VARIATIONAL PRINCIPLES AND METHODS IN THEORETICAL PHYSICS AND CHEMISTRY

ROBERT K. NESBET IBM Almaden Research Center



PUBLISHED BY THE PRESS SYNDICATE OF THE UNIVERSITY OF CAMBRIDGE The Pitt Building, Trumpington Street, Cambridge, United Kingdom

CAMBRIDGE UNIVERSITY PRESS The Edinburgh Building, Cambridge CB2 2RU, UK 40 West 20th Street, New York, NY 10011-4211, USA 477 Williamstown Road, Port Melbourne, VIC 3207, Australia Ruiz de Alarcón 13, 28014 Madrid, Spain Dock House, The Waterfront, Cape Town 8001, South Africa

http://www.cambridge.org

© Robert K. Nesbet 2003

This book is in copyright. Subject to statutory exception and to the provisions of relevant collective licensing agreements, no reproduction of any part may take place without the written permission of Cambridge University Press.

First published 2003

Printed in the United Kingdom at the University Press, Cambridge

Typeface Times 11/14 pt System $LATEX 2_{\mathcal{E}}$ [TB]

A catalogue record for this book is available from the British Library

Library of Congress Cataloguing in Publication data

Nesbet, R. K.

Variational principles and methods in theoretical physics and chemistry/Robert K. Nesbet.

p. cm. Includes bibliographical references and index. ISBN 0 521 80391 8

1. Calculus of variations. 2. Mathematical physics. 3. Chemistry, Physical and theoretical–Mathematics. I. Title.

QC20.7.C3 N48 2003 530.15'564-dc21 2002067614

ISBN 0 521 80391 8 hardback

Contents

	Preface page				
Ι	Cla	ssical	mathema	atics and physics	1
	1	Histo	ry of vari	ational theory	3
		1.1	The pri	nciple of least time	4
		1.2	The var	iational calculus	5
			1.2.1	Elementary examples	7
		1.3	The pri	nciple of least action	8
	2	Class	ical mecl	nanics	11
		2.1	Lagrang	gian formalism	11
			2.1.1	Hamilton's variational principle	12
			2.1.2	Dissipative forces	12
			2.1.3	Lagrange multiplier method for constraints	13
		2.2	Hamilto	onian formalism	14
			2.2.1	The Legendre transformation	14
			2.2.2	Transformation from Lagrangian to Hamiltonian	15
			2.2.3	Example: the central force problem	16
		2.3	Conser	vation laws	17
		2.4	Jacobi's principle		
		2.5	Special	relativity	20
			2.5.1	Relativistic mechanics of a particle	21
			2.5.2	Relativistic motion in an electromagnetic field	22
	3	Appli	ed mathe	ematics	25
		3.1	Linear	systems	25
		3.2	Simple	x interpolation	26
			3.2.1	Extremum in <i>n</i> dimensions	27
		3.3	Iterative	e update of the Hessian matrix	28
			3.3.1	The BFGS algorithm	29
		3.4	Geome	try optimization for molecules	30

viii	Contents				
		3.4.1	The GDIIS algorithm	31	
		3.4.2	The BERNY algorithm	31	
II	Bound sta	tes in qu	antum mechanics	33	
	4 Time	-independ	dent quantum mechanics	35	
	4.1	Variatio	onal theory of the Schrödinger equation	36	
		4.1.1	Sturm–Liouville theory	36	
		4.1.2	Idiosyncracies of the Schrödinger equation	38	
		4.1.3	Variational principles for the Schrödinger equation	40	
		4.1.4	Basis set expansions	41	
	4.2	Hellma	nn–Feynman and virial theorems	43	
		4.2.1	Generalized Hellmann–Feynman theorem	43	
		4.2.2	The hypervirial theorem	43	
		4.2.3	The virial theorem	44	
	4.3	The N-	electron problem	45	
		4.3.1	The N-electron Hamiltonian	45	
		4.3.2	Expansion in a basis of orbital wave functions	46	
		4.3.3	The interelectronic Coulomb cusp condition	48	
	4.4	Symme	try-adapted functions	49	
		4.4.1	Algorithm for constructing symmetry-adapted		
			functions	50	
		4.4.2	Example of the method	51	
	5 Indep	endent-e	lectron models	53	
	5.1	N-elect	ron formalism using a reference state	54	
		5.1.1	Fractional occupation numbers	55	
		5.1.2	Janak's theorem	56	
	5.2	Orbital	functional theory	57	
		5.2.1	Explicit components of the energy functional	57	
		5.2.2	Orbital Euler–Lagrange equations	58	
		5.2.3	Exact correlation energy	59	
	5.3	Hartree	–Fock theory	61	
		5.3.1	Closed shells – unrestricted Hartree–Fock (UHF)	61	
		5.3.2	Brillouin's theorem	62	
		5.3.3	Open-shell Hartree–Fock theory (RHF)	62	
		5.3.4	Algebraic Hartree–Fock: finite basis expansions	64	
		5.3.5	Multiconfiguration SCF (MCSCF)	64	
	5.4	The opt	imized effective potential (OEP)	65	
	- -	5.4.1	Variational formulation of OEP	67	
	5.5	Density	tunctional theory (DFT)	68	
		5.5.1	The Hohenberg–Kohn theorems	68	
		5.5.2	Kohn–Sham equations	70	

II

			Contents	ix
		5.5.3	Functional derivatives and local potentials	71
		5.5.4	Thomas–Fermi theory	72
		5.5.5	The Kohn–Sham construction	74
6	Time	-depende	nt theory and linear response	77
	6.1	The tim	ne-dependent Schrödinger equation for one electron	78
	6.2	The ind	lependent-electron model as a quantum field theory	79
	6.3	Time-d	ependent Hartree–Fock (TDHF) theory	81
		6.3.1	Operator form of Hartree–Fock equations	81
		6.3.2	The screening response	81
	6.4	Time-d	ependent orbital functional theory (TOFT)	83
		6.4.1	Remarks on time-dependent theory	83
		6.4.2	Exact linear response theory	84
		6.4.3	Definition of the response kernel	84
	6.5	Reconc	iliation of <i>N</i> -electron theory and orbital models	85
	6.6	Time-d	ependent density functional theory (TDFT)	86
~	6.7	Excitati	ion energies and energy gaps	89
Cor	tinuu	m states	and scattering theory	91
7 Multiple scattering theory for molecules and solids				
	7.1	Full-po	tential multiple scattering theory	95
		7.1.1	Definitions	96
		7.1.2	Two-center expansion	96
		7.1.3	Angular momentum representation	97
		7.1.4	I he surface matching theorem	99 100
		7.1.5	Surface integral formalism Muffin tin orbitals and atomic call orbitals	100
		7.1.0	Tail concellation and the clobal matching function	101
		7.1.7	Implementation of the theory	102
	7 2	Variatio	and principles	103
	1.2	721	Kohn_Rostoker variational principle	104
		7.2.1	Convergence of internal sums	104
		723	Schlosser–Marcus variational principle	108
		7.2.3	Elimination of false solutions	111
	7.3	Energy	-linearized methods	113
		7.3.1	The LMTO method	113
		7.3.2	The LACO method	115
		7.3.3	Variational theory of linearized methods	116
	7.4	The Po	isson equation	118
	7.5	Green f	functions	120
		7.5.1	Definitions	121
		7.5.2	Properties of the Green function	124

III

Contents

			7.5.3	Construction of the Green function	125
	8	Varia	tional me	ethods for continuum states	129
		8.1	Scatteri	ng by an N-electron target system	129
			8.1.1	Cross sections	132
			8.1.2	Close-coupling expansion	133
		8.2	Kohn v	ariational theory	134
			8.2.1	The matrix variational method	135
			8.2.2	The Hulthén–Kohn variational principle	137
			8.2.3	The complex Kohn method	139
		8.3	Schwin	ger variational theory	140
			8.3.1	Multichannel Schwinger theory	143
			8.3.2	Orthogonalization and transfer invariance	145
		8.4	Variatio	onal <i>R</i> -matrix theory	147
			8.4.1	Variational theory of the \mathcal{R} -operator	154
			8.4.2	The \mathcal{R} -operator in generalized geometry	156
			8.4.3	Orbital functional theory of the <i>R</i> -matrix	157
	9	Elect	ron-impa	ct rovibrational excitation of molecules	161
		9.1	The loc	al complex-potential (LCP) model	163
			9.1.1	The projection-operator method	164
		9.2	Adiaba	tic approximations	166
			9.2.1	The energy-modified adiabatic	
				approximation (EMA)	168
		9.3	Vibroni	c R-matrix theory	169
			9.3.1	Phase-matrix theory	172
			9.3.2	Separation of the phase matrix	173
			9.3.3	Phase-matrix formalism: EMAP	174
			9.3.4	Nonadiabatic theory: NADP	175
IV	Fiel	ld theo	ries		179
	10	Relati	ivistic La	grangian theories	181
		10.1	Classic	al relativistic electrodynamics	182
			10.1.1	Classical dynamical mass	184
			10.1.2	Classical renormalization and the Dirac equation	185
		10.2	Symme	try and Noether's theorem	186
			10.2.1	Examples of conservation laws	187
		10.3	Gauge	invariance	189
			10.3.1	Classical electrodynamics as a gauge theory	190
			10.3.2	Noether's theorem for gauge symmetry	191
			10.3.3	Nonabelian gauge symmetries	192
			10.3.4	Gauge invariance of the $SU(2)$ field theory	195

		Contents	xi
10.4	Energy	and momentum of the coupled fields	197
	10.4.1	Energy and momentum in classical	
		electrodynamics	197
	10.4.2	Energy and momentum in $SU(2)$ gauge theory	199
10.5	The Sta	ndard Model	201
	10.5.1	Electroweak theory (EWT)	202
	10.5.2	Quantum chromodynamics (QCD)	203
eferences	and bib	liography	205
ndex			225

History of variational theory

The principal references for this chapter are:

- [5] Akhiezer, N.I. (1962). The Calculus of Variations (Blaisdell, New York).
- [26] Blanchard, P. and Brüning, E. (1992). Variational Methods in Mathematical Physics (Springer-Verlag, Berlin).
- [78] Dieudonné, J. (1981). History of Functional Analysis (North-Holland, Amsterdam).
- [147] Goldstine, H.H. (1980). A History of the Calculus of Variations from the 17th through the 19th Century (Springer-Verlag, Berlin).
- [210] Lanczos, C. (1966). Variational Principles of Mechanics (University of Toronto Press, Toronto).
- [322] Pars, L.A. (1962). An Introduction to the Calculus of Variations (Wiley, New York).
- [436] Yourgrau, W. and Mandelstam, S. (1968). *Variational Principles in Dynamics and Quantum Theory*, 3rd edition (Dover, New York).

The idea that laws of nature should satisfy a principle of simplicity goes back at least to the Greek philosophers [436]. The anthropomorphic concept that the engineering skill of a supreme creator should result in rules of least effort or of most efficient use of resources leads directly to principles characterized by mathematical extrema. For example, Aristotle (*De Caelo*) concluded that planetary orbits must be perfect circles, because geometrical perfection is embodied in these curves: "... of lines that return upon themselves the line which bounds the circle is the shortest. That movement is swiftest which follows the shortest line". Hero of Alexandria (*Catoptrics*) proved perhaps the first scientific minimum principle, showing that the path of a reflected ray of light is shortest if the angles of incidence and reflection are equal.

The superiority of circular planetary orbits became almost a religious dogma in the Christian era, intimately tied to the idea of the perfection of God and of His creations. It was replaced by modern celestial mechanics only after centuries in which the concept of esthetic perfection of the universe was gradually superseded by a concept of esthetic perfection of a mathematical theory that could account for the actual behavior of this universe as measured in astronomical observations. Aspects of value-oriented esthetics lay behind Occam's logical "razor" (avoid unnecessary hypotheses), anticipating the later development of observational science and the search for an explanatory theory that was both as general as possible and as simple as possible. The path from Aristotle to Copernicus, Brahe, Kepler, Galileo, and Newton retraces this shift from *a priori* purity of concepts to mathematical theory solidly based on empirical science. The resulting theory of classical mechanics retains extremal principles that are the basis of the variational theory presented here in Chapter 2.

Variational principles have turned out to be of great practical use in modern theory. They often provide a compact and general statement of theory, invariant or covariant under transformations of coordinates or functions, and can be used to formulate internally consistent computational algorithms. Symmetry properties are often most easily derived in a variational formalism.

1.1 The principle of least time

The law of geometrical optics anticipated by Hero of Alexandria was formulated by Fermat (1601–1655) as a principle of least time, consistent with Snell's law of refraction (1621). The time for phase transmission from point P to point Q along a path $\mathbf{x}(t)$ is given by

$$T = \int_{P}^{Q} \frac{ds}{v(s)},\tag{1.1}$$

where ds is a path element, and v is the phase velocity. Fermat's principle is that the value of the integral T should be stationary with respect to any infinitesimal deviation of the path $\mathbf{x}(t)$ from its physical value. This is valid for geometrical optics as a limiting case of wave optics. The mathematical statement is that $\delta T = 0$ for all variations induced by displacements $\delta \mathbf{x}(t)$. In this and subsequent variational formulas, differentials defined by the notation $\delta \cdots$ are small increments evaluated in the limit that quadratic infinitesimals can be neglected. Thus for sufficiently small displacements $\delta \mathbf{x}(t)$, the integral T varies quadratically about its physical value. For planar reflection consider a ray path from P : (-d, -h) to the observation point Q : (-d, h) via an intermediate point (0, y) in the reflection plane x = 0. Elapsed time in a uniform medium is

$$T(y) = \left\{ \sqrt{d^2 + (h+y)^2} + \sqrt{d^2 + (h-y)^2} \right\} / v,$$
(1.2)

to be minimized with respect to displacements in the reflection plane parametrized

by y. The angle of incidence θ_i is defined such that

$$\sin \theta_i = \frac{h+y}{\sqrt{d^2 + (h+y)^2}}$$

and the angle of reflection θ_r is defined by

$$\sin \theta_r = \frac{h - y}{\sqrt{d^2 + (h - y)^2}}$$

The law of planar reflection, $\sin \theta_i = \sin \theta_r$, follows immediately from

$$\frac{\partial T}{\partial y} = (\sin \theta_i - \sin \theta_r)/v = 0.$$

To derive Snell's law of refraction, consider the ray path from point P : (-d, -h) to Q : (d, h) via point (0, y) in a plane that separates media of phase velocity v_i (x < 0) and v_r (x > 0). The elapsed time is

$$T(y) = v_i^{-1} \sqrt{d^2 + (h+y)^2} + v_r^{-1} \sqrt{d^2 + (h-y)^2}.$$
 (1.3)

The variational condition is

$$\frac{\partial T}{\partial y} = \sin \theta_i / v_i - \sin \theta_r / v_r = 0.$$

This determines parameter y such that

$$\frac{\sin \theta_i}{\sin \theta_r} = \frac{v_i}{v_r},\tag{1.4}$$

giving Snell's law for uniform refractive media.

1.2 The variational calculus

Derivation of a ray path for the geometrical optics of an inhomogeneous medium, given $v(\mathbf{r})$ as a function of position, requires a development of mathematics beyond the calculus of Newton and Leibniz. The elapsed time becomes a functional $T[\mathbf{x}(t)]$ of the path $\mathbf{x}(t)$, which is to be determined so that $\delta T = 0$ for variations $\delta \mathbf{x}(t)$ with fixed end-points: $\delta \mathbf{x}_P = \delta \mathbf{x}_Q = 0$. Problems of this kind are considered in the calculus of variations [5, 322], proposed originally by Johann Bernoulli (1696), and extended to a full mathematical theory by Euler (1744). In its simplest form, the concept of the variation $\delta \mathbf{x}(t)$ reduces to consideration of a modified function $\mathbf{x}_{\epsilon}(t) = \mathbf{x}(t) + \epsilon \mathbf{w}(t)$ in the limit $\epsilon \to 0$. The function $\mathbf{w}(t)$ must satisfy conditions of continuity that are compatible with those of $\mathbf{x}(t)$. Then $\delta \mathbf{x}(t) = \mathbf{w}(t) d\epsilon$ and the variation of the derivative function is $\delta \mathbf{x}'(t) = \mathbf{w}'(t) d\epsilon$.

1 History of variational theory

The problem posed by Bernoulli is that of the brachistochrone. If two points are connected by a wire whose shape is given by an unknown function y(x) in a vertical plane, what shape function minimizes the time of descent of a bead sliding without friction from the higher to the lower point? The mass of a bead moving under gravity is not relevant. It can easily be verified by trial and error that a straight line does not give the minimum time of passage. Always in such problems, conditions appropriate to physically meaningful solution functions must be specified. Although this is a vital issue in any mathematically rigorous variational calculus, such conditions will be stated as simply as possible here, strongly dependent on each particular application of the theory. Clearly the assumed wire in the brachistochrone problem must have the physical properties of a wire. This requires y(x) to be continuous, but does not exclude a vertical drop. Since no physical wire can have an exact discontinuity of slope, it is reasonable to require velocity of motion along the wire to be conserved at any such discontinuity, so that the hypothetical sliding bead does not come to an abrupt stop or bounce with undetermined loss of momentum. It can easily be verified that a vertical drop followed by a horizontal return to the smooth brachistochrone curve always increases the time of passage. Thus such deviations from continuity of the derivative function do not affect the optimal solution.

The calculus of variations [5, 322] is concerned with problems in which a function is determined by a stationary variational principle. In its simplest form, the problem is to find a function y(x) with specified values at end-points x_0, x_1 such that the integral $J = \int_{x_0}^{x_1} f(x, y, y') dx$ is stationary. The variational solution is derived from

$$\delta J = \int \left\{ \delta y \frac{\partial f}{\partial y} + \delta y' \frac{\partial f}{\partial y'} \right\} dx = 0$$

after integrating by parts to eliminate $\delta y'(x)$. Because

$$\int \delta y' \frac{\partial f}{\partial y'} dx = \delta y \left. \frac{\partial f}{\partial y'} \right|_{x_0}^{x_1} - \int \delta y \frac{d}{dx} \frac{\partial f}{\partial y'} dx,$$

 $\delta J = 0$ for fixed end-points $\delta y(x_0) = \delta y(x_1) = 0$ if

$$\frac{\partial f}{\partial y} - \frac{d}{dx} \frac{\partial f}{\partial y'} = 0.$$
(1.5)

This is a simple example of the general form of Euler's equation (1744), derived directly from a variational expression.

Blanchard and Brüning [26] bring the history of the calculus of variations into the twentieth century, as the source of contemporary developments in pure mathematics. A search for existence and uniqueness theorems for variational problems engendered deep studies of the continuity and compactness of mathematical entities that generalize the simple intuitive definitions assumed by Euler and Lagrange. The seemingly self-evident statement that, for free variations of the function y(x),

$$\int \left(\frac{\partial f}{\partial y} - \frac{d}{dx}\frac{\partial f}{\partial y'}\right)\delta y dx = 0$$

implies Euler's equation, was first proven rigorously by Du Bois-Reymond in 1879. With carefully stated conditions on the functions f and y, this made it possible to prove the fundamental theorem of the variational calculus [26], on the existence of extremal solutions of variational problems.

1.2.1 Elementary examples

A geodesic problem requires derivation of the shortest path connecting two points in some system for which distance is defined, subject to constraints that can be either geometrical or physical in nature. The shortest path between two points in a plane follows from this theory. The problem is to minimize

$$J = \int_{x_0}^{x_1} f(x, y, y') dx = \int_{x_0}^{x_1} dx \sqrt{1 + \left(\frac{dy}{dx}\right)^2},$$

where

$$\frac{\partial f}{\partial x} = 0, \quad \frac{\partial f}{\partial y} = 0, \quad \frac{\partial f}{\partial y'} = \frac{y'}{\sqrt{1 + y'^2}}$$

In this example, Euler's equation takes the form of the geodesic equation

$$\frac{d}{dx}\frac{y'}{\sqrt{1+{y'}^2}}=0.$$

The solution is y' = const, or

$$y(x) = y_0 \frac{x_1 - x}{x_1 - x_0} + y_1 \frac{x - x_0}{x_1 - x_0},$$

a straight line through the points x_0 , y_0 and x_1 , y_1 .

In Johann Bernoulli's problem, the brachistochrone, it is required to find the shape of a wire such that a bead slides from point 0, 0 to x_1 , y_1 in the shortest time T under the force of gravity. The energy equation $\frac{1}{2}mv^2 = -mgy$ implies $v = \sqrt{-2gy}$, so that

$$T = \int_0^{x_1} \frac{ds}{v} = \int_0^{x_1} f(y, y') \, dx,$$

where $f(y, y') = \sqrt{-(1 + y'^2)/2gy}$. Because $\partial f/\partial x = 0$, the identity

$$\frac{d}{dx}\left(y'\frac{\partial f}{\partial y'}-f\right)=y'\left(\frac{d}{dx}\frac{\partial f}{\partial y'}-\frac{\partial f}{\partial y}\right),$$

and the Euler equation imply an integral of motion,

$$y'\frac{\partial f}{\partial y'} - f = \frac{-1}{\sqrt{-2gy(1+y'^2)}} = const.$$

On combining constants into the single parameter *a* this implies

$$1 + \left(\frac{dy}{dx}\right)^2 = \frac{-2a}{y}.$$

The solution for a bead starting from rest at the coordinate origin is a cycloid, determined by the parametric equations $x = a(\phi - \sin \phi)$ and $y = a(\cos \phi - 1)$. This curve is generated by a point on the perimeter of a circle of radius *a* that rolls below the *x*-axis without slipping. The lowest point occurs for $\phi = \pi$, with $x_1 = \pi a$ and $y_1 = -2a$. By adding a constant ϕ_0 to ϕ , *a* can be adjusted so that the curve passes through given points x_0 , y_0 and x_1 , y_1 .

1.3 The principle of least action

Variational principles for classical mechanics originated in modern times with the principle of least action, formulated first imprecisely by Maupertuis and then as an example of the new calculus of variations by Euler (1744) [436]. Although not stated explicitly by either Maupertuis or Euler, stationary action is valid only for motion in which energy is conserved. With this proviso, in modern notation for generalized coordinates,

$$\delta \int_{P}^{Q} \mathbf{p} \cdot d\mathbf{q} = 0, \qquad (1.6)$$

for a path from system point P to system point Q.

For a particle of mass *m* moving in the (x, y) plane with force per mass (X, Y), instantaneous motion is described by velocity *v* along the trajectory. An instantaneous radius of curvature ρ is defined by angular momentum $\ell = mv\rho$ such that the centrifugal force mv^2/ρ balances the true force normal to the trajectory. Hence, following Euler's derivation, Newtonian mechanics implies that

$$\frac{v^2}{\rho} = \frac{Ydx - Xdy}{\sqrt{dx^2 + dy^2}}$$

along the trajectory. The principle of least action requires the action integral

per unit mass

$$\int v \, ds = \int v \, dx \sqrt{1 + \left(\frac{dy}{dx}\right)^2}$$

to be stationary. The variation of v along the trajectory is determined for fixed energy E = T + V by

$$v dv = -\frac{1}{m} \left(\frac{\partial V}{\partial x} dx + \frac{\partial V}{\partial y} dy \right) = X dx + Y dy.$$

Thus $v \frac{\partial v}{\partial x} = X$ and $v \frac{\partial v}{\partial y} = Y$. Euler's equation then takes the form

$$\frac{d}{dx}\left(\frac{vy'}{\sqrt{1+y'^2}}\right) - \frac{Y}{v}\sqrt{1+y'^2} = 0,$$

where y' = dy/dx. The local curvature of a trajectory is defined by

$$\frac{1}{\rho} = \frac{d}{dx} \left[y'/(1+y'^2)^{\frac{1}{2}} \right] = y''/(1+y'^2)^{\frac{3}{2}}.$$

Using this formula and $\frac{dv}{dx} = \frac{X + Yy'}{v}$, Euler's equation implies

$$\frac{v}{\rho} + \frac{(X + Yy')y'}{v\sqrt{1 + {y'}^2}} - \frac{Y}{v}\sqrt{1 + {y'}^2} = 0.$$

This reproduces the formula derived directly from Newtonian mechanics:

$$\frac{v^2}{\rho} = \frac{Y - Xy'}{\sqrt{1 + y'^2}} = \frac{Ydx - Xdy}{\sqrt{dx^2 + dy^2}}.$$

Euler's proof of the least action principle for a single particle (mass point in motion) was extended by Lagrange (c. 1760) to the general case of mutually interacting particles, appropriate to celestial mechanics. In Lagrange's derivation [436], action along a system path from initial coordinates P to final coordinates Q is defined by

$$A = \sum_{a} m_a \int_{P}^{Q} v_a ds_a = \sum_{a} m_a \int_{P}^{Q} \dot{\mathbf{x}}_a \cdot d\mathbf{x}_a.$$
(1.7)

Variations about a true dynamical path are defined by coordinate displacements $\delta \mathbf{x}_a$. Velocity displacements $\delta \dot{\mathbf{x}}_a$ are constrained so as to maintain invariant total energy. This implies modified time values at the displaced points [146]. The energy constraint condition is

$$\delta E = \sum_{a} \left(m_a \dot{\mathbf{x}}_a \cdot \delta \dot{\mathbf{x}}_a + \frac{\partial V}{\partial \mathbf{x}_a} \cdot \delta \mathbf{x}_a \right) = 0.$$

The induced variation of action is

$$\begin{split} \delta A &= \sum_{a} m_{a} \int_{P}^{Q} (\dot{\mathbf{x}}_{a} \cdot d\delta \mathbf{x}_{a} + \delta \dot{\mathbf{x}}_{a} \cdot d\mathbf{x}_{a}) \\ &= \sum_{a} m_{a} \dot{\mathbf{x}}_{a} \cdot \delta \mathbf{x}_{a} |_{P}^{Q} - \sum_{a} m_{a} \int_{P}^{Q} (d\dot{\mathbf{x}}_{a} \cdot \delta \mathbf{x}_{a} - \dot{\mathbf{x}}_{a} dt \cdot \delta \dot{\mathbf{x}}_{a}), \end{split}$$

on integrating by parts and using $d\mathbf{x}_a = \dot{\mathbf{x}}_a dt$. The final term here can be replaced, using the energy constraint condition. Then, using $d\dot{\mathbf{x}}_a = \ddot{\mathbf{x}}_a dt$,

$$\delta A = \sum_{a} m_{a} \dot{\mathbf{x}}_{a} \cdot \delta \mathbf{x}_{a} |_{P}^{Q} - \sum_{a} \int_{P}^{Q} \left(m_{a} \ddot{\mathbf{x}}_{a} + \frac{\partial V}{\partial \mathbf{x}_{a}} \right) \cdot \delta \mathbf{x}_{a} dt.$$

If the end-points are fixed, the integrated term vanishes, and *A* is stationary if and only if the final integral vanishes. Since $\delta \mathbf{x}_a$ is arbitrary, the integrand must vanish, which is Newton's law of motion. Hence Lagrange's derivation proves that the principle of least action is equivalent to Newtonian mechanics if energy is conserved and end-point coordinates are specified.