ods, see Ackermann (1995) and Plante *et al.* (1994), respectively.

The DMC and VMC Monte Carlo methods attempt to reduce the complexity problem for more complex systems by the use of random-sampling techniques. The DMC method takes advantage of the fact that the time-dependent Schrödinger equation is formally identical to the diffusion equation in imaginary time, and for large imaginary time, an arbitrary starting solution quickly decays to the ground state (see, e.g., Moskowitz *et al.*, 1982; Barnett *et al.*, 1995; and earlier references therein). A random sampling of initial configurations is then propagated forward in time to construct the wave function. The VMC method is more closely related to the standard variational techniques discussed in Sec. 3.3.4. The idea is to define a trial wave function Ψ_{tr} in terms of variational parameters, as in Sec. 3.3.4, and then to optimize them over a statistical distribution of sample points $\mathbf{r}_i$ by minimizing an expression for the variance such as

$$\frac{\sum_i (H\Psi_i - E_{\text{ref}}\Psi_i)^2/w_i}{\sum_i \Psi_i^2/w_i}, \tag{129}$$

or the energy variance given by

$$\frac{\sum_i (H\Psi_i - E_{\text{ref}}\Psi_i)^2 \Psi_i^2/w_i^2}{\left[\sum_i \Psi_i^2/w_i\right]^2}. \tag{130}$$

Here, $\Psi_i = \Psi_{\text{tr}}(\mathbf{r}_i)$ is the trial wave function evaluated at some particular set of values for the electronic coordinates collectively denoted by $\mathbf{r}_i$, and the weight function $w_i = w(\mathbf{r}_i)$ is the probability of choosing $\mathbf{r}_i$ if the sampling is nonuniform. The optimum strategy is to bias the sampling according to the value of a guiding function $g(\mathbf{r}_i)$ that resembles the actual Ψ^2 as closely as possible and to choose the reference energy E_{ref} as close as possible to the desired eigenvalue. Although the method could be applied to a direct optimization of $\langle H \rangle$, the advantage gained by optimizing the variance is that the sample space required for a given accuracy is much smaller. Several sample problems and illustrative examples are discussed by Alexander *et al.* (1991).

3.4 Variation–Perturbation Methods

For many problems, it is advantageous to split the Hamiltonian into two parts according to

$$H = H^{(0)} + gV, \tag{131}$$

where the eigenvalue problem for $H^{(0)}$ can be solved exactly (or to high precision), and V is a perturbation whose strength is controlled by the parameter g. If the wave functions and energies are similarly expanded,

$$\Psi = \Psi^{(0)} + g\Psi^{(1)} + g^2\Psi^{(2)} + \cdots, \tag{132}$$

$$E = E^{(0)} + gE^{(1)} + g^2E^{(2)} + \cdots, \tag{133}$$

and substituted into the Rayleigh–Ritz quotient (106), then the terms linear in g give

$$E^{(1)} = \frac{1}{\langle \Psi^{(0)}|\Psi^{(0)}\rangle}\left[\langle \Psi^{(0)}|V|\Psi^{(0)}\rangle + 2\langle \Psi^{(0)}|H^{(0)} - E^{(0)}|\Psi^{(1)}\rangle\right]. \tag{134}$$

This is stationary with respect to variations $\delta\Psi^{(0)}$ if $\Psi^{(1)}$ satisfies the first-order perturbation equation

$$(H^{(0)} - E^{(0)})|\Psi^{(1)}\rangle + (V - E^{(1)})|\Psi^{(0)}\rangle = 0. \tag{135}$$

Since by assumption

$$H^{(0)}|\Psi^{(0)}\rangle = E^{(0)}|\Psi^{(0)}\rangle, \tag{136}$$

it follows from Eq. (134) that

$$E^{(1)} = \langle \Psi^{(0)}|V|\Psi^{(0)}\rangle/\langle \Psi^{(0)}|\Psi^{(0)}\rangle. \tag{137}$$

The entire series of perturbation equations to all orders can be similarly generated from the Rayleigh–Ritz variational principle. Computational methods based on these results were first developed by Slater and Kirkwood (1931), and by Dalgarno and Lewis (1955, 1956) (see also Dalgarno and Stewart, 1956; Sternheimer, 1951, 1954, 1957; Schwartz, 1959). They have since been employed by numerous other authors for a wide variety of problems.

3.4.1 Variational Bounds A particular advantage of the variational derivation of the perturbation equations is its use in establish-

dent. For example, with the replacement $E^{(0)} \rightarrow i\hbar\partial/\partial t$, the variational condition

$$\delta\left[\left\langle \Psi^{(1)}(t)\middle| H^{(0)} - i\hbar\frac{\partial}{\partial t}\middle|\Psi^{(1)}(t)\right\rangle + 2\langle\Psi^{(1)}(t)|V(t)|\Psi^{(0)}(t)\rangle\right] = 0 \tag{154}$$

with respect to $\Psi^{(1)}(t)$ leads to the first-order time-dependent perturbation equation

$$\left(H^{(0)} - i\hbar\frac{\partial}{\partial t}\right)|\Psi^{(1)}(t)\rangle + V(t)|\Psi^{(0)}(t)\rangle = 0. \tag{155}$$

This can be solved by Dirac's method of variation of constants. Many other techniques have been developed, but these will not be further pursued here. See, for example, Dalgarno (1966).

4. THE GENERAL STURM–LIOUVILLE PROBLEM

Many of the variational techniques discussed in Sec. 3 were developed long before the invention of quantum mechanics, in connection with boundary-value problems in classical physics such as vibrating membranes. Any linear second-order differential equation (of which the radial Schrödinger equation is just one example) can be written in the Sturm–Liouville form

$$\frac{d}{dx}\left[K(x)\frac{dy}{dx}\right] - G(x)y = 0, \tag{156}$$

defined over some closed interval $[a,b]$, together with suitable boundary conditions. By application of the Euler–Lagrange equation with fixed end points, this equation follows from the variational condition

$$\delta\int_a^b\left[K(x)\left(\frac{dy}{dx}\right)^2 + G(x)y^2\right]dx, \tag{157}$$

and so all the techniques discussed thus far can be applied. With the choice

$$G(x) = -\lambda g(x) + l(x), \tag{158}$$

the Sturm–Liouville problem becomes an eigenvalue problem with λ adjusted to satisfy the boundary conditions.

4.1 The Oscillation Theorem

A great many theorems have been proven concerning the solutions to Sturm–Liouville problems (see, e.g., Ince, 1956). Of particular importance for physical applications is the oscillation theorem. Suppose that $K(x)$, $g(x)$, and $l(x)$ are all continuous, real, positive, monotonic decreasing functions of x in the interval $[a,b]$. It can then be proved that the two-point eigenvalue problem

$$\frac{d}{dx}\left[K(x)\frac{dy}{dx}\right] + [\lambda g(x) - l(x)]y = 0 \tag{159}$$

has an infinite sequence of increasing eigenvalues $\lambda_1, \lambda_2, \ldots$, with corresponding eigenvectors $y_1(x), y_2(x), \ldots$ such that $y_m(x)$ has exactly $m - 1$ zeros in the open interval $[a,b]$. The eigenvalues are entirely discrete. If $g(x)$ changes sign in the interval, then the sequence of eigenvalues becomes doubly infinite with both an increasing $(\lambda_m^{(+)})$ and a decreasing $(\lambda_m^{(-)})$ set. In either case, the solutions are orthogonal with respect to the weight function $g(x)$.

The importance of this theorem (and its extensions) is that the $y_m(x)$ form the basis for a generalized Fourier series in terms of which an arbitrary function $f(x)$ can be expanded in the form

$$f(x) = \sum_{m=1}^{\infty} c_m y_m(x) \tag{160}$$

with

$$c_m = \int_a^b f(x)g(x)dx. \tag{161}$$

Since the eigenvalues are entirely discrete, there is no integration over a continuum in Eq. (160). Such a basis is called a *Sturmian* basis set. Most of the mathematical apparatus developed for Fourier analysis can be carried over directly. In fact, a Fourier series just corresponds to the choices $K(x) = 1$, $g(x) = 1$, $l(x) = 0$.

4.2 Example: The Coulomb Problem

Consider the radial Schrödinger equation

$$\left[-\frac{1}{2r^2}\frac{d}{dr}r^2\frac{d}{dr}+\frac{l(l+1)}{2r^2}-\frac{Z}{r}\right]R(r)=ER(r) \tag{162}$$

for an electron moving in the field of a nucleus with charge Z. The quantum-mechanical eigenvalue problem is solved on the interval $[0,\infty]$ by holding Z fixed and varying E such that the boundary conditions

$$\lim_{r\to 0} rR(r)=0, \quad \lim_{r\to\infty} R(r)=0, \tag{163}$$

are satisfied for the infinity of bound states with $E<0$. There is in addition a continuum of scattering solutions with $E>0$.

The Sturmian eigenvalue problem differs in that E is held fixed at some negative value $-\epsilon$ with $\epsilon>0$, and Z is varied so as to satisfy the boundary conditions. Since the eigenvalues to the Coulomb problem are

$$E_n(Z)=-Z^2/2n^2, \tag{164}$$

it is clear that the Sturmian eigenvalue condition $E_n(Z)=-\epsilon$ can be satisfied infinitely many times by progressively increasing both n and Z. As Z increases, one eigenvalue after another from the original problem is pulled down through the value $-\epsilon$. The Sturmian eigenvalues are thus $Z_n=n\sqrt{\epsilon}$ and the corresponding eigenfunctions are

$$R_{nl}(r)=\frac{1}{(2l+1)!}\left(\frac{(n+l)!}{(n-l-1)!2n}\right)^{1/2}\times(2\alpha)^{3/2}(2\alpha r)^l e^{-\alpha r}\times F(-n+l+1,2l+2;2\alpha r), \tag{165}$$

where $\alpha=\sqrt{2\epsilon}$ and $F(a,b;z)$ is a confluent hypergeometric function. The $R_{nl}(r)$ form a complete set of finite Sturmian polynomials for $n\geq l+1$ that are orthogonal with respect to the potential $1/r$; i.e.

$$\int_0^\infty R_{n'l}(r)\frac{1}{r}R_{nl}(r)r^2dr=\epsilon\delta_{n',n}. \tag{166}$$

The Sturmian functions $R_{nl}(r)$ closely resemble the bound-state Coulomb wave functions. The main distinguishing feature is that α is a constant in the exponential factor instead of decreasing as $1/n$. The first N of them differ only by a transformation of the basis set from the functions used to construct a finite variational representation of $\Psi_{\rm tr}^{(1)}$ in Sec. 3.4.3. The theory of Sturmian functions therefore provides a rigorous foundation for the choice of basis functions in variational calculations, and their property of completeness ensures convergence to the correct answer as N increases.

5. APPLICATIONS TO ELECTRODYNAMICS

Consider an electromagnetic field propagating through a medium with a charge density $\rho(\mathbf{r})$ moving with velocity $\mathbf{v}(\mathbf{r})$. It follows from Maxwell's equations that the scalar and vector potentials introduced in Sec. 2.4.1 satisfy the equations

$$\nabla^2\mathbf{A}-\frac{1}{c^2}\frac{\partial^2\mathbf{A}}{\partial t^2}=-4\pi\rho\frac{\mathbf{v}}{\mathbf{c}}, \tag{167a}$$

$$\nabla^2\phi-\frac{1}{c^2}\frac{\partial^2\phi}{\partial t^2}=-4\pi\rho, \tag{167b}$$

provided that the Lorentz gauge condition

$$\nabla\cdot\mathbf{A}+\frac{1}{c}\frac{\partial\phi}{\partial t}=0 \tag{168}$$

is imposed. Many other gauge choices can be made that leave the physical fields $\mathbf{E}$ and $\mathbf{B}$ invariant, but this one is simplest for the present discussion.

Unlike problems involving point particles, we are now dealing with fields that vary continuously in space. Equations (167a) and (167b) can be derived from a variational principle if a Lagrangian density $\mathscr{L}$ is first defined such that

$$L=\int \mathscr{L}dxdydz. \tag{169}$$

The action integral in Hamilton's principle then assumes the four-dimensional form

$$J=\int \mathscr{L}dxdydzdt. \tag{170}$$

The condition $\delta J=0$ is obtained in a manner similar to that leading to Laplace's equation (31). The present case is an application of Eq. (23) with $f=\mathscr{L}$ and four independent

variables $t_1 = x$, $t_2 = y$, $t_3 = z$, $t_4 = t$. There will be four equations corresponding to $q_1 = A_1$, $q_2 = A_2$, $q_3 = A_3$, and $q_4 = \phi$. The choice of $\mathscr{L}$ is severely restricted for fields *in vacuo* by the requirement that it be quadratic in the field components (since the field equations are linear), and relativistically invariant. The only quantity satisfying both requirements is a term proportional to $E^2 - B^2$. The inhomogeneous interaction terms on the right-hand sides of Eqs. (167a) are also included with the definition

$$\mathscr{L} = \frac{1}{8\pi}\left[\left(-\nabla\phi - \frac{1}{c}\frac{\partial \mathbf{A}}{\partial t}\right)^2 - (\nabla \times \mathbf{A})^2 - \left(\nabla\cdot\mathbf{A} + \frac{1}{c}\frac{\partial\phi}{\partial t}\right)^2\right] + \rho\left(\mathbf{A}\cdot\frac{\mathbf{v}}{c} - \phi\right), \tag{171}$$

where the first two squared terms correspond to E^2 and $-B^2$, respectively, and the third term generates the Lorentz gauge condition (168). The last term is the interaction term. A straightforward application of Eq. (23) with the terms identified as described following Eq. (170) then yields Eqs. (167a) and (167b).

The Lagrangian density $\mathscr{L}$ gives the equations of motion for the fields in the presence of a predefined matter distribution $\rho(\mathbf{r},t)$. For comparison, the Lagrangian L defined by Eq. (96) gives the converse equations of motion for particles in the presence of predefined fields $\mathbf{A}$ and ϕ. The remarkable point emerging from a comparison of $\mathscr{L}$ and L is that the matter-field interaction term $\rho(\mathbf{A}\cdot\mathbf{v}/c - \phi)$ in $\mathscr{L}$ is very similar in form to the second and third terms in L. In fact, the terms become identical with the choice $\rho(\mathbf{r}) = q\delta(\mathbf{r} - \mathbf{r}')$, corresponding to a point particle of charge q at position $\mathbf{r}'$. This suggests that the two Lagrangians can be combined into a single Lagrangian

$$L_{\text{tot}} = L_0 + \int \mathscr{L}_0 dxdydz + L_{\text{int}}, \tag{172}$$

where L_0 and $\mathscr{L}_0$ are the Lagrangians for free particles and free fields, respectively, and L_{int} is the remaining interaction term common to both L and $\int \mathscr{L}\, d\mathbf{r}$. Hamilton's principle and the Euler–Lagrange equations then give the equations of motion for the combined system of interacting particles and fields.

The above is of course not a proof that the resulting equations of motion provide an exact description of nature. The derivation is based on the supposition that something like Hamilton's principle remains valid for the combined system of interacting particles and fields, and it ignores the quantum nature of both matter and fields. However, Eq. (172) provides a basis for combining a quantized description of matter fields and electromagnetic fields into a single theory called *quantum electrodynamics*, whose predictions have been verified to an extremely high degree of precision (see, e.g., Kinoshita and Yennie, 1990). It can safely be described as the most successful theory ever invented. However, further discussion of this topic would take us beyond the scope of this article (see Further Reading and the article QUANTUM ELECTRODYNAMICS).

6. FEYNMAN'S PATH INTEGRAL

This article would not be complete without at least a passing reference to Feynman's path integral because of the way in which it provides an underlying coherent formalism unifying classical mechanics, quantum mechanics, and optics.

Consider for simplicity the x coordinate of a particle moving in a potential. The aim is to construct a path integral giving the quantum-mechanical transition amplitude for the particle to move from position x_0 at time t_0 to position x_f at time t_f. Let the state vector corresponding to a particle at position x be denoted by $|x\rangle$. In the coordinate representation

$$\langle x'|x\rangle = \delta(x - x'), \tag{173}$$

and by closure,

$$\int |x\rangle\langle x| = \mathbf{1}, \tag{174}$$

where $\mathbf{1}$ is the identity operator. In the momentum representation,

$$\langle p|x\rangle = (2\pi\hbar)^{-1/2} e^{-px/\hbar} = \langle x|p\rangle^*. \tag{175}$$

The remaining ingredient is the time-evolution operator $e^{-iHt/\hbar}$. Its inverse defines states $|x,t\rangle$ in the Heisenberg representation such that

$$|x,t\rangle = e^{iHt/\hbar}|x\rangle. \tag{176}$$

With these preliminaries, an initial expression for the desired transition amplitude is

$$\begin{aligned} K(x_f,t_f;x_0,t_0) &= \langle x_f,t_f|x_0,t_0\rangle \\ &= \langle x_f|\exp[-iH(t_f - t_0)/\hbar]|x_0\rangle. \end{aligned} \tag{177}$$

The key idea in constructing a path integral is to suppose that the system passes through a large number N of intermediate states $|x_k,t_k\rangle$ in making the above transition from $|x_0,t_0\rangle$ to $|x_f,t_f\rangle$ such that $t_{k+1} = t_k + \epsilon$, with $\epsilon = (t_f - t_0)/(N + 1)$. This can be formally achieved by making repeated use of the closure relation (174) to write

$$\begin{aligned} &K(x_f,t_f;x_0,t_0) \\ &\quad = \int dx_1 \cdots dx_N \langle x_f,t_f|x_N,t_N\rangle \\ &\qquad \times \langle x_N,t_N|x_{N-1},t_{N-1}\rangle \cdots \langle x_1,t_1|x_0,t_0\rangle. \end{aligned} \tag{178}$$

Then for each intermediate step, the inner product is

$$\begin{aligned} &\langle x_k,t_k|x_{k-1},t_{k-1}\rangle \\ &\quad = \langle x_k|\exp[-i(t_k - t_{k-1})H/\hbar]|x_{k-1}\rangle \\ &\quad = \langle x_k|e^{-i\epsilon H/\hbar}|x_{k-1}\rangle. \end{aligned} \tag{179}$$

Using Eq. (175), this can be evaluated in the momentum representation to obtain (with symmetric or Weyl operator ordering)

$$\begin{aligned} &\langle x_k,t_k|x_{k-1},t_{k-1}\rangle \\ &\quad = \int \frac{dp_k}{2\pi\hbar} \exp\{i[p_k\Delta x_k - i\epsilon H(\bar{x}_k,p_k)]/\hbar\}, \end{aligned} \tag{180}$$

where $\Delta x_k = x_k - x_{k-1}$ and $\bar{x}_k = (x_k + x_{k-1})/2$. Substitution of this form into Eq. (178) then yields

$$K(x_f,t_f;x_0,t_0) = \int dx_1 \cdots dx_N \frac{dp_1}{2\pi\hbar} \cdots \frac{dp_{N+1}}{2\pi\hbar} e^{iS_N}, \tag{181}$$

where

$$S_N = \frac{\epsilon}{\hbar} \sum_{k=1}^{N+1} \left[\frac{p_k\Delta x_k}{\epsilon} - H(\bar{x}_k,p_k)\right]. \tag{182}$$

Consider now the limit $N \to \infty$, $\epsilon \to 0$. Although each x_k separately ranges over all possible values due to the integrations in Eq. (181) (see Fig. 5), the quantity $\Delta x_k/\epsilon \equiv (x_k - x_{k-1})/\epsilon$ contributes a large and rapidly varying phase that averages to zero unless $x_k \approx x_{k-1}$. We can therefore identify $\Delta x_k/\epsilon$ with $\dot{x}$ in the limit $\epsilon \to 0$ and write

$$\lim_{\epsilon\to 0} S_N = \frac{1}{\hbar}\int_{t_0}^{t_f} [p\dot{x} - H(x,p)]dt = \frac{1}{\hbar}\int_{t_0}^{t_f} L\, dt. \tag{183}$$

This result provides a version of the Feynman path integral with the path integrated over all possibilities (including discontinuous ones) in phase space. However, the result can be carried a step further by performing the momentum integrations in Eq. (181). For example, if H has the form

$$H(x,p) = p^2/2m + V(x), \tag{184}$$

then a typical momentum integral has the Gaussian form

$$\begin{aligned} &\int_{-\infty}^{\infty} \frac{dp_k}{2\pi\hbar} \exp\left\{-\frac{i\epsilon}{\hbar}\left[\frac{p_k^2}{2m} - \frac{p_k\Delta x_k}{\epsilon}\right]\right\} \\ &\quad = \left(\frac{m}{2\pi\hbar i\epsilon}\right)^{1/2} \exp\left[\frac{im\epsilon}{2\hbar}\left(\frac{\Delta x_k}{\epsilon}\right)^2\right]. \end{aligned} \tag{185}$$

Using this in Eq. (181) gives

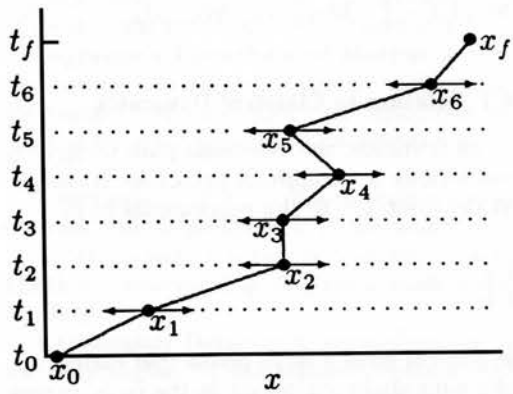

FIG. 5. A possible path for the Feynman integral with six intermediate states. Each of x_1 through x_6 varies independently over all possible values.

the Sturm–Liouville type. The theorem establishes that there is an infinite sequence of eigenvalues whose eigenfunctions have progressively more zeros between the boundary points, and hence progressively more oscillations.

Path Integral: The integral of a function $f(y(x))$ between given points in an xy plane (or its higher-dimensional generalizations) along a path specified by the function $y(x)$.

Perturbation Theory: A technique for the progressive approximation of more difficult problems involving the solution of differential equations (for example), starting from an exactly soluble simpler one. The difference between the two equations is called the perturbation term.

Principle of Least Action: A variational principle in classical dynamics, closely related to Hamilton's principle, which establishes a direct connection with Fermat's principle in geometrical optics.

Pseudostate: A member of a set of states obtained by diagonalization of the Hamiltonian matrix in a discrete variational basis set.

Quantum Electrodynamics: A quantized field theory describing the dynamical interactions of charged particles with electromagnetic fields.

Rayleigh–Ritz Variational Method: A method for the construction of an approximate wave function Ψ by expansion in a finite basis set of functions with expansion coefficients determined by the Rayleigh–Schrödinger variational principle.

Rayleigh–Schrödinger Variational Principle: A principle stating that the ratio $\langle\Psi|H|\Psi\rangle/\langle\Psi|\Psi\rangle$ is an upper bound to the lowest eigenvalue of H for any arbitrary (but normalizable) choice for the wave function Ψ.

Schrödinger Equation: A second-order partial differential wave equation that forms the basis of nonrelativistic quantum mechanics.

Sturmian Basis Set: The set of discrete eigenvalues and corresponding eigenfunctions obtained by solving a two-point eigenvalue problem of the Sturm–Liouville type.

Sturm–Liouville Problem: A class of second-order differential equations of the form $(d/dx)[K(x)dy/dx] - G(x)y = 0$, together with suitable boundary conditions.

Spectral Representation: A representation of the Green's function, or the terms in a perturbation series, in terms of explicit summations over the eigenvalue spectrum of the unperturbed problem.

Temple Bound: A method for constructing variational lower bounds to the energy based on the square of the Hamiltonian.

Variational Bound: An upper or lower bound on the energy or some other quantity obtained by means of a trial solution to the underlying differential equation, typically with parameters in the trial solution that can be adjusted to obtain the best possible solution.

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Further Reading

Techniques of the calculus of variations are covered in great detail by Courant and Hilbert (1966), and by Morse, P. M., and Feshbach, H. (1953), *Methods of Theoretical Physics,* New York: McGraw-Hill, along with most other books on the techniques of theoretical physics. The book by Yourgrau, W., and Mandelstam, S. (1968), *Variational Principles in Dynamics and Quantum Theory,* 3rd ed., Philadelphia: Saunders (Dover reprint 1979) provides an interesting and informative historical perspective.

Applications of variational principles to classical mechanics are covered in a very thorough, detailed, and readable manner by Goldstein, H. (1980), *Classical Mechanics,* 2nd ed., Reading, MA: Addison-Wesley. This book also contains a good pedagogical introduction to variational principles for continuous systems and fields. See also Lanczos, C. (1970), *The Variational Principles of Mechanics,* Toronto: University of Toronto Press (Dover reprint 1986).

The development of field theory from variational principles is covered in many recent books such as Ramond, P. (1981), *Field Theory, a Modern Primer,* Menlo Park, CA: Benjamin/Cummings; and Itzykson, C., and Zuber, J.-B. (1980), *Quantum Field Theory,* New York: McGraw-Hill. A good introduction to the Feynman path integral approach is given by Das, A. (1993), *Field Theory, a Path Integral Approach,* Singapore: World Scientific, and more detailed developments are contained in Rivers, R. J. (1987), *Path Integral Methods in Quantum Field Theory,* Cambridge, U.K.: Cambridge Univ. Press. The original development in Feynman, R. P., and Hibbs, A. R. (1965), *Quantum Mechanics and Path Integrals,* New York: McGraw-Hill, remains an authoritative source.

A wide variety of applications of variational principles in quantum-mechanical calculations can be found in numerous articles throughout Drake, G. W. F. (Ed.) (1996), *Atomic, Molecular, and Optical Physics Handbook,* New York: American Institute of Physics. In addition, the Kohn and Schwinger variational methods for scattering problems are covered in most books on scattering theory, such as Taylor, J. R. (1972), *Scattering Theory: The Quantum Theory on Nonrelativistic Collisions,* New York: Wiley. All of the above contain numerous other references to the literature and are intended only as a guide.