and the harmonic oscillator. We compare the lengths to their fundamental limits and evaluate the classical asymptote when the number of electrons becomes large. To do so requires that we first determine the energy difference E_{21} of the many-body system in terms of the single-particle state excitation energies. We also discuss the electron density to show that the asymptote meets our classical expectations and interpret the results in terms of classical concepts.

7.1 Particle in a Box

The particle in a box is the ideal system for studying length by virtue of its sharp walls. We have two choices for building a box. First, we can fix the box's size, then fill it with electrons. A more realistic model is to increase the size of the box in proportion to the number of electrons, which more closely reflects a real system such as a metal rod. With each added atom, the lattice become larger and simultaneously gains conduction electrons. We calculate both cases, starting with the simpler case of the fixed box size.

7.1.1 Fundamental Limit

We start by applying the fundamental limits to the particle in a box for N noninteracting electrons. The first step is to determine the energy difference E_{21} for the many-particle system in terms of the single-particle energies and the number of electrons. From this, we can calculate the scaling of the fundamental limit with number of electrons and evaluate the classical limit.

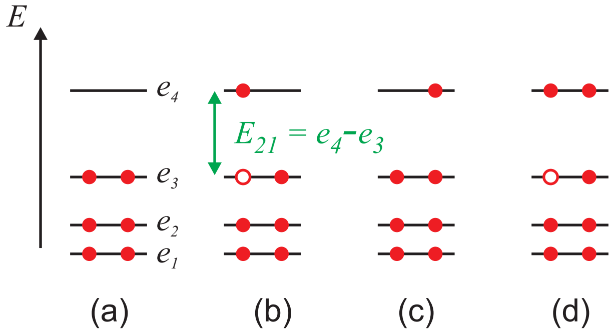


Figure 7.1: (a) The ground state and (b) the first excited state of N particles in a box when N is even; and, (c) ground state and (d) first excited state when N is odd.

The n^{th} eigenenergy of a single particle in a box of length a_0 is given by

$$e_n = \frac{n^2 \pi^2 \hbar^2}{2 m a_0^2}, \tag{7.1}$$

where we use the lowercase symbol for energy to denote a one-particle state and $n = 1$ is the single-particle ground state. Figure 7.1 shows a diagram of the electrons in the system's ground state and first excited state. In this example, since the electrons are non-interacting, $E_{21} = e_3 - e_4$ for both cases shown.

The sums in Equation 5.3 are over the filled states. Pauli exclusion demands that two electrons in the same single-electron state must be of opposite spin. This is imposed with the definition

$$|n\rangle = \begin{cases} \left|\frac{n+1}{2}, +\right\rangle & \text{for } n \text{ odd} \\ \left|\frac{n}{2}, -\right\rangle & \text{for } n \text{ even} \end{cases} . \tag{7.2}$$

In the ground state, then, there are two electrons in each single-particle energy eigenstate i up to the fermi energy. The pair of opposite spin states can be expressed as $|i, -\rangle$ and $|i, +\rangle$.

For the N-electron system, the highest-occupied state, n_h, is given by,

$$n_h = \begin{cases} \frac{N+1}{2} \text{ for } N \text{ odd} \\ \frac{N}{2} \text{ for } N \text{ even} \end{cases} . \tag{7.3}$$

For an even number of electrons, the lowest energy transition is the one that promotes the highest occupied electron to the first unoccupied state, as shown in Figures 7.1a and 7.1b. The situation is more complex for an odd number of electrons. For a particle in a box, the lowest-energy transition promotes the electron from the highest occupied state populated with two electrons to the state with one electron, as shown in Figures 7.1c and 7.1d. If the energy-level spacing decreases with increased energy, then the single electron in the highest-occupied state would be promoted.

Using Equation 7.3 and Equation 7.1, the energy difference for the N-electron system is given by $E_{21} = e_{n_h+1} - e_{n_h}$ for an even number of electrons and $E_{21} = e_{n_h} - e_{n_h-1}$ for an odd number of electrons, yielding

$$E_{21} = \begin{cases} \frac{(N+1)\pi^2\hbar^2}{2ma_0^2} & \text{for } N \text{ even} \\ \\ \frac{N\pi^2\hbar^2}{2ma_0^2} & \text{for } N (\neq 1) \text{ odd} \end{cases} . \tag{7.4}$$

Note that Equation 7.4 holds for $N > 1$. To calculate E_{21} for $N = 1$, simply evaluate the even case of Equation 7.4 using $N = 2$.

Substituting Equation 7.4 into Equation 6.10 yields the upper bound on the length of the box,

$$\boxed{L_{max} = \begin{cases} \frac{2}{\pi} \cdot a_0 \approx 0.64 a_0 & \text{for } N = 1 \\ \frac{2\sqrt{3}}{\pi} \sqrt{\frac{N}{N+1}} \cdot a_0 & \text{for } N \text{ even} \\ \frac{2\sqrt{3}}{\pi} \cdot a_0 \approx 1.1 a_0 & \text{for } N \neq 1 \text{ odd} \end{cases} . \quad \text{Particles in a Box Length Limits}} \tag{7.5}$$

Equation 3.3, which gives the *actual* quantum length of a single particle in a box of $L \approx 0.63 a_0$, falls a tad below the upper bound of the length $L_{max} \approx 0.64 a_0$ given by Equation 7.5. Interestingly, the even and odd electron limits both asymptote to $L_{max} \approx 1.1 a_0$ for large N, which is marginally larger than the box size a_0. As shown below, the actual quantum length falls short of these limits.

For the infinite well, the classical turning points are at the walls, well beyond the point where the probability density decreases rapidly for the case of the single electron. Thus, the quantum length for a single electron is shorter than what is expected for the classical limit.

A large number of electrons defines the classical limit, where the upper bound for the size asymptotes to a value that is slightly larger than the box size. The fact that the difference in size between the one-electron (quantum limit) and N-electron (classical limit) upper bound is within a factor of two is surprising. Mathematically, this behavior comes about because the energy difference between the ground state and first excited state scales in the large N limit in proportion to N. Thus, in the expression for the limit given by Equation 6.10, the energy denominator's growth is cancelled by the numerator.

Finally, the predicted upper bound of the length marginally exceeds the wall separation, a reasonable result because the actual size calculated is both less than the upper bounds and the wall separation.

The upper bound is determined from the actual energy difference E_{21} for a particle in a box. It is well known that multiple distinct Hamiltonians can yield the same energy spectrum, so it is possible that another quantum system may share the same energy spectrum with a particle in a box, but might be larger. However, there is no way of knowing if such a system does indeed exist. This ignorance was eloquently articulated in a paper by Kac in 1966 asking if it is possible to hear the shape of a drumhead.[9] The answer is no!

Next we consider a large box made by connecting smaller boxes together, as one would get when adding atoms to a lattice or bonds to a molecule. Figure 7.2a shows an energy-level diagram for the unit cell with one particle in its ground state and Figure 7.2b shows the first excited state. As in the case of the previous problem with fixed wall spacing, the energy difference between these to states is given by $E_{21} = e_2 - e_1$.

Each of these building blocks when placed end-to-end add both length and electrons. If each electron remains confined to its own cell, the length of the object is simply given by the quantum length of the cell multiplied by the number of cells. We later show that such classical additivity holds in the quantum limit. Alternatively, if all electrons are delocalized over the full length as unit cells are added, the system retains its quantum coherence into the classical regime.

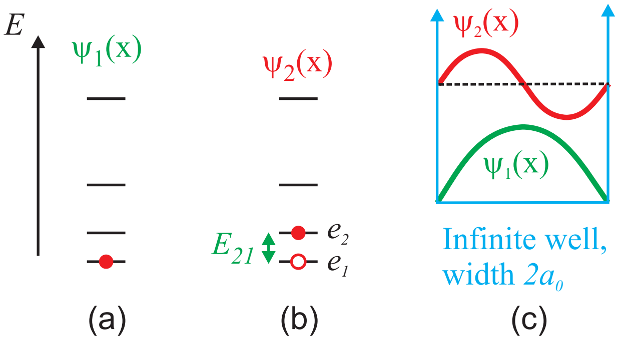


Figure 7.2: (a) The energy-level diagram of the ground state of a particle in a box, (b) the first excited state, and (c) the two lowest-energy eigenfunctions.

We treat this quantum case first and later consider the parsing of a ruler.

We will be evaluating matrix elements of the form $\langle n| f(x) |m\rangle$, where $f(x) = x$ and $f(x) = x^2$. When n is even and m is odd, the matrix elements can be expressed in terms of integers p and q, yielding,

$$\langle 2p| f(x) |2q+1\rangle = \langle p| f(x) |q\rangle \langle +| -\rangle = 0, \tag{7.6}$$

where we have used Equation 7.2. As such, the matrix elements of any function of the operator x vanishes when evaluated between an even and odd quantum number of the one-electron states because those correspond to opposite spins.

Assuming that there is one electron per unit cell (or per bond), and that the size of the unit cell is a_0, the ground and first excited state configurations are shown in Figure 7.3a for six electrons. The Pauli Exclusion principle allows two electrons per state. Since the energy spacing increases with quantum number n, the first excited state for seven electrons is the one where the electron from State 3 is excited to State 4, as shown in Figure 7.3b. Note that in this case, since adding the seventh electron makes the box larger, the energy spacing decreases. We again assume that the electrons do not otherwise interact so the energy difference for both cases is given by $E_{21} = e_4 - e_3$.

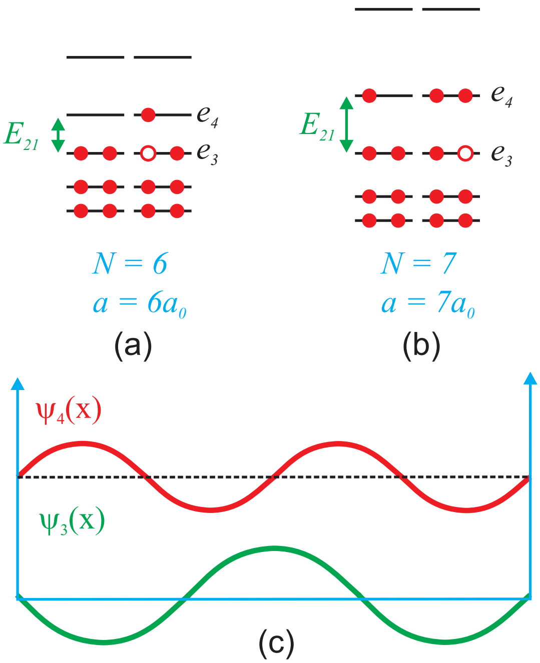


Figure 7.3: The energy-level diagrams of the ground state and first excited state of a box with (a) six electrons and (b) seven electrons. (c) A plot of the two one-particle wavefunctions at the fermi level.

This problem is identical to the case of the fixed box with the box width given by $a = Na_0$, so Equation 7.5 becomes

$$L^{\max}_{\left\{ \begin{array}{c} \text{even } N \\ \text{odd } N \end{array} \right\}} \leq Na_0 \cdot \frac{2\sqrt{3}}{\pi} \cdot \sqrt{\frac{N}{N + \frac{1}{2} \pm \frac{1}{2}}}, \tag{7.7}$$

which applies only to $N > 1$. Recall that the one-electron case is unique because the electron making the transition is simultaneously in the lowest-possible energy eigenstate and the highest occupied state. The classical limit $N \to \infty$ yields

$$L^{\max}_{N \to \infty} = \frac{2\sqrt{3}}{\pi} Na_0 \approx 1.1 Na_0, \tag{7.8}$$

in accord with the classical world; the length grows in proportion to the number of building blocks that are connected. However, the length change for each additional electron in the quantum regime varies depending on the number of electrons being even or odd.

7.1.2 Actual Quantum Length

In this section, we apply Equation 5.7 to calculate the quantum length of a particle in a box. To do so requires that we calculate $\langle n \,|\, x^2 \,|\, n \rangle$. For convenience, we place the left-hand side of the box at $x = 0$ and make it of length a, so

$$\langle n \,|\, x^2 \,|\, n \rangle = \frac{2}{a} \int_0^a dx\, x^2 \sin^2 \left(\frac{n\pi x}{a} \right). \tag{7.9}$$

Equation 7.9 can be integrated by making the trigonometric substitution $\sin^2\theta = (1 - \cos 2\theta)/2$; integrating the second term by parts, twice; and then using the fact that the sine function vanishes at the endpoints, which yields

$$\langle n \,|\, x^2 \,|\, n \rangle = a^2 \left(\frac{1}{3} - \frac{1}{2\pi^2 n^2} \right). \tag{7.10}$$

Equation 7.10 leads to the single-particle length in state n of

$$\boxed{\begin{array}{l} L_n = \sqrt{12 \left(\langle n \,|\, x^2 \,|\, n \rangle - \dfrac{a^2}{4} \right)} = a\sqrt{1 - \dfrac{6}{\pi^2 n^2}}, \\ \text{Length of a Single Particle in a Box in State } n \end{array}} \tag{7.11}$$

where we have used Equation 5.7 with $N = 1$ and $c = a/2$. Note that the excited-state length approaches the size of the box in the limit of large energy ($\lim_{n\to\infty} L_n = a$).

It is worthwhile to discuss the single-particle length of an excited state before proceeding to the many-electron case. The interpretation of the electron probability density as defining the system's size for an excited state can be analyzed as follows. Consider, for example, a particle in a box in state q, with a density as shown in Figure 7.4. Defining the average density over one period as

$$\left\langle |\psi(x)|^2 \right\rangle = \int_{x-\frac{L}{2q}}^{x+\frac{L}{2q}} |\psi(\xi)|^2 \, d\xi, \tag{7.12}$$

inside the well the density is constant if the range of integration is contained within the well and falls to zero outside the well over half a period, as shown by the dashed curve. The capped horizonal lines represent the range of integration and the points are the average density for several representative points near the left wall of the well.

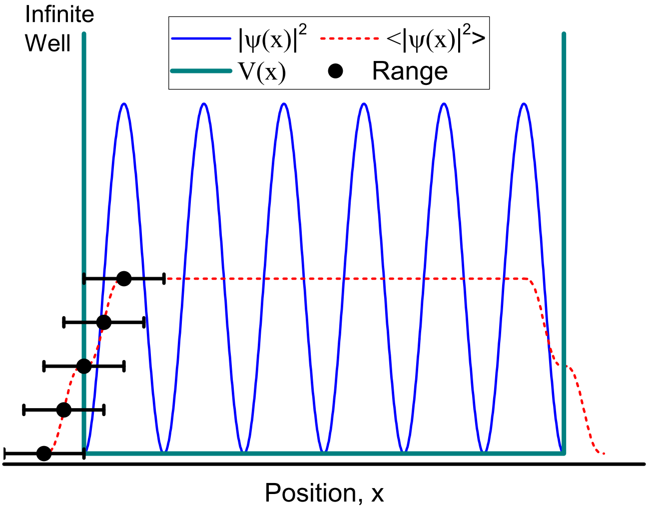


Figure 7.4: The density of a particle in a box in state $q = 6$ (solid curve) and the average density over one period (dashed curve). The horizontal lines represent the range of averaging and the points are the average values near the left wall of the well.

A higher-energy state has a wave function with more nodes than a lower energy one. Thus, at higher energies, there are many oscillations and the average density appears uniform inside the well and falls rapidly to zero at the walls, as we would expect in the classical limit. Thus, even though the microscopic view shows voids, they are not visible on macroscopic scales when the measurement resolution exceeds a period. As such, an excited state in the classical limit has uniform density and sharp edges.

Now we return to the problem at hand of calculating the length of the many particle ground sate. Substituting Equation 7.10 into Equation 5.7 and using the fact that the square well is a centrosymmetric potential centered at $a/2$ yields

$$\boxed{\begin{array}{c} L_N^2 = a^2 \left(1 - \frac{12}{\pi^2 N} \sum_{n=1}^{N/2} \frac{1}{n^2} \right). \\ \text{Length of N-particles in a box} \end{array}} \tag{7.13}$$

Here we have assumed that there are an even number of electrons and two electrons occupy each of the lowest-energy states. Equation 7.13 in the two-electron limit agrees with Equation 3.3. In the classical limit with many electrons, Equation 7.13 gives

$$\lim_{N\to\infty} L_N = \lim_{N\to\infty} a \sqrt{\left(1 - \frac{2}{N}\right)} = a, \tag{7.14}$$

where we have used the fact that $\sum_{n=1}^{\infty} n^{-2} = \pi^2/6$. This size, determined form the electron cloud, equals the distance between the classical turning points and the length is below the limits given by Equation 7.5.

If instead we build a system by adding electrons as we did in the calculations of the limits in Chapter 7.1.1, we make the substitution $a = a_0 N$ in Equation 7.13, and the length of the box for $N \to \infty$ asymptotically approaches $N a_0$. Again, the asymptote is given by the distance between the classical turning points.

7.1.3 Electron Density

The probability density from Equation 4.12 gives

$$\rho(x) = |\psi(x)|^2 = \frac{1}{N} \sum_{n=1}^{N} |\psi_n(x)|^2 . \tag{7.15}$$

Figure 7.5 shows a plot of the electron density as a function of position within a box of width a. Shown are electron densities for 2, 6, 18, 54, and 400 electrons; which fill states up to 1,3, 9, 27, 200 (2 electrons per state). This plot makes clear how the density becomes uniform and the edges sharp in the classical limit where the number of particles becomes large.

Figure 7.6 shows a plot of the electron density as a function of position inside a box using the same parameters as in Figure 7.5,

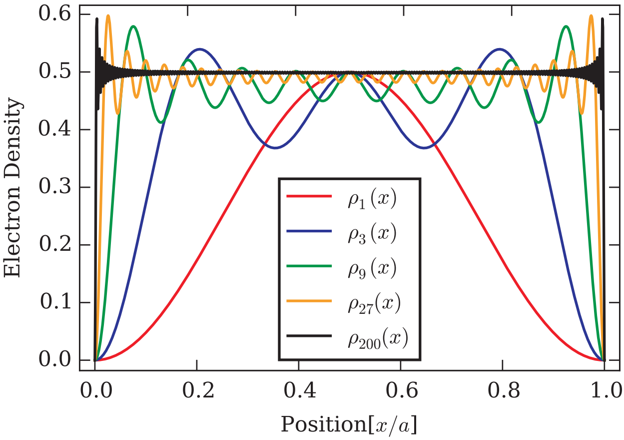


Figure 7.5: The electron density in a box as a function of the highest occupied state n =1, 3, 9, 27, and 200. In the classical limit, where the number of electrons becomes large, a uniform probability density with sharp edges is observed.

except the ground state is unoccupied. As a result, the electron density for small numbers of electrons is distorted so that it sags at the object's middle. However, a missing electron has little effect in the classical limit. The electron density is thus robust to missing electrons for an object with a large numbers of electrons.

Equation 7.5 is reminiscent of a mixed state – one that is viewed in terms of population fractions of separate particles rather than originating from an entangled state as represented by Equation 4.8. The density operator for a mixed state with N electrons populating N different states with equal probability is

$$\rho = \frac{1}{N} \sum_{n=1}^{N} |n\rangle \langle n| , \tag{7.16}$$

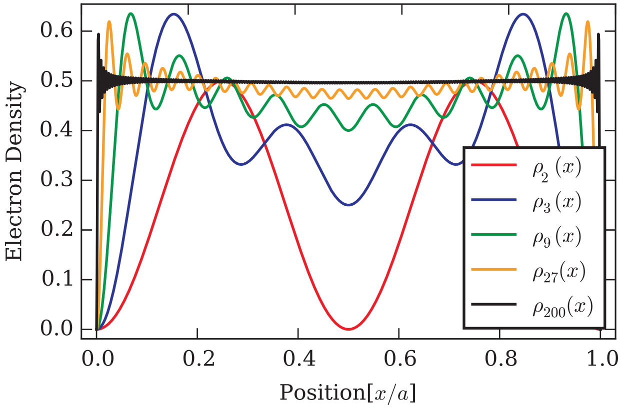


Figure 7.6: The electron density in a box as a function of the highest-occupied state n =2, 3, 9, 27, and 200 where the ground state is unoccupied.

which gives the electron density

$$\begin{aligned} \rho(x) \equiv \rho(x,x) &= \langle x \,|\, \rho \,|\, x \rangle = \frac{1}{N} \sum_{n=1}^{N} \langle x \,|\, n \rangle \langle n \,|\, x \rangle \\ &= \frac{1}{N} \sum_{n=1}^{N} |\psi_n(x)|^2 \,, \end{aligned} \tag{7.17}$$

the same as Equation 7.15.

The quantum entangled state and the mixed state represent very different objects. The entangled state is a pure quantum state in which the entanglement between all the electrons manifests in the state vector changing sign when any two electrons are interchanged. The density matrix, on the other hand, might for example represent N independent particles that are each in a different energy eigenstate. This smells of a classical system, where the particles are not entangled, as we see from the position matrix elements of the density matrix, which are not antisymmetric upon interchanging any two particles. So these two very different systems happen to give the same density.

The density operator given by Equation 7.16 is a very specific one, where the population of particles is equally distributed amongst the N states. More complex density operators are possible, which have distinct diagonal matrix elements as well as off-diagonal ones. Let's see if we can construct an N-particle system that gives the same result as would a density matrix. As we show below, we can construct a wave function to match any kind of density matrix with a superposition of states. What do such systems represent?

When electrons interact, the state vectors are more difficult to determine. However, without solving the problem, we know that the normalized ground state wave function can be expressed as a superposition of noninteracting state vectors of the form

$$|G\rangle = \sum_{n_1,\ldots,n_N} c_{n_1,\ldots,n_N} \left|n_1,\ldots,n_N\right\rangle, \tag{7.18}$$

where the sum is restricted to indices that are all distinct from each other.

The electron density calculated from Equation 7.18 as was done with Equation 4.6 yields

$$\rho(x) = \left|\langle x_1 \,|\, G\rangle\right|^2 = \left|\sum_{n_1,\ldots,n_N} c_{n_1,\ldots,N_n} \langle x \,|\, n_1\rangle \left|n_2,\ldots,n_N\right\rangle\right|^2, \tag{7.19}$$

where we use the fact that x is the same as x_1. Evaluating Equation 7.19 yields

$$\rho(x) = \sum_{n_1 n'_1} \sum_{n_2,\ldots,n_N} c^*_{n'_1,n_2\ldots,N_n} c_{n_1,n_2\ldots,N_n} \psi^*_{n'_1}(x)\psi_{n_1}(x), \tag{7.20}$$

where we have used that fact that states $|n_2,\ldots,n_N\rangle$ are orthonormal so the inner product between two such states vanishes unless all the same states are occupied in each. Defining

$$\rho_{n'_1,n_1} = \sum_{n_2,\ldots,n_N} c^*_{n'_1,n_2\ldots,N_n} c_{n_1,n_2\ldots,N_n}, \tag{7.21}$$

Equation 7.20 can be expressed as

$$\rho(x) = \sum_{n_1 n'_1} \rho_{n'_1,n_1} \psi^*_{n'_1}(x)\psi_{n_1}(x). \tag{7.22}$$

Equation 7.22 has the general form of a density matrix, where the coefficients depend on the interaction potentials between the electrons.

We interpreted Equation 7.16 in terms of classical populations, as do many textbooks. Landau, one of the earlier developers of the density matrix had this to say[10] "*The averaging by means of the statistical matrix* [this is his term for the more modern density matrix] ... *has a twofold nature. It comprises both the averaging due to the probabilistic nature of the quantum description (even when as compete as possible) and the statistical averaging necessitated by the incompleteness of our information concerning the object considered. Fore a pure state only the first averaging remains, but in the statistical cases both types of averaging are always present. It must be borne in mind, however, that these constituents cannot be separated; the whole averaging procedure is carried out as a single operation, and* **cannot be represented as the result of successive averaging, one purely quantum-mechanical and the other purely statistical**.)" The emphasis is mine to stress the importance of this last clause.

In calculating the probability density with the inner product of the position state vector of Particle #1 with the full state vector, we are using quantum mechanics in a single step. Alternatively, we might consider Particle #1 as the "system" and the rest of the particles as the "environment." Then we might treat the environment in some averaged way to get the density matrix without complete knowledge of the details. Landau is saying that quantum mechanics is the fundamental theory of nature. The density matrix appears along the way to calculating the length. This magical transition to a density matrix originates in the quantum probability density being calculable from the density of one specific electron. This transition can be scrutinized to understand how the two views are reconcilable.

7.2 Harmonic Oscillator

The harmonic oscillator is a unique system by virtue of the fact that the eigenenergies are equally spaced, so that

$$E_{21} = \hbar\omega, \tag{7.23}$$

where ω is the natural frequency of oscillation. This energy difference is the same for any pair of energetically adjacent eigenstates.

The position operator is given by

$$x = \sqrt{\frac{\hbar}{2m\omega}} \left(a + a^\dagger\right), \tag{7.24}$$

where a and $a^\dagger$ are the lowering and raising operators with the action $a\,|n\rangle = \sqrt{n-1}\,|n-1\rangle$ and $a^\dagger\,|n\rangle = \sqrt{n}\,|n+1\rangle$, where $|n\rangle$ is the n^{th} energy eigenvector. Note that we are using the unconventional notation that the ground state vector is $|1\rangle$ to make this book self consistent throughout. Then

$$\langle n|\, x\, |q\rangle = \sqrt{\frac{\hbar}{2m\omega}} \left(\sqrt{q-1}\delta_{n,q-1} + \sqrt{q}\delta_{n,q+1}\right), \tag{7.25}$$

and

$$\langle n|\, x^2\, |n\rangle = \frac{\hbar}{2m\omega}\left(2n-1\right). \tag{7.26}$$

Using Equation 5.3 for the quantum length, Equation 7.26 leads to

$$\boxed{\begin{array}{l} L_n = \sqrt{\dfrac{6\hbar}{m\omega}\,(2n-1)}. \\ \text{Excited State Length of Single Particle} \\ \text{Harmonic Oscilator in State } n \end{array}} \tag{7.27}$$

Unlike the particle in a box, a particle in a harmonic potential cannot be localized by sharp boundaries, so we use the turning points instead as an estimate of its size, which is determined from the two points in the particle's trajectory where the velocity vanishes. The zero-velocity condition for state n is met when the kinetic energy vanishes, leaving only potential energy, or

$$\hbar\omega(n - 1/2) = \frac{1}{2}m\omega^2 x_0^2(n). \tag{7.28}$$

We can then think of the distance between turning points as the classical length since the particle is confined to this region, and is calculated from Equation 7.28 to yield

$$\boxed{\begin{array}{l} L_n = 2x_0(n) = \sqrt{\dfrac{4\hbar}{m\omega}\,(2n-1)}. \\ \text{Distance Between Turning Points in a} \\ \text{Single-Particle Harmonic Oscillator in State } n \end{array}} \tag{7.29}$$

A comparison of Equation 7.29 and Equation 7.27 shows that the turning point separation and the quantum length of an excited state scales in the same way, but the quantum length is larger by $\sqrt{3/2}$. In contrast, the walls of an infinite well are the classical turning points, which also define the length in the limit of the many particle system.

Using Equation 6.14 for the excited state length, and recalling that the position operator connects only adjacent states, for one electron, we get

$$\frac{L_q^2}{12} \leq \frac{\hbar^2}{2mE_{q+1,q}} + \langle q|\, x \,|q-1\rangle \langle q-1|\, x \,|q\rangle \frac{E_{q+1,q-1}}{E_{q+1,q}}. \tag{7.30}$$

Evaluating the position matrix elements and the energies, we get

$$L_q \leq \sqrt{\frac{6\hbar}{m\omega}(2q-1)}. \tag{7.31}$$

Thus, the harmonic oscillator in an excited state, as given by Equation 7.27, is at its length limit.

This all meets with our classical expectations when we consider the classical turning points as a rough estimate of the length of a harmonic oscillator, which is defined by Equation 7.29.

7.2.1 Length Limit

The length limit for non-interacting electrons is calculated using Equation 7.23 with Equation 6.9, yielding

$$\boxed{L_{HO}^{\text{max}} = \sqrt{\frac{6\hbar N}{m\omega}}. \text{ N-Particle Harmonic Oscilator Length Limit}} \tag{7.32}$$

The particle in the highest-occupied state will have the largest oscillation amplitude. The fermi energy indexed by state number n corresponds to the highest occupied state, where $n = N/2$ for N even and $n = (N+1)/2$, for N odd, which using Equation 7.29 yields a distance between turning points of

$$\boxed{\begin{array}{l} L_N = 2x_0(N) = \begin{cases} \sqrt{\frac{4\hbar}{m\omega}N} & \text{for } N \text{ odd} \\ \\ \sqrt{\frac{4\hbar}{m\omega}(N-1)} & \text{for } N \text{ even} \end{cases} \\ \text{N-Particle Harmonic Oscilator Turning Point Length} \end{array}} \tag{7.33}$$

The length given by Equation 7.33 falls below the predicted length limit given by Equation 7.32, which for one electron or large N asymptotes to

$$\lim_{N\to\infty} \frac{L_N}{L_{HO}^{max}} = \lim_{N\to\infty} \sqrt{\frac{4N}{6N}} = \sqrt{\frac{2}{3}} = 0.82. \tag{7.34}$$

The quantum mechanical length limit of a harmonic oscillator exceeds the distance between turning points, as it should because the wave functions extend beyond the classical turning points. As for particles in a box, the quantum length for an even number of particles differs from the classical limit for a small number of electrons, and an even number of particles give a slightly different length per added particle. Finally, whereas the length of the electron cloud is constant in the classical limit of the fixed box size and increases as N with the number of electrons when unit cells are added, the harmonic oscillator length limit increases as $\sqrt{N}$.

7.2.2 Actual Quantum Length

Here, we determine the length of the harmonic oscillator using Equation 5.7. Since the coordinate system of the harmonic oscillator is centered at the symmetry point, $c = 0$ in Equation 5.7, so we need only to determine $\langle n \,|\, x^2 \,|\, n \rangle$.

Substituting Equation 7.26 into Equation 5.7 yields

$$L^2 = 12 \cdot \frac{1}{N} \cdot \sum_{n=1}^{N} \frac{\hbar}{2m\omega} \left(2n - 1\right). \tag{7.35}$$

The upper limit of the sum is given by the energy eigenstate indexed by n_h from Equation 7.3, the highest-occupied single-particle state.

If the highest occupied state is n_h, the sum in Equation 7.35 can be evaluated using Equation 7.26. For an even number of electrons, we get

$$\Sigma = 2 \cdot \sum_{n=1}^{n_h} (2n - 1) = 2n_h^2, \tag{7.36}$$

where the perfector of 2 accounts for the fact that there are 2 electrons in each state. Using Equation 7.3, for an even number of electrons, the sum in Equation 7.36 is

$$\Sigma_{even} = \frac{N^2}{2}. \tag{7.37}$$

For an odd number of electrons one of the spins occupies state n_h while the other spins occupy up to state $n_h - 1$. Thus, the sum splits into two parts:

$$\begin{aligned} \Sigma_{odd} &= \sum_{n=1}^{n_h}(2n-1) + \sum_{n=1}^{n_h-1}(2n-1) \\ &= (n_h - 1)^2 + n_h^2. \end{aligned} \tag{7.38}$$

Substituting Equation 7.3 into Equation 7.38 yields,

$$\Sigma_{odd} = \frac{N^2+1}{2}. \tag{7.39}$$

Summing Equation 7.26 with the help of Equations 7.37 and 7.39 yields

$$\sum_{n=1}^{\text{filled}} \langle n|\, x^2 \,|n\rangle = \begin{cases} \frac{\hbar(N^2+1)}{4m\omega} & \text{for } N \text{ odd} \\ \\ \frac{\hbar N^2}{4m\omega} & \text{for } N \text{ even.} \end{cases} \tag{7.40}$$

Substituting Equation 7.40 into Equation 7.35 yields the quantum length

$$\boxed{L = \sqrt{\frac{3\hbar}{m\omega}} \begin{cases} \sqrt{N + 1/N} & \text{for } N \text{ odd} \\ \\ \sqrt{N} & \text{for } N \text{ even.} \end{cases}} \tag{7.41}$$

N-Particle Harmonic Oscilator Length

Comparing Equation 7.41 with the upper limit given by Equation 7.32, we find that with $N = 1$ and $N = 2$, the actual length is at the upper bound but in the classical limit, the actual length asymptotes to $1/\sqrt{2}$ of the limit.

7.2.3 Electron Density

Figure 7.7 shows a plot of the probability density of a harmonic oscillator as a function of position normalized to the ground state turning

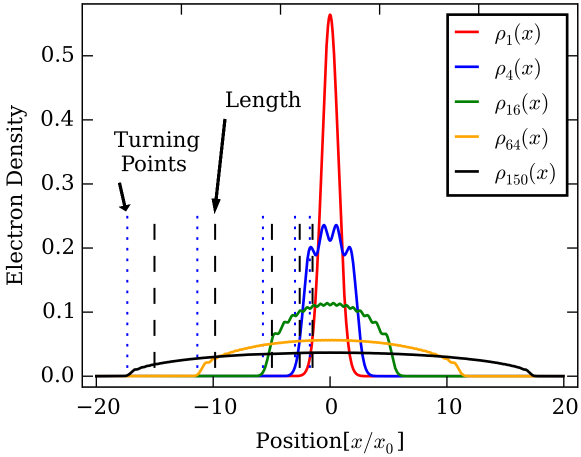


Figure 7.7: The electron density in a harmonic oscillator with highest occupied state number n =1, 4, 16, 64, and 150. In the classical limit, where the number of electrons becomes large, a smooth probability density develops. The vertical dotted lines give the classical turning points of the highest-occupied state and the dashed lines the edge as determined from the length calculation.

point when filled with one to 300 electrons. The plots are labelled by highest occupied state. The dotted vertical lines show the locations of the classical turning points as determined from Equation 7.23 and the position is normalized to the ground state turning point. The vertical dashed lines show the position of the edge of the oscillator as determined from the length calculation given by Equation 7.41. Both the quantum length and turning point lie within the calculated upper bound of the length.

For a few electrons, the probability density shows oscillations, but in the classical limit, the electron distribution becomes smooth and flat in the middle. The turning points defined by the highest occupied state straddle most of the electron density and the calculated length defines a region where the electron density is flat. This central flat region becomes wider in proportion to $\sqrt{N}$ as more electrons are added.

Chapter 8

Bosons

Let's next consider a system made of noninteracting bosons. Since the state vector is symmetric upon interchange of any two particles, the ground state is the one where all N particles occupy the single-particle ground state, or

$$|G\rangle = |1, 1, \ldots 1\rangle . \tag{8.1}$$

The upper bound for the length of a bosonic system is then given by Equation 6.10 with $E_{21} = e_{21}$, i.e. the single-particle energy difference represents the many-electron system's energy difference, or

$$L \leq \sqrt{\frac{6\hbar^2 N}{m e_{21}}}. \tag{8.2}$$

For a system with e_{21} equal to that of a particle in a box as given by Equation 7.1, Equation 8.2 gives a length limit of

$$L_{box} \leq \frac{2a}{\pi}\sqrt{N}. \tag{8.3}$$

This result disagrees with Equation 7.5 for fermions. Recall that for the particle in a box, the fermion upper limit gives a length that is less than the wall spacing for one particle and converges to a length about 10% larger than the separation between the walls in the classical limit. In contrast, the upper bound for the length of a material made of bosons increases without bound in proportion to $\sqrt{N}$. Thus, the length of a system of fermions with the energy spectrum of a box cannot increase as electrons are added, but a system of bosons might do so.

The actual length of a system of non-interacting bosons in a box is simple to compute using the single-particle method with the wave function given by Equation 8.1, yielding

$$L_{box} = a\sqrt{1 - \frac{6}{\pi^2}}, \tag{8.4}$$

which is independent of the number of bosons. Therefore, the actual length of the box is just a couple percent smaller than the length limit give by Equation 8.3 with $N = 1$. For a system of fermions in a box, the actual length for one particle is the same as for a boson, but increases when fermions are added, and converges to the distance between the walls.

For a harmonic oscillator energy spectrum, the length limit for N bosons is given by

$$L_{HO} \leq \sqrt{\frac{6\hbar N}{m\omega}}. \tag{8.5}$$

Equation 8.5 agrees with the fermion length limit as given by Equation 7.32. This is due to the fact that the energies are equally spaced, so the excitation energy is independent of the highest-energy occupied state.

The density of Particle 1 of the ground state of a collection of Bosons is given by

$$\rho(x_1) = \left|\langle x_1 \,|\, G\rangle\right|^2 = \left|\langle x_1 \,|\, 1, 1, \ldots 1\rangle\right|^2 = \left|\psi_1(x_1)\right|^2. \tag{8.6}$$

Thus, it is not surprising that the quantum length of the many-particle system of bosons in their ground state is the same as the single-particle result for any system. For a harmonic oscillator well filled with Bosons, the upper bound grows as $\sqrt{N}$ but the actual length remains constant as a function of the number of electrons, as it did for a particle in a box.

We saw for fermions that the particle density function in the large-particle-number limit approaches a step function for a particle in a box and is also flat near the origin for the harmonic oscillator. For bosons, the particle densities for the box and the harmonic oscillator potential are peaked functions, and the shape is independent of the number of particles. This behavior contradicts our intuition of how a system should behave because the materials with which we interact are are made of fermions. In a world of bosons, rulers would not have sharp ends so length would no longer have meaning in the classical limit.

Note that we could in principle construct a boson state vector that is of the same form as the fermion state vector given by Equation 4.9 except that the alternating signs given by the slater determinant for fermions are all positive signs for the bosons. Then, it is easy to show that the single-particle approach gives the same length for bosons as for fermions since the signs do not change the result. Then, the bosonic system would behave as we expect in the classical limit, making rulers with sharp boundaries. But, the system would be in an excited state. So, bosons can be prepared in a way that makes their classical limit appear fermion-like; but fermions cannot be prepared in a state that mimics bosons because of Pauli exclusion.

Chapter 9

Coherent States

A coherent state is described by the state vector $|\alpha\rangle$, which is an eigenstate of the annihilation operator a, or

$$a\,|\alpha\rangle = \alpha\,|\alpha\rangle \tag{9.1}$$

with complex eigenvalue α. Note that coherent states are useful for describing photons but are applicable to material systems, and were in fact originally studied by Schrödinger for the harmonic oscillator.[11] A coherent state is given by

$$\begin{aligned} |\alpha\rangle \qquad &= e^{i\delta} e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}}\,|n\rangle \\ &= e^{i\delta} e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{\alpha^n \left(a^\dagger\right)^n}{n!}\,|0\rangle \\ &= e^{i\delta - |\alpha|^2/2 + \alpha a^\dagger}\,|0\rangle\,, \end{aligned} \tag{9.2}$$

where δ is an arbitrary global phase that can be selected for convenience. The student can easily verify that Equation 9.2 is a coherent state by evaluating Equation 9.1. Note that we are here using the more common notation that $|0\rangle$ is the ground state. We do so only in this section.

The coherent state has been constructed so that the annihilation operator has the eigenvalue α; so, the expectation value of the annihilation operator is obviously given by

$$\langle \alpha\,|\,a\,|\,\alpha\rangle = \alpha \tag{9.3}$$

and the expectation value of the creation operator is then given by

$$\left\langle \alpha \,\middle|\, a^\dagger \,\middle|\, \alpha \right\rangle = \langle \alpha \,|\, a \,|\, \alpha \rangle^* = \alpha^*. \tag{9.4}$$

Similar manipulations trivially yield

$$\left\langle \alpha \,\middle|\, (a^\dagger)^n a^m \,\middle|\, \alpha \right\rangle = (\alpha^*)^n \alpha^m. \tag{9.5}$$

Coherent states are normalized but not orthonormal, with

$$\langle \alpha \,|\, \beta \rangle = e^{-(|\alpha|^2+|\beta|^2)/2} e^{\alpha^* \beta}. \tag{9.6}$$

A coherent state is an example of a very special kind of superposition of sates that gives the minimum uncertainty product $\Delta x \Delta p$. We start by calculating the single-particle length. The expectation of the position of a particle in a harmonic well is given by

$$\langle \alpha \,|\, x \,|\, \alpha \rangle = \sqrt{\frac{\hbar}{2m\omega}} \left\langle \alpha \,\middle|\, a + a^\dagger \,\middle|\, \alpha \right\rangle = \sqrt{\frac{\hbar}{2m\omega}} \Big(\alpha + \alpha^* \Big) \tag{9.7}$$

and the expectation of the square of the position is

$$\begin{aligned} \left\langle \alpha \,\middle|\, x^2 \,\middle|\, \alpha \right\rangle \quad &= \frac{\hbar}{2m\omega} \left\langle \alpha \,\middle|\, a^2 + \left(a^\dagger\right)^2 + 2a^\dagger a + 1 \,\middle|\, \alpha \right\rangle \\ &= \frac{\hbar}{2m\omega} \Big(\alpha^2 + (\alpha^*)^2 + 2\,|\alpha|^2 + 1 \Big). \end{aligned} \tag{9.8}$$

Using the definition of length given by Equation 2.4, the length of the coherent state in state $|\alpha\rangle$ is calculated using Equation 9.7 and 9.8, and is given by

$$L_\alpha = \sqrt{\frac{6\hbar}{m\omega}}. \tag{9.9}$$

The length is independent of the eigenvalue α of the state and is just above the distance between the classical turning points of the ground state.

To understand this result, recall that Equation 7.29 gives the length of a harmonic oscillator in state n as the distance distance between the classical turning points. The expectation value of energy of a coherent state is given by

$$\langle \alpha \,|\, H \,|\, \alpha \rangle = \hbar\omega \left\langle \alpha \,\middle|\, a^\dagger a + 1/2 \,\middle|\, \alpha \right\rangle = \hbar\omega(\alpha^* \alpha + 1/2). \tag{9.10}$$

Setting the energy to the potential energy at the turning point yields

$$\boxed{\begin{array}{l} L'_\alpha = 2x_0(n) = \sqrt{\dfrac{4\hbar}{m\omega}\,(2\alpha^*\alpha - 1)}. \\ \text{Distance Between Turning Points in a Single-} \\ \text{Particle Harmonic Oscilator Coherent State } |\alpha\rangle \end{array}} \tag{9.11}$$

Equation 9.9 shows that the length of the coherent state is independent of α but the distance between turning points given by Equation 9.11 does. Since the coherent state is a localized wave packet that resembles a particle, the length given by Equation 9.9 is the width of the wave packet and is thus the size of the particle itself. The distance between turning points, on the other hand, is the excursion amplitude of the particle in the harmonic well. This example serves to show that the general length definition $\sqrt{12}\Delta x$ gives the wave packet's width, which describes the size of the particle. The distance between the turning points is only an estimate of the length when the wave function is delocalized over the well, as it is when a single particle is in an excited state – as given by Equation 7.27, or when many particle are in the ground state – as given by Equation 7.41.

Clearly, one can construct a fully antisymmetrized state vector for several particles, each in a coherent state. The length of this system of particles will be a complicated function of the motions of the particles, and might lead to interesting behavior, but is beyond the scope of this book.

Chapter 10

Discussion

This Chapter focuses on the use of a ruler, the ramifications of making subdivisions, its accuracy, and the implications of entanglement between a ruler and the object being measured. A boson ruler is also discussed.

10.1 Rulers

There is a connection between a measure of length with a line of stones and the spread of a quantum mechanical electron cloud. Figure 10.1 shows a length determined by the congruence of the ends of the object and the number of identical stones that fit between its ends. Doing so requires that the object be well-enough defined to locate its edges.

A ruler operates on the same principle. Rather than making lots of small identical rods, a single object is marked at uniform intervals to signify the points of contact of a stack of many tiny rods of equal length. If the markings are to be resolvable, the de Broglie wavelength of the electrons in the ruler material must be shorter than the width of the markings. Otherwise, the markings would not indiscernible. Thus, a ruler with markings must obey the same quantum physics as a stack of rods with localized electrons in each one. We choose to use a stack of rods as the paradigm for ruler segments, each represented by electrons in a box, and separated by a quantum length.

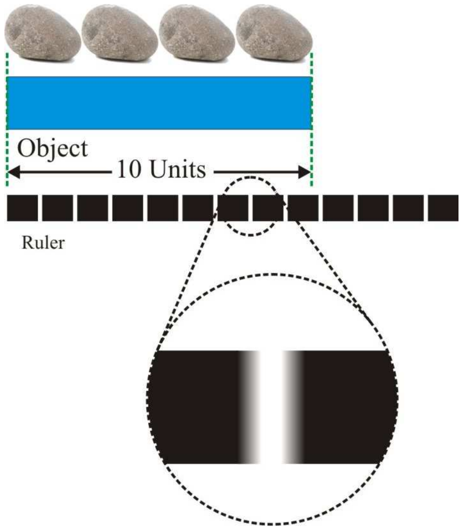


Figure 10.1: An object's length determined using it's equivalence in number of stones; and using a ruler made of small pieces or a single piece with markings.

The bottom portion of Figure 10.1 shows a ruler and a magnified view of the point of contact. We will assume that the length of a segment is given by its quantum length and when stacked, the overall length is given by the sum of the individual segment lengths. This property of additivity applies when the electrons are delocalized only over each small segment. If the electrons are delocalized over the whole rod, it would behave as a single unit rather than a composite of parts, and no demarcations would be defined – making it useless as a ruler.

Consider a rod of length L that is determined to be of the same size as the object that is being measured. When the electrons are delocalized over the rod, we model it as particles in a single large box that is made of N unit cells each of length a_0 and each contributing one electron, for a total of N electrons. The length of the N-electron box is given by the spread of the electron density. In the limit of many electrons, the length is $L = Na_0$, which coincides with the walls of the full box. The length of a unit cell in isolation, which contains one electron, is given by Equation 3.3.

Next, we divide the rod into R equal cells, where $R \leq N$, to construct a ruler where the contact points between the segments define the markings of the ruler. We assume that the electrons are localized in their own segments; and, when the segments are pressed together, the length will be the sum of the quantum lengths of the segments, an assumption we treat later.

Using Equation 7.13, the length of one segment is

$$\Delta L_R(N) = \sqrt{\frac{(Na_0/R)^2}{(N/R)/2} \sum_{n=1}^{N/2R} \left(1 - \frac{6}{\pi^2 n^2}\right)}, \tag{10.1}$$

where we have used $N \to N/R$ and $a = Na_0/R$. Thus, the box size defining the rulings decreases in proportion to R. Obviously N/R must be an integer since unit cells cannot be subdivided. The length of the rulings is then given by $L_R = R\Delta L_R$, which using Equation 10.1 yields

$$L_R(N) = a_0 N \sqrt{1 - \frac{12}{\pi^2} \cdot \frac{R}{N} \cdot \sum_{n=1}^{N/2R} \frac{1}{n^2}}, \tag{10.2}$$

where we have used the fact that $\sum_1^{N/2R} 1 = N/2R$ to evaluate the first term in the parentheses in Equation 10.1. When $R = 1$ and N is large, Equation 10.2 gives the length $L_R = Na_0$, as we would expect for a rod with N unit cells.

For ruler segments of unit cell size with one electron in each, the ruler's length is

$$L_{R=N}(N) = a_0 N \sqrt{1 - \frac{6}{\pi^2}} \approx 0.63 a_0 N. \tag{10.3}$$

Thus, chopping the ruler into the smallest possible segments and recombining them makes the ruler over a third shorter than its monolithic form. Using the classical assumption that the length remains constant under such an operation would lead to an overestimate of the length of the object that is being measured.

An interesting artifact of chopping a rod into segments is that the process leads to a change in the energy of the rod. The ground state energy of the rod with fully delocalized electrons is given by

$$E_G = 2\sum_{n=1}^{N/2} \frac{h^2 n^2}{8mN^2 a_0^2} = \frac{h^2(N+2)(N+1)N}{96mN^2a_0^2}. \tag{10.4}$$

The ground state energy of the R segments after cutting is given by

$$E'_G = 2R\sum_{n=1}^{N/2R} \frac{h^2 R^2 n^2}{8mN^2 a_0^2} = \frac{h^2(N+2R)(N+R)N}{96mN^2a_0^2}. \tag{10.5}$$

The reader can easily verify that in the limiting case where $R = 1$, the ruler is whole and Equation 10.5 is the same as Equation 10.4. If the ruler is cut into its smallest possible parts, $R = N$ and $E'_G/E_G = 6$ when $N \to \infty$. Thus, the net amount of work done in cutting up the ruler is five times the ground state energy of the single rod.

10.2 Ruler Reliability

Next we consider a user of a ruler who assumes that its length is independent of the number of subdivisions, as would be the case within the realm of common experience. As long as the classical limit is maintained, the precision of the measurement increases as more rulings are made. Since the object being measured is large and behaves classically, it's edges are sharp and can be located to within one division, or L/R, the spacing between markings. However, as the rulings are made closer together and quantum effects take hold, the systematic overestimate of the object's length grows.

The length measurement is most true when the increase in resolution from making smaller segments is offset by the greater overestimate of the object's length – the condition given by $Na_0 - L_R(N) = Na_0/R$. Using Equation 10.2, this condition gives,

$$1 - \sqrt{1 - \frac{12}{\pi^2}\cdot\frac{R}{N}\cdot\sum_{n=1}^{N/2R}\frac{1}{n^2}} = \frac{1}{R}. \tag{10.6}$$

If R/N is small, the second term under the square root in Equation 10.6 is necessarily small. Since the sum converges to $\pi^6/6$ for an infinite number of terms, the second term can be approximated by this value is $2R/N \ll 1$. Then, the square root can be expanded in a series with R/N small, giving the condition

$$\boxed{\begin{array}{l} R = \sqrt{N} = \sqrt{L/a_0}. \\ \text{Ideal Number of Rulings} \\ \text{for Maximum Accuracy} \\ \Delta L = \dfrac{L}{R} = \sqrt{a_0 L} \\ \text{Optimum Size of Rulings} \end{array}} \qquad (10.7)$$

Thus, for a ruler of 10 cm length made of a material with lattice constant $a_0 = 1\text{Å}$, the most accurate resolution is for $3\,\mu m$ rulings.

These results may seem suspicious given that optical microscopes have a resolution of 1 μm and electron microscopes are much better than that. The reason is that here we are dealing with a single line of atoms. Most objects are much thicker than that, so ones gets added precisions from the statistics of adding together many side-by-side rulers.

10.3 Classical Versus Quantum Parsing

We have calculated the length of a single ruler and of the individual sections quantum mechanically. However, when combining the sections, we are using the classical notion of the length, that is, the ruler length is taken to be the sum of the pieces. This requires that two issues be resolved. First, the assumption that the ruler segments can be stacked as if each piece is of the calculated quantum length leads to an overlap in the wave functions between them. This is of no consequence if the electrons are noninteracting, as we have assumed from the start. A second more interesting issue is that the classical construction ignores the requirement that the ruler segments must remain entangled.

To avoid undue complexity, we consider a ruler with N electrons and N segments with one electron per segment. Then, in the global ground state, each segment will also be found in it's ground state. If the single-particle ground statevector of the i^{th} segment containing one electron is designated by $\left|1^{(i)}\right\rangle$, the fully antisymmetric entangled state vector of the segmented ruler is given by

$$|G\rangle = \frac{1}{\sqrt{N}} \sum_{i=1}^{N} \left|1^{(i)}\right\rangle \left|\overline{1^{(i)}}\right\rangle . \tag{10.8}$$

The decomposition given by Equation 10.8 is analogous to Equation 4.11, but rather than forming an entanglement of single particle states of different energies, the energies are the same and the entanglement is between the spatially-separated segments.

Using Equation 10.8 to get the probability density yields

$$\rho(x_1) = \left| \frac{1}{\sqrt{N}} \sum_{i=1}^{N} \left\langle x_1 \,\middle|\, 1^{(i)} \right\rangle \left|\overline{1^{(i)}}\right\rangle \right|^2 = \frac{1}{N} \sum_{i=1}^{N} \rho_1^{(i)}(x_1), \tag{10.9}$$

where $\rho_1^{(i)}(x_1)$ is the probability density of segment i in its ground state. Note the similarity between Equation 10.9 and Equation 4.12. Equation 4.12 is the average density of N particles in different energy eigenstates of the same box, but Equation 10.9 is the average density of one particle in each of N wells, all in the single-particle ground states.

Proceeding with the length calculation in the usual way by substituting Equation 10.9 into Equation 2.6 yields

$$L^2 = \frac{12}{N} \sum_{i=1}^{N} \int_{-\infty}^{+\infty} dx \left(x^2 - \langle x \rangle^2 \right) \rho_1^{(i)}(x) \tag{10.10}$$

The probability density can be expressed by a sum over the individual segments via

$$\rho_1(x) = \frac{1}{N} \sum_{i=1}^{N} \rho_1^{(i)}(x) = \frac{1}{N} \sum_{i=1}^{N} \rho_1^{(1)} \left(x - (i-1)L_1 \right), \tag{10.11}$$

where the second summation uses the fact that each segment is identical. Then, the probability density of each segment is equivalent to the first one, but shifted by iL_1 to get the contribution from the i^{th} one, i.e. $\rho_1^{(i)}(x) = \rho_1^{(1)}(x - (i-1)L_1)$. This procedure is an implementation of the classical notion that the full length is the sum of its parts. However, we leave L_1 arbitrary and solve for it self-consistently by demanding that the full length L is given by NL_1.

This will test the classical notion of additivity assumed in Equations 10.1 and 10.2 are valid. But first we must evaluate the integral given by Equation 10.10.

Consider the length formula given by Equation 5.7. The term under the square root is the average of the length variance contributions from each of the occupied states. This procedure makes sense for a monolithic object in which every electron is delocalized over the full length of the object. Then, the probability density is the average of the contributions from each state. This is precisely the kind of probability density that is depicted in Figures 7.5, 7.6 and 7.7.

When the ruler is made by cutting a rod into segments, each segment localizes electrons. The ground state configuration of the system has each segment in its ground state. Figure 10.2 shows a reconstruction of the full density when the segments are placed end-to-end with a spacing of L_1. The density is then calculated using Equation 10.11. Figure 10.2 is in essence representing the probability density in the same way as in Figure 7.5, except the system is made of segments, with each contributing to the probability density in the local well as opposed to particles in different states of the same larger well. We evaluate Equation 10.11 for the probability density in Figure 10.2 as follows.

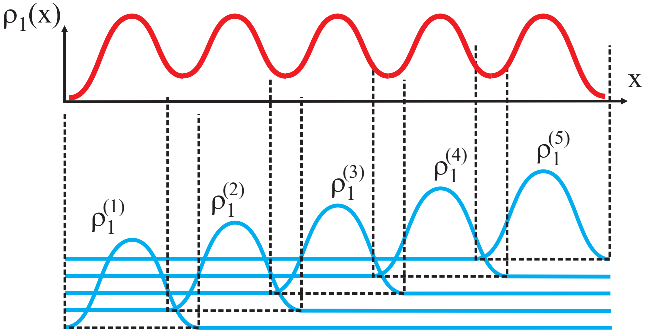


Figure 10.2: The bottom curves show the probability density due to each segment, with each plot offset slightly upwards for readability. The dashed lines show the infinite well walls and the solid curve at the top the system's probability density.

First, we need to determine how to calculate the expectation of a function $f(x)$ for a probability density that is made of a sum of functions shifted by L_1 as shown in Figure 10.3. The expectation values for two such pieces can be separated into integrals of three separate regions as follows:

$$\begin{aligned}\langle f(x)\rangle = &\int_0^{L_1} f(x)\rho(x)\,dx \\ &+ \int_{L_1}^{a} f(x)\left(\rho(x)+\rho(x-L_1)\right)\,dx \\ &+ \int_{a}^{L_1+a} f(x)\rho(x-L_1)\,dx, \end{aligned} \tag{10.12}$$

where we have used the fact that the probability density $\rho(x)$ is non-vanishing only in the interval a. Combining the first line of Equation 10.12 with the first term in parentheses of the second line, and grouping the second term in parentheses of the second line with the third line, yields

$$\langle f(x)\rangle = \int_0^{a} f(x)\rho(x)\,dx + \int_{L_1}^{L_1+a} f(x)\rho(x-L_1)\,dx. \tag{10.13}$$

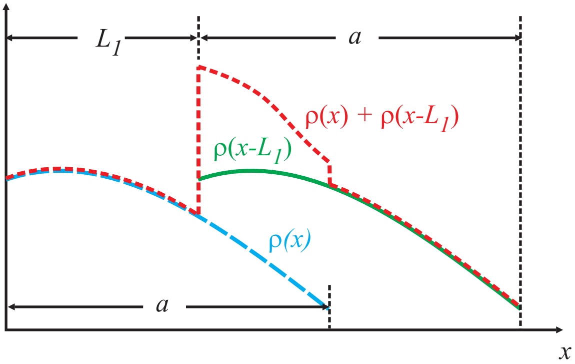


Figure 10.3: The function $\rho(x)$ (long dashed curve), the shifted function $\rho(x-L_1)$ (solid curve), and the sum of the two (short dashed curve).

We can now evaluate the length using Equation 2.6 by casting Equation 10.11 in the form of Equation 10.13 with $f(x) = x^2 - \langle x\rangle^2$, which yields the square of the length

$$L^2 = \frac{12}{N}\sum_{i=1}^{N}\int_{(i-1)L_1}^{(i-1)L_1+a} dx\, \Big(x^2 - \langle x\rangle^2\Big)\, \rho_1^{(1)}\big(x-(i-1)L_1\big). \quad (10.14)$$

Because the well is centrosymmetric, Equation 5.6 shows that the expectation $\langle x\rangle$ of a segment is just the position of its center. For the i^{th} segment, the center position is given by $\langle x\rangle_i = L_1(i-1)+a/2$. $\langle x\rangle$ is thus given by

$$\begin{aligned}\langle x\rangle &= \frac{1}{N}\sum_{i=1}^{N}\int_{(i-1)L_1}^{(i-1)L_1+a} dx\, x\rho_1^{(1)}\big(x-(i-1)L_1\big)\\ &= \frac{1}{N}\sum_{i=1}^{N}\langle x\rangle_i = \frac{1}{N}\sum_{i=1}^{N}\Big(L_1(i-1)+a/2\Big). \end{aligned} \quad (10.15)$$

Evaluating the sum yields

$$\langle x\rangle = \frac{(N-1)L_1 + a}{2}. \quad (10.16)$$

Equation 10.14 then becomes,

$$\begin{aligned}L^2 &= \frac{12}{N}\sum_{i=1}^{N}\int_{(i-1)L_1}^{(i-1)L_1+a} dx\, x^2\rho_1^{(1)}\big(x-(i-1)L_1\big)\\ &\quad - 3\big((N-1)L_1+a\big)^2\\ &\equiv \frac{12}{N}\sum_{i=1}^{N} I_i - 3\big((N-1)L_1+a\big)^2. \end{aligned} \quad (10.17)$$

To evaluate the integral I_i in Equation 10.17, we make the substitution $y = x-(i-1)L_1$, yielding

$$\begin{aligned}I_i &= \int_0^a dy\,(y+(i-1)L_1)^2\,\rho_1^{(1)}(y)\\ &= \int_0^a dy\,\big(y^2 + 2y(i-1)L_1 + (i-1)^2L_1^2\big)\,\rho_1^{(1)}(y)\,. \end{aligned} \quad (10.18)$$

The first term in Equation 10.18 is evaluated using Equation 7.10 with $n=1$. The second term can be evaluated using $\langle y\rangle = a/2$ and the last term by noting that an integral over the probability density is unity by virtue of normalization. Putting it all together, Equation 10.18 becomes

$$I_i = a^2\left(\frac{1}{3} - \frac{1}{2\pi^2}\right) + a(i-1)L_1 + (i-1)^2 L_1^2. \tag{10.19}$$

Next we group the terms in Equation 10.19 so as to yield a polynomial in i, yielding

$$\begin{aligned} I_i = {} & \left[L_1^2\right] i^2 + \left[aL_1 - 2L_1^2\right] i \\ & + \left[a^2\left(\frac{1}{3} - \frac{1}{2\pi^2}\right) + L_1^2 - aL_1\right], \end{aligned} \tag{10.20}$$

where the terms in brackets are the coefficients. Using $\sum_{i=1}^{N} 1 = N$, $\sum_{i=1}^{N} i = N(N+1)/2$ and

$$\sum_{i=1}^{N} i^2 = N(N+1)(2N+1)/6, \tag{10.21}$$

after some algebra, Equation 10.19 sums to

$$\begin{aligned} \frac{1}{N}\sum_{i=1}^{N} I_i = {} & \left(\frac{1}{3} - \frac{1}{2\pi^2}\right) a^2 + \frac{N-1}{2} aL_1 \\ & + \frac{(2N-1)(N-1)}{6} L_1^2. \end{aligned} \tag{10.22}$$

Finally, substituting Equation 10.22 into Equation 10.17 yields

$$L^2 = \left(\frac{1}{3} - \frac{1}{2\pi^2}\right) a^2 + \left(N^2 - 1\right) L_1^2. \tag{10.23}$$

Recall that L_1 – the yet-to-be determined length of the first segment – also prescribes the shift of each segment when combining the pieces to make the ruler. Calling upon symmetry to demand that each segment is of the same length and that the full length is thus given by $L = NL_1$, Equation 10.23 yields

$$N^2 L_1^2 = \left(\frac{1}{3} - \frac{1}{2\pi^2}\right) a^2 + \left(N^2 - 1\right) L_1^2. \tag{10.24}$$

Solving Equation 10.24 for L_1 yields

$$L_1 = a\sqrt{\frac{1}{3} - \frac{1}{2\pi^2}}. \tag{10.25}$$

Equation 10.25 is the length of a single particle in a box in the ground state, as given by Equation 7.11. This shows that quantum parsing acts in the way we would expect from classical arguments.

In conclusion, a ruler can be made by stacking individual pieces with spacing given by the quantum length of each piece. While this type of parsing appears to be a classical construct, the same result is obtained through a self-consistent fully quantum calculation with the requirement that the length is given by the number of segments times the number of times they are shifted. The quantum nature is evident from the length being shorter than the box size, but the classical act of stacking the segments is consistent with the quantum description.

10.4 Bosons

The same analysis applies to Bosons. Equation 8.4 gives the length of a box filled with bosons in their ground state. With $a = Na_0$, this gives a length of

$$L_N = a_0 N\sqrt{1 - \frac{6}{\pi^2}}. \tag{10.26}$$

If the box is chopped into R pieces, the length of the individual pieces will be given by Equation 8.4 with $a = Na_0/R$, or

$$L_{N/R} = \frac{a_0 N}{R}\sqrt{1 - \frac{6}{\pi^2}} \tag{10.27}$$

and the total length is $L_R = RL_{N/R}$, given by

$$L_R = a_0 N\sqrt{1 - \frac{6}{\pi^2}}. \tag{10.28}$$

Thus for bosons, chopping the ruler into pieces and recombining them gives the same length, as is verified by the equality between Equations 10.26 and 10.28.

Unlike the case of the fermion, where there is an ideal cutting interval, the boson ruler becomes more reliable as it is cut into more sections. The length is always smaller than the size of the box that defines the potential. Since the ruler is defined by the electron cloud, this is the length that matters.

Finally, we calculate the ground state energy of the uniform ruler and one made by chopping it into sections. The monolithic ruler energy for each particle is simply the energy of a particle in a box of length Na_0, so the total energy is N times the single particle energy, yielding

$$E_G = \frac{h^2}{8mNa_0^2}. \tag{10.29}$$

The ground state energy of each of the R segments is of the form of Equation 10.29 with $N \to N/R$, and the total energy is R times the segment energy, yielding

$$E'_G = \frac{h^2R^2}{8mNa_0^2}. \tag{10.30}$$

Thus, the energy grows quadratically with the number of segments, requiring substantial work in producing each slice. Thus, increased accuracy comes at a cost of increased energy.

Finally, we note that the boson system can be placed into a superposition with two particles per state to mimic the ground state fermion system, albeit with all positive signs upon particle exchange. In this configuration, the signs are irrelevant, leading to the same results obtained for fermions. Thus, bosons can be manipulated into many more configurations of energy equal to or less than the fermion ground state energy, leading to a richer set of possibilities. We leave these configurations for future study.

10.5 Entanglement of Ruler and Object

The electrons in a ruler and the object being measured are entangled because the exchange of any two electrons changes the sign of the joint wave function. This section expresses the quantum state of the ruler and object as a jointly entangled wave function to determine the consequences.

For N noninteracting particles in a box of length Na_0, where a_0 is the length of the unit cell and contains one electron, the energy of

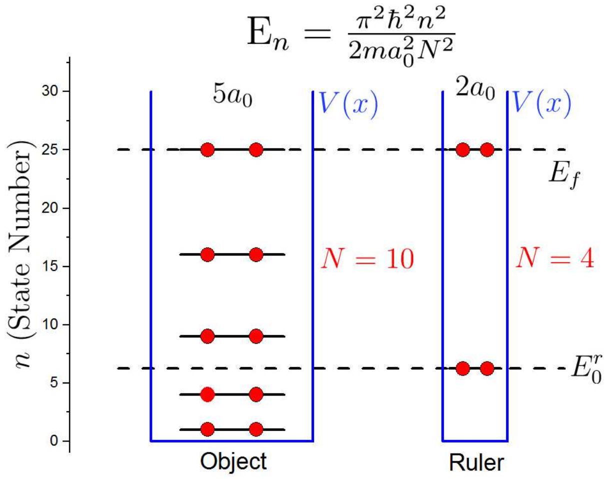


Figure 10.4: The object and ruler segment as an entangled quantum system.

single-particle state n is

$$E_n = \frac{\pi^2\hbar^2 n^2}{2ma_0^2N^2}. \tag{10.31}$$

The Fermi energy for a box with an even number of electrons is calculated from Equation 10.31 with $n = N/2$, yielding

$$E_f = \frac{\pi^2\hbar^2}{8ma_0^2}. \tag{10.32}$$

Equation 10.32 shows that the Fermi energy is independent of the size of the box since an electron is added with each unit cell. Figure 10.4 shows an object and a ruler that are made of the same material so the unit cells in each are the same size. Since the ruler segment is smaller than the object, its ground state energy E_0^r is higher than that of the object. Furthermore, the energy levels of the object are more densely spaced than in the ruler. We have arbitrarily chosen a ruler with 4 electrons and an object with 10 electrons for illustration.

Since the state vector of the 14-electron composite system must be antisymmetric upon interchange of any two of them, the electrons in a universe made of only the ruler and the object are necessarily entangled, independent of the distance between them. As such, we will express the state vector of the combined system as

$$\begin{aligned} |\Psi\rangle &= |1, 2, \ldots, 10, 1', \ldots 4'\rangle \\ &= \frac{1}{\sqrt{14}} \left(\sum_{n=1}^{10} |n\rangle\, |\overline{n}\rangle + \sum_{n'=1}^{4} |n'\rangle\, |\overline{n}'\rangle \right), \end{aligned} \tag{10.33}$$

where the primes indicate the state number of the ruler and the unprimed ones the state index of the object. The barred index refers to the state that excludes that state and is the fully anisymmetrized one of all other state indices of both the ruler and the object.

Up to this point we have assumed that the object and ruler can be placed side by side and the measurement made by eye. When the objects are made smaller they can be viewed under a microscope. The comparison between ruler and object is essentially made with a scattering experiment, where the scattered light is measured by eye or with an instrument. At ever smaller sizes, shorter wavelengths of the electromagnetic spectrum can be used as well as particle beams.

With enough spatial resolution, the object and the ruler appear separate because the electron distribution is confined to one box or the other even though the electrons are entangled. An image of the ruler is obtained from the probability density $|\langle x' \,|\, \Psi\rangle|^2$, which is defined by

$$\begin{aligned} \rho(x') = |\langle x' \,|\, \Psi\rangle|^2 &= \left| \frac{1}{\sqrt{4}} \sum_{n'=1}^{4} \langle x' \,|\, n'\rangle\, |\overline{n}'\rangle \right|^2 \\ &= \frac{1}{4} \sum_{n'=1}^{4} |\langle x' \,|\, n'\rangle|^2, \end{aligned} \tag{10.34}$$

where we use the fact that $\langle x' \,|\, n\rangle\, |\overline{n}\rangle = 0$. This is so because the position state vector of the ruler, indicated with a prime, is in an orthogonal space to the object's state vector. Note that the probability density needs to be renormalized when calculating the length from this subsystem. This primed part of the state vector is experimentally probed by blocking the object so that light scatters only from the ruler. Alteratively, the light can be focused onto only the ruler. Thus, the probability density given by Equation 10.34 will yield the length of the ruler. The same process can be applied to the object, and the two compared. Clearly, the ruler can be eliminated and the illuminated pixels of the camera used as the segments of a ruler to characterize the object's size. Then, the electrons in the pixels and the object are entangled. The fact that the two objects are entangled does not lead to any weirdness in that spatial distinguishably holds because the probability density of each will be well separated from the other as long as the distance between objects is more than a unit cell.

Things become more interesting when the ruler and object are made of different materials, making it possible for the unit cell size in each to be different. Let the lattice spacings of the ruler and object be b_0 and a_0. For the rest of the discussion, we assume that when the object and ruler are well separated, the object has 10 electrons and the ruler has 4 electrons as in Figure 10.4.

With different lattice constants, the fermi energies are unequal as are the single-particle ground state energies. The diagram in Table 10.1a shows an example of the case when the unit cell of the ruler is smaller than that of the object. The horizontal dashed lines show the lowest-energy single-particle state and the occupied state at the fermi energy. The shaded parts represent all of the discrete occupied states in between these two extremes.

The lowest unoccupied state energy of the object E_l^o is given by Equation 10.31 with $n = 6$, yielding

$$E_l^o = \frac{9\pi^2\hbar^2}{50ma_0^2}. \tag{10.35}$$

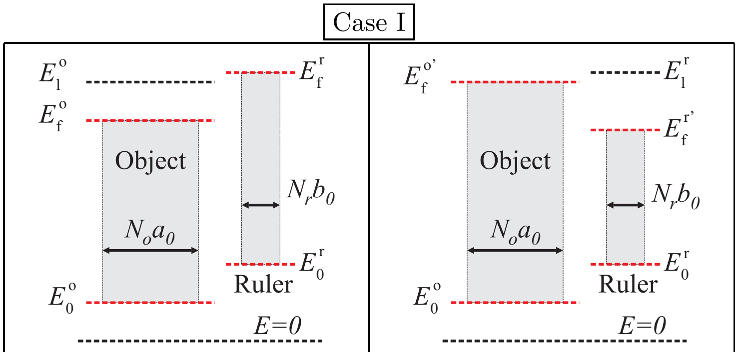
The Fermi energy of the ruler E_f^r, given by Equation 10.32 with lattice spacing b_0 will match the highest unoccupied state energy E_l^o given by Equation 10.35 when

$$E_f^r = E_l^o \quad \Rightarrow \quad \frac{9\pi^2\hbar^2}{50ma_0^2} = \frac{\pi^2\hbar^2}{8mb_0^2}, \tag{10.36}$$

or

$$\frac{a_0}{b_0} = \frac{6}{5}. \tag{10.37}$$

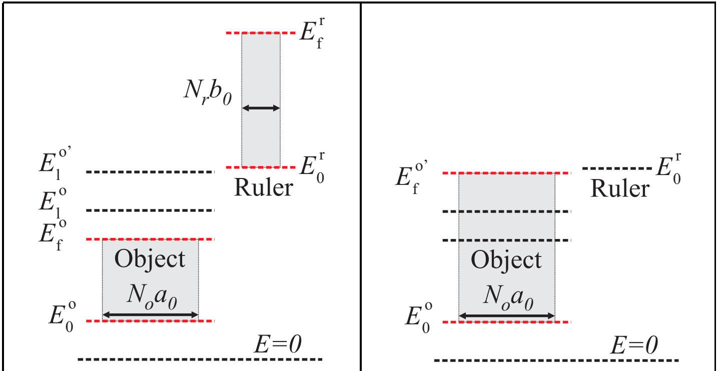
The energy-level diagram in Table 10.1a is for a ratio that is slightly larger than $\frac{a_0}{b_0} = \frac{6}{5}$.



$\frac{a_0}{b_0} > \frac{6}{5}$	$\frac{a_0}{b_0} > \frac{6}{5}$
$\frac{N_o}{N_r} = \frac{10}{4}$	$\frac{N'_o}{N'_r} = \frac{12}{2}$
Classical: $\frac{N_o a_0}{N_r b_0} = 3$	$\frac{N_o a_0}{N_r b_0} = 3$
Quantum: $\frac{L^o_{10}}{L^r_4} = 3.45$	$\frac{L^o_{12}}{L^r_2} = 4.41$
(a)	(b)

Table 10.1: Energy level diagram of an object and ruler segment. The gray shaded areas represent the occupied states. (a) A ruler with fermi energy E^r_f that is above the highest unoccupied state energy of the object, E^o_l, is not in it's true ground state. (b) The two electrons at the fermi level of the ruler shown in Table 10.1a de-excite into the lowest unoccupied state of the object, leading to the true ground state of the system. The rows below the figures show, from top to bottom, the ratio of the lattice constant of the object and ruler a_0/b_0, the ratio of the number of lattice periods of the object to the number of lattice periods of the ruler N_0/N_r, the ratio of the classical lengths $N_0 a_o/N_r b_0$, and the ratio of the quantum lengths calculated from Equation 7.13. n in the subscript of L^o_n is the number of electrons in the object and L^r_n the number of electrons in the ruling. Note that the lattice spacing does not change when an electron jumps from the ruler to the object because the nuclei that define the potential are assumed to remain fixed.

Case II



$\frac{a_0}{b_0} > \frac{12}{5}$	$\frac{a_0}{b_0} > \frac{12}{5}$
$\frac{N_o}{N_r} = \frac{10}{4}$	$\frac{N'_o}{N'_r} = \frac{14}{0}$
$\frac{N_o a_0}{N_r b_0} = 6$	$\frac{N_o a_0}{N_r b_0} = 6$
$\frac{L^o_{10}}{L^r_4} = 6.91$	$\frac{L^o_{14}}{L^r_0} = \text{N.D.}$
(c)	(d)

Table 10.2: Energy level diagram of an object and ruler segment in the same form as Table 10.1. (c) All four electrons in the ruler segment are above the two lowest unoccupied states of the object. (d) In the lowest energy configuration of the system shown in Table 10.2c, all of the electrons leave the ruler, rendering it invisible.

When $b_0 < 5a_0/6$, the Fermi energy of the ruler is higher than the lowest-energy unoccupied state of the object. In this situation, the entangled ruler/object system is in an excited state. If the electrons are noninteracting as assumed from the start, a system so prepared will remain in this excited state. However, a weak perturbation that couples the two can cause the two electrons at the Fermi level of the ruler to jump to the object. As a result, the object will become longer and the ruler will become shorter, as depicted in Table 10.1b. If the nuclei, which define the potential remain fixed, the lattice constant and therefore the well size stays the same. In reality, the lengths change because molecular bonds originate in the electron clouds, complications which we ignore here.

Before we proceed, it is worthwhile to dwell on the strangeness of this state of affairs. Viewing an object and ruler as each being electrically neutral and independent of the other places the system as a whole in an excited state. Thus, our classical world being made of many objects, is in a highly-excited state. When the objects are brought together, the interactions will cause them to de-excite and emit photons. However, these energy differences are small compared to the composite energy, so the effect is not obvious unless the rulers and objects become small.

The numbers in Table 10.1 summarize the results that follow. N_o and N_r are the number of unit cells that form the object and the ruler. The classical size is given by the number of unit cells times the unit cell size, which is given by the width of the box. The ruler determines the length of the object by counting the number of segments placed end-to-end across the object. In the classical case, this ratio is $\frac{N_o a_0}{N_r b_0} = 3$. Thus, we would say that the object size is three ruler segments.

The quantum length of the object before the electrons transfer to the object is given by Equation 7.13 with $N = 10$ and lattice constant a_0, and the ruler length is given by Equation 7.13 with $N = 4$ and lattice constant b_0 yielding the ratio $L_{10}^o / L_4^r = 3.45$. In the quantum case, the object is said to be 3.45 units in length.

After the system relaxes into its ground state, the object has 12 electrons and the ruler has 2, as shown in Table 10.1b. As a result, the object's Fermi energy has increased and the ruler's Fermi energy has decreased. The quantum lengths of the ruler and the object have both changed, resulting in the conclusion that the object's length is

4.41 units. Thus, there are several quantum effects at play. First, the quantum length and classical length are different. Secondly, the length determined from a standard measurement is affected by the fact that the electron and ruler are not independent systems, and that they share electrons. As a result, both the object and the ruler can change length.

What configuration is being characterized by the measurement? Is it the one in which the ruler and the object are independent, or the one in which electrons are exchanged? Electron transfer can in principle be verified with the detection of emitted photons of energy $\hbar\omega$ given by the difference between the Fermi energies, or $\hbar\omega = E_f^r - E_f^0$. Though not discussed here, the emission of a single photon of this energy is a signal that only one electron is exchanged, so the ruler and object would each have an odd number of electrons, yielding yet a different measure of the length.

An even more peculiar configuration is one in which all of the energy levels of the ruler are above vacant states of the object. Table 10.1c show the case where the lowest-energy occupied state of the ruler is above the lowest unoccupied state of the object, or $E_0^r > E_l^o$; and, the ruler's Fermi energy is above the second unoccupied state of the object, or $E_f^r > E_l^{o'}$. The classical length of the object is 6 ruler units before the electrons are exchanged, and the quantum length is 6.91 ruler units. However, once the electrons are exchanged, the ruler disappears because there are no longer any electrons in the segment.

In a real system, the material is held together by bonds that are mediated by interactions between the electrons and the nuclei. If all electrons were to leave the ruler, it would fly apart. The configurations of real materials do not have the required energetics for this to happen, nor are the lattice constants independent of the number of electrons. However, the model systems presented here do not violate any quantum principles, illustrating the bizarre consequences of measuring length and the classical notion that the length is an additive inviolable property.

Other examples can be contrived. For example, electrons can be made to transfer to the ruler from the object, leading to the evaporation of the object in the process of its length being measured. Of course, a ruler with markings that are septated by larger intervals than the object size makes for a useless ruler. In the quantum realm, there is no distinction between the ruler and the object, and the two remain entangled through the electrons from which they are made and through which we detect them.

Chapter 11

Conclusion

This book started by defining the quantum length under the condition that it be consistent with the classical length in the many-electron limit. This definition was used to study the length of a particle in a box, which yields the expected uniform density and sharp edges for many electrons. The Harmonic oscillator yields a length that is proportional to the distance between the classical turning points. In contrast, the length calculation for a coherent state yields the width of the wave packet, whose excursions sweep out the region between the turning points.

With these fundamentals established, the length calculation was applied to bosons, showing that the upper limit of the resulting length goes well beyond the size of the box – an intuitively unexpected result. Furthermore, the ground state of a boson ruler does not approach uniform density with sharp edges in the classical unit; but, it is possible to construct a particular superposition that has that property. There is no reason to believe that our experience with ordinary matter, whose properties are dominated by fermions and the statistics that they follow, would inform us of how a ruler made of bosons would act.

Classical reasoning would lead us to conclude that rulers become more precise when the gradations are made smaller. This is true unless quantum effects become important, at which point the length of the ruler made of slices is shorter than the original monolithic one. Thus, the length is not the sum of its classically-determined parts, though additivity of the quantum lengths holds. In such finely graded rules, quantum corrections need to be taken into account to get the object's length. This interplay between increasing resolution of the ruler and the onset of nonadditivity of the *classical quantities* leads to an optimum number of ruler parsings, equal to the square root of the number of unit cells from which the ruler is constructed. Since slicing the ruler takes work, the increased accuracy comes at an energy cost.

The length definition has its origins at the quantum level, so the upper bound of an object's length can be determined from the number of electrons and the energy difference between the two-lowest eigen energies. This purely quantum-derived limit survives in the classical realm, though it probably overestimates the length to a larger degree.

There are no weird consequences arising from the entanglement of electrons that are shared by the ruler and the object to be measured when they are made of the same material. Then, the occupied states in the ruler and in the object are no different than if the two were unentangled objects, thus agreeing with the classical picture of distinct objects. However, if the two are made of different materials with differing unit cell sizes, the Fermi energies no longer match. When the size of the ruler segment is small enough to bring its Fermi energy above the energy of the lowest unoccupied state of the object, an electron can jump from the ruler to the object, affecting the length of each, changing the nature of the measurement and making the result ill-defined. In the extreme case of large unit-cell size mismatch, all of the electrons can jump from the ruler to the object, in essence causing it to disappear since the electrons with which light interacts are absent. The ruler and object can be reversed to make electrons jump to the ruler, leading to similar weirdness. However, in this case, the rulings in the ruler would be larger than the size of the object – not a useful ruler.

Table 11 shows a summary of all the various lengths for Fermions and Bosons in boxes and harmonic potentials, the length limit for a box spectrum and harmonic oscillator spectrum. The classical limit can be determined by taking $N \to \infty$.

When we think of observables such as position and momentum, they are characterized by points. In contrast, we saw that the length is given by the spread in the probability density, which in turn is related to the uncertainty range of the position. Classically, we think of the length as the distance between two points at an objects ends. In the classical limit, both of these views are seen to converge. However, the spread of the wave function is the more rigourous definition.

Central to the classical definition of size is one-to-one correspondence between the segments of a ruler and points on the object. Such correspondence between the two assumes that numbers are agnostic with regards to the composition of the objects that they are quantifying. In the quantum realm, the composition of the material can affect the measurement of its length. Furthermore, on small enough scales, objects are no longer distinct. This suggests that one-to-one correspondence is a classical approximation that holds on human size scales, but requires a more nuanced analysis when an object is made of only a few electrons.

Counting is the basis of mathematics, so it is amazing that the quantum realm – where one-to-one correspondence is ill-defined – is so well described by a theory based on counting. This narrative has shown when size is a useful focus for studying one-to-one correspondence and when it becomes murky.

The quantum definition of length has no affect on our day to day interactions with the world, but enriches our imagination as we struggle to understand the subtleties of nature and attempt to reconcile our findings with intuition.

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	Fermion	Boson
General Limit:	$L_{max} = \sqrt{\frac{6\hbar^2 N}{mE_{FG}}}$	$L_{max} = \sqrt{\frac{6\hbar^2 N}{me_{21}}}$
Box Spectrum Limit:	$L_{\text{max}}^{\text{box}} = \begin{cases} \frac{2}{\pi} \cdot a \approx 0.64a & \text{N} = 1 \\ \frac{2\sqrt{3}}{\pi}\sqrt{\frac{N}{N+1}} \cdot a & N \text{ even} \\ \frac{2\sqrt{3}}{\pi} \cdot a \approx 1.1a & N \text{ odd} \end{cases}$	$L_{\text{max}}^{\text{box}} = \frac{2a}{\pi}\sqrt{N}$
Actual Box Length:	$L^{\text{box}} = a\left(1 - \frac{12}{\pi^2 N}\sum_{n=1}^{N/2}\frac{1}{n^2}\right)^{1/2}$	$L^{\text{box}} = a\sqrt{1 - \frac{6}{\pi^2}}$
HO Spectrum Limit:	$L_{\text{max}}^{HO} = \sqrt{\frac{6\hbar N}{m\omega}}$	$L_{\text{max}}^{HO} = \sqrt{\frac{6\hbar N}{m\omega}}$
Actual HO Length:	$L^{HO} = \sqrt{\frac{3\hbar N}{m\omega}}$	$L^{HO} = \sqrt{\frac{3\hbar}{m\omega}}$

Table 11.1: Summary of lengths and limits for fermions and bosons in textbook potentials.

Appendix A

The Sum Rules

The sum rules are derived from the commutator $[x,[x,H]]$, where x is the position operator and H the Hamiltonian. The commutator is evaluated directly using the fact that for a mechanical Hamiltonian $[x,H]=\left[x,\frac{p^2}{2m}\right]=i\hbar\frac{p}{m}$, which yields

$$[x,[x,H]]=-\frac{\hbar^2}{m}, \tag{A.1}$$

where m is the mass of the particle. Usually the particle is an electron in an atom, molecule, crystal or nanostructure.

The commutator can be explicitly expressed as

$$[x,[x,H]]=x^2H+Hx^2-2xHx. \tag{A.2}$$

Setting Equations A.1 and A.2 equal to each other, and taking the expectation with respect to the ground state energy eigenket $|1\rangle$ yields

$$\langle 1|\, x^2 \,|1\rangle\, E_1 + E_1 \,\langle 1|\, x^2 \,|1\rangle - 2\,\langle 1|\, xHx \,|1\rangle = -\frac{\hbar^2}{m}, \tag{A.3}$$

where we have used $H\,|1\rangle = E_1\,|1\rangle$.

Inserting closure, given by Equation 6.3, between each pair of position operators x in the three terms of Equation A.3 and collecting like terms yields

$$\sum_n \langle 1|\, x \,|n\rangle \,\langle n|\, x \,|1\rangle \,(E_n - E_1) = \frac{\hbar^2}{2m}, \tag{A.4}$$

where $|n\rangle$ is an energy eigenstate with $H|n\rangle = E_n |n\rangle$.

To treat a system with N electrons, we calculate $[X,[X,H]]$, with Equation 6.7 defining X and the commutator $[X,H]$ given by

$$[X,H] = \left[X, \sum_{i=1}^{N} \frac{p_i^2}{2m}\right] = \frac{1}{2m}\sum_{i=1}^{N}\left[x_i, p_i^2\right] = i\hbar \sum_{i=1}^{N} \frac{p_i}{m}, \tag{A.5}$$

where p_i is the momentum operator of the i^{th} electron.

Using Equation A.5, the double commutator becomes

$$[X,[X,H]] = i\frac{\hbar}{m}\sum_{i=1}^{N}[x_i, p_i] = -\frac{N\hbar^2}{m}. \tag{A.6}$$

The sum rules are calculated following the same procedure as in the one-electron case, yielding

$$\sum_n \langle 1| X |n\rangle \langle n| X |1\rangle (E_n - E_1) = \frac{N\hbar^2}{2m}. \tag{A.7}$$

Equation A.7 is the general result for a system of N electrons and since it is calculated without approximation, it must hold far any quantum system made of a collection of particles governed by a mechanical Hamiltonian coupled to electromagnetic fields.[12]

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