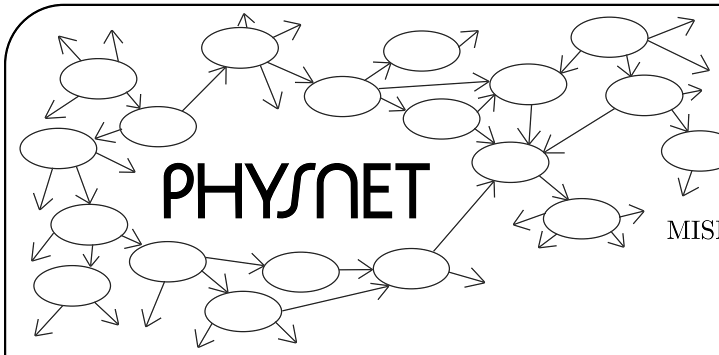

MISN-0-386

HARMONIC OSCILLATOR I

Quantum Physics

Project PHYSNET Physics Bldg. Michigan State University East Lansing, MI

HARMONIC OSCILLATOR I
by
R. Spital

Title: **Harmonic Oscillator I**

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Version: 2/1/2000 Evaluation: Stage B0

Length: 2 hr; 9 pages

Input Skills:

1. Vocabulary: polynomial, Taylor expansion, power series.
2. Be able to take partial derivatives.
3. Unknown: assume (MISN-0-385).

Output Skills (Knowledge):

K1. Write the S-equation for the harmonic oscillator and transform it to dimensionless form.

K2. Propose a form for the solution involving a decaying exponential and a power series.

K3. Obtain recursion relations among the coefficients of the power series and show that the power series must terminate.

K4. Write down a rule for obtaining the Hermite polynomials through a sequence of differentiations.

Output Skills (Rule Application):

R1. Use the requirement in K3 to determine the energy eigenvalues of the Hamiltonian.

R2. Use the recursion relations to derive the first few Hermite polynomials given that $H_0(q) = 1$, $H_1(q) = 2q$.

R3. Use the rule of K4 to obtaining the normalization of the harmonic oscillator wave functions, and express these wave functions in terms of the coordinate x. Also use the rule to show that any two different harmonic oscillator wave functions are orthogonal.

R4. Obtain $< x >$, $< P_x >$, $< T >$, and $< v >$ from simple symmetry arguments without integration and verify these results for the lowest two energy eigenstates.

R5. Solve problems such as 5-18a.

External Resources (Required):

1. E. E. Anderson, *Modern Physics and Quantum Mechanics*, W. B. Saunders (1971).

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1. Introduction

Next in our study of the one-dimensional S-equation, we come to the harmonic oscillator. Here the potential is given by $V = 1/2kx^2$, where we recognize the constant k as the familiar Hooke's law constant of classical mechanics. Since nearly all potential wells can be approximated by parabolas near their minima, the harmonic oscillator can be used to approximate the low-lying energy levels of many systems. It is also of the greatest importance in the theoretical treatment of statistical mechanics and quantum field theory.

2. Procedures

1. Read section 5.5 through equation 5-20. Equation 5.20 is the required dimensionless form.

2. Read the arguments leading to equation 5.22. The proposed form is $e^{-q^2/2}H(q)$. If the arguments for this form don't seem convincing, then regard it as simply a good guess. After all, the method by which one finds the solution to a differential equation is irrelevant as long as the solution works!

3. Read the remainder of section 5.5. The recursion relations are obtained by demanding that the coefficients of each power of q vanish separately.

   Make sure you understand the steps leading to equation 5.23. The general result (for arbitrary k) can be proved by induction (try this if you know how and are ambitious). You must be able to get the results for $k = 0, 1$ and 2 on your own.

   Read carefully the argument that the series must terminate. (Implicit here is the requirement that the wave function must not diverge as $q \Rightarrow \infty$. What is the physical reason for this?) Starting from

   $$\frac{a_{k+2}}{a_k} \Rightarrow \frac{2}{k},$$

   you should be able to complete the argument.

4. The requirement that the series terminate means that $\epsilon - 1 - 2k = 0$, or $\epsilon = 2k + 1$. Use the definition of ϵ to show that the possible energies of the system are $E_k = (2k + 1)\hbar\omega/2$. This is more usually written as $E_n = (n + 1)\hbar\omega/2$. Note that the ground state energy $E_0 = 1/2\hbar\omega$. This can be understood from the uncertainty principle in much the same way as the fact that the "particle in a box" ground state also has $E_0 \neq 0$.

   Notice that both here and in the infinite square well, the *boundary conditions* have led to quantization of the energy levels; i. e. the boundary conditions can only be satisfied for certain discrete energies. This is in sharp contrast to our classical intuition!

5. Read section 5.6 through the top of page 181. Then using $a_0 = 1$, $a_1 = 2$, find H_3, H_4 and $H + 5$ from the recursion relations.

   The "oddness and evenness" properties of $H_n(q)$ remind us of the similar properties of the square well wave functions. The *parity* of a wave function is defined to be +1 if $\psi(x) = \psi(-x)$ and −1 if $\psi(x) = -\psi(-x)$. It turns out that if $V(x) = V(-x)$, it is always possible to demand that an energy eigenstate be either even or odd (have definite parity). This is because the parity operator, defined by $Pf(x) = f(-x)$, commutes with the Hamiltonian. We shall return to this in MISN-0-388.

   The remainder of section 5.6 is optional.

6. The rule is equation 5.35.

7. Read section 5.7 through equation 5.38. Make sure you understand and can reproduce every step. Then derive eauation 5.40 by using the definition of q in terms of x.

   Two wave functions ψ_1 and ψ_2 are said to be orthogonal if and only if

   $$\int \psi_1^*(\vec{r})\psi_2(\vec{r})d\tau = 0\,.$$

   The orthogonality of the different eigenstates of the Hamiltonian is no accident. It turns out that so long as the eigenstates correspond to *different* energies, they must be orthogonal. (In fact this holds for any *observable* operator.) More on this in Unit 8. The remainder of section 5.7 is optional. As an exercise check the orthogonality and normalizations of ψ_0 and ψ_1.

8. Looking at the Hamiltonian, you see that it is completely symmetric about $x = 0$ and $p_x = 0$; and moreover, no other values of x and p_x have the same status. What then do you predict for $< x >$ and $< p_x >$?

   Let $p' = p_x/\sqrt{m}$ and let $q' = \sqrt{k}x$. Then the Hamiltonian is $1/2(p'^2 + q'^2)$ and $T = 1/2p'^2$, $V = 1/2q'^2$. Note that $\mathcal{H}$ is completely symmetric in p' and q'. How then do you expect the energy to be apportioned between T and V? Use this to obtain $< T >$ and $< V >$.

   While the above arguments are not proofs (the eigenstates do *not* always have the symmetries of the Hamiltonian), there could be no physical justification for a breakdown of these arguments in this simple system. Of course, the vindication of our intuition lies in the calculations. Verify your results for ψ_0 and ψ_1.

9. To introduce the application of our results to molecular vibrations, read section 5.8 and solve problem 5.18a.

   To see how the harmonic oscillator is used to approximate more complicated potentials, do the following exercise:

   Let the potential $V(x)$ have a minimum at $x = x_0$. Expand V in a Taylor series about x_0 and identify the appropriate "spring constant" to use if we wish to approximate V in the neighborhood of by a quadratic potential. What will the constant term in the expansion do to the oscillator energy levels?

Acknowledgments

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