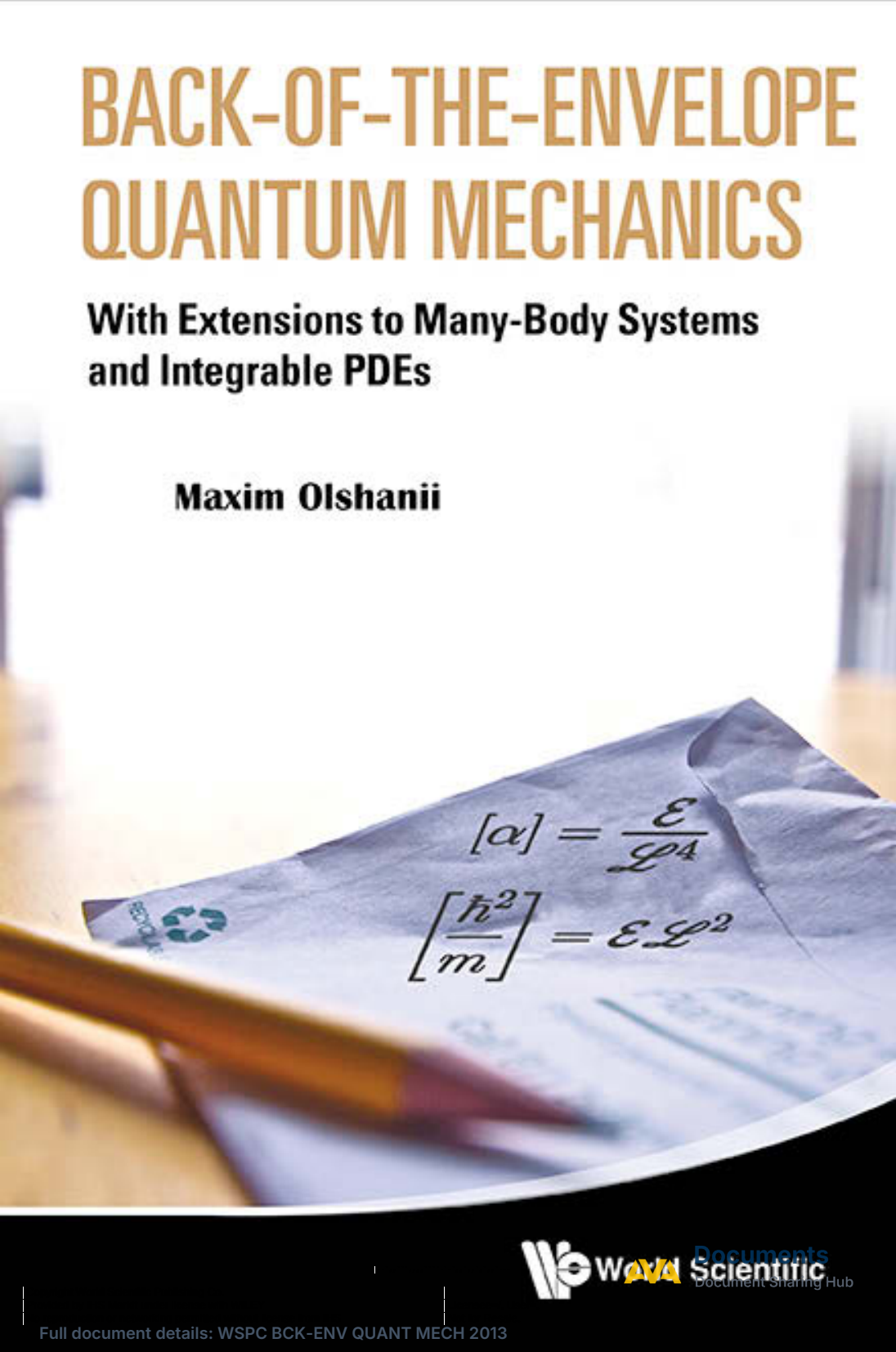


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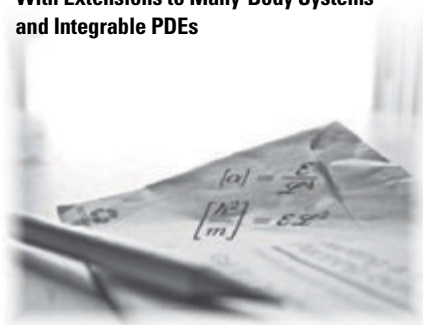
**With Extensions to Many-Body Systems
and Integrable PDEs**

Maxim Olshanii


$$[\alpha] = \frac{\mathcal{E}}{\mathcal{L}^4}$$
$$\left[\frac{\hbar^2}{m}\right] = \mathcal{E} \mathcal{L}^2$$

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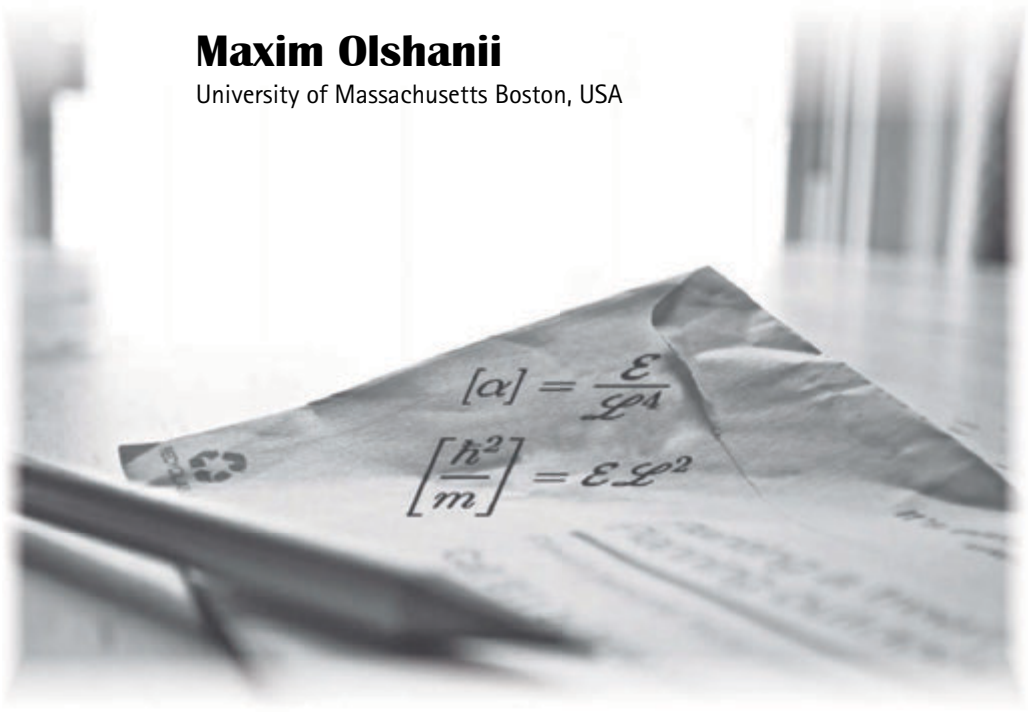
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**With Extensions to Many-Body Systems
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Maxim Olshanii

University of Massachusetts Boston, USA


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$$\left[\frac{\hbar^2}{m} \right] = E \hbar^2$$



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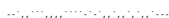
Preface

As I come to realize, this book was uniquely inspired by Professor Krainov's course on qualitative methods in physical kinetics that I attended at the Moscow Engineering Physics Institute (National Research Nuclear University MEPhI nowadays) thirty years ago. As we students learnt in a more rigorous class to follow, in physical kinetics, even the most basic results require laborious multi-page derivations. But Krainov's course and his book published later by the American Institute of Physics taught us that if one is *not* interested in the exact values of prefactors, then ten pages of calculations can be replaced by two short lines on the *back of an envelope*; in some cases, even a postal stamp would suffice.

The book you are about to read is based on the problems assigned in a graduate course in quantum mechanics that I have been teaching at the University of Massachusetts Boston for many years. Similar to the physical kinetics classes I attended at the MEPhI, the discussion on any new topic in my class would invariably start from a series of qualitative problems. When I realized I had more than fifty of them, I decided to assemble them in a book.

In this book, I clearly *distinguish between the dimensional and the order-of-magnitude estimates*. Dimensional analysis is a powerful method to analyze new unexplored equations, but it fails when there are too many dimensionless parameters involved. In an order-of-magnitude estimate—a calculation where all angles are 90° , all numbers are unity, and all integrals are just “height times width”—one needs to understand the physics behind the process really well; as a reward, the method is nearly universal.

Approximately half of the book is devoted to the estimates based on either semi-classical approximation or on perturbation theory expansions



in *elementary quantum mechanics*. Thanks to a reduced number of independent dimensionful parameters in the domains of applicability of these theories, both dimensional and order-of-magnitude approaches are ideally suited there.

A sequence of variational problems is also included. The breadth and elegance of variational reasoning makes it a valuable tool in a preliminary analysis of a problem; determination of the parity of the ground state in a well is a good example. Furthermore, even the quantitative results obtained from simple one-parametric variational ansatzes still fit on an envelope.

Similarly, I could not resist including several powerful results produced by applying the Hellmann-Feynman theorem to *integrable many-body quantum systems*. Unlike other methods considered, it produces exact answers; those can also be obtained in a few lines.

The *integrable partial differential equations* serve as an example of a field where there are no innate measurement units, and yet dimensional analysis can be deployed; the dependence of the size of a Korteweg-de Vries soliton on its speed is a typical application of the method.

This book contains both solved problems and exercises. The order of the solved problems is important: the sequence gradually prepares the reader for the problems without solutions. Minimal theoretical background is provided as well. Several lesser known theoretical facts are attached to the respective “Background” sections as “Problems linked to the ‘Background’”. Various approximate and qualitative methods are compared in three case studies: of a hybrid, harmonic-quartic oscillator, of a “halved” harmonic oscillator, and of a gravitational well.

This book would not have been possible without input from all the students I have taught in my quantum mechanics courses at UMass Boston and at the University of Southern California before it. Special thanks to Vladimir Pavlovich Krainov for introducing me to qualitative methods, first as a professor and, later on, as my first research project adviser. Further interactions with my mentors, Vladimir Minogin and Yvan Castin, inspired many new problems for the book and shaped its structure.

A good half of this book was compiled during quiet Mediterranean nights, profiting from the free internet in the lobby of the Galil Hotel in Netanya, Israel. Many thanks to its staff for the cookies they were incessantly feeding me throughout those nights.

This is an appropriate place to thank my friends—Vincent Lorent, Lana Jitomirskaya, Vanja Dunjko, Lena Dotsenko, and Paul Gron—for standing by my side in good and in bad times.

I am immensely grateful to Zaijong Hwang and Vanja Dunjko for a thorough critical reading of the manuscript.

Finally, I would like to thank my wife Milena Gueorguieva for correcting commas, articles, and awkward sentences and my son Mark Olchanyi for producing the cover art.

Maxim Olshanii
Boston, Massachusetts
January 14, 2013

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Contents

Preface	vii
1. Ground State Energy of a Hybrid Harmonic-Quartic Oscillator: A Case Study	1
1.1 Solved problems	1
1.1.1 Dimensional analysis and why it fails in this case	1
1.1.2 Dimensional analysis: the harmonic oscillator alone	9
1.1.3 Order-of-magnitude estimate: full solution	10
1.1.4 An afterthought: boundary between regimes from dimensional considerations	13
1.1.5 A Gaussian variational solution	14
2. Bohr-Sommerfeld Quantization	17
2.1 Solved problems	17
2.1.1 A semi-classical analysis of the spectrum of a harmonic oscillator: the exact solution, an order-of-magnitude estimate, and dimensional analysis	17
2.1.2 WKB treatment of a “straightened” harmonic oscillator	19
2.1.3 Ground state energy in power-law potentials	21
2.1.4 Spectrum of power-law potentials	22



2.1.5	The number of bound states of a diatomic molecule	23
2.1.6	Coulomb problem at zero angular momentum	25
2.1.7	Quantization of angular momentum from WKB	29
2.1.8	From WKB quantization of 4D angular momentum to quantization of the Coulomb problem	30
2.2	Problems without provided solutions	32
2.2.1	Size of a neutral meson in Schwinger's toy model of quark confinement	32
2.2.2	Bohr-Sommerfeld quantization for periodic boundary conditions	33
2.2.3	Ground state energy of multi-dimensional power-law potentials	33
2.2.4	Ground state energy of a logarithmic potential	33
2.2.5	Spectrum of a logarithmic potential	33
2.2.6	1D box as a limit of power-law potentials	34
2.2.7	Spin-1/2 in the field of a wire	34
2.2.8	Dimensional analysis of the time-dependent Schrödinger equation for a hybrid harmonic-quartic oscillator	35
2.3	Background	35
2.3.1	Bohr-Sommerfeld quantization	35
2.3.2	Multi-dimensional WKB	37
2.4	Problems linked to the "Background"	37
2.4.1	Bohr-Sommerfeld quantization for one soft turning point and a hard wall	37
2.4.2	Bohr-Sommerfeld quantization for two hard walls	40
3.	"Halved" Harmonic Oscillator: A Case Study	43
3.1	Solved Problems	44
3.1.1	Dimensional analysis	44
3.1.2	Order-of-magnitude estimate	44
3.1.3	Another order-of-magnitude estimate	45
3.1.4	Straightforward WKB	46
3.1.5	Exact solution	46

4. Semi-Classical Matrix Elements of Observables and Perturbation Theory	49
4.1 Solved problems	49
4.1.1 Quantum expectation value of x^6 in a harmonic oscillator	49
4.1.2 Expectation value of r^2 for a circular Coulomb orbit	50
4.1.3 WKB approximation for some integrals involving spherical harmonics	52
4.1.4 Ground state wavefunction of a one-dimensional box	54
4.1.5 Eigenstates of the harmonic oscillator at the origin: how a factor of two can restore a quantum-classical correspondence	55
4.1.6 Probability density distribution in a “straightened” harmonic oscillator	58
4.1.7 Eigenstates of a quartic potential at the origin	60
4.1.8 Perturbation theory with exact and semi-classical matrix elements for a harmonic oscillator perturbed by a quartic correction or ...	61
4.1.9 ...or by a cubic correction	63
4.1.10 Shift of the energy of the first excited state	65
4.1.11 Impossible potentials	67
4.1.12 Correction to the frequency of a harmonic oscillator as a perturbation	70
4.1.13 Outer orbital of sodium atom	72
4.1.14 Relative contributions of the expectation values of the unperturbed Hamiltonian and the perturbation to the first and the second order perturbation theory correction to energy	76
4.2 Problems without provided solutions	79
4.2.1 A perturbation theory estimate	79
4.2.2 Eigenstates of a two-dimensional harmonic oscillator at the origin	79

4.2.3	Approximate WKB expressions for matrix elements of observables in a harmonic oscillator	81
4.2.4	Off-diagonal matrix elements of the spatial coordinate for a particle in a box	81
4.2.5	Harmonic oscillator perturbed by a δ -potential, ...	82
4.2.6	...and by a uniform field	82
4.2.7	Perturbative expansion of the expectation value of the perturbation itself and the virial theorem	82
4.2.8	A little theorem	83
4.3	Background	83
4.3.1	Matrix elements of operators in the WKB approximation	83
4.3.2	Perturbation theory: a brief summary	86
4.3.3	Non-positivity of the second order perturbation theory shift of the ground state energy	88
5.	Variational Problems	89
5.1	Solved problems	89
5.1.1	Inserting a wall	89
5.1.2	Parity of the eigenstates	90
5.1.3	Simple variational estimate for the ground state energy of a harmonic oscillator	90
5.1.4	A property of variational estimates	91
5.1.5	Absence of nodes in the ground state	93
5.1.6	Absence of degeneracy of the ground state energy level	95
5.2	Problems without provided solutions	95
5.2.1	Do stronger potentials always lead to higher ground state energies?	95
5.2.2	Variational analysis meets perturbation theory	95
5.2.3	Another variational estimate for the ground state energy of a harmonic oscillator	96
5.2.4	...and yet another	96
5.2.5	Gaussian- and wedge- variational ground state energy of a quartic oscillator	96

5.3	Background	96
5.3.1	Variational analysis	96
5.4	Problems linked to the “Background”	98
5.4.1	Complex vs. real variational spaces	98
5.4.2	A proof that the $(\psi')^2$ energy functional does not have minima with discontinuous derivatives	100
6.	Gravitational Well: A Case Study	103
6.1	Solved problems	104
6.1.1	Bohr-Sommerfeld quantization	104
6.1.2	A WKB-based order-of-magnitude estimate for the spectrum	104
6.1.3	A WKB-based dimensional estimate for the spectrum	105
6.1.4	A perturbative calculation of the shift of the energy levels under a small change in the coupling constant. The first order	106
6.1.5	A dimensional estimate for the perturbative correction to the spectrum	107
6.1.6	A perturbative calculation of the shift of the energy levels under a small change in the coupling constant. The second order	108
6.1.7	A simple variational treatment of the ground state of a gravitational well	110
7.	Miscellaneous	113
7.1	Solved problems	113
7.1.1	A dimensional approach to the question of the number of bound states in δ -potential well	113
7.1.2	... and in a Pöschl-Teller potential	114
7.1.3	Existence of lossless eigenstates in the $1/x^2$ -potential	115
7.1.4	On the absence of the unitary limit in two dimensions	116

8. The Hellmann-Feynman Theorem	119
8.1 Solved problems	119
8.1.1 Lieb-Liniger model	119
8.1.2 Expectation values of $1/r^2$ and $1/r$ in the Coulomb problem, using the Hellmann-Feynman theorem	121
8.1.3 Expectation value of the trapping energy in the ground state of the Calogero system	123
8.1.4 Virial theorem from the Hellmann-Feynman theorem	124
8.2 Problems without provided solutions	126
8.2.1 Virial theorem for the logarithmic potential and its corollaries	126
8.3 Background	127
8.3.1 The Hellmann-Feynman theorem	127
9. Local Density Approximation Theories	129
9.1 Solved problems	129
9.1.1 A Thomas-Fermi estimate for the atom size and total ionization energy	129
9.1.2 The size of an ion	130
9.1.3 Time-dependent Thomas-Fermi model for cold bosons	132
9.2 Problems without provided solutions	134
9.2.1 The quantum dot	134
9.2.2 Dimensional analysis of an atom beyond the Thomas-Fermi model	134
10. Integrable Partial Differential Equations	135
10.1 Solved problems	135
10.1.1 Solitons of the Korteweg-de Vries equation	135
10.1.2 Breathers of the nonlinear Schrödinger equation	137
10.1.3 Healing length	138
10.1.4 Dimensional analysis of the projectile problem as a prelude to a discussion on the Kadomtsev-Petviashvili solitons	140

10.1.5	Kadomtsev-Petviashvili equation	142
10.2	Problems without provided solutions	144
10.2.1	Stationary solitons of the nonlinear Schrödinger equation	144
10.2.2	Solitons of the sine-Gordon equation	144
	Further Reading	145
	Subject Index	147
	Author Index	151



Some notations

$[a]$	Units in which an observable a is measured
$[\mathcal{L}], [\mathcal{T}], [\mathcal{M}], [\mathcal{E}], \dots$	Units of length, time, mass, energy, ...
$\mathcal{L}, \mathcal{T}, \mathcal{M}, \mathcal{E}, \dots$	Length scale, time scale, mass scale, energy scale, ...
$P_1, P_2, \dots$	Independent dimensionless parameters of a given problem
$\mathcal{A}[\psi(\cdot)]$	A functional $\mathcal{A}$ acting on a wavefunction $\psi(x)$
$\mathfrak{V}$	A variational space $\mathfrak{V}$

Chapter 1

Ground State Energy of a Hybrid Harmonic-Quartic Oscillator: A Case Study

Introduction

Consider the Schrödinger equation for a one-dimensional particle moving in a combination of harmonic potential of frequency ω and a quartic potential of strength β :

$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x) + \frac{m\omega^2}{2} x^2 \psi(x) + \beta x^4 \psi(x) = E \psi(x), \quad (1.1)$$

where m is the particle's mass. We will be mainly interested in determining the ground state energy. The Eq. (1.1) does not allow for an exact solution. However, the major features of the dependence of the ground state energy on the system parameters can be determined via elementary methods, such as dimensional analysis, order-of-magnitude estimates, and simple variational bounds. The goal of this chapter is to illustrate the application of these methods using the ground state problem (1.1) as an example.

1.1 Solved problems

1.1.1 Dimensional analysis and why it fails in this case

The assignment is: perform dimensional analysis of the problem and show that from a dimensional point of view the problem is underdetermined: no estimate for the ground state energy can be produced. However, some information about the structure of the expression for the ground state energy can still be extracted, on purely dimensional grounds.

Solution: The dimensional procedure for finding the ground state energy $E_{g.s.}$ (or assessing the impossibility of a complete dimensional solution) is



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as follows:

- Begin by identifying the *principal units* of measurement for the problem, *i.e.* the minimal set of units sufficient to describe all input parameters of the problem. For stationary problems in quantum mechanics, the units of length, $[\mathcal{L}]$, and energy, $[\mathcal{E}]$, have been proven to provide a handy set;
- Identify the *input parameters* and units used to measure them;
- Determine the *maximal set of independent dimensionless parameters*: the set will include only the parameters that are generally either much greater or much less than unity. These include both the dimensionless parameters present in the problem *a priori* (such as the quantum number n), and the dimensionless combinations of the dimensionful input parameters. If the set is empty, the unknown quantities can be determined almost completely, *i.e.* up to a numerical prefactor of the order of unity. If some dimensionless parameters are present, the class of possible relationships between the unknowns and the input parameters can be narrowed down, but the order of magnitude of the unknown quantities can not be determined.
- For each of the principal units, choose a *scale*: a combination of the input parameters measured using the unit in question;
- Express the unknown quantities as a multi-power-law of principal scales, times an arbitrary function of all dimensionless parameters, if any. If no dimensionless parameters are present, the arbitrary function is replaced by an arbitrary constant, presumed to be of the order of unity.

In our case, the above procedure gives:

- *The principal units—the units of length and the units of energy:*

$$[\mathcal{L}], \quad [\mathcal{E}];$$

- *The input parameters and their units:*

$$[\eta] = [\mathcal{L}]^2 [\mathcal{E}]$$

$$[\Upsilon] = [\mathcal{L}]^{-2} [\mathcal{E}]$$

$$[\beta] = [\mathcal{L}]^{-4} [\mathcal{E}],$$

where $\eta \equiv \hbar^2/m$, and $\Upsilon \equiv m\omega^2$;

- *The set of independent dimensionless parameters =*

$$\left\{ P_1 \equiv \frac{\hbar\beta}{m^2\omega^3} \right\}.$$

(1.2)



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It is represented by a single element. Let us prove that. First, there are no *a priori* dimensionless parameters in this problem. Assume now that P is a dimensionless parameter that is derived from the dimensionful input parameters. It must be represented as a multi-power law of the input parameters:

$$P = \text{const} \times \eta^{\xi_1} \Upsilon^{\xi_2} \beta^{\xi_3}.$$

Units for P are given by

$$\begin{aligned} [P] &= [\eta]^{\xi_1} [\Upsilon]^{\xi_2} [\beta]^{\xi_3} \\ &= ([\mathcal{L}]^2 [\mathcal{E}])^{\xi_1} ([\mathcal{L}]^{-2} [\mathcal{E}])^{\xi_2} ([\mathcal{L}]^{-4} [\mathcal{E}])^{\xi_3} \\ &= [\mathcal{L}]^{2\xi_1 - 2\xi_2 - 4\xi_3} [\mathcal{E}]^{\xi_1 + \xi_2 + \xi_3}. \end{aligned}$$

On the other hand, P is supposed to be dimensionless:

$$[P] = [\mathcal{L}]^0 [\mathcal{E}]^0.$$

Thus, the powers ξ_1, ξ_2, ξ_3 must obey the following system of linear homogeneous algebraic equations:

$$\hat{M} \cdot \begin{pmatrix} \xi_1 \\ \xi_2 \\ \xi_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \quad (1.3)$$

where

$$\hat{M} = \begin{pmatrix} 1 & 1 & 1 \\ 2 & -2 & -4 \end{pmatrix}. \quad (1.4)$$

The number of independent dimensionless parameters will be given by

$$\begin{aligned} &(\# \text{ of independent dimensionless parameters}) \\ &= \underbrace{(\# \text{ of independent } a\text{-priori-dimensionless parameters})}_0 \\ &\quad + \underbrace{(\# \text{ of independent dimensionful parameters})}_3 \\ &\quad - \underbrace{\text{rank}(\hat{M})}_2 \\ &= 1. \end{aligned} \quad (1.5)$$

The dimensionless parameter P_1 can be found by solving the system (1.3). It gives

$$\begin{pmatrix} \xi_1 \\ \xi_2 \\ \xi_3 \end{pmatrix} = \text{const} \times \begin{pmatrix} \frac{1}{2} \\ -\frac{3}{2} \\ 1 \end{pmatrix},$$

leading to

$$\begin{aligned} P_1 &= \text{const} \times \frac{\beta\sqrt{\eta}}{\Upsilon^{3/2}} \\ &= \text{const} \times \frac{\beta\hbar}{m^2\omega^3}; \end{aligned}$$

— The principal scales—the length scale and the energy scale, examples of:

$$\begin{aligned} \mathcal{L} &= \sqrt{\frac{\hbar}{m\omega}} \\ \mathcal{E} &= \hbar\omega. \end{aligned}$$

The principal scales above are defined as examples of observables measured in principal units, $[\mathcal{L}]$ and $[\mathcal{E}]$ in our case. To derive the above expression for the length scale, let us represent this scale as

$$\mathcal{L} = \text{const} \times \eta^{\nu_1} \Upsilon^{\nu_2} \beta^{\nu_3}.$$

The corresponding units are related as

$$\begin{aligned} [\mathcal{L}] &= [\eta]^{\nu_1} [\Upsilon]^{\nu_2} [\beta]^{\nu_3} \\ &= \left([\mathcal{L}]^2 [\mathcal{E}]\right)^{\nu_1} \left([\mathcal{L}]^{-2} [\mathcal{E}]\right)^{\nu_2} \left([\mathcal{L}]^{-4} [\mathcal{E}]\right)^{\nu_3} \\ &= [\mathcal{L}]^{2\nu_1 - 2\nu_2 - 4\nu_3} [\mathcal{E}]^{\nu_1 + \nu_2 + \nu_3}. \end{aligned}$$

The powers ν_1 , ν_2 , ν_3 obviously obey a system of linear inhomogeneous algebraic equations given by

$$\hat{M} \cdot \begin{pmatrix} \nu_1 \\ \nu_2 \\ \nu_3 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad (1.6)$$

where M is given by the expression (1.4). Any particular solution of Eq. (1.6) (and in this particular case we have a one-dimensional family of them) can be chosen to represent a length scale; this choice is a

matter of convenience. We choose the scale associated uniquely with the harmonic oscillator,

$$\begin{pmatrix} \nu_1 \\ \nu_2 \\ \nu_3 \end{pmatrix} = \begin{pmatrix} \frac{1}{4} \\ -\frac{1}{4} \\ 0 \end{pmatrix},$$

or, for example,

$$\begin{aligned} \mathcal{L} &= \left(\frac{\beta\eta}{\Upsilon} \right)^{1/4} \\ &= \sqrt{\frac{\hbar}{m\omega}}. \end{aligned}$$

The energy scale $\mathcal{E}$, given by the expression (1.6), can be obtained the same way. The only difference is the right hand side of equation (1.6): it should read $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$;

— *Solution for the unknown:*

$$[E_{\text{g.s.}}] = [\mathcal{E}] \Rightarrow E_{\text{g.s.}} = \Phi(P_1) \times \mathcal{E} = \Phi\left(\frac{\hbar\beta}{m^2\omega^3}\right) \times \hbar\omega, \quad (1.7)$$

where $\Phi(P)$ is an arbitrary function.

To summarize,

$$\begin{aligned} E_{\text{g.s.}} &= \Phi\left(\frac{\hbar\beta}{m^2\omega^3}\right) \times \hbar\omega \\ \Phi(\cdot) &= \text{any function} \end{aligned}$$

This solution does narrow the class of possible expressions for the ground state energy, but does not allow one to determine it, not even its order of magnitude.

If needed, analogous expressions for other observables can be readily obtained. For the observables measured in combinations of principal units only, one should combine the principal scales to form a scale for the observable of interest. The full dimensional prediction for this observable will be given, as before, as a product of an arbitrary function of all dimensionless parameters and the scale. For example, the r.m.s. force acting on our particle in the ground state will be given by

$$F_{\text{g.s.}} = \Phi_2(P_1) \times \mathcal{F} = \Phi_2\left(\frac{\hbar\beta}{m^2\omega^3}\right) \times \sqrt{m\hbar\omega^3},$$

where

$$\mathcal{F} \equiv \frac{\mathcal{E}}{\mathcal{L}} = \sqrt{m\hbar\omega^3}$$

is the force scale, and $\Phi_2(P)$ is another arbitrary function.

For the observables measured in units that do not belong to the principal set (the minimal set of units to describe all input parameters), other scales must be invented if needed. For example, the inverse harmonic frequency, $1/\omega$, provides a useful time scale:

$$\mathcal{T} = \frac{1}{\omega}.$$

In mechanics problems, both classical and quantum, no more than three independent scales are ever necessary. For example, the r.m.s. ground state velocity is given by

$$v_{\text{g.s.}} = \Phi_3(P_1) \times \mathcal{V} = \Phi_3\left(\frac{\hbar\beta}{m^2\omega^3}\right) \times \sqrt{\hbar\omega/m},$$

with

$$\mathcal{V} \equiv \frac{\mathcal{L}}{\mathcal{T}} = \sqrt{\hbar\omega/m}$$

being the velocity scale.

1.1.1.1 Side comment: dimensional analysis and approximations

Often, when an exact theory is replaced by an approximate one, the number of independent dimensionful parameters decreases, thus shifting the counting (1.5) in favor of accurate up-to-a-prefactor dimensional predictions. In what follows, we will encounter several examples of such reduction. For example, in semi-classical theory, considered in Chapter 2, the Planck constant $\hbar$ and the level index n fuse into a single entity, the classical canonical action $\tilde{\hbar}$:

$$\begin{array}{c} \hbar \\ \searrow \\ \hbar(n + 1/2) \equiv \tilde{\hbar} \\ \nearrow \\ n \end{array}$$

This reduction is a consequence of the absence of the quantization of action in classical mechanics. Another example is the Thomas-Fermi theory, Chapter 9. There, the number of electrons Z and the electron charge $|e|$

unite and form a total charge Q , never appearing separately:

$$\begin{array}{c} Z \\ \searrow \\ Z|e| \equiv Q \\ \nearrow \\ |e| \end{array}$$

The physical reason for such a merger is that in mean-field theories—such as the Thomas-Fermi theory—the number of electrons is no longer quantized, and a continuous field of electron number density $n(\vec{r})$ is used instead of the individual electron positions. A similar reduction happens when solutions of a many-body Schrödinger equation for an ensemble of bosonic particles are approximated using solutions of a one-body nonlinear Schrödinger equation (See Problem 10.1.3).

Yet another example of a reduction of the number of input parameters under an approximation is provided by perturbation theory (Chapter 4). Here, in the n -th order of perturbation theory, the power of a dimensionful prefactor in front of the perturbation is fixed to n , effectively removing the prefactor from the list of independent parameters. See, specifically, Problems 4.1.8 and 4.1.9.

1.1.1.2 *Side comment: how to recast input equations in a dimensionless form*

Prior to involved analytical or numerical calculations, equations are often expressed in a “dimensionless form”, the advantage being a reduced number of parameters and an absence of numbers that are too large or too small.

The recipe is as follows:

- Several input parameters, as many as there are principal units, are replaced by unity;
- The remaining input parameters retain their notations, but their numerical dimensionful values are replaced by dimensionless numbers given by the ratios between the original values of the parameters and the corresponding “scales”;
- Likewise, in the end the numerical values of the answers are multiplied by the corresponding scales.

A well-defined formal procedure is hidden behind. It consists of two elements. (a) The parameters to be set to unity are chosen as principal scales;

(b) these scales and their multi-power combinations are used as new units of measurement.

In our example, we can choose $[\eta]$ and $[\Upsilon]$ as the “principal units” and η and Υ themselves as the “principal scales”. Obviously, in this system of units, η and Υ assume unit values. Also, for moderate values of the remaining dimensionless parameters, all answers we get become of the order of unity.

Conventionally, this system of units is denoted as

$$\frac{\hbar^2}{m} = m\omega^2 = 1,$$

or even more often

$$\hbar = m = \omega = 1. \quad (1.8)$$

The appearance of three scales is not an accident. The recipe (1.8) (a) does not lead to any ambiguities in time-independent problems; (b) allows one to fix all the scales, not only the principal ones; (c) prepares ground for time-dependent problems.

According to the recipe (1.8), the original Schrödinger equation (1.1) becomes

$$-\frac{1}{2} \frac{\partial^2}{\partial x^2} \psi(x) + \frac{1}{2} x^2 + \beta x^4 \psi(x) = E \psi(x). \quad (1.9)$$

In short, according to this recipe, instead of the original Eq. (1.1) we deal with its dimensionless form (1.9), ready for analytic or numerical work: the way to obtain (1.9) is to replace each of the parameters $\hbar^2/m$ and $m\omega^2$ by unity, and replace the parameter β by $\frac{\beta\hbar}{m^2\omega^3}$; the latter will further become a number, say 2.74, if some numerical answers are required:

$$\begin{aligned} \hbar^2/m &\rightarrow 1 \\ m\omega^2 &\rightarrow 1 \\ \beta &\rightarrow \frac{\beta\hbar}{m^2\omega^3} \xrightarrow{\text{in numerics}} 3.74 \rightsquigarrow \dots \end{aligned}$$

Imagine that we solved numerically the Eq. (1.9) for some value of β and obtained $E_{\text{g.s.}} = 1.14 \dots$. To return to the usual system of units, we have to simply multiply this result by the energy scale $\hbar\omega$ —*i.e.* the only parameter with units of energy that can be constructed out of $\hbar$, m , and ω :

$$\dots \rightsquigarrow E_{\text{g.s.}} = 1.14 \dots \rightarrow E_{\text{g.s.}} = 1.14 \dots \times \hbar\omega.$$

The true reason why the whole procedure looks mysterious at first is that formally speaking it severely abuses notations: for example, $E_{\text{g.s.}} = 1.14$

and $E_{\text{g.s.}} = 1.14 \dots \times \hbar\omega$ should be denoted by different symbols—but they are *not*. The practical advantages of this convention, however, compensate for the difficulties experienced at the learning stage.

1.1.2 Dimensional analysis: the harmonic oscillator alone

Now, let us try to produce a dimensional solution for the ground state energy of the harmonic oscillator alone:

$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x) + \frac{m\omega^2}{2} x^2 = E\psi(x). \quad (1.10)$$

Solution: The procedure goes as follows:

- The principal units—the units of length and the units of energy:

$$[\mathcal{L}], \quad [\mathcal{E}];$$

- The input parameters and their units:

$$[\eta] = [\mathcal{L}]^2 [\mathcal{E}]$$

$$[\Upsilon] = [\mathcal{L}]^{-2} [\mathcal{E}],$$

where again $\eta \equiv \hbar^2/m$, and $\Upsilon \equiv m\omega^2$;

- The set of independent dimensionless parameters = $\emptyset$. Indeed, assume there exists a dimensionless parameter P expressed as a product of powers of principal scales:

$$P = \text{const} \times \eta^{\xi_1} \Upsilon^{\xi_2}.$$

Its units are now

$$\begin{aligned} [P] &= [\eta]^{\xi_1} [\Upsilon]^{\xi_2} \\ &= ([\mathcal{L}]^2 [\mathcal{E}])^{\xi_1} ([\mathcal{L}]^{-2} [\mathcal{E}])^{\xi_2} \\ &= [\mathcal{L}]^{2\xi_1 - 2\xi_2} [\mathcal{E}]^{\xi_1 + \xi_2}. \end{aligned}$$

The analogue of Eq. (1.3) is

$$\hat{M} \cdot \begin{pmatrix} \xi_1 \\ \xi_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \quad (1.11)$$

where

$$\hat{M} = \begin{pmatrix} 1 & 1 \\ 2 & -2 \end{pmatrix}. \quad (1.12)$$

Now, according to the rule (1.5), this problem has *no dimensionless parameters at all*. This is exactly the situation where dimensional analysis produces the most complete solutions, accurate up to an unknown numerical prefactor;

- *The principal scales—the length scale and the energy scale, examples of:*

$$\mathcal{L} = \sqrt{\frac{\hbar}{m\omega}}$$

$$\mathcal{E} = \hbar\omega.$$

They are exactly the same as in the full harmonic-quartic problem;

- *Solution for the unknown:*

$$[E_{\text{g.s.}}] = [\mathcal{E}] \Rightarrow E_{\text{g.s.}} = \text{const} \times \mathcal{E} = \text{const} \times \hbar\omega,$$

where const is a number of the order of unity. Its precise value is inaccessible for dimensional methods. Recall that the exact value of this constant is 1/2.

Finally,

$$E_{\text{g.s.}} \sim \hbar\omega.$$

1.1.3 Order-of-magnitude estimate: full solution

1.1.3.1 Order-of-magnitude estimates vis-a-vis dimensional analysis

The dimensional analysis exemplified above is a formal method. It requires almost no understanding of the physics of the problem at hand. It has the advantage of being potentially applicable when a poorly understood physical phenomenon is studied; for example, in Chapter 10, we will deploy the dimensional machinery to analyze properties of integrable partial differential equations, under an explicit assumption that the reader either did not have any prior experience with the Kortewg-de Vries and sine-Gordon equations, or tries his or her best to pretend he or she didn't. The drawback of dimensional analysis is its limited scope of applicability. It applies only to problems with a small enough number of not-of-the-order-unity input parameters.

Conversely, order-of-magnitude estimates require a deep understanding of the physics behind the problem. Two principal stages of the solution

can be identified. At the first stage, the space of input parameters is split into regions of approximate applicability of simpler models. Often, the position of the boundary between the regimes becomes clear only after the simpler models are solved. At the second stage, these models are solved approximately: typically the geometry of the problem is rendered on a rectangular grid (“every closed trajectory is a rectangle, every angle is 90° , and integrals are height times width”), and all numbers of the order of unity are replaced by unity.

Our goal is to give an order of magnitude estimate of the ground state energy of the harmonic-quartic system (1.1).

A detailed solution to this problem is presented on the next two pages.

1.1.3.2 Harmonic vs. quartic regimes

It is obvious that for sufficiently small values of the quartic potential strength β , the ground state energy will be dominated by the harmonic part. It is equally obvious that if the value of β is too large, the harmonic contribution to the potential can be neglected. What is less obvious is that the boundary $\beta_{\text{between domains of applicability}}$ between the domains of applicability (“regimes”) of the harmonic and quartic theories must lie at a point $\beta_{\text{comparable predictions}}$ where these theories give comparable predictions:

$$\beta_{\text{between domains of applicability}} \sim \beta_{\text{comparable predictions}}.$$

To prove the latter assertion one should rely on the assumption that the ground state energy is a *continuous* function of the quartic strength β . Let us assume now that the boundary between regimes lies far below the point of comparable predictions, $\beta_{\text{between domains of applicability}} \ll \beta_{\text{comparable predictions}}$, and let us try to arrive at a contradiction. Indeed for $\beta \lesssim \beta_{\text{between domains of applicability}}$, the prediction of the harmonic theory applies, and for $\beta \gtrsim \beta_{\text{between domains of applicability}}$, the quartic theory applies. But since we are far from the point where the predictions of the two theories are comparable, at around $\beta_{\text{between domains of applicability}}$, the ground state energy as a function of β will have a discontinuity, that we disallowed. The identical reasoning applies for the case of $\beta_{\text{between domains of applicability}} \gg \beta_{\text{comparable predictions}}$. Thus, we arrive at a contradiction, *Q.E.D.*

The point of comparable predictions $\beta_{\text{comparable predictions}}$ is still unknown. But on both sides of this boundary, the models are much simpler than the original one: there, the ground state energy can be easily

estimated. These estimates will be used to determine the boundary between regimes β_{between} domains of applicability.

1.1.3.3 The harmonic oscillator alone

To estimate the ground state energy of the harmonic oscillator,

$$\hat{H}_{\text{HO}} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}x^2, \quad (1.13)$$

assume that the ground state has a spatial width Δx . It is known that in the ground state, the Heisenberg uncertainty inequality becomes an approximate equality,

$$\Delta p \sim \frac{\hbar}{\Delta x}, \quad (1.14)$$

where Δp is the momentum width. The ground state energy can then be estimated as

$$E_{\text{g.s.}} \sim A \frac{\hbar^2}{m(\Delta x)^2} + Bm\omega^2(\Delta x)^2 \quad (1.15)$$

$$A \sim B \sim 1, \quad (1.16)$$

where A and B are unknown entities of the order of unity. Now, it is also known that the ground state energy minimizes the expectation value of energy among all possible states. In particular, it should do so among states that yield an approximate Heisenberg equality (1.14). Thus the ground state energy is represented by the minimum of the energy (1.16) considered as a function of the width Δx . This minimum is given by

$$E_{\text{g.s.,HO}} \sim \hbar\omega, \quad (1.17)$$

and it is reached at

$$(\Delta x)_{\text{g.s.,HO}} \sim \sqrt{\frac{\hbar}{m\omega}}.$$

1.1.3.4 The quartic oscillator alone

The analysis of the ground state of a quartic oscillator,

$$\hat{H}_{\text{QO}} = \frac{\hat{p}^2}{2m} + \beta x^4, \quad (1.18)$$

is identical to the analysis of the harmonic one. The result is

$$E_{\text{g.s.,QO}} \sim \left(\frac{\hbar^2}{m}\right)^{2/3} \beta^{1/3}, \quad (1.19)$$

at

$$(\Delta x)_{\text{g.s.,QO}} \sim \left(\frac{\hbar^2}{m}\right)^{1/6} \frac{1}{\beta^{1/6}}.$$

1.1.3.5 The boundary between the regimes and the final result

Setting the ground state energy predictions, (1.17) and (1.19), equal,

$$E_{\text{g.s.,HO}} \sim E_{\text{g.s.,QO}},$$

we get

$$\beta_{\text{between domains of applicability}} \sim \frac{m^2 \omega^3}{\hbar}.$$

The final prediction for the ground state energy of a harmonic-quartic oscillator (1.1) reads

$$E_{\text{g.s.}} \sim \begin{cases} \hbar\omega & \text{for } \beta \lesssim \frac{m^2 \omega^3}{\hbar} \\ \left(\frac{\hbar^2}{m}\right)^{2/3} \beta^{1/3} & \text{for } \beta \gtrsim \frac{m^2 \omega^3}{\hbar} \end{cases}$$

1.1.4 An afterthought: boundary between regimes from dimensional considerations

It turns out that if we knew *a priori* there was a boundary between two regimes we would be able to get it on dimensional grounds. So the problem is: *find* $\beta_{\text{between domains of applicability}}$ *dimensionally*.

Solution: The dimensionless parameter P_1 (see (1.2)) is the only dimensionless number that controls how deep into the harmonic or quartic regime the system is. The transition between the regimes must happen at some special value of this parameter. *A priori*, for a non-negative dimensionless number, there exist only three special values: 0, 1, and $+\infty$. We know that the first corresponds to a deep harmonic regime, and the last corresponds to the quartic one. Thus, the transition between regimes must happen when the parameter P_1 reaches a value of the order of unity:

$$P_1|_{\beta \sim \beta_{\text{between domains of applicability}}} \sim \frac{\hbar \beta_{\text{between domains of applicability}}}{m^2 \omega^3} \sim 1.$$

An estimate for the boundary between regimes immediately follows:

$$\beta_{\text{between domains of applicability}} \sim \frac{m^2 \omega^3}{\hbar}$$

It is necessary to stress that this estimate does not imply that a harmonic-to-quartic transition exists. To show that, we have to go beyond dimensional analysis.

1.1.5 A Gaussian variational solution

Variational methods, introduced in Chapter 5, provide another simple but powerful tool that allows one to quickly estimate the result of a problem. Unlike dimensional and order-of-magnitude arguments, variational methods produce numerical answers, usually close to the exact result. *The assignment is: using a Gaussian variational ansatz, find the unknown function $\Phi(P_1)$ in Eq. (1.7).*

Solution: The exact ground state $\psi_{\text{g.s.,exact}}$ minimizes the energy functional

$$\mathcal{E}[\psi(\cdot)] = \int dx \left\{ \frac{\hbar^2}{2m} |\psi'(x)|^2 + \left(\frac{m\omega^2}{2} x^2 + \beta x^4 \right) |\psi(x)|^2 \right\}$$

on the space of smooth functions normalized to unity. The minimum of this functional on a one-parametric Gaussian manifold,

$$\psi(x, \sigma) \equiv \frac{1}{(2\pi\sigma^2)^{1/4}} e^{-x^2/(4\sigma^2)}$$

constitutes a Gaussian variational estimate for the true ground state energy.

The variational solution to the ground state energy is given by

$$\begin{aligned} E_{\text{g.s.}} &\stackrel{\text{variational}}{=} \Phi(P_1) \times \hbar\omega, \\ \text{with} \\ \Phi(P_1) &= \frac{6f(\phi(P_1))^2 + f(\phi(P_1))^3 + 1944P_1^2}{432f(\phi(P_1))P_1} \\ f(\phi) &= \phi + \frac{1}{\phi} - 1 \\ \phi(P_1) &= (486P_1^2 + 18\sqrt{729P_1^4 - 3P_1^2} - 1)^{1/3} \\ P_1 &= \frac{\hbar\beta}{m^2\omega^3} \end{aligned}$$

This result, along with the purely harmonic and purely quartic predictions, is presented in Fig. 1.1. As expected, for $P_1 \gtrsim 2$, the variational value is

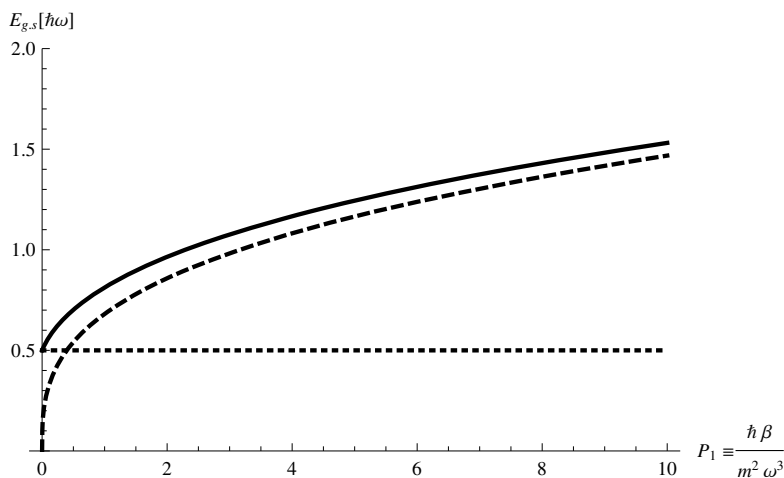


Fig. 1.1 A Gaussian variational solution for the ground state energy of a hybrid harmonic-quartic oscillator (1.1), as a function of the strength β of the quartic part of the potential (solid line). P_1 is the only dimensionless parameter of the problem. Exact energy for a purely harmonic oscillator (short-dashed line), and a Gaussian energy for a purely quartic oscillator (long-dashed line) are shown for comparison.

fairly close to the quartic prediction. On the other hand, for $P_1 \lesssim 0.25$, the ground state energy is close to the one for the harmonic oscillator.

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Chapter 2

Bohr-Sommerfeld Quantization

2.1 Solved problems

2.1.1 *A semi-classical analysis of the spectrum of a harmonic oscillator: the exact solution, an order-of-magnitude estimate, and dimensional analysis*

(a) Using the Bohr-Sommerfeld quantization rule,

$$\oint p(x|E_n) dx = 2\pi\hbar(n + 1/2)$$

$$n = 0, 1, 2, \dots, \quad (2.1)$$

where

$$p(x|E) \equiv \pm \sqrt{2m(E - V(x))}$$

$$\oint p(x|E) dx \equiv 2 \int_{x_{min}}^{x_{max}} |p(x|E)| dx,$$

determine the energy spectrum of a harmonic oscillator;

Solution: The WKB integral

$$A = \oint \sqrt{2m \left(E - \frac{m\omega^2 x^2}{2} \right)} dx$$

is nothing else but the area, $A = \pi r_x r_p$, of an ellipse with the half-axes $r_x = \sqrt{2E/(m\omega^2)}$ and $r_p = \sqrt{2mE}$. Thus, this integral is given by $A = 2\pi E/\omega$. Finally

$$E_n = \hbar\omega \left(n + \frac{1}{2} \right)$$

(b) Pretending you do not know how to compute the integral in Eq. (2.1), estimate E_n .

Solution: Replacing the ellipse by a rectangle, we get $A \approx r_x r_p \sim \sqrt{E/(m\omega^2)} \sqrt{mE} = E/\omega$. Finally, we get

$$E_n \sim \hbar\omega(n + 1/2)$$

(c) Pretending you do not even know what an “integral” is—just that its symbol “ $\oint$ ” is a dimensionless entity—estimate E_n using dimensional analysis.

Solution: The Bohr-Sommerfeld quantization rule again reads

$$\oint \sqrt{2m \left(E_n - \frac{m\omega^2 x^2}{2} \right)} dx = 2\pi\hbar(n + 1/2)$$

$$n = 0, 1, 2, \dots; \quad (2.2)$$

but this time around, we pretend that the integral is some obscure, poorly understood mathematical operation, and all we know is units the participants of the Eq. (2.2) are measured in.

Notice however that the state index n enters (2.2) *only* as one of the two factors of the product $\hbar(n + 1/2)$. This allows us to introduce a new dimensionful parameter, $\tilde{\hbar}$. Furthermore, we realize that only two independent dimensionful parameters are needed: $\tilde{\eta} \equiv \tilde{\hbar}^2/m$ and $\Upsilon \equiv m\omega^2$. The quantization rule now reads:

$$\oint \sqrt{2 \left(E_n - \frac{\Upsilon x^2}{2} \right)} dx = 2\pi\sqrt{\tilde{\eta}}$$

$$n = 0, 1, 2, \dots$$

Performing dimensional analysis we get

— The principal units—the units of length and the units of energy:

$$[\mathcal{L}], \quad [\mathcal{E}];$$

— The input parameters and their units:

$$[\tilde{\eta}] = [\mathcal{L}]^2 [\mathcal{E}]$$

$$[\Upsilon] = [\mathcal{L}]^{-2} [\mathcal{E}];$$

— The set of independent dimensionless parameters = $\emptyset$;



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— The principal scales—the length scale and the energy scale, examples of:

$$\mathcal{L} = \sqrt{\frac{\hbar}{m\omega}}$$

$$\mathcal{E} = \hbar\omega;$$

— Solution for the unknown:

$$E_n \sim \sqrt{\hbar}\Upsilon = \tilde{\hbar}\omega.$$

Finally,

$$E_n \sim \hbar\omega(n + 1/2)$$

2.1.2 WKB treatment of a “straightened” harmonic oscillator

Consider a “straightened” harmonic oscillator potential

$$V(x) = \begin{cases} \frac{m\omega^2(x + L/2)^2}{2} & \text{for } x < -L/2 \\ 0 & \text{for } -L/2 \leq x < +L/2 \\ \frac{m\omega^2(x - L/2)^2}{2} & \text{for } x \geq +L/2 \end{cases},$$

see Fig. 2.1.

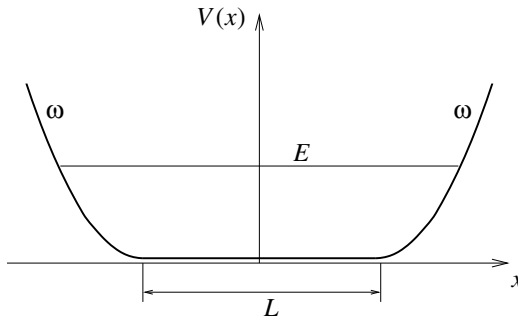


Fig. 2.1 Straightened harmonic oscillator.

Derive a WKB expression for the energy levels E_n .

Useful integral:

$$\int_0^1 \sqrt{1-t^2} dt = \frac{\pi}{4}.$$

Solution: The Bohr-Sommerfeld quantization rule reads:

$$S(E_n) = 2\pi\hbar \left(n + \frac{1}{2} \right) \\ n = 0, 1, 2, \dots, \quad (2.3)$$

where

$$S(E) = 2 \int_{x_1}^{x_2} dx \sqrt{2m(E - V(x))}$$

is the so-called classical full-cycle abbreviated action. Here x_1 and x_2 are the left and right classical turning points respectively.

In our case

$$S(E) = S_{\text{HO}}(E) + S_{\text{free}}(E),$$

where

$$\begin{aligned} S_{\text{HO}}(E) &= 2 \int_{-L/2 - \sqrt{2E/(m\omega^2)}}^{-L/2} dx \sqrt{2m(E - m\omega^2(x + L/2)^2/2)} \\ &\quad + 2 \int_{+L/2}^{+L/2 + \sqrt{2E/m\omega^2}} dx \sqrt{2m(E - m\omega^2(x - L/2)^2/2)} \\ &= 2 \int_{-\sqrt{2E/(m\omega^2)}}^{+\sqrt{2E/(m\omega^2)}} dx \sqrt{2m(E - m\omega^2 x^2/2)} \\ &= \frac{2\pi E}{\omega} \end{aligned}$$

and

$$S_{\text{free}}(E) = 2\sqrt{2mEL}.$$

Substitution of the above to the quantization rule (2.3) leads to

$$E_n = E_{\text{HO},n} + 2 \left(\mathcal{E} - \sqrt{\mathcal{E}(E_{\text{HO},n} + \mathcal{E})} \right) \\ n = 0, 1, 2, \dots,$$

where

$$E_{\text{HO},n} = \hbar\omega \left(n + \frac{1}{2} \right) \\ \mathcal{E} = \frac{1}{2\pi^2} m\omega^2 L^2$$

Interestingly, in the limit of the infinitely strong oscillator where $\omega \rightarrow \infty$, the energy spectrum reduces to

$$E_n \xrightarrow{\omega \rightarrow \infty} \frac{\hbar^2}{2m} \left(\frac{\pi}{L} \right)^2 \left(n + \frac{1}{2} \right)^2$$

$$n = 0, 1, 2, \dots,$$

which is nothing else but the spectrum of a box with “soft walls”—sharp boundaries where, at the same time, the spatial derivative of potential remains finite. Compare with the hard-wall box result,

$$E_{\text{hard-wall box}, n} = \frac{\hbar^2}{2m} \left(\frac{\pi}{L} \right)^2 (n+1)^2$$

$$n = 0, 1, 2, \dots$$

Note also, that when we remove the flat region of our potential (*i.e.* set $L = 0$) the spectrum reduces to the usual spectrum of the harmonic oscillator:

$$E_n \stackrel{L=0}{=} \hbar\omega \left(n + \frac{1}{2} \right)$$

$$n = 0, 1, 2, \dots,$$

2.1.3 Ground state energy in power-law potentials

Consider the Schrödinger equation for a particle in a “ $2q$ -tic” potential:

$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x) + K_q x^{2q} \psi(x) = E \psi(x)$$

$$q = 1, 2, 3, \dots$$

(a) *Using the Heisenberg uncertainty principle, estimate the ground state energy;*

Solution: The momentum and position uncertainties read

$$\frac{(\Delta p)^2}{m} \sim E_{\text{g.s.}} \Rightarrow \Delta p \sim \sqrt{mE}$$

$$K_q (\Delta x)^{2q} \sim E_{\text{g.s.}} \Rightarrow \Delta x \sim \left(\frac{E}{K_q} \right)^{\frac{1}{2q}}.$$

The ground state minimizes the Heisenberg uncertainty:

$$\Delta p \Delta x \sim \hbar.$$

Hence,

$$E_{\text{g.s.}} \sim \left(\frac{\hbar^2}{m} \right)^{\frac{q}{q+1}} K_q^{\frac{1}{q+1}}$$

(b) *The same as the above, but using dimensional analysis.*

Solution: The input parameters are $\hbar^2/m \equiv \eta$ and K_q . Their units are given by $[\eta] = \mathcal{E}\mathcal{L}^2$ and $[K_q] = \mathcal{E}/\mathcal{L}^{2q}$. The units for the ground state energy $E_{\text{g.s.}}$ are $[E_{\text{g.s.}}] = \mathcal{E}$. Thus,

$$E_{\text{g.s.}} \sim \left(\frac{\hbar^2}{m} \right)^{\frac{q}{q+1}} K_q^{\frac{1}{q+1}}$$

2.1.4 Spectrum of power-law potentials

Consider the Schrödinger equation for a particle in a “2q-tic” potential:

$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x) + K_q x^{2q} \psi(x) = E \psi(x).$$

(a) *Give an order-of-magnitude estimate for the spectrum E_n ; use the WKB quantization rule as a starting point.*

Solution: WKB quantization reads

$$\oint p(x|E_n) dx = 2\pi\hbar \left(n + \frac{1}{2} \right).$$

Estimating the WKB integral as

$$\oint p(x|E_n) dx \sim \underbrace{\sqrt{mE_n}}_{\Delta p} \underbrace{(E_n/K_q)^{\frac{1}{2q}}}_{\Delta x},$$

we get

$$\sqrt{mE_n}^{\frac{q+1}{2q}} \frac{1}{K_q^{\frac{1}{2q}}} \sim \hbar(n + 1/2),$$

or

$$E_n \sim \left(\frac{\hbar^2}{m} \right)^{\frac{q}{q+1}} K_q^{\frac{1}{q+1}} (n + 1/2)^{\frac{2q}{q+1}}$$

(b) Estimate the spectrum E_n using dimensional analysis applied to the WKB quantization rule.

Solution: In this case, the method of solution is completely analogous to the one used in Problem 2.1.1. Consider WKB quantization at large n :

$$\oint \sqrt{2m(E_n - K_q x^{2q})} dx = 2\pi\hbar(n + 1/2).$$

We can identify two input parameters: $(\hbar(n + 1/2))^2/m \equiv \tilde{\eta}$ and K_q , with $[\tilde{\eta}] = \mathcal{E}\mathcal{L}^2$ and $[K_q] = \mathcal{E}/\mathcal{L}^{2q}$. Here, K_q plays a role of Υ for the harmonic oscillator (Problem 2.1.1). The eigenenergies E_n , which have the dimension of energy, are given by

$$E_n \sim \left(\frac{\hbar^2}{m}\right)^{\frac{q}{q+1}} K_q^{\frac{1}{q+1}} (n + 1/2)^{\frac{2q}{q+1}} \quad (2.4)$$

Remark: A rigorous WKB quantization gives

$$E_n = C_q \left(\frac{\hbar^2}{m}\right)^{\frac{q}{q+1}} K_q^{\frac{1}{q+1}} (n + 1/2)^{\frac{2q}{q+1}},$$

where

$$C_q = \left(\frac{\pi}{2}\right)^{\frac{q}{q+1}} \left(\frac{\Gamma[\frac{3q+1}{2q}]}{\Gamma[\frac{2q+1}{2q}]}\right)^{\frac{2q}{q+1}}, \quad (2.5)$$

and $\Gamma[z]$ is the gamma-function.

2.1.5 The number of bound states of a diatomic molecule.

Consider two atoms with masses m_1 and m_2 , interacting via a “hard-core Van der Waals potential”,

$$V(r) = \begin{cases} -\frac{C_6}{r^6}, & r \geq R \\ +\infty, & r < R \end{cases}. \quad (2.6)$$

(a) Using dimensional analysis and the WKB approximation, estimate the total number N of the s -wave bound states ($l = 0$) of a diatomic molecule consisting of these two atoms.

Recall that the relative motion is the one of a single particle of the so-called reduced mass $\mu = m_1 m_2 / (m_1 + m_2)$, moving in the potential (2.6).

Solution: The only dimensionless combination one can form out of the set $\hbar^2/\mu$, C_6 , and R is

$$\xi \equiv \frac{\hbar^2 R^4}{\mu C_6}.$$

Therefore the (dimensionless) number N can only have the form

$$N = \Phi\left(\frac{\hbar^2 R^4}{\mu C_6}\right), \quad (2.7)$$

where $\Phi(\xi)$ is an unknown dimensionless function.

At the level of the Schrödinger equation, Eq. (2.7) constitutes the absolute maximum of the information one can extract from the dimensional analysis. However, at the WKB level, the level indices enter only as a factor in the product $\hbar(n - 1/4)$ (, where $n = 1, 2, 3, \dots$)¹, the physical reason being that in the limit $n \gg 1$, all the appearances of Planck's constant must be absorbed in the classical action, $I = \oint p dx = \hbar(n - 1/4)$. On the other hand, N is an upper bound for such indices, and therefore, any relation it is involved in should only contain functions of $\hbar(N - 1/4)$ as a whole. This limits $\Phi(\xi)$ to

$$\Phi(\xi) = \text{const} \times \frac{1}{\sqrt{\xi}} + 1/4.$$

Thus, finally

$$N - 1/4 \sim \frac{\sqrt{mC_6}}{\hbar R^2}$$

(b) *Compute this number exactly, within WKB.* Recall that for the hard-wall/soft-wall combination the Bohr-Sommerfeld rule reads

$$\oint p(x | E_n) dx = 2\pi\hbar \left(n + \frac{3}{4}\right), \quad n = 0, 1, 2, \dots \quad (2.8)$$

Solution: The upper bound n_{max} can be obtained from the Bohr-Sommerfeld quantization rule (2.8) by setting E_n to zero. The integral can then be easily computed, and it gives

$$N = \left\lfloor \frac{1}{\sqrt{2\pi}} \frac{\sqrt{mC_6}}{\hbar R^2} + \frac{1}{4} \right\rfloor$$

where $\lfloor \dots \rfloor$ is the floor function.

¹Here, we apply the quantization rule (2.17) corresponding to one “hard” and one “soft” turning point.

2.1.6 Coulomb problem at zero angular momentum

The zero-angular-momentum motion of an electron in the field of an atomic nucleus is described by the one-dimensional Schrödinger equation

$$\begin{aligned}
 -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial r^2} \chi(r) - \frac{\alpha}{r} \chi(r) &= E \chi(r) \\
 0 < r < \infty \\
 \chi(r \rightarrow 0) &= 0,
 \end{aligned}
 \tag{2.9}$$

where $\alpha = Ze^2$, e is the electron charge, and Z is the number of protons in the nucleus².

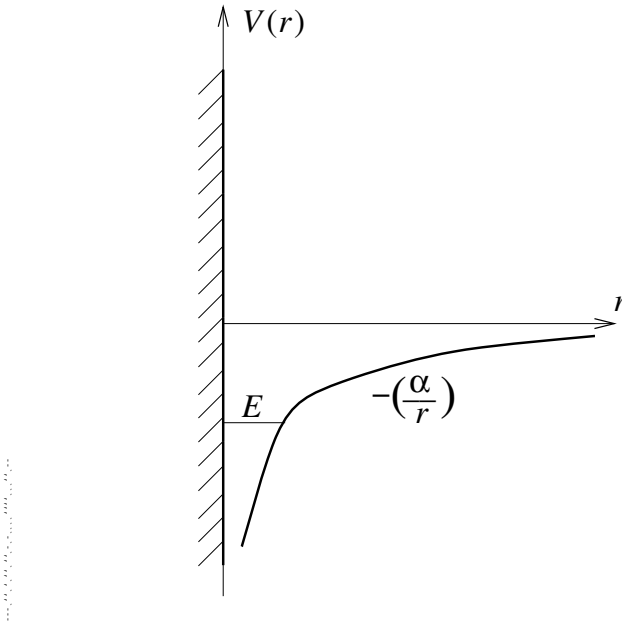


Fig. 2.2 Coulomb problem at zero angular momentum.

- (a) Find the ground state energy E_1 in three ways:
 (i) From the dimensional analysis;

²The effective one-dimensional wavefunction $\chi(r)$ is related to actual solutions $\Psi(r, \Theta, \phi)$ of the three-dimensional Coulomb problem $-\frac{\hbar^2}{2m} \nabla^2 \Psi(r, \Theta, \phi) - \frac{\alpha}{r} \Psi(r, \Theta, \phi) = E \Psi(r, \Theta, \phi)$ as $\Psi(r, \Theta, \phi) = r^{-1} \chi_l(r) Y_{l,m}(\Theta, \phi)$, where l and m are the azimuthal and magnetic quantum numbers respectively, and $Y_{l,m}$ are the spherical harmonics.

Solution:

- The principal units—the units of length and the units of energy.

$$[\mathcal{L}], \quad [\mathcal{E}];$$

- The input parameters and their units:

$$[\tilde{\eta} \equiv \hbar^2/m] = [\mathcal{L}]^2 [\mathcal{E}]$$

$$[\alpha] = [\mathcal{L}] [\mathcal{E}] ;$$

- The set of independent dimensionless parameters = $\emptyset$;

- The principal scales—the length scale and the energy scale, examples of:

$$\mathcal{L} = \frac{\hbar}{m\alpha}$$

$$\mathcal{E} = \frac{m\alpha^2}{\hbar} ;$$

- Solution for the unknown:

$$E_1 \sim \mathcal{E} = \frac{m\alpha^2}{\hbar}.$$

We get finally

$$E_1 \sim \frac{m\alpha^2}{\hbar^2}$$

(ii) From the Heisenberg uncertainty principle:

- (α) Estimate the spatial extent Δr of the motion at a given energy E ;
 (β) Estimate the momentum spread Δp using dimensional analysis³;
 (γ) Obtain the ground state energy E_1 using the fact that the Heisenberg inequality $\Delta p \Delta r \gtrsim \hbar$ becomes an (approximate) equality $\Delta p \Delta r \sim \hbar$ in the ground state.

³Estimating Δp from the phase-space trajectory (as we do usually) is not straightforward, because the momentum diverges at $r = 0$.

Solution:

(α) A classical estimate for the apogee gives

$$\frac{\alpha}{\Delta r} \sim E \Rightarrow \Delta r \sim \frac{\alpha}{E}.$$

(β) A classical dimensional analysis (no $\hbar$, energy E instead) gives

$$\Delta p \sim \sqrt{mE}.$$

(γ) In the ground state, the Heisenberg inequality becomes close to an equality:

$$\Delta p(E_1) \Delta r(E_1) \sim \hbar.$$

Thus

$$E_1 \sim \frac{m\alpha^2}{\hbar^2}$$

(iii) From the Bohr-Sommerfeld rule⁴:

$$\oint p(r) dr = 2\pi\hbar(n + \delta) \quad (2.10)$$

$$n = 0, 1, 2, 3, \dots$$

⁴We deliberately leave δ undefined. The question of a proper WKB quantization of a three-dimensional radially symmetric potential, including Coulomb problems at both non-zero and zero angular momenta, has a long and convoluted history. A rigorous analysis of the question is presented in a comprehensive book on WKB by Heading [M. A. Heading, *An Introduction to Phase-Integral Methods* (John Wiley, New York (1962))]. The currently most accepted quantization recipe is based on the classic paper by Langer [R. E. Langer, On the connection formulas and the solutions of the wave equation, *Phys. Rev.* **51**, 669 (1937)]. In short, Langer's WKB prescription for a potential $V(r)$ at angular momentum l is as follows:

$$\oint p_{\text{eff.}}(r) dr = 2\pi\hbar(n_r + 1/2)$$

$$n_r = 0, 1, 2, 3, \dots$$

$$p_{\text{eff.}}(r) \equiv \sqrt{2m(E_{n_r} - V_{\text{eff.}}(r))}$$

$$V_{\text{eff.}}(r) \equiv V(r) + \frac{\hbar^2(l + 1/2)^2}{2mr^2};$$

notice the replacement $l(l + 1) \rightarrow (l + 1/2)^2$ (the so-called Langer correction). The rule applies to both regular and singular potentials for any value of the angular momentum, including $l = 0$.

Useful integral:

$$\int_0^1 \sqrt{1/t - 1} dt = \frac{\pi}{2}.$$

Solution:

$$\begin{aligned} \int_0^{r_2(E)} dr \sqrt{2m(-|E| + \alpha/r)} &= \sqrt{2m|E|} r_2(E) \int_0^1 \sqrt{1/t - 1} \\ &= \frac{\sqrt{2m\alpha} \pi}{\sqrt{|E|}} \frac{1}{2}. \end{aligned}$$

Here, $r_2(E) = \alpha/|E|$ is the right turning point (the apogee point for the Coulomb case). On the other hand

$$\int_0^{r_2(E_n)} \sqrt{2m(-|E_n| + \alpha/r)} = \pi \hbar (n + \delta).$$

We get

$$\begin{aligned} E_n &= -\frac{(m\alpha^2/\hbar^2)}{2(n + \delta)^2} \\ n &= 0, 1, 2, 3, \dots \end{aligned}$$

For the ground state energy we have

$$E_1 = \left(-\frac{1}{2}\right) \frac{m\alpha^2}{\hbar^2} \frac{1}{\delta^2}$$

(b) Verify that

$$\chi_1(r) = \frac{2}{\sqrt{a_Z}} (r/a_Z) \exp(-r/a_Z) \quad (2.11)$$

obeys the Schrödinger equation (2.9). Here, $a_Z = a_B/Z$, and $a_B = \hbar^2/(me^2)$ is the Bohr radius. Find the corresponding energy E_1 . Since (2.11) has the least number of the nodes allowed by the boundary conditions in (2.9), it corresponds to the ground state, and thus the energy E_1 you will infer from (2.11) is the exact ground state energy. Compare the exact E_1 you will get with the WKB prediction from sub-problem (a)-(iii).

Solution: Substitution of the state (2.11) into the Schrödinger equation (2.9) makes the latter an equality for

$$E_1 = \left(-\frac{1}{2}\right) \frac{m\alpha^2}{\hbar^2}$$

2.1.7 Quantization of angular momentum from WKB

Consider a particle of mass m moving on a surface of a sphere of radius R . The energy of the particle is determined by its azimuthal quantum number l :

$$E_{l,m} = \frac{\hbar^2 l(l+1)}{2mR^2}.$$

At large energies (thus at short de Broglie wavelengths), one may assume that the particle's wavefunction becomes less sensitive to the curvature of the sphere, and the problem can be approximately replaced by a *flat* billiard of the same area as the sphere. According to this interpretation,

$$P \equiv \frac{\hbar l}{R}$$

becomes the magnitude of the linear momentum of the particle, and the energy,

$$E_{l,m} \stackrel{E_{l,m} \gg \hbar^2/(mR^2)}{\approx} \frac{(\hbar l/R)^2}{2m} = \frac{P^2}{2m},$$

becomes reinterpreted as the particle's kinetic energy.

(a) Using the multi-dimensional WKB quantization rule (see Weyl law in Sec. (2.3.2)), determine $\bar{N}(E)$ —the number of eigenstates with energy below or equal to some energy E ;

Solution: For a given energy E , the phase space volume occupied by points with energy less than or equal to E is

$$\begin{aligned} W(\text{energy} \leq E) &= \underbrace{2\text{D-Volume}(\text{surface of 3D-sphere, coordinates})}_{4\pi R^2} \\ &\quad \times \underbrace{2\text{D-Volume}(\text{2D-ball, momenta})}_{\pi P^2} \\ &= 4\pi^2 R^2 P^2. \end{aligned}$$

Now, according to the Weyl law,

$$\bar{N}(E) \stackrel{E \gg \hbar^2/(mR^2)}{\approx} \frac{W(\text{energy} \leq E)}{(2\pi\hbar)^2}.$$

We get:

$$\boxed{\bar{N}(E) \stackrel{E \gg \hbar^2/(mR^2)}{\approx} 2 \frac{E}{\hbar^2/(mR^2)} \stackrel{E \gg \hbar^2/(mR^2)}{\approx} l^2}$$

where $E = (\hbar l/R)^2/2m \stackrel{E \gg \hbar^2/(mR^2)}{\approx} E_{l,m}$.

(b) Using the exact quantization of the motion on a sphere, $E_{l,m} = \hbar^2 l(l+1)/(2mR^2)$, $l = 0, 1, \dots$; $m = -l, -l+1, \dots, +l$, find an expression for $\bar{N}_l$ —the number of angular momentum eigenstates with the azimuthal quantum number l' less than or equal to l and compare it with your result from part (a).

Solution:

$$\bar{N}_l = \sum_{l'=0}^l \sum_{m=-l}^{+l} 1,$$

or

$$\bar{N}_l = (l+1)^2$$

The agreement between (a) and (b) is quite remarkable.

2.1.8 From WKB quantization of 4D angular momentum to quantization of the Coulomb problem

It is not well-known⁵ that there exists a map between the eigenstates $|n, l, m\rangle$ of the (three-dimensional) Coulomb problem $\hat{H} = p^2/(2m) - \alpha/r$ and the eigenstates $|l_{4D}, l_{3D}, m\rangle$ of a particle moving on a surface of a *four-dimensional* sphere of radius R . In this map, the quantum number n is related to the four-dimensional azimuthal quantum number l_{4D} as $n = l_{4D} + 1$. Likewise, $l = l_{3D}$. The energy on the 4D sphere is quantized as

$$E_{l_{4D}, l_{3D}, m} = \frac{\hbar^2 l_{4D}(l_{4D} + 2)}{2mR^2}. \quad (2.12)$$

Similarly to the three-dimensional case of Problem 2.1.7, we would assume that high energies, the 3D “surface” of the 4D-sphere will look almost flat, and the surface can be un-bent to a 3D Cartesian billiard. Again, analogously to the Problem 2.1.7 case,

$$P \equiv \frac{\hbar l_{4D}}{R}$$

⁵V. Fock, Zur Theorie des Wasserstoatoms, Z. Physik **98**, 145 (1935) [English translation: V. Fock, On the theory of the hydrogen atom, in: Dynamical Groups and Spectrum Generating Algebras, vol. 1, p. 411, A. Bohm, Y. Neeman, A. O. Barut (eds.) (World Scientific, Singapore (1988)).

should be interpreted as momentum, and

$$E_{l_{4D}, l_{3D}, m} \stackrel{E_{l_{4D}, l_{3D}, m} \gg \hbar^2/(mR^2)}{\approx} \frac{(\hbar l_{4D}/R)^2}{2m} = \frac{P^2}{2m}$$

as kinetic energy.

(a) Using Weyl's multi-dimensional WKB quantization rule (Sec. 2.3.2)), determine the number $\bar{N}(E)$, which is the of number the eigenstates of the four-dimensional sphere with energy below or equal some energy E , reinterpret your result in terms of the Coulomb spectrum, and find the number $\bar{N}_C(E_C)$ defined as the number of the eigenstates of the Coulomb problem with energies not exceeding E_C .

Useful information: in four dimensions, the 3D-surface of a sphere of radius R is $S_3 = 2\pi^2 R^3$. The 4D-volume of a four-dimensional ball of radius R is $V_4 = (\pi^2/2)R^4$.

Solution: For a given energy E , the phase space volume occupied by the points with energy less or equal E is

$$\begin{aligned} W(\text{energy} \leq E) &= \underbrace{\text{3D-Volume}(\text{surface of 4D-sphere, coordinates})}_{2\pi^2 R^3} \\ &\times \underbrace{\text{3D-Volume}(\text{3D-ball, momenta})}_{\frac{4}{3}\pi P^3} = \frac{8\pi^3}{3} R^3 P^3. \end{aligned}$$

Thus,

$$\begin{aligned} \bar{N}(E) &\stackrel{E \gg \hbar^2/(mR^2)}{\approx} \frac{W(\text{energy} \leq E)}{(2\pi\hbar)^3} \\ &\stackrel{E \gg \hbar^2/(mR^2)}{\approx} \frac{2}{3} \left(\frac{E}{\hbar^2/(mR^2)} \right)^{3/2} \\ &\stackrel{E \gg \hbar^2/(mR^2)}{\approx} \frac{1}{3} l_{4D}^3. \end{aligned}$$

Now, observe that (a) the eigenenergies of the 4D-sphere, given by Eq. (2.12), represent a monotonically increasing function of l_{4D} ; (b) Coulomb eigenenergies,

$$E_{C;n,l,m} = -\frac{m\alpha^2/\hbar^2}{2n^2},$$

increase monotonically with n , and (c) according to Fock's map described above, $n \stackrel{l_{4D} \gg 1}{\approx} l_{4D}$. Thus,

$$\bar{N}_C(E_{C;n \approx l_{4D}, l, m}) \approx \bar{N}(E_{l_{4D}, l_{3D}, m}).$$