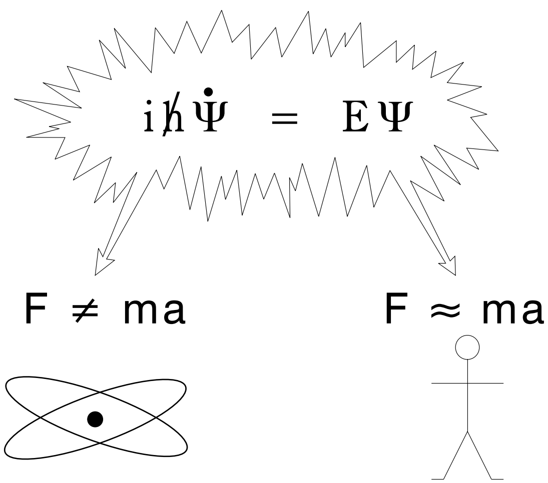
PHYSNET

MISN-0-248

NEWTON'S SECOND LAW FROM QUANTUM PHYSICS



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

NEWTON'S SECOND LAW FROM QUANTUM PHYSICS

by

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Input Skills:

1. Explain deBroglie waves, their probabilistic interpretation and their wave-particle duality (MISN-0-240).
2. State the time-independent Schrodinger Equation and define the momentum operator (MISN-0-243)).
3. Integrate by parts (any calculus textbook).
4. Calculate quantum mechanical mean values from wave functions (MISN-0-243).
5. Expand a function about a point using a Taylor series (MISN-0-4).

Output Skills (Knowledge):

K1. Discuss the reason(s) why any wave packet in a constant force field must obey classical particle physics.

K2. Given the Time-Dependent Schrodinger Equation, derive Newton's Second Law and the first correction term to it.

K3. Show and discuss the condition(s) under which Newton's Second Law is a good approximation, including the details of how the condition(s) would be evaluated in practice if you were given a wave packet and force law.

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1. Introduction

1a. A Time-Dependent Equation Needed. Although the time-independent version of the Schrödinger equation has had astonishing successes in the domains of atomic, molecular, nuclear, and solid state physics, and in chemistry, it cannot describe systems which change with time; it cannot deal with transition rates, spectral line intensities, tunneling, or scattering. For such cases we need the equation which tells us how wave functions change with time. Then, from the resulting time-dependent wave function all observable quantities will be calculable.

1b. When Classical and Quantum Mechanics Coincide. In order to justify the time-dependent equation found by Schrödinger, we will argue that quantum mechanics and classical particle mechanics must coincide for certain cases. Then we will derive Newton's Second Law as the first term in a power series and will examine the next (correction) term to determine the circumstances under which Newton's Second Law is a good approximation. Thus it will be apparent that quantum mechanics is a more general theory than classical particle mechanics since the latter is included within it.

2. Constant Force: Classical Behavior

When will an electron, say, act like a classical particle and when like a quantum mechanical wave? One commonly given answer[1] is that it will act like a wave when its deBroglie wavelength is large compared to the structural dimensions in an object with which it is interacting. Another answer is that it will act like a classical particle when the size of its wave packet is small compared to interacting structural dimensions. These two statements are not very satisfactory, being vague[2] and not entirely equivalent. We will find a precise statement based on the Schrödinger equation for the case where the above-stated wave packet condition becomes exact; namely, in the case of a constant force field. A constant field has no structure at all and hence there is no way we can say whether a wave packet in it is "large" or "small." This means that in a constant force we may regard the wave packet as being as small as we wish so classical mechanics must apply exactly. Of course quantum mechanics must also apply exactly because quantum mechanics is the fundamental overall theory.

[1]See "deBroglie Waves" (MISN-0-240).

[2]What is a Gaussian wave packet's "deBroglie wavelength?" Perhaps, its RMS uncertainty in position—but is that obvious? To what distance should the hydrogen-atom-electron's deBroglie wavelength be compared? To its non-existent orbital radius; or perhaps to the size of the proton with which it interacts, a number 10^7 times smaller?

3. Mean Position as Particle "Position"

We have said that under a constant force a wave packet of any size or shape must act like a classical particle, obeying Newton's laws exactly. But what part of the wave packet is it that is to obey, say, Newton's Second Law? Is it the leading edge of the wave packet, its trailing edge, its middle? Since quantum mechanics deals with mean values,[3] it would seem natural to try the assumption that it is the wave packet's mean position which exactly obeys Newton's Second Law for a constant force. In one dimension, Newton's Second Law for a wave packet's mean position is:

$$F(\bar{x}) = m\frac{d^2\bar{x}}{dt^2}\,, \qquad (F = ma) \tag{1}$$

which says that the force at the particle's position is to be equal to the particle's mass times the second time derivative of its position. Here "position" means "mean position."

4. Mean Velocity & Velocity of Mean Position

4a. The Time-Dependent Schrödinger Equation. The first step in obtaining Newton's Second Law is to obtain the particle's velocity, the velocity of its mean position:[4]

$$\dot{\bar{x}} \equiv \frac{d\bar{x}}{dt} = \frac{d}{dt}\int_{-\infty}^{\infty} \psi^*(x,t)x\psi(x,t)\,dx = \int_{-\infty}^{\infty}\left[\frac{d\psi^*}{dt}x\psi + \psi^* x\frac{d\psi}{dt}\right]dx. \tag{2}$$

One would expect that for a free packet or for one in a constant force field, where classical mechanics holds, the right hand side of Eq. (2) would be

[3]See "Wave Functions, Probability, and Mean Values."(MISN-0-243).

[4]We denote the time derivative of a symbol by a dot over it. This is a common notation.

equal to the mean momentum divided by the mass, which we shall call the mean velocity:

$$\dot{\bar{x}} = \bar{p}/m = \bar{v}; \qquad \text{constant force.} \tag{3}$$

Schrödinger discovered that the way to construct this equality was to write the time-dependence of the wave function as:

$$i\hbar \frac{d\psi(x,t)}{dt} = -\frac{\hbar^2}{2m}\frac{d^2\psi(x,t)}{dx^2} + V(x)\psi(x,t). \tag{4}$$

In the usual succinct notation this is:

$$i\hbar\dot{\psi} = -(\hbar^2/2m)\psi'' + V\psi. \tag{5}$$

This is an addition to the rules for construction of the Schrödinger equation,[5] added for cases where one wishes to see a wave function's time dependence. Equations (5) is called the Time-Dependent Schrödinger Equation.

4b. Velocity of Mean Position Equals Mean Velocity. Substituting Eq. (3) and its complex conjugate[6] into Eq. (2), we obtain:

$$\dot{\bar{x}} = \frac{\hbar}{2im}\int_{-\infty}^{\infty} \psi^{*\prime\prime}x\psi - \psi^* x\psi''\,dx.$$

Integrating by parts or, equivalently, making the substitution

$$\psi^{*\prime\prime}x\psi - \psi^* x\psi'' = \frac{d}{dx}(\psi^{*\prime}x\psi - \psi^* x\psi') - (\psi^{*\prime}\psi - \psi^*\psi'),$$

and assuming the usual boundary conditions at infinity, we find:[7]

$$\dot{\bar{x}} = \frac{\hbar}{2im}\int_{-\infty}^{\infty} (\psi^{*\prime}\psi - \psi^*\psi')\,dx. \qquad [S-5] \tag{6}$$

The first term on the right hand side can be converted to the form of the second term using another integration by parts and again applying boundary conditions at infinity:[8]

$$\int_{-\infty}^{\infty} \psi^{*\prime}\psi\,dx = -\int_{-\infty}^{\infty} \psi^*\psi'\,dx.$$

[5] See "The Schrödinger Equation in One Dimension: Quantization of Energy" (MISN-0-242).

[6] See "Some Simple Functions in the Complex Plane" (MISN-0-59).

[7] The notation [S-3] at the end of the equation indicates that help is available in sequence [S-3] in this module's *Special Assistance Supplement*.

[8] For wave packets whose probability is confined to finite distances from the origin, $\psi(\pm\infty) = 0 = \psi'(\pm\infty)$. See Appendix A, this unit, and "Wave Functions, Probability, and Mean Values" (MISN-0-243).

This converts equation (6) to:

$$\dot{\bar{x}} = \frac{1}{m}\int_{-\infty}^{\infty} (\psi^*(x,t)\left[-i\hbar\frac{d}{dx}\right]\psi(x,t)\,dx, \tag{7}$$

hence:

$$\dot{\bar{x}} = \bar{p}/m \equiv \bar{v}. \tag{8}$$

Thus the velocity of the particle's mean position is exactly equal to its mean velocity. Note that we made no restriction on the potential function, $V(x)$, and so the result, Eq. (8), is valid for any force, constant or not.

5. Force at Mean Pos. & Accel. of Mean Position

5a. Acceleration of Mean Position. To derive Newton's Second Law we need the acceleration of the mean position, for which we can differentiate equation (7) with respect to time:

$$\ddot{\bar{x}} \equiv \frac{d^2\bar{x}}{dt^2} = -\frac{i\hbar}{m}\int_{-\infty}^{\infty} (\dot{\psi}^{*\prime}\psi' + \psi^*\dot{\psi}')\,dx.$$

Then by integration by parts and use of the boundary conditions at infinity:

$$\ddot{\bar{x}} = -\frac{i\hbar}{m}\int_{-\infty}^{\infty} (\dot{\psi}^{*\prime}\psi' - \psi^{*\prime}\dot{\psi})\,dx. \qquad [S-1]$$

Substituting the time dependent Schrödinger equation, Eq. (3), and its complex conjugate, and integrating by parts, we obtain the acceleration of the particle's mean position:

$$a = \ddot{\bar{x}} = -\frac{1}{m}\int \psi^* V'\psi\,dx = -\frac{1}{m}\overline{\left[\frac{dV}{dx}\right]} \equiv +\overline{F(x)}/m. \qquad [S-2] \tag{9}$$

5b. A Constant Force ⇒ Classical Mechanics. For a constant force,

$$\overline{F(x)} = F(\bar{x}) = F = \text{ constant},$$

hence Newton's Second Law is obeyed:

$$F = ma; \qquad (F = \text{ constant}).$$

We conclude that, as anticipated, Newton's Second Law is exactly obeyed by a quantum mechanical wave packet in a constant force field.

5c. The Case of a General Force. For a general force we need to relate the mean force in (8) to the force at the mean position. To do this we expand F(x) in a power series about the mean position of the wave packet and then take the mean of the whole expansion. The expansion:

$$F(x) = F(\bar{x}) + F'(\bar{x})(x - \bar{x}) + \frac{1}{2}F''(\bar{x})(x - \bar{x})^2 + \dots$$

Then taking the mean:

$$\overline{F(x)} = F(\bar{x}) + \frac{1}{2}F''(\bar{x})\Delta_x^2 + \dots \qquad [S-8] \qquad (10)$$

Here Δ_x is the root-mean-square deviation of the wave packet from its mean.[9] Combining (9) and (10) we get:

$$ma \equiv m\ddot{\bar{x}} = F(\bar{x}) + \frac{1}{2}F''(\bar{x})\Delta_x^2 + \dots \qquad (11)$$

and the first term on the right side is the proper force for Newton's Second Law. For that term alone to be a good approximation, the next term must be much smaller:

$$\Delta_x^2 F''(\bar{x}) \ll F(\bar{x}),$$

or:

$$\text{If} \qquad \Delta_x^2 \ll \frac{F(\bar{x})}{F''(\bar{x})} \qquad \text{then} \qquad F \approx ma. \qquad (12)$$

Equation (12) says that, for Newton's Second Law to be valid, the size of the wave packet must be much smaller than structure in the force field, here represented by the relative inverse of the second spatial derivative.

6. Two Examples: $F = ma$ and $F \neq ma$

6a. The Simple Harmonic Oscillator. As a very simple example consider the one-dimensional simple harmonic oscillator, which has a linear force:

$$F(x) = -kx.$$

The second derivative, F'' , is zero and hence Eq. (11) becomes:

$$ma \equiv m\ddot{\bar{x}} = F(\bar{x}),$$

[9]See "Wave Functions, Probability, and Mean Values" (MISN-0-243).

and Newton's Second Law is obeyed exactly. One can envision some wave packet oscillating back and forth in this harmonic oscillator potential, continually changing its shape, but with an exactly sinusoidal mean position:

$$\bar{x}(t) = A \sin \omega_0 t; \qquad \omega_0 = \sqrt{k/m}.$$

6b. Coulomb Force: Hydrogen Atom Ground State. Now consider the ground state of hydrogen, where $\bar{r}^2 = a_0^2$, $\Delta_r^2 = (3/4)a_0^2$, with $a_0 \equiv \hbar^2/(me^2) \approx 0.05\,\text{nm}$.[10] Then:

$$F(\bar{r}) = -k_e \frac{e^2}{\bar{r}^2} = -k_e \frac{e^2}{a_0^2}\,,$$

$$F''(\bar{r}) = -6k_e \frac{e^2}{\bar{r}^4} = -k_e \frac{6e^2}{a_0^4}\,.$$

Putting these together, condition (12) is not met. Thus the electron in the normal hydrogen atom (the ground state) does not obey Newton's Second Law. That statement is in correspondence with the fact that the ground state wave function is spread out all around the nucleus. This would appear to be a far cry from a classical picture where the electron would have to be a tiny wave packet circling the nucleus.

▷ In a footnote to Section 2, a question is asked about the nuclear dimension to which a hydrogen atom electron's wave packet should be compared. What is the answer to that question?

It is interesting that condition (12) *is* met for the hydrogen atom for $n \gg 4$, where n is the principal quantum number. For such states there is very little probability near the nucleus. See for example, *Introduction to Quantum Mechanics*, L. Pauling and R. Wilson, McGraw-Hill (1935).

▷ Show that the hydrogen atom electron will obey Newton's Second Law for $n \gg 4$, $\ell = 0$, using the hydrogen wave functions found in almost any Quantum Mechanics textbook.

Acknowledgments

I wish to thank William Lane, Edward Spurlock, Jim Krebs, and Steve Smith, who provided valuable feedback on an earlier version. The

[10]For these values of Δ_r^2 and $\bar{r}^2$, see any quantum mechanics text. For example: *Introduction to Quantum Mechanics*, L. Pauling and R. Wilson, McGraw-Hill (1935).

basic expansion came from D. I. Blokhintsev.[11] Preparation of this module was supported in part by the National Science Foundation, Division of Science Education Development and Research, through Grant #SED 74-20088 to Michigan State University.

A. Boundary Conditions At Infinity

In quantum mechanics one frequently encounters integrals of the type:

$$I \equiv \int_{-\infty}^{\infty} \frac{d}{dx}(\psi^{*\prime} x\psi - \psi^* x\psi')\, dx = (\psi^{*\prime} x\psi - \psi^* x\psi')|_{-\infty}^{+\infty}. \tag{13}$$

For a wave packet whose probability is confined to finite distances from the origin, both terms are generally zero. For example, consider the wave function for the simple harmonic oscillator:

$$\psi(x) = cxe^{-ax^2/2},$$

where c and a are constants. The first term in equation (13) is:

$$|c|^2(1-ax^2)^2 e^{-ax^2} x^2 \Big|_{-\infty}^{+\infty}.$$

Since a decreasing exponential (or Gaussian) eventually falls off faster than any polynomial, we have that:

$$\lim_{x\to\infty}(1-ax^2)^2 x^2 e^{-ax^2} \to 0.$$

Thus the integral I of Eq. (13) is zero. Note that for any real wave function (one without an imaginary part) the two terms of the integrand in (13) add to zero and hence the integral is zero. This is true for the Gaussian wave function used in the example.

[11] D, I. Blokhintsev, *Principles of Quantum Mechanics*, Allyn and Bacon, Boston (1964), pp. 122-128. Blokhintsev also considers these phenomena in the transition to classical mechanics: spreading of the wave packet, derivation of the Hamilton-Jacobi Equation, and analogies to mechanics and optics.

SPECIAL ASSISTANCE SUPPLEMENT

S-1 *(from TX-5a)*

Only the second term of the integrand has been transformed. The process is similar to that used in deriving Eq. (6).

S-2 *(from TX-5a)*

Substitute $\dot\psi$ from Eq. (3), $\dot\psi^*$ from the complex conjugate of Eq. 3. Rearranging terms and factors, this gives:

$$\ddot{\bar{x}} = -\frac{1}{m}\int_{-\infty}^{\infty}\left[\frac{\hbar^2}{2m}(\psi^{*\prime\prime}\psi' - \psi^{*\prime}\psi'')(\psi^* V\psi' + \psi^{*\prime} V\psi)\right] dx.$$

Now the first term can be written:

$$(\psi^{*\prime\prime}\psi' - \psi^{*\prime}\psi'') = \frac{d}{dx}(\psi^{*\prime}\psi'), \qquad \textit{Help: [S-3]}$$

and the second term:

$$(\psi^* V\psi' + \psi^{*\prime} V\psi) = \frac{d}{dx}(\psi^* V\psi) - \psi^* V'\psi. \qquad \textit{Help: [S-3]}$$

S-3 *(from [S-2])*

$$\int_{-\infty}^{\infty}\frac{d}{dx}[\psi^* f(x)\psi]\, dx = |\psi^* f\psi|_{-\infty}^{\infty} = 0,$$

because there is no probability at infinity or (in cases you have not yet met) $\psi^* f\psi$ is the same at $+\infty$ as it is at $-\infty$. Similarly, quantities involving ψ' will also be zero. Also, see Appendix A.

S-4 *(from TX-5c)*

$F(x) = F(\bar x) + F'(\bar x)(x - \bar x) + \dots$

Take the average of both sides. Since the average is an integral (*see MISN-0-243*), use the properties of integrals to write:

$\overline{F(x)} = F(\bar x) + F'(\bar x)(\overline{x - \bar x}) + \dots$

where $F(x)$ and $F'(\bar x)$ are constants. Again, use the summative properties of integrals to see that:

$\overline{(x - \bar x)} = \bar x - \bar x = 0.$

$\boxed{\text{S-5}}$ *(from TX-4b)*

(i) make the suggested substitution; (ii) evaluate the argument of the perfect differential on the boundaries ($\pm\infty$) to get zero for that term. The remainder is the result shown in Eq. (6).