

Nine formulations of quantum mechanics

Daniel F. Styer,^{a)} Miranda S. Balkin, Kathryn M. Becker, Matthew R. Burns, Christopher E. Dudley, Scott T. Forth, Jeremy S. Gaumer, Mark A. Kramer, David C. Oertel, Leonard H. Park, Marie T. Rinkoski, Clait T. Smith, and Timothy D. Wotherspoon

Department of Physics, Oberlin College, Oberlin, Ohio 44074

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Nine formulations of nonrelativistic quantum mechanics are reviewed. These are the wavefunction, matrix, path integral, phase space, density matrix, second quantization, variational, pilot wave, and Hamilton–Jacobi formulations. Also mentioned are the many-worlds and transactional interpretations. The various formulations differ dramatically in mathematical and conceptual overview, yet each one makes identical predictions for all experimental results. © 2002 American

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I. WHY CARE ABOUT VARIOUS FORMULATIONS?

A junior-level classical mechanics course devotes a lot of time to various formulations of classical mechanics—Newtonian, Lagrangian, Hamiltonian, least action, and so forth (see Appendix A). But not a junior-level quantum mechanics course! Indeed, even graduate-level courses emphasize the wavefunction formulation almost to the exclusion of all variants. It is easy to see why this should be so—learning even a single formulation of quantum mechanics is difficult enough—yet at the same time students must wonder why it is so important to learn several formulations of classical mechanics but not of quantum mechanics. This article surveys nine different formulations of quantum mechanics. It is a project of the Spring 2001 offering of Oberlin College’s Physics 412, “Applied Quantum Mechanics.”

Why should one care about different formulations of mechanics when, in the end, each provides identical predictions for experimental results? There are at least three reasons. First, some problems are difficult in one formulation and easy in another. For example, the Lagrangian formulation of classical mechanics allows generalized coordinates, so it is often easier to use than the Newtonian formulation. Second, different formulations provide different insights.¹ For example, the Newtonian and least action principles provide very different pictorializations of “what’s really going on” in classical mechanics. Third, the various formulations are variously difficult to extend to new situations. For example, the Lagrangian formulation extends readily from conservative classical mechanics to conservative relativistic mechanics, whereas the Newtonian formulation extends readily from conservative classical mechanics to dissipative classical mechanics. In the words of the prolific chemist E. Bright Wilson:²

“I used to go to [J. H. Van Vleck] for quantum mechanical advice and found him always patient and ready to help, sometimes in a perplexing flow of mixed wave mechanical, operator calculus, and matrix language which often baffled this narrowly Schrödinger-equation-oriented neophyte. I had to learn to look at things in these alternate languages and, of course, it was indispensable that I do so.”

Any attempt to enumerate formulations must distinguish between “formulations” and “interpretations” of quantum

mechanics. Our intent here is to examine only distinct mathematical formulations, but the mathematics of course influences the conceptual interpretation, so this distinction is by no means clear cut,³ and we realize that others will draw boundaries differently. Additional confusion arises because the term “Copenhagen interpretation” is widely used but poorly defined: For example, of the two primary architects of the Copenhagen interpretation, Werner Heisenberg maintained that⁴ “observation of the position will alter the momentum by an unknown and undeterminable amount,” whereas Niels Bohr⁵ “warned specifically against phrases, often found in the physical literature, such as ‘disturbing of phenomena by observation.’”

II. CATALOG OF FORMULATIONS

A. The matrix formulation (Heisenberg)

The matrix formulation of quantum mechanics, developed by Werner Heisenberg in June of 1925, was the first formulation to be uncovered. The wavefunction formulation, which enjoys wider currency today, was developed by Erwin Schrödinger about six months later.

In the matrix formulation each mechanical observable (such as the position, momentum, or energy) is represented mathematically by a matrix (also known as “an operator”). For a system with N basis states (where in most cases $N = \infty$) this will be an $N \times N$ square Hermitian matrix. A quantum state $|\psi\rangle$ is represented mathematically by an $N \times 1$ column matrix.

Connection with experiment. Suppose the measurable quantity \mathcal{A} is represented by the operator \hat{A} . Then for any function $f(x)$ the expectation value for the measurement of $f(\mathcal{A})$ in state $|\psi\rangle$ is the inner product

$$\langle \psi | f(\hat{A}) | \psi \rangle. \quad (1)$$

Because the above statement refers to $f(\mathcal{A})$ rather than to \mathcal{A} alone, it can be used to find uncertainties [related to $f(\mathcal{A}) = \mathcal{A}^2$] as well as expectation values. Indeed, it can even produce the eigenvalue spectrum, as follows:⁶ Consider a set of real values a_1, a_2, a_3, \dots , and form the non-negative function

$$g(x) \equiv (x - a_1)^2 (x - a_2)^2 (x - a_3)^2 \cdots \quad (2)$$

Then the set a_1, a_2, a_3, \dots , constitutes the eigenvalues of \mathcal{A} if and only if

$$\langle \psi | g(\hat{A}) | \psi \rangle = 0 \text{ for all states } |\psi\rangle. \quad (3)$$

The matrix formulation places great emphasis on operators, whence eigenproblems fall quite naturally into its purview. This formulation finds it less natural to calculate time-dependent quantities or to consider the requirements for identical particles. Such problems fall more naturally into the second quantization formulation discussed below.

Time development. The operator corresponding to the mechanical observable energy is called the Hamiltonian and represented by \hat{H} . Any operator $\hat{A}(t)$ changes in time according to

$$\frac{d\hat{A}(t)}{dt} = -\frac{i}{\hbar} [\hat{A}(t), \hat{H}] + \frac{\partial \hat{A}}{\partial t}. \quad (4)$$

The states do not change with time.

Applications. For many (perhaps most) applications, the wavefunction formulation is more straightforward than the matrix formulation. An exception is the simple harmonic oscillator, where most problems are more cleanly and easily solved through the operator factorization technique (with raising and lowering operators) than through arcane manipulations involving Hermite polynomials. Similar matrix techniques are invaluable in the discussion of angular momentum. More general factorization methods (described in the book by Green, below) can solve more general problems, but often at such a price in complexity that the wavefunction formulation retains the advantage of economy.

Recommended references. Most contemporary treatments of quantum mechanics present an amalgam of the wavefunction and matrix formulations, with an emphasis on the wavefunction side. For treatments that emphasize the matrix formulation, we recommend

1. H. S. Green, *Matrix Mechanics* (P. Noordhoff, Ltd., Groningen, The Netherlands, 1965).
2. T. F. Jordan, *Quantum Mechanics in Simple Matrix Form* (Wiley, New York, 1986).

History. Matrix mechanics was the first formulation of quantum mechanics to be discovered. The founding papers are

3. W. Heisenberg, "Über die quantentheoretische Umdeutung kinematischer und mechanischer Beziehungen," ("Quantum-theoretical re-interpretation of kinematic and mechanical relations"), *Z. Phys.* **33**, 879–893 (1925).
4. M. Born and P. Jordan, "Zur Quantenmechanik," ("On quantum mechanics"), *Z. Phys.* **34**, 858–888 (1925).
5. M. Born, W. Heisenberg, and P. Jordan, "Zur Quantenmechanik II," *Z. Phys.* **35**, 557–615 (1926).

These three papers (and others) are translated into English in

6. B. L. van der Waerden, *Sources of Quantum Mechanics* (North-Holland, Amsterdam, 1967).

The uncertainty principle came two years after the formal development of the theory

7. W. Heisenberg, "Über den anschaulichen Inhalt der quantentheoretischen Kinematik und Mechanik," ("The physical content of quantum kinematics and mechanics"), *Z. Phys.* **43**, 172–198 (1927) [English translation in J. A. Wheeler and W. H. Zurek, editors, *Quantum Theory and Measurement* (Princeton University Press, Princeton, NJ, 1983), pp. 62–84].

B. The wavefunction formulation (Schrödinger)

Compared to the matrix formulation, the wavefunction formulation of quantum mechanics shifts the focus from "measurable quantity" to "state." The state of a system with two particles (ignoring spin) is represented mathematically by a complex function in six-dimensional configuration space, namely

$$\psi(\mathbf{x}_1, \mathbf{x}_2, t). \quad (5)$$

Alternatively, and with equal legitimacy, one may use the mathematical representation in six-dimensional momentum space:

$$\begin{aligned} \tilde{\psi}(\mathbf{p}_1, \mathbf{p}_2, t) = & \frac{1}{\sqrt{(2\pi\hbar)^6}} \int_{-\infty}^{+\infty} d^3x_1 \\ & \times \int_{-\infty}^{+\infty} d^3x_2 e^{-i(\mathbf{p}_1 \cdot \mathbf{x}_1 + \mathbf{p}_2 \cdot \mathbf{x}_2)/\hbar} \psi(\mathbf{x}_1, \mathbf{x}_2, t). \end{aligned} \quad (6)$$

Schrödinger invented this formulation in hopes of casting quantum mechanics into a "congenial" and "intuitive" form⁷—he was ultimately distressed when he found that his wavefunctions were functions in configuration space and did not actually exist out in ordinary three-dimensional space.⁸ The wavefunction should be regarded as a mathematical tool for calculating the outcomes of observations, not as a physically present entity existing in space such a football, or a nitrogen molecule, or even an electric field. (See also Appendix B.)

Time development. The configuration-space wavefunction changes in time according to

$$\begin{aligned} \frac{\partial \psi(\mathbf{x}_1, \mathbf{x}_2, t)}{\partial t} = & -\frac{i}{\hbar} \left[-\frac{\hbar^2}{2m_1} \nabla_1^2 \psi(\mathbf{x}_1, \mathbf{x}_2, t) \right. \\ & -\frac{\hbar^2}{2m_2} \nabla_2^2 \psi(\mathbf{x}_1, \mathbf{x}_2, t) \\ & \left. + V(\mathbf{x}_1, \mathbf{x}_2) \psi(\mathbf{x}_1, \mathbf{x}_2, t) \right], \end{aligned} \quad (7)$$

where the particle masses are m_1 and m_2 , and where $V(\mathbf{x}_1, \mathbf{x}_2)$ is the classical potential energy function. Equivalently, the momentum-space wavefunction changes in time according to

$$\begin{aligned} \frac{\partial \tilde{\psi}(\mathbf{p}_1, \mathbf{p}_2, t)}{\partial t} = & -\frac{i}{\hbar} \left[\frac{p_1^2}{2m_1} \tilde{\psi}(\mathbf{p}_1, \mathbf{p}_2, t) + \frac{p_2^2}{2m_2} \tilde{\psi}(\mathbf{p}_1, \mathbf{p}_2, t) \right. \\ & + \int_{-\infty}^{\infty} d^3p'_1 \int_{-\infty}^{\infty} d^3p'_2 \tilde{V}(\mathbf{p}'_1, \mathbf{p}'_2) \\ & \left. \times \tilde{\psi}(\mathbf{p}_1 + \mathbf{p}'_1, \mathbf{p}_2 + \mathbf{p}'_2, t) \right], \end{aligned} \quad (8)$$

where the Fourier transform of the potential energy function is

$$\begin{aligned} \tilde{V}(\mathbf{p}_1, \mathbf{p}_2) \\ = & \frac{1}{(2\pi\hbar)^6} \int_{-\infty}^{+\infty} d^3x_1 \int_{-\infty}^{+\infty} d^3x_2 e^{i(\mathbf{p}_1 \cdot \mathbf{x}_1 + \mathbf{p}_2 \cdot \mathbf{x}_2)/\hbar} V(\mathbf{x}_1, \mathbf{x}_2). \end{aligned} \quad (9)$$

After the measurement of a quantity, the wavefunction “collapses” to an appropriate eigenfunction of the operator corresponding to that quantity.

Energy eigenstates. Most states do not have a definite energy. Those that do⁹ satisfy the eigenequation

$$\left[-\frac{\hbar^2}{2m_1}\nabla_1^2 - \frac{\hbar^2}{2m_2}\nabla_2^2 + V(\mathbf{x}_1, \mathbf{x}_2, t) \right] \eta_n(\mathbf{x}_1, \mathbf{x}_2) = E_n \eta_n(\mathbf{x}_1, \mathbf{x}_2). \quad (10)$$

The energy spectrum may be either discrete (“quantized”) or continuous, depending upon the potential energy function $V(\mathbf{x}_1, \mathbf{x}_2, t)$ and the energy eigenvalue E_n .

Identical particles. If the two particles are identical, then the wavefunction is symmetric or antisymmetric under label interchange,

$$\psi(\mathbf{x}_1, \mathbf{x}_2, t) = \pm \psi(\mathbf{x}_2, \mathbf{x}_1, t), \quad (11)$$

depending upon whether the particles are bosons or fermions. A precisely parallel statement holds for the momentum–space wavefunction.

Recommended references. Most treatments of quantum mechanics emphasize the wavefunction formulation. Among the many excellent textbooks are

8. L. D. Landau and E. M. Lifshitz, *Quantum Mechanics: Non-Relativistic Theory*, translated by J. B. Sykes and J. S. Bell, 3rd ed. (Pergamon, New York, 1977).
9. A. Messiah, *Quantum Mechanics* (North-Holland, New York, 1961).
10. D. J. Griffiths, *Introduction to Quantum Mechanics* (Prentice–Hall, Englewood Cliffs, New Jersey, 1995).
11. R. W. Robinett, *Quantum Mechanics: Classical Results, Modern Systems, and Visualized Examples* (Oxford University Press, New York, 1997).

History. Schrödinger first wrote down the configuration-space form of the energy eigenequation (10) in

12. E. Schrödinger, “Quantisierung als Eigenwertproblem (Erste Mitteilung),” (“Quantization as a problem of paper values (part I)”), *Annalen der Physik* **79**, 361–376 (1926).

He wrote down the time-development equation (7) (which he called “the true wave equation”) five months later in

13. E. Schrödinger, “Quantisierung als Eigenwertproblem (Vierte Mitteilung),” (“Quantization as a problem of proper values (part IV)”), *Annalen der Physik* **81**, 109–139 (1926).

English translations appear in

14. E. Schrödinger, *Collected Papers on Wave Mechanics* (Chelsea, New York, 1978).

C. The path integral formulation (Feynman)

The path integral formulation (also called the sum-over-histories formulation) shifts the focus yet again—from “state” to “transition probability.”

Suppose, for example, that a single particle is located at point \mathbf{x}_i when the time is t_i , and we wish to find the probability that it will be located at \mathbf{x}_f when the time is t_f . This probability is calculated as follows:

- Enumerate all classical paths from the initial to the final state.
- Calculate the classical action $S = \int (\text{Lagrangian}) dt$ for each path.
- Assign each path a “transition amplitude” proportional to $e^{iS/\hbar}$. (The proportionality constant is adjusted to assure normalization.)

- Sum the amplitude over all paths. (Because there is a continuum of paths, this “sum” is actually a particular kind of integral called a “path integral.”)

- The resulting sum is the transition amplitude, and its square magnitude is the transition probability.

For different problems—such as a particle changing from one momentum to another, or for an initial state that has neither a definite position nor a definite momentum—variations on this procedure apply.

Applications. The path integral formulation is rarely the easiest way to approach a straightforward problem in nonrelativistic quantum mechanics. On the other hand, it has innumerable applications in other facets of physics and chemistry, particularly in quantum and classical field theory and in statistical mechanics. For example, it is a powerful tool in the Monte Carlo simulation of quantal systems:

15. M. H. Kalos and P. A. Whitlock, *Monte Carlo Methods* (Wiley, New York, 1986), Chap. 8.

In addition, many find this formulation appealing because the mathematical formalism is closer to experiment: the center stage is occupied by transition probabilities rather than by the unobservable wavefunction. For this reason it can be effective in teaching:

16. E. F. Taylor, S. Vokos, J. M. O’Meara, and N. S. Thornber, “Teaching Feynman’s sum over paths quantum theory,” *Comput. Phys.* **12**, 190–199 (1998).

Identical particles. The path integral procedure generalizes in a straightforward way to collections of several non-identical particles or of several identical bosons. (The term “path” now means the trajectories of the several particles considered collectively.) Thus it must *not* generalize in the same straightforward way to identical fermions, because if it did then bosons and fermions would behave in the same way!

The proper procedure for identical fermions involves a single additional step. When enumerating classical paths from the initial situation at time t_i to the final situation at time t_f (as in Fig. 1), notice that some of the paths interchange the particles relative to other paths. (In Fig. 1, the particles are interchanged in paths III and IV but not in paths I and II.) The assignment of amplitude to a fermion path proceeds exactly as described above except that, in addition, any amplitude associated with an interchanging path is multiplied by -1 before summing. (This rule is the Pauli principle: In your mind, slide the two particles at the final time t_f towards each other. As the separation vanishes, the amplitude associated with path I approaches the amplitude associated with path III. Similarly, each other direct path approaches an interchange path. Because of the factor of -1 , the amplitudes exactly cancel upon summation. Thus two fermions cannot move to be on top of each other.)

This sign adjustment is not difficult for humans, but it poses a significant challenge—know as “the fermion sign problem”—for computers. This important standing problem in quantum Monte Carlo simulation is discussed in, for example,

17. N. Makri, “Feynman path integration in quantum dynamics,” *Comput. Phys. Commun.* **63**, 389–414 (1991).
18. S. Chandrasekharan and U.-J. Wiese, “Meron-cluster solution of fermion sign problems,” *Phys. Rev. Lett.* **83**, 3116–3119 (1999).

Recommended references.

19. R. P. Feynman and A. R. Hibbs, *Quantum Mechanics and Path Integrals* (McGraw-Hill, New York, 1965).

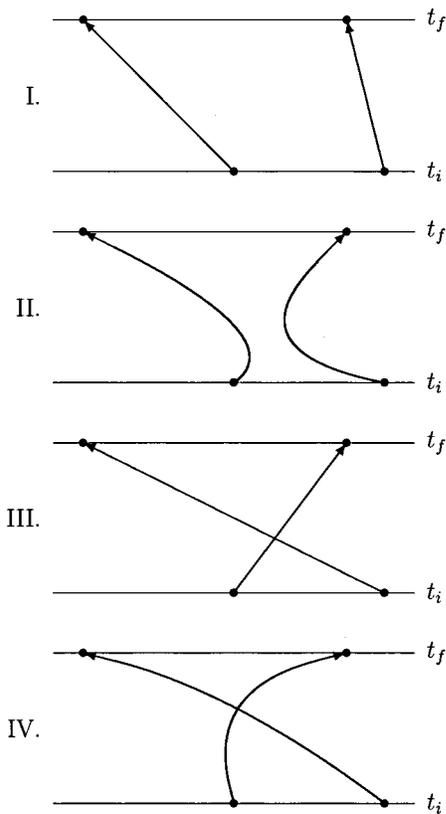


Fig. 1. If the two particles are identical fermions, then the amplitudes associated with interchanging paths, such as III and IV, must be multiplied by -1 before summing.

20. D. F. Styer, “Additions and corrections to Feynman and Hibbs,” <http://www.oberlin.edu/physics/dstyer/TeachQM/Supplements.html>.

21. L. S. Schulman, *Techniques and Applications of Path Integration* (Wiley, New York, 1981).

History. This formulation was developed by

22. R. P. Feynman, “Space–time approach to non-relativistic quantum mechanics,” *Rev. Mod. Phys.* **20**, 367–387 (1948).

D. Phase space formulation (Wigner)

For a single particle restricted to one dimension, the Wigner phase-space distribution function is

$$W(x, p, t) = \frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} \psi^*(x - \frac{1}{2}y, t) \times \psi(x + \frac{1}{2}y, t) e^{-ipy/\hbar} dy. \quad (12)$$

This function has a number of useful properties:

- It is pure real, but may be positive or negative.
- The integral over momentum gives the probability density in position:

$$\int_{-\infty}^{+\infty} W(x, p, t) dp = |\psi(x, t)|^2. \quad (13)$$

- The integral over position gives the probability density in momentum:

$$\int_{-\infty}^{+\infty} W(x, p, t) dx = |\tilde{\psi}(p, t)|^2. \quad (14)$$

- If the wavefunction ψ is altered by a constant phase factor, the Wigner function is unaltered.

- Given $W(x, p, t)$, one can find the wavefunction through a two-step process. First, find the Fourier transform

$$\begin{aligned} \tilde{W}(x, y, t) &= \frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} W(x, p, t) e^{ipy/\hbar} dp \\ &= \frac{1}{2\pi\hbar} \psi^*(x - \frac{1}{2}y, t) \psi(x + \frac{1}{2}y, t). \end{aligned} \quad (15)$$

Second, select an arbitrary point x_0 where $\tilde{W}(x_0, 0, t)$ does not vanish, and find

$$\psi(x, t) = \sqrt{\frac{2\pi\hbar}{\tilde{W}(x_0, 0, t)}} \tilde{W}(\frac{1}{2}(x+x_0), x-x_0, t). \quad (16)$$

The Wigner function is not a probability density in phase space—according to Heisenberg’s uncertainty principle, no such entity can exist. Yet it has several of the same properties, whence the term “distribution function” is appropriate.

Time development.

$$\begin{aligned} \frac{\partial W(x, p, t)}{\partial t} &= -\frac{p}{m} \frac{\partial W(x, p, t)}{\partial x} \\ &\quad - \int_{-\infty}^{+\infty} K(x, p') W(x, p+p', t) dp', \end{aligned} \quad (17)$$

where the kernel $K(x, p)$ is

$$K(x, p) = \frac{1}{2\pi\hbar^2} \int_{-\infty}^{+\infty} [V(x - \frac{1}{2}y) - V(x + \frac{1}{2}y)] \sin(py/\hbar) dy. \quad (18)$$

Identical particles. If the wavefunction is either symmetric or antisymmetric under interchange, then the Wigner function is symmetric:

$$W(x_1, p_1, x_2, p_2) = W(x_2, p_2, x_1, p_1). \quad (19)$$

This does not, of course, mean that bosons and fermions behave identically in this formulation: the wave-functions produced through Eq. (16) will exhibit the correct symmetry under interchange. It does mean that the type of interchange symmetry is more difficult to determine in the phase-space formulation than it is in the wavefunction formulation.

Applications. For an N -state system (where N may equal ∞), the wavefunction is specified by N complex numbers with an overall phase ambiguity, that is, by $2N-1$ real numbers. For this same system the Wigner function requires N^2 real numbers. Clearly the Wigner function is *not* the most economical way to record information on the quantal state. The Wigner function is useful when the desired information is more easily obtained from the redundant Wigner form than from the economical wavefunction form. (For example, the momentum density is obtained from the Wigner function through a simple integral over position. The momentum density is obtained from the configuration-space wavefunction through the square of a Fourier transform.)

A number of problems, particularly in quantum optics, fall into this category. See, for example, the following:

23. D. Leibfried, T. Pfau, and C. Monroe, “Shadows and mirrors: Reconstructing quantum states of atom motion,” *Phys. Today* **51**, 22–28 (1998).

24. Y. S. Kim and W. W. Zachary, editors, *The Physics of Phase Space* (Springer-Verlag, Berlin, 1987).

Recommended references.

25. Y. S. Kim and E. P. Wigner, "Canonical transformation in quantum mechanics," *Am. J. Phys.* **58**, 439–448 (1990).
 26. M. Hillary, R. F. O'Connell, M. O. Scully, and E. P. Wigner, "Distribution functions in physics: Fundamentals," *Phys. Rep.* **106**, 121–167 (1984).

History. The phase space formulation was invented by

27. E. P. Wigner, "On the quantum correction for thermodynamic equilibrium," *Phys. Rev.* **40**, 749–759 (1932).

E. Density matrix formulation

The density matrix corresponding to a pure state $|\psi\rangle$ is the outer product

$$\hat{\rho} = |\psi\rangle\langle\psi|. \tag{20}$$

Given the density matrix $\hat{\rho}$, the quantal state $|\psi\rangle$ can be found as follows: First select an arbitrary state $|\phi\rangle$. The (unnormalized) ket $|\psi\rangle$ is $\hat{\rho}|\phi\rangle$ (as long as this quantity does not vanish).

The density matrix is more properly but less frequently called "the density operator." As with any quantum mechanical operator, the operator is independent of basis whereas the matrix elements $\rho_{ij} = \langle i|\hat{\rho}|j\rangle$ do depend on the basis selected.

The density matrix formulation is particularly powerful in dealing with statistical knowledge. For example, if the exact state of a system is unknown, but it is known to be in one of three states—state $|\psi\rangle$ with probability p_ψ , state $|\phi\rangle$ with probability p_ϕ , or state $|\chi\rangle$ with probability p_χ —then the system is said to be in a "mixed state" (in contrast to a "pure state"). A mixed state *cannot* be represented by something like

$$c_\psi|\psi\rangle + c_\phi|\phi\rangle + c_\chi|\chi\rangle,$$

because this represents another pure state that is a superposition of the three original states. Instead, the mixed state is represented by the density matrix

$$p_\psi|\psi\rangle\langle\psi| + p_\phi|\phi\rangle\langle\phi| + p_\chi|\chi\rangle\langle\chi|. \tag{21}$$

All of the results that follow in this section apply to both pure and mixed states.

Connection with experiment. The density matrix is always Hermitian. If the measurable quantity \mathcal{A} is represented by the operator \hat{A} , then the expectation value for the measurement of $f(\mathcal{A})$ is the trace

$$\text{tr}\{f(\hat{A})\hat{\rho}\}. \tag{22}$$

Time development. The density matrix evolves in time according to

$$\frac{d\hat{\rho}(t)}{dt} = + \frac{i}{\hbar} [\hat{\rho}(t), \hat{H}], \tag{23}$$

where \hat{H} is the Hamiltonian operator. (Note that this formula differs in sign from the time-development formula in the matrix formulation.)

Identical particles. The density matrix, like the Wigner phase-space distribution function, remains unchanged under interchange of the coordinates of identical particles, whether bosons or fermions. As with the Wigner distribution, this does not mean that symmetric and antisymmetric wavefunc-

tions behave identically; it simply means that the different behaviors are buried in the density matrix rather than readily visible.

Applications. For an N -state system (where N may equal ∞), a pure-state wavefunction is specified by N complex numbers with an overall phase ambiguity, that is, by $2N - 1$ real numbers. For this same system the density matrix requires N real diagonal elements plus $N(N - 1)/2$ complex above-diagonal elements for a total of N^2 real numbers. Thus the density matrix is *not* the most economical way to record information about a pure quantal state. Nevertheless, the ready availability of this information through the trace operation, plus the ability to treat mixed states, make the density matrix formulation valuable in several areas of physics. In particular, the formula

$$\frac{\text{tr}\{\hat{A}e^{-\hat{H}/kT}\}}{\text{tr}\{e^{-\hat{H}/kT}\}} \tag{24}$$

is something of a mantra in quantum statistical mechanics.

Recommended references.

28. U. Fano, "Description of states in quantum mechanics by density matrix and operator techniques," *Rev. Mod. Phys.* **29**, 74–93 (1957).
 29. K. Blum, *Density Matrix Theory and Applications*, 2nd ed. (Plenum, New York, 1996).

History. The density matrix was introduced by the following:

30. J. von Neumann, "Wahrscheinlichkeitstheoretischer Aufbau der Quantenmechanik," ("Probability theoretical arrangement of quantum mechanics"), *Nachr. Ges. Wiss. Goettingen*, 245–272 (1927), reprinted in *Collected Works* (Pergamon, London, 1961), Vol. 1, pp. 208–235.

F. Second quantization formulation

This formulation features operators that create and destroy particles. It was developed in connection with quantum field theory, where such actions are physical effects (for example, an electron and a positron are destroyed and a photon is created). However, the formulation has a much wider domain of application and is particularly valuable in many-particle theory, where systems containing a large (but constant) number of identical particles must be treated in a straightforward and reliable manner.

The unfortunate name of this formulation is due to a historical accident—from the point of view of nonrelativistic quantum mechanics, a better name would have been the "occupation number formulation."

The second-quantized creation operator a_ψ^\dagger "creates" a particle in quantum state $|\psi\rangle$. A one-particle state is formed by having a_ψ^\dagger act upon a state with no particles, the so-called "vacuum state" $|0\rangle$. Thus the following are different expressions for the same one-particle state:

$$|\psi\rangle, \quad \psi(x), \quad \tilde{\psi}(p), \quad a_\psi^\dagger|0\rangle. \tag{25}$$

Thus as far as one-particle systems are concerned, the second quantization formulation is equivalent to the wavefunction formulation, although somewhat more cumbersome.

What about many-particle systems? Suppose $|\psi\rangle$, $|\phi\rangle$, and $|\chi\rangle$ are orthonormal one-particle states. Then a state with two identical particles is produced by creating two particles from the vacuum: for example $a_\phi^\dagger a_\psi^\dagger|0\rangle$. If the particles are bosons, then

$$a_\phi^\dagger a_\psi^\dagger|0\rangle = a_\psi^\dagger a_\phi^\dagger|0\rangle, \tag{26}$$

whereas for fermions

$$a_{\phi}^{\dagger} a_{\psi}^{\dagger} |0\rangle = -a_{\psi}^{\dagger} a_{\phi}^{\dagger} |0\rangle. \quad (27)$$

This illustrates the general rule that bosonic creation operators commute:

$$[a_{\phi}^{\dagger}, a_{\psi}^{\dagger}] = 0, \quad (28)$$

whereas fermionic creation operators anticommute:

$$\{a_{\phi}^{\dagger}, a_{\psi}^{\dagger}\} = 0. \quad (29)$$

(The anticommutation notation means $\{\hat{A}, \hat{B}\} = \hat{A}\hat{B} + \hat{B}\hat{A}$.)

The advantages of second-quantized notation for many-particle systems are becoming apparent. Most physicists would agree that of the two equivalent forms

$$a_{\phi}^{\dagger} a_{\psi}^{\dagger} |0\rangle \quad \text{and} \quad \frac{1}{\sqrt{2}} [\psi(x_1)\phi(x_2) \pm \psi(x_2)\phi(x_1)], \quad (30)$$

it is easier to work with the one on the left. And nearly all physicists find it easier to work with

$$a_{\chi}^{\dagger} a_{\phi}^{\dagger} a_{\psi}^{\dagger} |0\rangle \quad (31)$$

than with the equivalent

$$(1/\sqrt{3!}) [+\psi(x_1)\phi(x_2)\chi(x_3) \pm \psi(x_1)\phi(x_3)\chi(x_2) \\ + \psi(x_3)\phi(x_1)\chi(x_2) \pm \psi(x_3)\phi(x_2)\chi(x_1) \\ + \psi(x_2)\phi(x_3)\chi(x_1) \pm \psi(x_2)\phi(x_1)\chi(x_3)]. \quad (32)$$

Yet the greatest advantage of second quantization is not mere compactness of notation. The wavefunction formulation allows you—indeed, it almost *invites* you—to write down expressions such as

$$\psi(x_1)\phi(x_2),$$

expressions that are neither symmetric nor antisymmetric under interchange, and hence expressions that do not correspond to any quantal state for identical particles. Yet the wavefunction formulation provides no overt warning that this expression is an invitation to ruin. By contrast, in the second quantized formulation it is impossible to even write down a formula such as the one above—the symmetrization (or antisymmetrization) happens automatically through the commutation (or anticommutation) of creation operators, so only legitimate states can be expressed in this formulation. For this reason, the second quantization formulation is used extensively in many-particle theory.

Recommended references.

31. H. J. Lipkin, *Quantum Mechanics: New Approaches to Selected Topics* (North-Holland, Amsterdam, 1986), Chap. 5.
32. V. Ambegaokar, “Second quantization,” in *Superconductivity*, edited by R. D. Parks (Marcel Dekker, New York, 1969), pp. 1359–1366.
33. W. E. Lawrence, “Algebraic identities relating first- and second-quantized operators,” *Am. J. Phys.* **68**, 167–170 (2000).

An extensive discussion of applications is

34. G. D. Mahan, *Many-Particle Physics*, 3rd ed. (Kluwer Academic, New York, 2000).

History. Second quantization was developed by Dirac for photons, then extended by Jordan and Klein to massive bosons, and by Jordan and Wigner to fermions:

35. P. A. M. Dirac, “The quantum theory of the emission and absorption of radiation,” *Proc. R. Soc. London, Ser. A* **114**, 243–265 (1927).

36. P. Jordan and O. Klein, “Zum Mehrkörperproblem der Quantentheorie,” (“On the many-body problem in quantum theory”), *Z. Phys.* **45**, 751–765 (1927).

37. P. Jordan and E. Wigner, “Über das Paulische Äquivalenzverbot,” (“On the Pauli valence line prohibition”), *Z. Phys.* **47**, 631–651 (1928).

The Dirac and Jordan–Wigner papers are reprinted in

38. J. Schwinger, editor, *Selected Papers on Quantum Electrodynamics* (Dover, New York, 1958).

G. Variational formulation

The “variational formulation” must not be confused with the more-commonly-encountered “variational method,” which provides a bound on the ground state energy. Instead the variational formulation provides a full picture describing any state—not just the ground state—and dictating its full time evolution—not just its energy. It is akin to Hamilton’s principle in classical mechanics.

The central entity in this formulation remains the wavefunction $\psi(\mathbf{x}_1, \mathbf{x}_2, t)$, but the rule for time evolution is no longer the Schrödinger equation. (We again consider a non-relativistic two-particle system ignoring spin.) Of all possible normalized wavefunctions $\psi(\mathbf{x}_1, \mathbf{x}_2, t)$, the correct wavefunction is the one that minimizes the “action integral” over time and configuration space, namely

$$\int dt \int d^3x_1 \int d^3x_2 \mathcal{L}(\mathbf{x}_1, \mathbf{x}_2, t), \quad (33)$$

where the “Lagrangian density” is

$$\mathcal{L}(\mathbf{x}_1, \mathbf{x}_2, t) = \hbar \operatorname{Im} \left\{ \psi^* \frac{\partial \psi}{\partial t} \right\} + \frac{\hbar^2}{2m_1} \nabla_1 \psi^* \cdot \nabla_1 \psi \\ + \frac{\hbar^2}{2m_2} \nabla_2 \psi^* \cdot \nabla_2 \psi + V(\mathbf{x}_1, \mathbf{x}_2) \psi^* \psi, \quad (34)$$

and $\operatorname{Im}\{z\}$ means the imaginary part of z . It is not difficult to show that this minimization criterion is equivalent to the Schrödinger time-development equation (7).

Applications. On the practical side, this formulation is directly connected to the invaluable variational method for estimating ground state energies. (Apply the principle to the class of time-independent trial wavefunctions, and the variational method tumbles right out.)

On the fundamental side, we note that field variational techniques often provide formulations of physical law that are manifestly Lorentz invariant. This role is exploited for electricity and magnetism in

39. J. Schwinger, L. L. DeRaad, Jr., K. A. Milton, and W. Tsai, *Classical Electrodynamics* (Perseus Books, Reading, MA, 1998), especially Chaps. 8 and 9,

for general relativity (“Hilbert’s formulation”) in

40. C. W. Misner, K. S. Thorne, and J. A. Wheeler, *Gravitation* (Freeman, San Francisco, 1973), Chap. 21,

and for quantum field theory in

41. C. Itzykson and J.-B. Zuber, *Quantum Field Theory* (McGraw-Hill, New York, 1980).

For this reason, such variational formulations are now the preferred instrument of attack for extending physics to new domains, for example to supersymmetric strings or membranes:

42. E. Witten, “Reflections on the fate of spacetime,” *Phys. Today* **49**, 24–30 (April 1996).

43. E. Witten, "Duality, spacetime and quantum mechanics," *Phys. Today* **50**, 28–33 (May 1997).

However, these roles are not played directly by the formulation discussed here which is (i) intrinsically nonrelativistic and which (ii) involves integration over time and configuration space rather than time and physical space.

Recommended reference.

44. P. M. Morse and H. Feshbach, *Methods of Theoretical Physics* (McGraw-Hill, New York, 1953), pp. 314–316 and 341–344.

[Caution! This reference defines a Lagrangian density with the opposite sign of Eq. (34), so the Morse and Feshbach action integral is maximized, not minimized, by the correct wavefunction.]

History. This formulation originated in the following:

45. P. Jordan and O. Klein, "Zum Mehrkörperproblem der Quantentheorie," ("On the many-body problem in quantum theory"), *Z. Phys.* **45**, 751–765 (1927).

(The same paper that introduced second quantization for massive bosons!)

H. The pilot wave formulation (de Broglie–Bohm)

We outline the pilot wave formulation through the example of an electron and a proton (ignoring spin). In classical mechanics this system is represented mathematically by two points tracing out trajectories in three-dimensional physical space. In the wavefunction formulation this system is represented mathematically by a complex-valued wavefunction evolving in six-dimensional configuration space. In the pilot wave formulation this system is represented mathematically by *both* the two points in physical space *and* the wavefunction in configuration space. The wavefunction is called the "pilot wave" and it (along with the classical potential energy function) provides information telling the two points how to move.

The most frequently cited version of the pilot wave formulation is that of Bohm (but see also the version by Dürr, Goldstein, and Zanghí, cited below). In Bohm's version, the wavefunction is written in terms of the (real) magnitude and phase functions as

$$\psi(\mathbf{x}_1, \mathbf{x}_2, t) = R(\mathbf{x}_1, \mathbf{x}_2, t) e^{iS(\mathbf{x}_1, \mathbf{x}_2, t)/\hbar}. \quad (35)$$

If one defines the state-dependent "quantum potential"

$$Q(\mathbf{x}_1, \mathbf{x}_2, t) = -\frac{\hbar^2}{2m_1} \frac{\nabla_1^2 R}{R} - \frac{\hbar^2}{2m_2} \frac{\nabla_2^2 R}{R}, \quad (36)$$

then the pilot wave evolves in time according to

$$\frac{\partial S}{\partial t} = -\frac{(\nabla_1 S)^2}{2m_1} - \frac{(\nabla_2 S)^2}{2m_2} - V(\mathbf{x}_1, \mathbf{x}_2) - Q(\mathbf{x}_1, \mathbf{x}_2, t) \quad (37)$$

and

$$\frac{\partial P}{\partial t} + \frac{1}{m_1} \nabla_1 \cdot (P \nabla_1 S) + \frac{1}{m_2} \nabla_2 \cdot (P \nabla_2 S) = 0, \quad (38)$$

where

$$P(\mathbf{x}_1, \mathbf{x}_2, t) = R^2(\mathbf{x}_1, \mathbf{x}_2, t). \quad (39)$$

The first equation resembles a Hamilton–Jacobi equation; the second acts such as a continuity equation in which P represents a probability density.

The two point particles move with accelerations

$$m_1 \frac{d\mathbf{v}_1}{dt} = -\nabla_1 V - \nabla_1 Q \quad \text{and} \quad m_2 \frac{d\mathbf{v}_2}{dt} = -\nabla_2 V - \nabla_2 Q. \quad (40)$$

In other words, the force is given not only by the gradient of the classical potential, but by the gradient of the quantum potential as well. The initial positions of the point particles are uncertain: for an ensemble of systems the probability density of initial positions is given by $P(\mathbf{x}_1, \mathbf{x}_2, 0)$. Thus both the particle corresponding to the proton and the particle corresponding to the electron have a definite position and a definite momentum; however the initial ensemble uncertainty and the quantum potential work together to ensure that any set of measurements on a collection of identically prepared systems will satisfy $\Delta x \Delta p \geq \hbar/2$.

The quantum potential $Q(\mathbf{x}_1, \mathbf{x}_2, t)$ changes instantaneously throughout configuration space whenever the wavefunction changes, and this mechanism is responsible for the nonlocal correlations that are so characteristic of quantum mechanics. A rather natural mechanism prevents human beings from tapping into this instantaneous change for the purpose of faster-than-light communications.

Applications. To use the pilot wave formulation one must keep track of both trajectories and wavefunctions, so it is not surprising that this formulation is computationally difficult for most problems. For example the phenomenon of two-slit interference, often set as a sophomore-level modern physics problem using the wavefunction formulation, requires a computational *tour de force* in the pilot wave formulation:

46. C. Philippidis, C. Dewdney, and B. J. Hiley, "Quantum interference and the quantum potential," *Nuovo Cimento Soc. Ital. Fis.*, B **52**, 15–28 (1979).

In contrast, the pilot wave formulation is effective in raising questions concerning the general character of quantum mechanics. For example, John Bell's epoch-making theorem concerning locality and the quantum theory was inspired through the pilot wave formulation.¹⁰ And many astute observers find the pilot wave formulation intuitively insightful. For example:

47. J. S. Bell, "Six possible worlds of quantum mechanics," in *Possible Worlds in Humanities, Arts and Sciences: Proceedings of Nobel Symposium 65*, 11–15 August 1986, edited by S. Allén (Walter de Gruyter, Berlin, 1989), pp. 359–373. Reprinted in J. S. Bell, *Speakable and Unsayable in Quantum Mechanics* (Cambridge University Press, Cambridge, UK, 1987), Chap. 20, pp. 181–195.
48. H. P. Stapp, "Review of 'The Undivided Universe' by Bohm and Hiley," *Am. J. Phys.* **62**, 958–960 (1994).

Recommended references.

49. D. Bohm, B. J. Hiley, and P. N. Kaloyerou, "An ontological basis for the quantum theory," *Phys. Rep.* **144**, 321–375 (1987).
50. D. Bohm and B. J. Hiley, *The Undivided Universe: An Ontological Interpretation of Quantum Theory* (Routledge, London, 1993).
51. D. Dürr, S. Goldstein, and N. Zanghí, "Quantum equilibrium and the origin of absolute uncertainty," *J. Stat. Phys.* **67**, 843–907 (1992).

History. Louis de Broglie proposed the germ of this approach which was discussed at, for example, the Solvay Congress of 1927. But the substantial development of these ideas began with

52. D. Bohm, "A suggested interpretation of the quantum theory in terms of 'hidden' variables, I and II," *Phys. Rev.* **35**, 166–179 and 180–193 (1952).

I. The Hamilton–Jacobi formulation

The classical Hamilton–Jacobi formulation systematically finds changes of variable such that the resulting equations of motion are readily integrated. In particular, if this results in a new set of variables of the so-called “action-angle” form, one can find the period of a repetitive motion without actually finding the motion itself.

Classical Hamilton–Jacobi theory provided important inspiration in the development of quantum mechanics. (Dirac’s “transformation theory” places a similar emphasis on strategic changes of variable, and the Wilson–Sommerfeld version of old quantum theory relies on action-angle variables.) But it was not until 1983 that Robert Leacock and Michael Padgett produced a treatment extensive enough to be regarded as a full Hamilton–Jacobi formulation of quantum mechanics. The central entity of this formulation is “Hamilton’s principal function” $S(\mathbf{x}_1, \mathbf{x}_2, t)$ such that

$$\psi(\mathbf{x}_1, \mathbf{x}_2, t) = \exp[iS(\mathbf{x}_1, \mathbf{x}_2, t)/\hbar]. \quad (41)$$

[Caution: This function may be complex...it is not the same S as in the pilot-wave defining Eq. (35).] Hamilton’s principal function satisfies the quantum Hamilton–Jacobi equation,

$$\frac{\partial S}{\partial t} = i \frac{\hbar}{2m_1} \nabla_1^2 S - \frac{1}{2m_1} \nabla_1 S \cdot \nabla_1 S + i \frac{\hbar}{2m_2} \nabla_2^2 S - \frac{1}{2m_2} \nabla_2 S \cdot \nabla_2 S - V(\mathbf{x}_1, \mathbf{x}_2). \quad (42)$$

[Caution: The name “quantum Hamilton–Jacobi equation” is applied both to this equation and to the pilot wave equation (37).]

If the resulting change in variables is of action-angle form, then this formulation can find the energy eigenvalues without needing to find the eigenfunctions.

Recommended references.

53. R. A. Leacock and M. J. Padgett, “Hamilton–Jacobi/action-angle quantum mechanics,” *Phys. Rev. D* **28**, 2491–2502 (1983).
54. R. S. Bhalla, A. K. Kapoor, and P. K. Panigrahi, “Quantum Hamilton–Jacobi formalism and the bound state spectra,” *Am. J. Phys.* **65**, 1187–1194 (1997).
55. J.-H. Kim and H.-W. Lee, “Canonical transformations and the Hamilton–Jacobi theory in quantum mechanics,” *Can. J. Phys.* **77**, 411–425 (1999).

J. Summary and conclusions

We have discussed nine distinct formulations of quantum mechanics. Did we learn anything in the process? The most profound lesson is already familiar from classical mechanics, and indeed from everyday life: “There is no magic bullet.” Each of these formulations can make some application easier or some facet of the theory more lucid, but no formulation produces a “royal road to quantum mechanics.” Quantum mechanics appears strange to our classical eyes, so we employ mathematics as our sure guide when intuition fails us. The various formulations of quantum mechanics can repack-age that strangeness, but they cannot eliminate it.

The *matrix formulation*, the first formulation to be discovered, is useful in solving harmonic oscillator and angular momentum problems, but for other problems it is quite difficult. The ever-popular *wavefunction formulation* is standard for problem solving, but leaves the conceptual misimpression that wavefunction is a physical entity rather than a mathematical tool. The *path integral formulation* is physically appealing and generalizes readily beyond the domain of nonrelativistic quantum mechanics, but is laborious in most

standard applications. The *phase space formulation* is useful in considering the classical limit. The *density matrix formulation* can treat mixed states with ease, so it is of special value in statistical mechanics. The same is true of *second quantization*, which is particularly important when large numbers of identical particles are present. The *variational formulation* is rarely the best tool for applications, but it is valuable in extending quantum mechanics to unexplored domains. The *pilot wave formulation* brings certain conceptual issues to the fore. And the *Hamilton–Jacobi formulation* holds promise for solving otherwise-intractable bound state problems.

We are fortunate indeed to live in a universe where nature provides such bounty.

III. ADDITIONAL ISSUES

This section treats two interpretations of quantum mechanics that might instead be considered formulations, then goes on to briefly discuss four miscellaneous items.

A. The many-worlds interpretation (Everett)

The many-worlds interpretation is close to the boundary between a “formulation” and an “interpretation”—indeed its founder, Hugh Everett, called it “the relative state formulation,” while it is most widely known under Bryce DeWitt’s name of “the many-worlds interpretation.”

In this interpretation there is no such thing as a “collapse of the wavefunction.” At the same time, the question changes from “What happens in the world?” to “What happens in a particular story line?” This change in viewpoint is best demonstrated through an example: Suppose a scientist cannot make up her mind whether to marry or to break off her engagement. Rather than flip a coin, she sends a single circularly-polarized photon into a sheet of polaroid. If a photon emerges (linearly polarized) from the polaroid, a photo-detector will register and an attached bell will chime. The scientist decides beforehand that if the bell chimes, she will marry. Otherwise, she will remain single. In the Bohr version of quantum mechanics, the question is “What happens?” and the answer is that the scientist has a 50% chance of marriage and a 50% chance of breaking her engagement. In the Everett version, this is not the right question: There is one story line in which the photon emerges, the bell rings, and the marriage occurs. There is another story line in which the photon is absorbed, silence reigns, and the engagement terminates. Each story line is consistent. To find out which story line we are living in, we simply check on the marital status of the scientist. If she is married, we are living in the story line where a linearly polarized photon emerged and the bell rang. Otherwise, we live in the other story line. The question “What happens?” is ill-posed—one must ask instead “What happens in a particular story line?” (Just as the question “How far is Chicago?” is ill-posed—one must ask instead “How far is Chicago from San Francisco?”)

In the relative state formulation, the wavefunction never collapses—it merely continues branching and branching. Each branch is consistent, and no branch is better than any of the other branches. (In the many-worlds version, one speaks of coexisting branching universes rather than of multiple story lines.) In summary, the relative state formulation places the emphasis on *correlations* and avoids *collapse*.

Applications. The relative state formulation is mathematically equivalent to the wavefunction formulation, so there can be no technical reason for preferring one formulation

over the other. On the other hand, some find that the conceptual orientation of the relative state formulation produces insights in what would otherwise be fallow ground. For example, David Deutsch's 1985 paper, which founded the enormously fertile field of quantum computing, expressed his opinion that "The intuitive explanation of these properties places an intolerable strain on all interpretations of quantum theory other than Everett's."

56. D. Deutsch, "Quantum theory, the Church-Turing principle and the universal quantum computer," *Proc. R. Soc. London, Ser. A* **400**, 97–117 (1985).

Recommended references.

57. H. Everett III, " 'Relative state' formulation of quantum mechanics," *Rev. Mod. Phys.* **29**, 454–462 (1957).
 58. B. S. DeWitt and N. Graham, in *The Many-Worlds Interpretation of Quantum Mechanics* (Princeton University Press, Princeton, NJ, 1973).
 59. Y. Ben-Dov, "Everett's theory and the 'many-worlds' interpretation," *Am. J. Phys.* **58**, 829–832 (1990).
 60. B. S. DeWitt, "Quantum mechanics and reality," *Phys. Today* **23**, 30–35 (September 1970).
 61. L. E. Ballentine, P. Pearle, E. H. Walker, M. Sachs, T. Koga, J. Gerver, and B. DeWitt, "Quantum mechanics debate," *Phys. Today* **24**, 36–44 (April 1971).

B. The transactional interpretation (Cramer)

This interpretation (or formulation) is coherent and valuable, but it is difficult to describe in brief compass, so many who have inspected it only briefly consider it simply bizarre. If our short description here leaves you with that misimpression, we urge you to consult the recommended references.

In the transactional interpretation sources and detectors of, say, electrons emit both retarded waves (moving forward in time) and advanced waves (moving backward in time). An electron moving from a source to a detector involves an "offer wave" (corresponding to ψ) from the source and a "confirmation wave" (corresponding to ψ^*) from the detector which interfere to produce "a handshake across space-time."¹¹ Destructive interference between these two waves assures that the electron cannot arrive at the detector before it leaves its source.

Applications. According to John Cramer,¹² "the transactional interpretation...makes no predictions that differ from those of conventional quantum mechanics [that is, the wavefunction formulation]... We have found it to be more useful as a guide for deciding which quantum-mechanical calculations to perform than as an aid in the performance of such calculations... The main utility of the transactional interpretation is [as] a conceptual model which provides the user with a way of clearly visualizing complicated quantum processes and of quickly analyzing seemingly 'paradoxical' situations... It also seems to have considerable value in the development of intuitions and insights into quantum phenomena that up to now have remained mysterious."

Identical particles. Discussions of the transactional interpretation are usually carried out in the context of one-particle quantum mechanics. It is not clear to us whether, in a two-particle system, there are two "handshakes across space-time" or one "handshake across configuration-space-time." Consequently, we cannot report on how the transactional formulation differentiates between bosons and fermions.

Recommended references.

62. J. G. Cramer, "The transactional interpretation of quantum mechanics," *Rev. Mod. Phys.* **58**, 647–687 (1986).

63. J. G. Cramer, "An overview of the transactional interpretation of quantum mechanics," *Int. J. Theor. Phys.* **27**, 227–236 (1988).

History. This interpretation originated in

64. J. G. Cramer, "Generalized absorber theory and the Einstein–Podolsky–Rosen paradox," *Phys. Rev. D* **22**, 362–376 (1980).

C. Miscellaneous items

Most physicists interested in formulations will also be interested in density functional theory, in decoherence, in the consistent histories interpretation, and in the possibility of continuous spontaneous localization, so these matters are briefly touched upon here.

The *density functional theory* of Hohenberg and Kohn is a powerful quantum-theoretic tool, but it is not a formulation...it deals only with the ground state. (Admittedly, this is the only state of interest for much of chemistry and condensed matter physics.)

65. R. G. Parr and W. Yang, *Density-Functional Theory of Atoms and Molecules* (Oxford University Press, New York, 1989).

From the birth of quantum mechanics, everyone recognized the importance of a correct classical limit. Results such as Ehrenfest's famous theorem assure that some quantal states behave nearly classically. But this does not completely answer the need: It is also true that other quantal states behave far from classically. Why do we never encounter such states in the day-to-day world? The phenomenon of *decoherence* attempts to explain this absence. The vast technical literature is best approached through the two reviews

66. W. H. Zurek, "Decoherence and the transition from quantum to classical," *Phys. Today* **44**, 36–44 (October 1991).
 67. S. Haroche, "Entanglement, decoherence and the quantum/classical boundary," *Phys. Today* **51**, 36–42 (July 1998).

Robert Griffiths's *consistent histories* interpretation is not a formulation, but provides an interesting point of view. See

68. R. B. Griffiths and R. Omnès, "Consistent histories and quantum measurements," *Phys. Today* **52**, 26–31 (August 1999).

The idea of *continuous spontaneous localization* deals with wavefunction collapse and the classical limit by modifying the Schrödinger equation in such a way that extended quantal states naturally collapse, as if under their own weight. There are several such schemes, the most prominent of which is

69. G. C. Ghirardi, A. Rimini, and T. Weber, "Unified dynamics for microscopic and macroscopic systems," *Phys. Rev. D* **34**, 470–491 (1986).

Finally, everyone should be aware of the two wide-ranging reviews

70. S. Goldstein, "Quantum theory without observers," *Phys. Today* **51**, 42–46 (March 1998) and *ibid.* 38–42 (April 1998).
 71. F. Laloë, "Do we really understand quantum mechanics? Strange correlations, paradoxes, and theorems," *Am. J. Phys.* **69**, 655–701 (2001).

APPENDIX A: FORMULATIONS OF CLASSICAL MECHANICS

The formulations of classical mechanics known to us are the following:

Newtonian
 Lagrangian
 Hamiltonian

Hamilton's principle (called by Feynman and Landau "the principle of least action")

the Maupertuis principle of least action (also associated with the names of Euler, Lagrange, and Jacobi)
 least constraint (Gauss)
 least curvature (Hertz)
 Gibbs–Appell
 Poisson brackets
 Lagrange brackets
 Liouville
 Hamilton–Jacobi

These formulations are discussed to a greater or lesser extent in any classical mechanics textbook. The definitive scholarly work appears to be

72. E. T. Whittaker, *A Treatise on the Analytical Dynamics of Particles and Rigid Bodies*, 4th ed. (Cambridge University Press, Cambridge, UK, 1937).

APPENDIX B: GAUGE TRANSFORMATIONS

The wavefunction plays such a central role in most discussions of quantum mechanics that one is easily trapped into thinking of it as a physical entity rather than a mathematical tool. Anyone falling into this trap will be dissuaded by the following argument. Consider a single particle of charge q moving in an electromagnetic field described by scalar potential $\phi(\mathbf{x}, t)$ and vector potential $\mathbf{A}(\mathbf{x}, t)$. Then the configuration-space Schrödinger equation is

$$\frac{\partial \psi(\mathbf{x}, t)}{\partial t} = -\frac{i}{\hbar} \left[\frac{1}{2m} \left(-i\hbar \nabla - \frac{q}{c} \mathbf{A}(\mathbf{x}, t) \right)^2 + q\phi(\mathbf{x}, t) \right] \psi(\mathbf{x}, t). \quad (\text{B1})$$

On the other hand, we can describe exactly the same system using the gauge-transformed potentials:

$$\mathbf{A}'(\mathbf{x}, t) = \mathbf{A}(\mathbf{x}, t) + \nabla \chi(\mathbf{x}, t), \quad (\text{B2})$$

$$\phi'(\mathbf{x}, t) = \phi(\mathbf{x}, t) - \frac{1}{c} \frac{\partial \chi(\mathbf{x}, t)}{\partial t}. \quad (\text{B3})$$

One can easily show that the wavefunction obtained using these new potentials is related to the original wavefunction by

$$\psi'(\mathbf{x}, t) = e^{iq\chi(\mathbf{x}, t)/\hbar c} \psi(\mathbf{x}, t). \quad (\text{B4})$$

This gauge transformation has not changed the system at all, and any experimental result calculated will be the same regardless of which gauge is employed. Yet the wavefunction has changed dramatically. (Indeed, although the probability density cannot and does not change through a gauge trans-

formation, the all-important phase—responsible for all interference effects—can be selected at will.)

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^{a)}Electronic mail: Dan.Styer@oberlin.edu

¹To our classical sensibilities, the phenomena of quantum mechanics—interference, entanglement, nonlocal correlations, and so forth—seem weird. The various formulations package that weirdness in various ways, but none of them can eliminate it because the weirdness comes from the facts, not the formalism.

²E. B. Wilson, “Some personal scientific reminiscences,” *International Journal of Quantum Chemistry: Quantum Chemistry Symposium*, Proceedings of the International Symposium held at Flagler Beach, Florida, 10–20 March 1980, Vol. 14, pp. 17–29, 1980 (see p. 21). Wilson co-authored one of the very earliest quantum mechanics textbooks, namely L. Pauling and E. B. Wilson, *Introduction to Quantum Mechanics* (McGraw-Hill, New York, 1935).

³C. A. Fuchs and A. Peres, “Quantum theory needs no ‘interpretation’,” *Phys. Today* **53**, 70–71 (March 2000); D. Styer, “Quantum theory—interpretation, formulation, inspiration [letter],” *ibid.* **53**, 11 (September 2000); C. A. Fuchs and A. Peres, “Reply,” *ibid.* **53**, 14,90 (September 2000).

⁴W. Heisenberg, *The Physical Principles of the Quantum Theory*, translated by Carl Eckart and F. C. Hoyt (University of Chicago Press, Chicago, 1930), p. 20.

⁵N. Bohr, “Discussion with Einstein on epistemological problems in atomic physics,” in *Albert Einstein, Philosopher–Scientist*, edited by P. A. Schilpp (Library of Living Philosophers, Evanston, IL, 1949), p. 237. Reprinted in N. Bohr, *Atomic Physics and Human Knowledge* (Wiley, New York, 1958), pp. 63–64.

⁶N. David Mermin, unpublished lectures given at Cornell University.

⁷Schrödinger used both words in his first 1926 paper (Ref. 12 in the text). In the translation (Ref. 14 in the text), “congenial” appears on p. 10 and “intuitive” on p. 9. The latter corresponds to the German *anschaulich*, which has been variously translated as “intuitive,” “pictorial,” or “visualizable.”

⁸See, for example, A. Pais, *Inward Bound* (Clarendon, Oxford, UK, 1986), p. 256.

⁹We represent arbitrary wavefunctions by $\psi(\mathbf{x})$ or by $\phi(\mathbf{x})$, and energy eigenfunctions by $\eta(\mathbf{x})$, because the Greek letter η suggests “e” (as in “energy eigenfunction” and as in “eta”). This admirable convention was established by D. T. Gillespie, in *A Quantum Mechanics Primer* (International Textbook Company, Scranton, PA, 1970).

¹⁰J. Bernstein, *Quantum Profiles* (Princeton University Press, Princeton, NJ, 1991), pp. 72–77.

¹¹Cramer, Ref. 63 in the text, p. 661.

¹²Cramer, Ref. 63 in the text, p. 663.