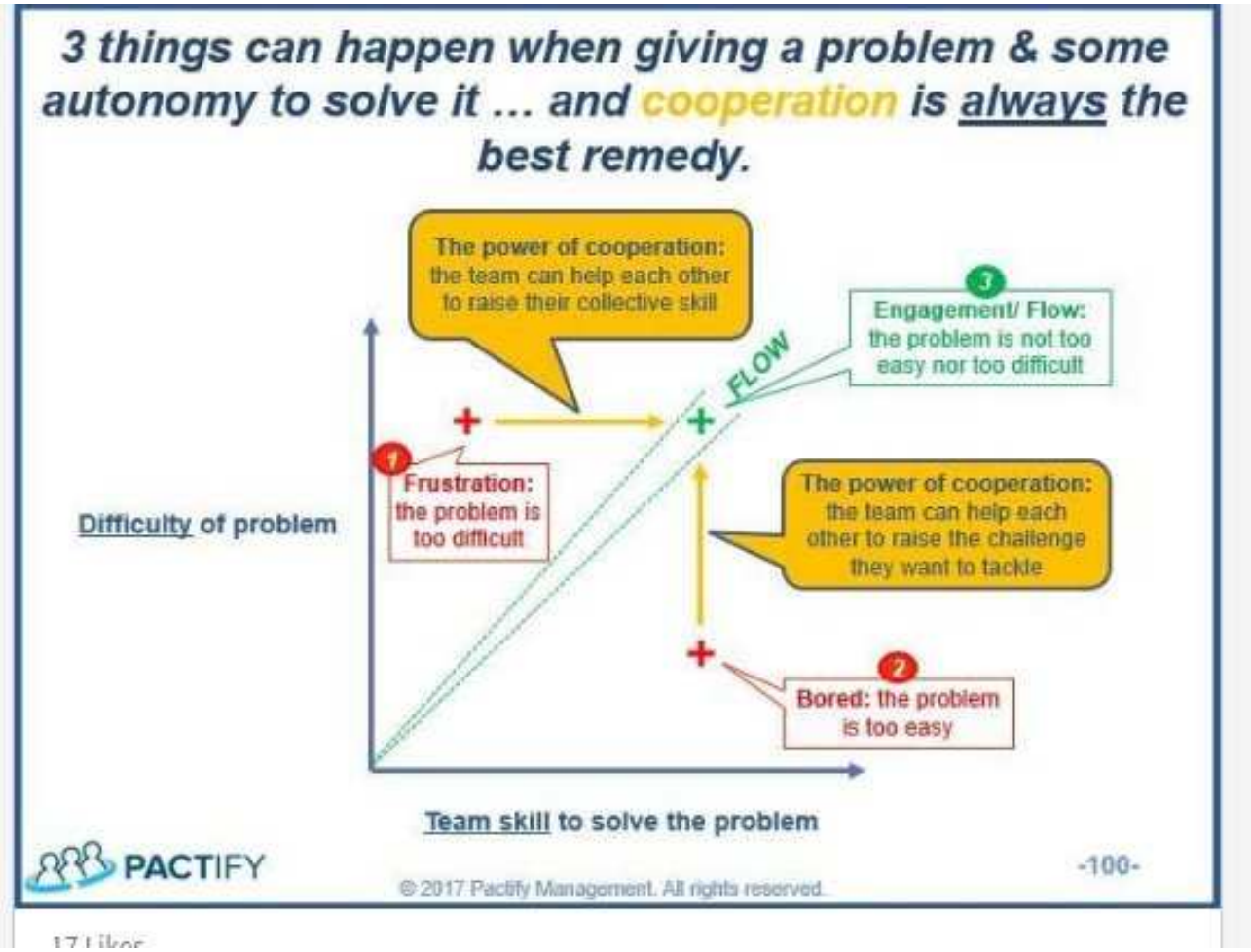
Project: THE ANHARMONIC OSCILLATOR and WAVE PACKETS

- **Coaches:** Corneel Casert and Frederic Van Assche
- **Responsible lecturer:** Jan Ryckebusch
- **Questions with regard to this project?** Please put your question in an e-mail addressed to the two coaches and the responsible lecturer.



The following rules apply:

1. You can work on this project for two consecutive days of eight working hours. It can happen that you face some difficulties in completing some parts of the project. In those situations, please sketch the efforts you have made and the difficulties you have encountered.

2. By 7pm on the second day you are expected to upload the following files to the "Documents > RESULTS" directory of your "Exam Group" on Minerva

   (1) A presentation (in pdf format) of about 10-15 pages. The presentation provides a summary of the obtained results. There is one presentation for the whole group. On the first page of the presentation it is mentioned who has been in charge for the different parts of the project. For example, Ms. Y and Mr. X took care of most of the programming, Ms. Z has made most of the figures. Mr. A and Ms. B mostly worked on the second part of the project . . . .

   (2) A copy of the computer programs that were developed during the course of project work. It is perfectly legitimate to build on programs that were part of the course material (theory and problem sessions). Please clearly mention the additions or modifications to existing programs that have been made by adding comments of the type
   "⟶ START OF MODIFICATION"
   . . .
   "⟵ END OF MODIFICATION"

3. The project work is evaluated by at least two qualified researchers on an individual basis according to the following criteria

   (a) the quality of the presentation (including the quality and originality of the figures)

   (b) the degree of displayed inititiative and creativity, demonstrated ability to work independently

   (c) a proper research attitude is important: careful, structured work aimed at finding new solutions, as well as critical attitude towards the results obtained

   (d) the mastery of the technical aspects of the topics covered in the project, including mastery of the numerical methods and the physical assumptions that underlie the methods that were used *(for example, how well have the computer programs been tested and displayed attention for the efficiency of the algorithms)*

   (e) quality of the answers to the questions of the evaluators during the oral exam

THE ANHARMONIC OSCILLATOR

We wish to study the quantum behaviour of an electron with a Hamiltonian of the type

$$H(x, p_x) = \frac{p_x^2}{2m} - \frac{a^2 V_0}{a^2 + x^2} \; . \tag{1}$$

This so-called anharmonic oscillator is most often a more realistic description of an oscillator than a linear harmonic oscillator. One reason is that it takes only a finite amount of energy to break a real object, so $V(x \to +\infty)$ should be finite, which is obviously not the situation for a linear harmonic oscillator.

Neither in classical mechanics nor in quantum mechanics, the equations-of-motion for the anharmonic oscillator are exactly solvable. In this project, you will work out numerical solutions for both the "classical" and "quantum mechanical" anharmonic oscillator.

QUESTIONS

CLASSICAL 1: Use the Euler and velocity Verlet method to determine the dynamics of the anharmonic oscillator in classical (Newtonian) mechanics.

CLASSICAL 2: Design and implement a methodology to compute the classical probability distribution $P_{CL}(x)$ for the position x of an anharmonic oscillator. Thereby, you may find some parts of the paper of R.W. Robinett in Am. J. .Phys. 65(3) (1993) 190 (appended) useful.

QUANTUM 1: Use the variational method to determine the eigenvalues and eigenfunctions of the anharmonic oscillator. Perform some tests that clearly illustrate that your results have the expected behaviour with increasing basis set size in linear variational calculus.

QUANTUM 2: Compare the classical $P_{CL}(x)$ and quantum mechanical $P_{QM}(x)$ probability distributions for the anharmonic oscillator. In how far do you retrieve the well-known correspondence principle from Bohr? This principle states that in the limit of large quantum numbers the quantum mechanical predictions approach the classical ones.

QUANTUM 3: For a one-dimensional harmonic oscillator the Heisenberg uncertainty principle adopts the form

$$\Delta x \Delta p_x = \left(n + \frac{1}{2} \right) \hbar \; ,$$

with n the quantum number of the bound state. Use appropriate numerical methods to compute $\Delta x \Delta p_x$ for the anharmonic oscillator and evaluate the difference with the harmonic situation for the different values of n. Are your results in line with the expectations? In how far do your results differ from the harmonic situation? Do you retrieve the analytic predictions for $\Delta x \Delta p_x$ for combinations of (V_0, a) that approach the harmonic situation?

QUANTUM 4: An alternate method to find the solutions of the time-independent Schrödinger equation (TISE) is based on the approximation detailed below and for example explained on physics stackexchange [1]. The technique allows one to turn the TISE into a finite matrix equation and then to use a numerical linear algebra package to find the eigenvalues and eigenvectors.

1. The second-order derivative can be approximated by

$$\frac{d^2\psi(x)}{dx^2} \approx \frac{1}{h^2}\left[\psi(x+h) + \psi(x-h) - 2\psi(x)\right]$$

   where h is a small increment in the position x.
2. Consider a finite grid of position variables $x_n = nh$ ($n \in \mathbb{Z}$).
3. Define the wave function $\psi(x)$ and the potential $V(x)$ in the grid of position variables: $\psi(x+h) = \psi((n+1)h) \equiv \psi_{n+1}$ and $V(x+h) = V((n+1)h) \equiv V_{n+1}$.
4. With these approximations the TISE becomes the eigenvalue equation of a tridiagonal matrix (this is a matrix with non-zero elements on the leading diagonal, above this diagonal and below this diagonal)

(Q3a) Use the above method to find the eigenvalues and eigenfunctions of the anharmonic oscillator.
(Q3b) Is the behaviour of accuracy of the solutions under $h \to \frac{h}{2} \to \frac{h}{4} \to \ldots$ in line with your expectations? Please explain your answer.

QUANTUM 5: An experiment places an electron with a definite momentum k_0 in a one-dimensional region of space the size of an atom. A convenient wave function $\Psi(x, t=0)$ describing this situation is a Gaussian multiplying a plane wave $\exp ik_0x$. The electron is confined to a specific region in space by an anharmonic oscillator potential. You are expected to determine the resultant electron behaviour in time ($t > 0$) and space. To this end you can build on the methodology outlined in Sections 18.5-18.9 of the book "A Survey of Computational Physics" by Rubin H. Landau. For your convenience the corresponding sections of this book are appended to this questionnaire –PLEASE CHECK THE DERIVATIONS AS THERE ARE TYPOS.

[1] https://physics.stackexchange.com/questions/170546/

Average value of position for the anharmonic oscillator: Classical versus quantum results

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The evaluation of the average value of the position coordinate, $\langle x \rangle$, of a particle moving in a harmonic oscillator potential ($V(x)=kx^2/2$) with a small anharmonic piece ($V'(x)=-\lambda kx^3$) is a standard calculation in classical Newtonian mechanics and statistical mechanics where the problem has relevance to thermal expansion. In each case, the calculation is most easily done using a perturbative expansion. In this note, we perform the same computation of $\langle x \rangle$ in quantum mechanics using time-independent perturbation theory and the ladder operator formalism to show how similar results are obtained. We also indicate how a semiclassical calculation using a classical probability distribution can also be used to obtain the same result. © *1997 American Association of Physics Teachers.*

I. INTRODUCTION

The simple harmonic oscillator is one of the most often discussed problems in all of classical, statistical, and quantum mechanics.[1] In addition to its direct connections to important physical systems, one of its most useful features is that at every stage of development, from elementary classical mechanics to quantum field theory, it is exactly soluble and so can be easily used as a closed-form analytic example.

Many interesting physical phenomena, however, rely directly on small deviations away from the simple form of the quadratic potential of the harmonic oscillator. As an example, even introductory texts[2–4] often stress the fact that the thermal expansion observed in many materials is due to a lack of symmetry about the minimum in the intermolecular potential. Such a feature of realistic potentials can be modeled by the addition of a small anharmonic term of the form $V'(x)=-\lambda kx^3$ to the usual harmonic piece, $V(x)=kx^2/2$. The average value of position, $\langle x \rangle$, in such an oscillator can then be calculated using classical Newtonian mechanics (see, e.g., Ref. 5) or statistical mechanics (see, e.g., Ref. 6) with the familiar result that $\langle x \rangle$ increases linearly with amplitude squared, energy, or temperature in contrast to the case of the pure oscillator where $\langle x \rangle = 0$.

Many texts on quantum mechanics consider the effects of small anharmonicities on the energy spectrum of the harmonic oscillator. A quadratic term of the form $V'(x)=ax^4$ is often discussed (see, e.g., Refs. 7–11) in the context of perturbation theory where there is a nontrivial first-order effect; such calculations are also often used as an illustration of the power of operator methods and raising/lowering operator techniques are used to evaluate the required matrix elements. In contrast, the $V'(x)=-\lambda kx^3$ term is presented (see, e.g., Refs. 10–13) as an example where the first-order correction vanishes (due to the symmetry of the problem and the perturbation) and a second-order calculation is required. In a few cases, the first-order correction to the wave function itself has also been explicitly presented (Refs. 10 and 13), but no physical information is extracted from it.

In this note, we extend these very familiar analyses to evaluate, using perturbation theory and operator techniques, the average value of position for the standard oscillator problem perturbed by a small cubic anharmonic term and make comparisons with the classical and statistical mechanical results. In addition, we also present a derivation of the same effect using classical probability distributions, $P_{\rm CL}(x)$, which are also discussed in many elementary texts and make a nice connection between the classical Newtonian solutions and the probabilistic quantum mechanical derivation using $P_{\rm QM}(x)=|\psi(x)|^2$. In Sec. II we very briefly review the classical and statistical mechanical results and their relevance to thermal expansion, while Sec. III presents the main quantum mechanical and semiclassical results.

II. CLASSICAL RESULTS

In classical Newtonian mechanics, a potential energy given by

$$U(x)=\tfrac{1}{2}kx^2-\lambda kx^3 \tag{1}$$

corresponds to a force

$$F(x)=-kx+3\lambda kx^2 \tag{2}$$

so that Newton's law reads

$$\ddot{x}(t)=-\omega^2x(t)+3\lambda\omega^2x^2(t), \tag{3}$$

where $\omega=\sqrt{k/m}$ as usual. A perturbative solution of the form

$$x(t)=x_0(t)+(\lambda A)x_1(t)+(\lambda A)^2x_2(t)+\cdots, \tag{4}$$

where $x_0(t)=A\cos(\omega t)$ is the lowest-order result with amplitude A, gives the differential equation

$$\ddot{x}_1(t)=-\omega^2x_1(t)+3\omega^2A\cos^2(\omega t) \tag{5}$$

for the $\mathcal{O}(\lambda)$ term. This can be easily solved for $x_1(t)$ using standard techniques to give

$$x(t)=A\cos(\omega t)+\frac{\lambda A^2}{2}(3-\cos(2\omega t)). \tag{6}$$

The average value of position can be defined via

$$\langle x(t)\rangle_\tau=\frac{\int_0^\tau x(t)dt}{\int_0^\tau dt}=\frac{1}{\tau}\int_0^\tau x(t)dt \tag{7}$$

using, for example, τ as the period of the unperturbed motion or in the limit that $\tau\to\infty$. In either case, the averaging process singles out the ''dc'' component only, giving

$$\langle x\rangle=\frac{3}{2}\lambda A^2. \tag{8}$$

In order to make connections with thermal expansion, we note that the total energy of the (unperturbed) oscillator system is given by $E_{\rm tot}=kA^2/2$. For the one-dimensional oscillator with two quadratic degrees of freedom, this energy will also correspond to $E=2[k_BT/2]=k_BT$, where k_B is Boltzmann's constant. In this way we find that Eq. (8) implies that

$$\langle x\rangle=\frac{3\lambda}{k}(E)=\frac{3\lambda}{k}(k_BT), \tag{9}$$

so that the average separation increases with temperature.

This last result can be seen more directly (see, e.g., Ref. 6) by using the Boltzmann distribution (which is proportional to $\exp(-\beta U(x))$, where $\beta=1/k_BT$) in the thermodynamic average value given by

$$\begin{aligned}\langle x\rangle&=\frac{\int_{-\infty}^{+\infty}xe^{-\beta U(x)}dx}{\int_{-\infty}^{+\infty}e^{-\beta U(x)}dx}\\&\approx+\lambda k\beta\frac{\int_{-\infty}^{+\infty}x^4e^{-\beta kx^2/2}\,dx}{\int_{-\infty}^{+\infty}e^{-\beta kx^2/2}\,dx}\\&=\frac{3\lambda}{k\beta}=\frac{3\lambda}{k}(k_BT),\end{aligned} \tag{10}$$

where we have used the expansion

$$e^{-\beta U(x)}\approx e^{-\beta kx^2/2}(1+\beta\lambda kx^3+\cdots). \tag{11}$$

III. QUANTUM MECHANICAL AND SEMICLASSICAL RESULTS

In quantum mechanics, information on the average value of position is most easily extracted from the position-space stationary state wave functions, in this case labeled $\psi_n(x)$. The average value of position in the unperturbed system is given by

$$\langle x\rangle^{(0)}=\langle\psi_n^{(0)}|x|\psi_n^{(0)}\rangle=0, \tag{12}$$

which vanishes because of the parity properties of the energy eigenfunctions. The first-order shift in the energy eigenvalue also vanishes since

$$\begin{aligned}\Delta E&=E_n^{(1)}-E_n^{(0)}=\langle\psi_n^{(0)}|V'(x)|\psi_n^{(0)}\rangle\\&=-\lambda k\langle\psi_n^{(0)}|x^3|\psi_n^{(0)}\rangle=0\end{aligned} \tag{13}$$

for the same reason.

The first-order wave function is given by

$$\psi_n^{(1)}=\psi_n^{(0)}+\sum_{j\neq n}c_{jn}\psi_j^{(0)}, \tag{14}$$

where

$$c_{jn}=\frac{\langle\psi_j^{(0)}|V'(x)|\psi_n^{(0)}\rangle}{(E_n^{(0)}-E_j^{(0)})}=\frac{\mathsf{V}'_{jn}}{(E_n^{(0)}-E_j^{(0)})}. \tag{15}$$

Using the anharmonic piece, $V'(x)=-\lambda kx^3$, as the perturbing potential, we require the values of

$$\mathsf{V}'_{jn}=-\lambda k\langle\psi_j^{(0)}|x^3|\psi_n^{(0)}\rangle. \tag{16}$$

To evaluate these, we use the formalism of raising and lowering operators which satisfy

$$\hat{A}^\dagger\psi_n^{(0)}=\sqrt{n+1}\,\psi_{n+1}^{(0)}\quad\text{and}\quad\hat{A}\psi_n^{(0)}=\sqrt{n}\,\psi_{n-1}^{(0)} \tag{17}$$

in terms of which the position coordinate is given by

$$x=\sqrt{\frac{\hbar}{2m\omega}}(\hat{A}^\dagger+\hat{A}). \tag{18}$$

The matrix elements are given by[9,10,12,13]

$$\begin{aligned}\langle\psi_j^{(0)}|x^3|\psi_n^{(0)}\rangle=\left(\frac{\hbar}{2m\omega}\right)^{3/2}[&\sqrt{n(n-1)(n-2)}\,\delta_{j,n-3}\\&+3n^{3/2}\delta_{j,n-1}+3(n+1)^{3/2}\delta_{j,n+1}\\&+\sqrt{(n+1)(n+2)(n+3)}\,\delta_{j,n+3}].\end{aligned} \tag{19}$$

One then has for the first-order wave functions (Refs. 10 and 13)

$$\begin{aligned}\psi_n^{(1)}=\psi_n^{(0)}-\left(\frac{\lambda k}{3\hbar\omega}\right)\left(\frac{\hbar}{2m\omega}\right)^{3/2}[&\sqrt{n(n-1)(n-2)}\,\psi_{n-3}^{(0)}\\&+9n^{3/2}\psi_{n-1}^{(0)}-9(n+1)^{3/2}\psi_{n+1}^{(0)}\\&-\sqrt{(n+1)(n+2)(n+3)}\,\psi_{n+3}^{(0)}].\end{aligned} \tag{20}$$

Using the perturbed wave function, we find the average value of position to first-order in λ is given by

$$\langle x\rangle^{(1)}=\langle\psi_n^{(1)}|x|\psi_n^{(1)}\rangle=\sqrt{\frac{\hbar}{2m\omega}}\,\langle\psi_n^{(1)}|\hat{A}^\dagger+\hat{A}|\psi_n^{(1)}\rangle. \tag{21}$$

We once again make use of raising and lowering operators to find [to $\mathcal{O}(\lambda)$]

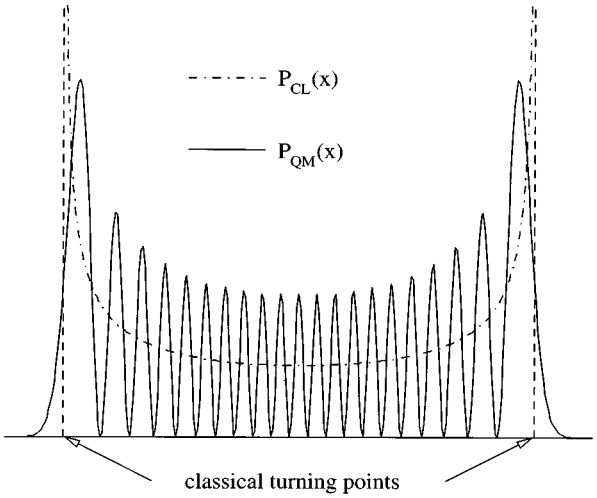

Fig. 1. Quantum mechanical (solid) and classical (dot–dash) probability distributions, $P_{\rm QM}(x)=|\psi_n^{(0)}(x)|^2$ and $P_{\rm CL}^{(0)}(x)$ vs x. The state corresponding to $n=20$ is shown and the vertical dashed lines indicate the locations of the classical turning points at $\pm A$ given by $E_n=(n+1/2)\hbar\omega=kA^2/2$.

$$\langle \psi_n^{(1)}|\hat{A}^\dagger|\psi_n^{(1)}\rangle=\langle \psi_n^{(1)}|\hat{A}|\psi_n^{(1)}\rangle$$

$$=6\left(\frac{\lambda k}{\hbar\omega}\right)\left(\frac{\hbar}{2m\omega}\right)^{3/2}\left(n+\frac{1}{2}\right) \tag{22}$$

so that the average value of position can be written as

$$\langle x\rangle^{(1)}=\frac{3\lambda}{m\omega^2}\left[\left(n+\frac{1}{2}\right)\hbar\omega\right]=\frac{3\lambda}{k}\,E_n^{(0)}, \tag{23}$$

since $k=m\omega^2$. If we then associate the (unperturbed) energy eigenvalues, $E_n^{(0)}$, via

$$E_n^{(0)} \Leftrightarrow \tfrac{1}{2}kA^2, \tag{24}$$

we do indeed reproduce the result of Eq. (8), namely,

$$\langle x\rangle^{(1)}=\tfrac{3}{2}\lambda A^2. \tag{25}$$

To better visualize how the probability is ''shifted around'' in response to the anharmonic perturbation to yield a nonvanishing value of $\langle x\rangle$, we first plot in Fig. 1 a standard image of the quantum mechanical probability density $P_{\rm QM}(x)=|\psi_n(x)|^2$ (solid curve) for the case $n=20$. For later comparison, the corresponding classical expression, $P_{\rm CL}(x)$, (dot–dashed curve) and the classical turning points (vertical dashed lines) are also shown. The *difference* in probability densities corresponding to the unperturbed oscillator and the result including the effect of the cubic perturbation to first order [given by Eq. (20)] is given by

$$\Delta P_{\rm QM}(x)=|\psi_n^{(1)}(x)|^2-|\psi_n^{(0)}(x)|^2\propto-\lambda\,\psi_n^{(0)}(x)$$
$$\times[\sqrt{n(n-1)(n-2)}\,\psi_{n-3}^{(0)}+9n^{3/2}\psi_{n-1}^{(0)}$$
$$-9(n+1)^{3/2}\psi_{n+1}^{(0)}$$
$$-\sqrt{(n+1)(n+2)(n+3)}\,\psi_{n+3}^{(0)}]. \tag{26}$$

This is seen to be an odd function of x for all values of n and is plotted in Fig. 2 for the same $n=20$ case. The classical connection is better realized by suitably averaging locally over the obvious rapid oscillations in the quantum case, and in Fig. 3 we show the same probability density, but now

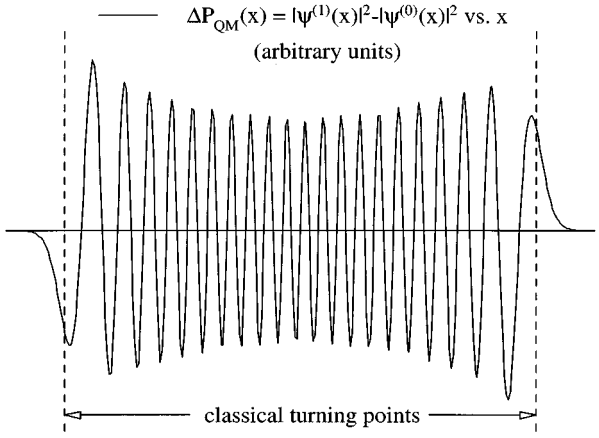

Fig. 2. The difference in probability densities [defined in Eq. (26)], $\Delta P_{\rm QM}(x)$ vs x between the first-order wave function $\psi_n^{(1)}(x)$ of Eq. (20) and the zeroth order result $\psi_n^{(0)}(x)$. We use the same value of $n=20$ as in Fig. 1.

binned into finite intervals. The shift in probability density from left to right near both the classical turning points is quite similar to what would be expected from classical arguments.

One final way to derive these results is to use semiclassical probability distributions. These are often discussed in elementary texts on quantum mechanics (see, e.g., Ref. 14), where the (unperturbed) harmonic oscillator is the standard example (as in Fig. 1), but which can be applied to many other systems as well.[15] We recall that the average value of a function of the position coordinate can obtained by generalizing Eq. (7) to yield

$$\langle f(x)\rangle=\frac{1}{\tau}\int_0^\tau f(x(t))dt\rightarrow\left(\frac{2}{\tau}\right)\int_{x_-}^{x_+}f(x)\,\frac{dx}{v(x)}$$

$$=\int_{x_-}^{x_+}f(x)P_{\rm CL}(x)dx, \tag{27}$$

where we have used the connection $v(x)=dx/dt$ and defined the classical probability distribution via

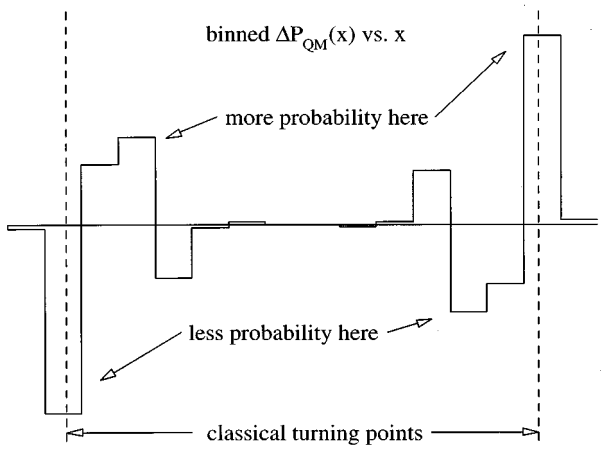

Fig. 3. The difference in probability densities, $\Delta P_{\rm QM}(x)$, between the zeroth- and first-order results vs x integrated over small bins in the position coordinate; we use the same value of $n=20$ as in Figs. 1 and 2. Note that the probability has been shifted slightly from left to right near both classical turning points as expected from a classical picture.

$$P_{\rm CL}(x)=\frac{2}{\tau}\frac{1}{v(x)}. \tag{28}$$

The integral is now taken between the classical turning points, i.e., in the range (x_-,x_+), which is over only half the period, $\tau/2$. The local speed is related to the potential energy functions via

$$E=\tfrac{1}{2}mv^2(x)+U(x). \tag{29}$$

For the harmonic oscillator, the standard result is

$$P^{(0)}_{\rm CL}(x)=\frac{1}{\pi\sqrt{A^2-x^2}}, \tag{30}$$

which satisfies

$$\int_{-A}^{+A}P_{\rm CL}(x)dx=1 \tag{31}$$

as it should; this is the classical result reproduced in Fig. 1.

For the perturbed oscillator, the turning points are determined by the roots of the cubic equation

$$\tfrac{1}{2}kA^2=E=\tfrac{1}{2}\,kx^2-\lambda kx^3 \quad \text{or} \quad x^2-2\lambda x^3-A^2=0. \tag{32}$$

The two roots which represent the actual turning points of the classical motion in the (slightly) modified well are given by

$$x_+=+A\pi(+\epsilon) \quad \text{and} \quad x_-=-A\rho(-\epsilon), \tag{33}$$

where $\epsilon\equiv\lambda A$ and $\rho(\epsilon)$ has the series expansion

$$\rho(\epsilon)=1+\epsilon+\tfrac{5}{2}\epsilon+8\epsilon^3+112\epsilon^4+\cdots\,. \tag{34}$$

[The third (extraneous) root, which is due to the eventual ''turnover'' of the potential caused by the cubic piece, is given by $x_3=1/2\lambda-2A^2\lambda+\mathcal{O}(A^3\lambda^2)$ and properly is ''pushed to infinity'' when $\lambda\to0$.]

With these changes in turning points and potential, we can write the expectation value of the position coordinate in the form

$$\begin{aligned}\langle x\rangle&=\int_{x_-}^{x_+}\frac{x}{v(x)}\,dx\Bigg/\int_{x_-}^{x_+}\frac{1}{v(x)}\,dx\\&=\int_{-A\rho(-\epsilon)}^{+A\rho(+\epsilon)}x\,\frac{dx}{\sqrt{A^2-(x^2-2\lambda x^3)}}\Bigg/\int_{-A\rho(-\epsilon)}^{+A\rho(+\epsilon)}\frac{dx}{\sqrt{A^2-(x^2-2\lambda x^3)}}\\&=A\left\{\int_{-\rho(-\epsilon)}^{+\rho(+\epsilon)}z\,\frac{dz}{\sqrt{1-(z^2-2\epsilon z^3)}}\Bigg/\int_{-\rho(-\epsilon)}^{+\rho(+\epsilon)}z\,\frac{dz}{\sqrt{1-(z^2-2\epsilon z^3)}}\right\}\\&\equiv AI(\epsilon)\\&\equiv AR(\epsilon)\epsilon,\end{aligned} \tag{35}$$

where we have defined $R(\epsilon)=I(\epsilon)/\epsilon$ in the expectation that the integral giving information on the shift in the average value of position will have an expansion in ϵ starting with ϵ^1.

Our first inclination might be to attempt to expand both required integrals using the standard calculus result for the differentiation of definite integrals, namely,

$$\frac{d}{d\epsilon}\left[\int_{a(\epsilon)}^{b(\epsilon)}f(x,\epsilon)dx\right]=f(b,\epsilon)\,\frac{db(\epsilon)}{d\epsilon}-f(a,\epsilon)\,\frac{da(\epsilon)}{d\epsilon}+\int_{a(\epsilon)}^{b(\epsilon)}\frac{\partial}{\partial\epsilon}\,f(x,\epsilon)dx. \tag{36}$$

The singular nature of the integrands near the classical turning points, however, makes such an expansion far from obviously convergent. To explicitly check the behavior of $I(\epsilon)$ for $\epsilon\ll1$, we perform the necessary integrals numerically (in this case, using MATHEMATICA®) for several values of ϵ and the results are shown in Table I.

For smaller values of ϵ, the numerical integration results are not reliable and even for $\epsilon=0.0001$ we are somewhat ''in the noise.'' Over this range, however, it certainly seems that the integral is well described by the expansion $I(\epsilon)\approx3\epsilon/2$ and this implies, of course, that the expectation value of position satisfies

$$\langle x\rangle\approx A\left(\frac{3}{2}\,\epsilon\right)=\frac{3}{2}\,\lambda A^2, \tag{37}$$

as expected from all our earlier results. (Using values of ϵ in the range 0.001–0.01, it also seems likely that the next term in the expansion is $9\epsilon^2/4$.)

We can attempt to extract these results in a more analytic fashion using some rather formal properties of the integrals involved. For example, we can argue that the new classical probability distribution can actually be written in the form

$$P^{(1)}_{\rm CL}(x)=\frac{1}{\pi\sqrt{A^2-(x^2-2\lambda x^3)}} \tag{38}$$

with the same normalization (to order λ or ϵ) as before. This can be justified by calculating

$$\begin{aligned}1&\overset{?}{=}\int_{-A\rho(-\epsilon)}^{+A\rho(+\epsilon)}P^{(1)}_{\rm CL}(x)dx\\&=\int_{-\rho(-\epsilon)}^{+\rho(+\epsilon)}\frac{dz}{\pi\sqrt{1-(z^2-2\epsilon z^3)}}\\&=\int_{0}^{+\rho(+\epsilon)}\frac{dz}{\pi\sqrt{1-(z^2-2\epsilon z^3)}}+\int_{-\rho(-\epsilon)}^{0}\frac{dz}{\pi\sqrt{1-(z^2-2\epsilon z^3)}}\\&=\int_{0}^{+\rho(+\epsilon)}\frac{dz}{\pi\sqrt{1-(z^2-2\epsilon z^3)}}+\int_{0}^{+\rho(-\epsilon)}\frac{dy}{\pi\sqrt{1-(y^2+2\epsilon y^3)}}\\&\equiv F(\epsilon)+F(-\epsilon)\approx2F(0)+\mathcal{O}(\epsilon^2)\\&=1+\mathcal{O}(\epsilon^2),\end{aligned} \tag{39}$$

where $x=Az$ and $y=-z$ and we have assumed a series expansion for $F(\epsilon)$; one can perform this normalization integral

Table I. Results of the numerical integration of Eq. (35) for various values of ϵ.

ϵ	$I(\epsilon)/\epsilon-3/2$	$(R(\epsilon)-3/2))/\epsilon^2$
0.0001	6×10^{-7}	60
0.001	2.26×10^{-6}	2.26
0.01	2.26×10^{-4}	2.26
0.1	2.26×10^{-2}	2.26
0.5	0.653	2.61

numerically (as mentioned above) for several small values of ϵ and fit to a lower-power polynomial in ϵ and one indeed finds the result $1+\epsilon^2+\mathcal{O}(\epsilon^4)$. This implies that the normalization of $P_{\rm CL}(x)$ is unchanged (in this case, at least) by a first-order change in the potential; this is similar to the quantum result where first-order changes in $\psi(x)$ only change the normalization of $|\psi(x)|^2$ to second order.

Using this notation, we find that the average value of position in the perturbed oscillator is given by

$$\begin{aligned}\langle x\rangle &= \int_{x_-}^{x_+} x P^{(1)}_{\rm CL}(x)\,dx \\ &= \int_{-A\rho(-\epsilon)}^{+A\rho(+\epsilon)} \frac{x}{\pi\sqrt{A^2-(x^2-2\lambda x^3)}}\,dx \\ &= \frac{A}{\pi}\left[\int_0^{+\rho(+\epsilon)} \frac{z}{\sqrt{1-(z^2-2\epsilon z^3)}}\,dz \right. \\ &\quad \left. + \int_{-\rho(-\epsilon)}^{0} \frac{z}{\sqrt{1-(z^2-2\epsilon z^3)}}\,dz\right] \\ &= \frac{A}{\pi}\left[\int_0^{+\pi(+\epsilon)} \frac{z}{\sqrt{1-(z^2-2\epsilon z^3)}}\,dz \right. \\ &\quad \left. - \int_0^{+\rho(-\epsilon)} \frac{y}{\sqrt{1-(y^2+2\epsilon y^3)}}\,dy\right] \\ &= \frac{A}{\pi}\,[G(\epsilon)-G(-\epsilon)] \\ &\approx \frac{2A}{\pi}\,\epsilon G'(0), \end{aligned} \tag{40}$$

where we also assume that $G(\epsilon)$ has a series expansion. We can extract information on $G(\epsilon)$ by writing

$$\begin{aligned} G(\epsilon) &= \int_0^{+\rho(+\epsilon)} \frac{z}{\sqrt{1(z^2-2\epsilon z^3)}}\,dz \\ &= -\frac{1}{2}\int_0^{+\rho(+\epsilon)} \frac{[-2z+(6\epsilon z^2-6\epsilon z^2)]}{\sqrt{1-(z^2-2\epsilon z^3)}}\,dz \\ &= -\frac{1}{2}\int_0^{+\rho(+\epsilon)} \frac{-2z+6\epsilon z^2}{\sqrt{1-(z^2-2\epsilon z^3)}}\,dz \\ &\quad +3\epsilon\int_0^{+\rho(+\epsilon)} \frac{z^2}{\sqrt{1-(z^2-2\epsilon z^3)}}\,dz \\ &= H_1(\epsilon)+3\epsilon H_2(\epsilon). \end{aligned} \tag{41}$$

The first integral can be performed yielding

$$H_1(\epsilon) = -\tfrac{1}{2}(2\sqrt{1-(z^2-2\epsilon z^3)})_0^{\rho(+\epsilon)} = +1, \tag{42}$$

since $\rho(\epsilon)$ defines the classical turning point where the integral vanishes. The second integral can be evaluated with $\epsilon=0$ since this term is already explicitly of order ϵ; this results in

$$H_2(0) = \int_0^{+1} \frac{z^2}{\sqrt{1-z^2}}\,dz = \frac{\pi}{4}. \tag{43}$$

This implies that $G'(0)=3H_2(0)=3\pi/4$ and from Eq. (40) we find

$$\langle x\rangle \approx \frac{2A}{\pi}\,\epsilon\left(\frac{3\pi}{4}\right) = \frac{3}{2}\,\lambda A^2, \tag{44}$$

as expected. Once again, one can perform this integral numerically and fit to powers of ϵ and this result is confirmed.

The assumption that we can systematically expand all of these semiclassical quantities in powers of ϵ is, perhaps, only justified to leading order in ϵ as that corresponds, in some sense, to the use of first-order perturbation theory. Higher-order terms in ϵ, which would correspond to second-order (and higher) perturbation theory would arise from truly quantum mechanical effects (coupling to different states, weighted by energy differences) and cannot necessarily be expected to be reproduced by purely classical arguments.

ACKNOWLEDGMENTS

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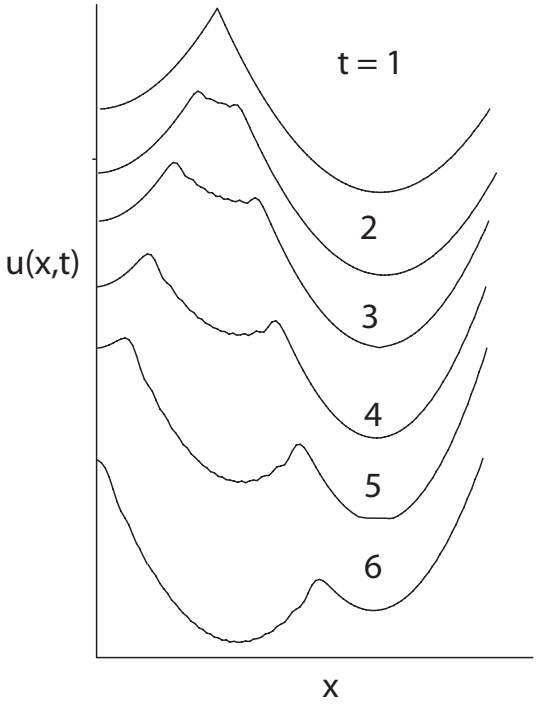

Figure 18.6 The wave motion of a plucked catenary with friction. (Courtesy of Juan Vanegas.)

7. Try the first two normal modes for a uniform string as the initial conditions for the catenary. These should be close to, but not exactly, normal modes.
8. We derived the normal modes for a uniform string after assuming that $k(x) = \omega/c(x)$ is a constant. For a catenary without too much x variation in the tension, we should be able to make the approximation

$$c(x)^2 \simeq \frac{T(x)}{\rho} = \frac{T_0 \cosh(x/d)}{\rho}.$$

See if you get a better representation of the first two normal modes if you include some x dependence in k. ▌

18.5 Unit II. Quantum Wave Packets

Problem: An experiment places an electron with a definite momentum and position in a 1-D region of space the size of an atom. It is confined to that region by some kind of attractive potential. Your **problem** is to determine the resultant electron behavior in time and space.

18.6 Time-Dependent Schrödinger Equation (Theory)

Because the region of confinement is the size of an atom, we must solve this problem quantum mechanically. Nevertheless, it is different from the problem of a particle confined to a box considered in Chapter 9, "Differential Equation Applications," because now we are starting with a particle of definite momentum and position. In Chapter 9 we had a time-independent situation in which we had to solve the eigenvalue problem. Now the definite momentum and position of the electron imply that the solution is a wave packet, which is not an eigenstate with a uniform time dependence of $\exp(-i\omega t)$. Consequently, we must now solve the time-dependent Schrödinger equation.

We model an electron initially localized in space at $x = 5$ with momentum k_0 ($\hbar = 1$ in our units) by a wave function that is a wave packet consisting of a Gaussian multiplying a plane wave:

$$\psi(x, t = 0) = \exp\left[-\frac{1}{2}\left(\frac{x-5}{\sigma_0}\right)^2\right] e^{ik_0 x}. \tag{18.38}$$

To solve the **problem** we must determine the wave function for all later times. If (18.38) were an eigenstate of the Hamiltonian, its $\exp(-i\omega t)$ time dependence can be factored out of the Schrödinger equation (as is usually done in textbooks). However, $\tilde{H}\psi \neq E\psi$ for this ψ, and so we must solve the full time-dependent Schrödinger equation. To show you where we are going, the resulting wave packet behavior is shown in Figures 18.7 and 18.8.

The time and space evolution of a quantum particle is described by the 1-D time-dependent Schrödinger equation,

$$i\,\frac{\partial \psi(x,t)}{\partial t} = \tilde{H}\psi(x,t) \tag{18.39}$$

$$i\,\frac{\partial \psi(x,t)}{\partial t} = -\frac{1}{2m}\frac{\partial^2 \psi(x,t)}{\partial x^2} + V(x)\psi(x,t), \tag{18.40}$$

where we have set $2m = 1$ to keep the equations simple. Because the initial wave function is complex (in order to have a definite momentum associated with it), the wave function will be complex for all times. Accordingly, we decompose the wave function into its real and imaginary parts:

$$\psi(x,t) = R(x,t) + i\,I(x,t), \tag{18.41}$$

$$\Rightarrow \quad \frac{\partial R(x,t)}{\partial t} = -\frac{1}{2m}\frac{\partial^2 I(x,t)}{\partial x^2} + V(x)I(x,t), \tag{18.42}$$

$$\frac{\partial I(x,t)}{\partial t} = +\frac{1}{2m}\frac{\partial^2 R(x,t)}{\partial x^2} - V(x)R(x,t), \tag{18.43}$$

where $V(x)$ is the potential acting on the particle.

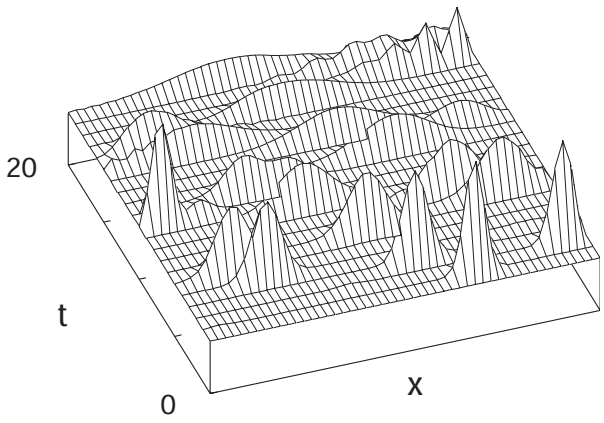

Figure 18.7 The position as a function of time of a localized electron confined to a square well (computed with the code `SqWell.java` available on the instructor's CD). The electron is initially on the right with a Gaussian wave packet. In time, the wave packet spreads out and collides with the walls.

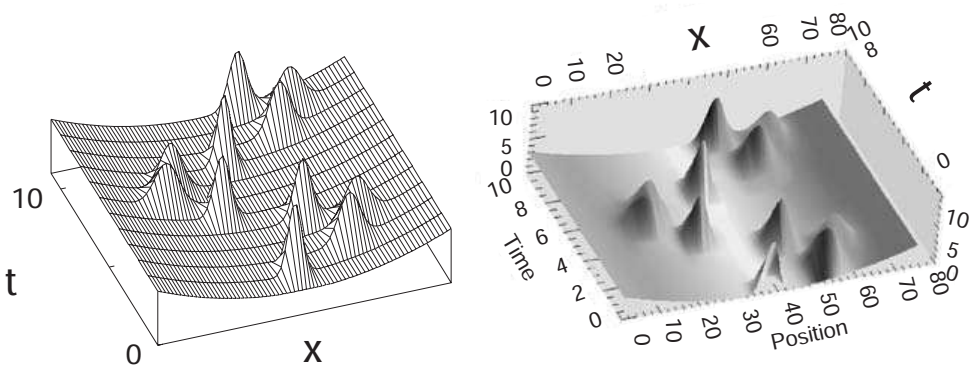

Figure 18.8 The probability density as a function of time for an electron confined to a 1-D harmonic oscillator potential well. On the left is a conventional surface plot from Gnuplot, while on the right is a color visualization from OpenDX.

18.6.1 Finite-Difference Algorithm

The time-dependent Schrödinger equation can be solved with both implicit (large-matrix) and explicit (leapfrog) methods. The extra challenge with the Schrödinger equation is to ensure that the integral of the probability density $\int_{-\infty}^{+\infty} dx\ \rho(x,t)$ remains constant (conserved) to a high level of precision for all time. For our project we use an *explicit* method that improves the numerical conservation of probability by solving for the real and imaginary parts of the wave function at slightly different or "staggered" times [Ask 77, Viss 91, MLP 00]. Explicitly, the real part R is determined at times $0, \Delta t, \ldots$, and the imaginary part I at $\frac{1}{2}\Delta t, \frac{3}{2}\Delta t, \ldots$. The algorithm

is based on (what else?) the Taylor expansions of R and I:

$$R\left(x, t+\frac{1}{2}\Delta t\right) = R\left(x, t-\frac{1}{2}\Delta t\right) + [4\alpha + V(x)\,\Delta t]I(x,t)$$
$$-2\alpha[I(x+\Delta x, t) + I(x-\Delta x, t)], \tag{18.44}$$

where $\alpha = \Delta t/2(\Delta x)^2$. In discrete form with $R^{t=n\Delta t}_{x=i\Delta x}$, we have

$$R_i^{n+1} = R_i^n - 2\left\{\alpha\left[I_{i+1}^n + I_{i-1}^n\right] - 2\left[\alpha + V_i\,\Delta t\right] I_i^n\right\}, \tag{18.45}$$

$$I_i^{n+1} = I_i^n + 2\left\{\alpha\left[R_{i+1}^n + R_{i-1}^n\right] - 2\left[\alpha + V_i\,\Delta t\right] R_i^n\right\}, \tag{18.46}$$

where the superscript n indicates the time and the subscript i the position.

The probability density ρ is defined in terms of the wave function evaluated at three different times:

$$\rho(t) = \begin{cases} R^2(t) + I\left(t+\frac{\Delta t}{2}\right)I\left(t-\frac{\Delta t}{2}\right), & \text{for integer } t, \\ I^2(t) + R\left(t+\frac{\Delta t}{2}\right)R\left(t-\frac{\Delta t}{2}\right), & \text{for half-integer } t. \end{cases} \tag{18.47}$$

Although probability is not conserved exactly with this algorithm, the error is two orders higher than that in the wave function, and this is usually quite satisfactory. If it is not, then we need to use smaller steps. While this definition of ρ may seem strange, it reduces to the usual one for $\Delta t \to 0$ and so can be viewed as part of the art of numerical analysis. You will investigate just how well probability is conserved. We refer the reader to [Koon 86, Viss 91] for details on the stability of the algorithm.

18.6.2 Wave Packet Implementation and Animation

In Listing 18.2 you will find the program `Harmos.java` that solves for the motion of the wave packet (18.38) inside a harmonic oscillator potential. The program `Slit.java` on the instructor's CD solves for the motion of a Gaussian wave packet as it passes through a slit (Figure 18.10). You should solve for a wave packet confined to the square well:

$$V(x) = \begin{cases} \infty, & x < 0, \text{ or } x > 15, \\ 0, & 0 \le x \le 15. \end{cases}$$

1. Define arrays `psr[751][2]` and `psi[751][2]` for the real and imaginary parts of ψ, and `Rho[751]` for the probability. The first subscript refers to the x position on the grid, and the second to the present and future times.

2. Use the values $\sigma_0 = 0.5$, $\Delta x = 0.02$, $k_0 = 17\pi$, and $\Delta t = \frac{1}{2}\Delta x^2$.
3. Use equation (18.38) for the initial wave packet to define psr[j][1] for all j at $t = 0$ and to define psi[j][1] at $t = \frac{1}{2}\Delta t$.
4. Set Rho[1] = Rho[751] = 0.0 because the wave function must vanish at the infinitely high well walls.
5. Increment time by $\frac{1}{2}\Delta t$. Use (18.45) to compute psr[j][2] in terms of psr[j][1], and (18.46) to compute psi[j][2] in terms of psi[j][1].
6. Repeat the steps through all of space, that is, for $i = 2$–750.
7. Throughout all of space, replace the present wave packet (second index equal to 1) by the future wave packet (second index 2).
8. After you are sure that the program is running properly, repeat the time-stepping for $\sim$5000 steps.

```
//  Harmos.java: t-dependent Schro eqn, for wavepacket in harmonic oscillator V
import java.io.*;

public class Harmos  {

  public static void main(String[] argv) throws IOException, FileNotFoundException  {
    PrintWriter w =  new PrintWriter(new FileOutputStream("Harmos.dat"), true);
    double psr[][] = new double[751][2], psi[][] = new double[751][2];
    double p2[] = new double[751], v[] = new double[751], dx=0.02, k0, dt, x, pi;
    int i, n, max = 750;
    pi   = 3.14159265358979323846;  k0 = 3.0*pi;   dt = dx*dx/4.0;   x = -7.5;// i.c.
    for( i=0; i < max; i++)  {
      psr[i][0] = Math.exp(-0.5*(Math.pow((x/0.5), 2.))) * Math.cos(k0*x);  // RePsi
      psi[i][0] = Math.exp(-0.5*(Math.pow((x/0.5), 2.))) * Math.sin(k0*x);  // ImPsi
      v[i] = 5.0*x*x;                                                       // Potential
      x    = x + dx;
    }
    for ( n=0; n < 20000; n++)  {                                  // Propagate in time
      for( i=1; i < max-1; i++ )  {                                       // RePsi
        psr[i][1] = psr[i][0] - dt*(psi[i+1][0] + psi[i-1][0]
                    -2.*psi[i][0])/(dx*dx)+dt*v[i]*psi[i][0];
        p2[i] = psr[i][0]*psr[i][1]+psi[i][0]*psi[i][0];
      }
      for ( i=1; i < max-1; i++ )  { psi[i][1] = psi[i][0] + dt*(psr[i+1][1]
           + psr[i-1][1] -2.*psr[i][1])/(dx*dx)-dt*v[i]*psr[i][1]; }       // ImPsi
      if ( (n == 0) || (n%2000 == 0) ) {                  // Output every 2000 steps
        for( i=0; i<max; i=i+10 ) w.println(""+(p2[i]+0.0015*v[i])+"");
        w.println("");
      }
      for ( i=0; i<max; i++ )   {psi[i][0] = psi[i][1]; psr[i][0] = psr[i][1];}
    }
    System.out.println("data saved in Harmos.dat");
} }
```

Listing 18.2 Harmos.java solves the time-dependent Schrödinger equation for a particle described by a Gaussian wave packet moving within a harmonic oscillator potential.

1. **Animation:** Output the probability density after every 200 steps for use in animation.
2. Make a surface plot of probability *versus* position *versus* time. This should look like Figure 18.7 or 18.8.
3. Make an animation showing the wave function as a function of time.

CD

4. Check how well the probability is conserved for early and late times by determining the integral of the probability over all of space, $\int_{-\infty}^{+\infty} dx\, \rho(x)$, and seeing by how much it changes in time (its specific value doesn't matter because that's just normalization).
5. What might be a good explanation of why collisions with the walls cause the wave packet to broaden and break up? (*Hint:* The collisions do not appear so disruptive when a Gaussian wave packet is confined within a harmonic oscillator potential well.) ▌

18.7 Wave Packets in Other Wells (Exploration)

1-D Well: Now confine the electron to lie within the harmonic oscillator potential:

$$V(x) = \frac{1}{2}x^2 \quad (-\infty \le x \le \infty).$$

Take the momentum $k_0 = 3\pi$, the space step $\Delta x = 0.02$, and the time step $\Delta t = \frac{1}{4}\Delta x^2$. Note that the wave packet broadens yet returns to its initial shape!

2-D Well ⊙: Now confine the electron to lie within a 2-D parabolic tube (Figure 18.9):

$$V(x,y) = 0.9x^2, \quad -9.0 \le x \le 9.0, \quad 0 \le y \le 18.0.$$

The extra degree of freedom means that we must solve the 2-D PDE:

$$i\,\frac{\partial \psi(x,y,t)}{\partial t} = -\left(\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2}\right) + V(x,y)\psi. \tag{18.48}$$

Assume that the electron's initial localization is described by the 2-D Gaussian wave packet:

$$\psi(x,y,t=0) = e^{ik_{0x}x}\, e^{ik_{0y}y}\, \exp\left[-\frac{(x-x_0)^2}{2\sigma_0^2}\right] \exp\left[-\frac{(y-y_0)^2}{2\sigma_0^2}\right]. \tag{18.49}$$

Note that you can solve the 2-D equation by extending the method we just used in 1-D or you can look at the next section where we develop a special algorithm.

18.8 Algorithm for the 2-D Schrödinger Equation

One way to develop an algorithm for solving the time-dependent Schrödinger equation in 2-D is to extend the 1-D algorithm to another dimension. Rather than do that, we apply quantum theory directly to obtain a more powerful algorithm

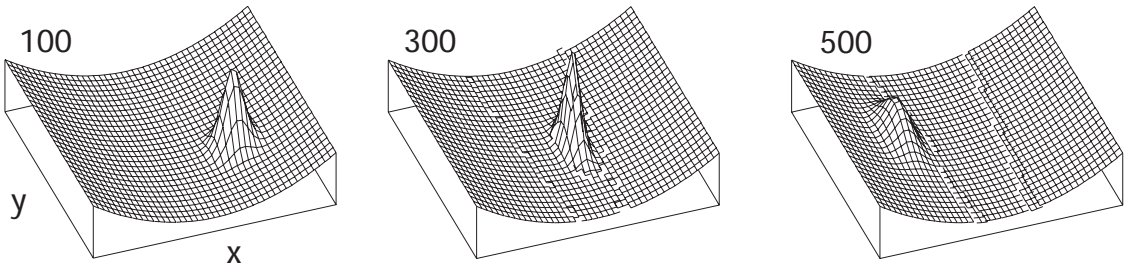

Figure 18.9 The probability density as a function of *x* and *y* of an electron confined to a 2-D parabolic tube. The electron's initial localization is described by a Gaussian wave packet in both the *x* and *y* directions. The times are 100, 300, and 500 steps.

[MLP 00]. First we note that equation (18.48) can be integrated in a formal sense [L&L,M 76] to obtain the operator solution:

$$\psi(x,y,t) = U(t)\psi(x,y,t=0) \tag{18.50}$$

$$U(t) = e^{-i\tilde{H}t}, \quad \tilde{H} = -\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) + V(x,y),$$

where $U(t)$ is an operator that translates a wave function by an amount of time t and $\tilde{H}$ is the Hamiltonian operator. From this formal solution we deduce that a wave packet can be translated ahead by time Δt via

$$\psi_{i,j}^{n+1} = U(\Delta t)\psi_{i,j}^{n}, \tag{18.51}$$

where the superscripts denote time $t = n\,\Delta t$ and the subscripts denote the two spatial variables $x = i\Delta x$ and $y = j\Delta y$. Likewise, the inverse of the time evolution operator moves the solution back one time step:

$$\psi^{n-1} = U^{-1}(\Delta t)\psi^{n} = e^{+i\tilde{H}\Delta t}\psi^{n}. \tag{18.52}$$

While it would be nice to have an algorithm based on a direct application of (18.52), the references show that the resulting algorithm is not stable. That being so, we base our algorithm on an indirect application [Ask 77], namely, the relation between the difference in ψ^{n+1} and ψ^{n-1}:

$$\psi^{n+1} = \psi^{n-1} + [e^{-i\tilde{H}\Delta t} - e^{+i\tilde{H}\Delta t}]\psi^{n}, \tag{18.53}$$

where the difference in sign of the exponents is to be noted. The algorithm derives from combining the $O(\Delta x^2)$ expression for the second derivative obtained from

the Taylor expansion,

$$\frac{\partial^2\psi}{\partial x^2} \simeq -\frac{1}{2}\left[\psi^n_{i+1,j} + \psi^n_{i-1,j} - 2\psi^n_{i,j}\right], \tag{18.54}$$

with the corresponding-order expansion of the evolution equation (18.53). Substituting the resulting expression for the second derivative into the 2-D time-dependent Schrödinger equation results in[2]

$$\psi^{n+1}_{i,j} = \psi^{n-1}_{i,j} - 2i\left[\left(4\alpha + \tfrac{1}{2}\Delta t V_{i,j}\right)\psi^n_{i,j} - \alpha\left(\psi^n_{i+1,j} + \psi^n_{i-1,j} + \psi^n_{i,j+1} + \psi^n_{i,j-1}\right)\right],$$

where $\alpha = \Delta t/2(\Delta x)^2$. We convert this complex equations to coupled real equations by substituting in the wave function $\psi = R + iI$,

$$R^{n+1}_{i,j} = R^{n-1}_{i,j} + 2\left[\left(4\alpha + \tfrac{1}{2}\Delta t V_{i,j}\right) I^n_{i,j} - \alpha\left(I^n_{i+1,j} + I^n_{i-1,j} + I^n_{i,j+1} + I^n_{i,j-1}\right)\right],$$
$$I^{n+1}_{i,j} = I^{n-1}_{i,j} - 2\left[\left(4\alpha + \tfrac{1}{2}\Delta t V_{i,j}\right) R^n_{i,j} + \alpha\left(R^n_{i+1,j} + R^n_{i-1,j} + R^n_{i,j+1} + R^n_{i,j-1}\right)\right].$$

This is the algorithm we use to integrate the 2-D Schrödinger equation. To determine the probability, we use the same expression (18.47) used in 1-D.

18.8.0.1 EXPLORATION: A BOUND AND DIFFRACTED 2-D PACKET

1. Determine the motion of a 2-D Gaussian wave packet within a 2-D harmonic oscillator potential:

$$V(x,y) = 0.3(x^2 + y^2), \quad -9.0 \le x \le 9.0, \quad -9.0 \le y \le 9.0. \tag{18.55}$$

2. Center the initial wave packet at $(x, y) = (3.0, -3)$ and give it momentum $(k_{0x}, k_{0y}) = (3.0, 1.5)$.
3. Young's single-slit experiment has a wave passing through a small slit with the transmitted wave showing interference effects. In quantum mechanics, where we represent a particle by a wave packet, this means that an interference pattern should be formed when a particle passes through a small slit. Pass a Gaussian wave packet of width 3 through a slit of width 5 (Figure 18.10) and look for the resultant quantum interference.

[2] For reference sake, note that the constants in the equation change as the dimension of the equation changes; that is, there will be different constants for the 3-D equation, and therefore our constants are different from the references!

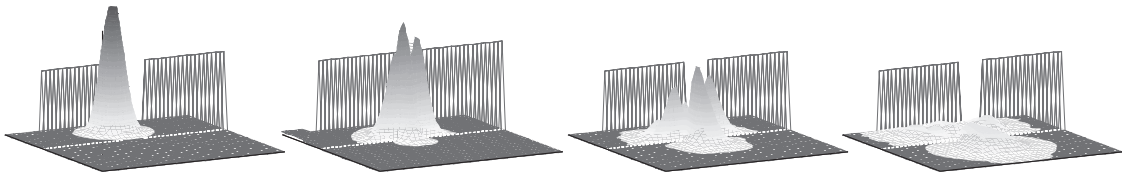

Figure 18.10 The probability density as a function of position and time for an electron incident upon and passing through a slit.

18.9 Unit III. E&M Waves via Finite-Difference Time Domain ⊙

Problem: You are given a 1-D resonant cavity with perfectly conducting walls. An initial electric pulse with the shape

$$E_x(z=3) = \exp\left[\frac{1}{2}\left(\frac{40-t}{12}\right)^2\right]\cos(2\pi f t), \quad 0 \le t \le T, \tag{18.56}$$

is placed in this cavity. Determine the motion of this pulse at all later times for $T = 10^{-8}$ s and $f = 700$ MHz.

Simulations of electromagnetic waves are of tremendous practical importance. Indeed, the fields of nanotechnology and spintronics rely heavily upon such simulations. The basic techniques used to solve for electromagnetic waves are essentially the same as those we used in Units I and II for string and quantum waves: Set up a grid in space and time and then step the initial solution forward in time one step at a time. For E&M simulations, this technique is known as the finite difference time domain *(FDTD) method. What is new for E&M waves is that they are vector fields, with the variations of one generating the other, so that the components of* $\mathbf{E}$ *and* $\mathbf{B}$ *are coupled to each other. Our treatment of FDTD does not do justice to the wealth of physics that can occur, and we recommend [Sull 00] for a more complete treatment and [Ward 04] (and their Web site) for modern applications.*

18.10 Maxwell's Equations

The description of electromagnetic (EM) waves via Maxwell's equations is given in many textbooks. For propagation in just one dimension (z) and for free space with no sinks or sources, four coupled PDEs result:

$$\vec{\nabla}\cdot\mathbf{E} = 0 \;\Rightarrow\; \frac{\partial E_x(z,t)}{\partial x} = 0 \tag{18.57}$$

$$\vec{\nabla}\cdot\mathbf{H} = 0 \;\Rightarrow\; \frac{\partial H_y(z,t)}{\partial y} = 0, \tag{18.58}$$

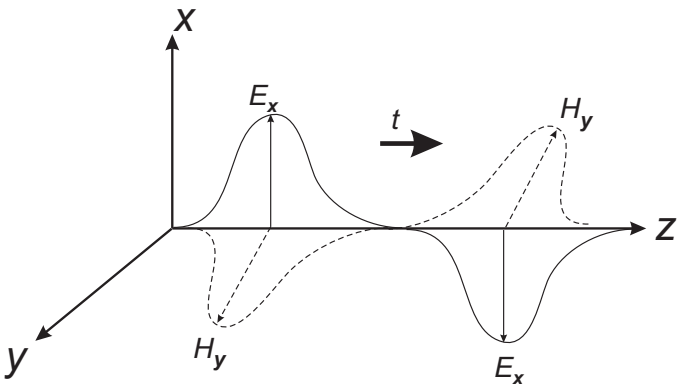

Figure 18.11 A single electromagnetic pulse traveling along the *z* axis. The two pulses correspond to two different times, and the coupled electric and magnetic fields are indicated by solid and dashed curves, respectively.

$$\frac{\partial \mathbf{E}}{\partial t} = +\frac{1}{\epsilon_0}\vec{\nabla} \times \mathbf{H} \;\Rightarrow\; \frac{\partial E_x}{\partial t} = -\frac{1}{\epsilon_0}\frac{\partial H_y(z,t)}{\partial z}, \tag{18.59}$$

$$\frac{\partial \mathbf{H}}{\partial t} = -\frac{1}{\mu_0}\vec{\nabla} \times \mathbf{E} \;\Rightarrow\; \frac{\partial H_y}{\partial t} = -\frac{1}{\mu_0}\frac{\partial E_x(z,t)}{\partial z}. \tag{18.60}$$

As indicated in Figure 18.11, we have chosen the electric field $\mathbf{E}(z,t)$ to oscillate (be polarized) in the x direction and the magnetic field $\mathbf{H}(z,t)$ to be polarized in the y direction. As indicated by the bold arrow in Figure 18.11, the direction of power flow for the assumed transverse electromagnetic (TEM) wave is given by the right-hand rule for $\mathbf{E} \times \mathbf{H}$. Note that although we have set the initial conditions such that the EM wave is traveling in only one dimension (z), its electric field oscillates in a perpendicular direction (x) and its magnetic field oscillates in yet a third direction (y); so while some may call this a 1-D wave, the vector nature of the fields means that the wave occupies all three dimensions.

18.11 FDTD Algorithm

We need to solve the two coupled PDEs (18.59) and (18.60) appropriate for our problem. As is usual for PDEs, we approximate the derivatives via the central-difference approximation, here in both time and space. For example,

$$\frac{\partial E(z,t)}{\partial t} \simeq \frac{E(z,t+\frac{\Delta t}{2}) - E(z,t-\frac{\Delta t}{2})}{\Delta t}, \tag{18.61}$$