BRILLOUIN–WIGNER METHODS FOR MANY-BODY SYSTEMS
Progress in Theoretical Chemistry and Physics

VOLUME 21

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Brillouin–Wigner Methods for Many-Body Systems

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PROGRESS IN THEORETICAL CHEMISTRY
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A series reporting advances in theoretical molecular and material sciences, including theoretical, mathematical and computational chemistry, physical chemistry and chemical physics

Aim and Scope

Science progresses by a symbiotic interaction between theory and experiment: theory is used to interpret experimental results and may suggest new experiments; experiment helps to test theoretical predictions and may lead to improved theories. Theoretical Chemistry (including Physical Chemistry and Chemical Physics) provides the conceptual and technical background and apparatus for the rationalisation of phenomena in the chemical sciences. It is, therefore, a wide ranging subject, reflecting the diversity of molecular and related species and processes arising in chemical systems. The book series *Progress in Theoretical Chemistry and Physics* aims to report advances in methods and applications in this extended domain. It will comprise monographs as well as collections of papers on particular themes, which may arise from proceedings of symposia or invited papers on specific topics as well as initiatives from authors or translations.

The basic theories of physics – classical mechanics and electromagnetism, relativity theory, quantum mechanics, statistical mechanics, quantum electrodynamics – support the theoretical apparatus which is used in molecular sciences. Quantum mechanics plays a particular role in theoretical chemistry, providing the basis for the spectroscopic models employed in the determination of structural information from spectral patterns. Indeed, Quantum Chemistry often appears synonymous with Theoretical Chemistry: it will, therefore, constitute a major part of this book series. However, the scope of the series will also include other areas of theoretical chemistry, such as mathematical chemistry (which involves the use of algebra and topology in the analysis of molecular structures and reactions); molecular mechanics, molecular dynamics and chemical thermodynamics, which play an important role in rationalizing the geometric and electronic structures of molecular assemblies and polymers,
clusters and crystals; surface, interface, solvent and solid-state effects; excited-state
dynamics, reactive collisions, and chemical reactions.

Recent decades have seen the emergence of a novel approach to scientific research,
based on the exploitation of fast electronic digital computers. Computation provides
a method of investigation which transcends the traditional division between theory
and experiment. Computer-assisted simulation and design may afford a solution to
complex problems which would otherwise be intractable to theoretical analysis, and
may also provide a viable alternative to difficult or costly laboratory experiments.
Though stemming from Theoretical Chemistry, Computational Chemistry is a field
of research in its own right, which can help to test theoretical predictions and may
also suggest improved theories.

The field of theoretical molecular sciences ranges from fundamental physical ques-
tions relevant to the molecular concept, through the statics and dynamics of isolated
molecules, aggregates and materials, molecular properties and interactions, and the
role of molecules in the biological sciences. Therefore, it involves the physical basis
for geometric and electronic structure, states of aggregation, physical and chemical
transformation, thermodynamic and kinetic properties, as well as unusual properties
such as extreme flexibility or strong relativistic or quantum-field effects, extreme
conditions such as intense radiation fields or interaction with the continuum, and the
specificity of biochemical reactions.

Theoretical chemistry has an applied branch – a part of molecular engineering,
which involves the investigation of structure–property relationships aiming at the
design, synthesis and application of molecules and materials endowed with spe-
cific functions, now in demand in such areas as molecular electronics, drug design
or genetic engineering. Relevant properties include conductivity (normal, semi- and
supra-), magnetism (ferro- or ferri-), optoelectronic effects (involving nonlinear
response), photochromism and photoreactivity, radiation and thermal resistance,
molecular recognition and information processing, and biological and pharmaceutical
activities; as well as properties favouring self-assembling mechanisms, and combina-
tion properties needed in multifunctional systems.

Progress in Theoretical Chemistry and Physics is made at different rates in these
various research fields. The aim of this book series is to provide timely and in-depth
coverage of selected topics and broad-ranging yet detailed analysis of contemporary
theories and their applications. The series will be of primary interest to those whose
research is directly concerned with the development and application of theoretical
approaches in the chemical sciences. It will provide up-to-date reports on theoretical
methods for the chemist, thermodynamician or spectroscopist, the atomic, molec-
ular or cluster physicist, and the biochemist or molecular biologist who wishes to
employ techniques developed in theoretical, mathematical or computational chem-
istry in their research programmes. It is also intended to provide the graduate student
with a readily accessible documentation on various branches of theoretical chemistry,
physical chemistry and chemical physics.
This book is dedicated
to the late J. Mášik
and to our children,
Michelle, Jonathan & James,
& grandchildren,
Nathael & Kierann.
The purpose of this book is to provide a detailed description of Brillouin–Wigner methods and their application to the many-body problem in atomic and molecular physics and quantum chemistry. Recently there has been a renewal of interest in Brillouin–Wigner methods. This interest is fuelled by the need to develop robust, yet efficient multireference theoretical approaches to the electron correlation problem in molecules together with associated algorithms. Such theories are an essential ingredient of the quantum mechanical description of most dissociative processes in molecules, of excited states, and of ionization and electron attachment processes.

This volume contains a concise, systematic and self-contained account of the Brillouin–Wigner methods. Chapter 1 is introductory giving the historical background to the Brillouin–Wigner methods and their application to atomic and molecular structure. Chapter 2 uses the partitioning technique to develop both single reference and multireference Brillouin–Wigner methods in a systematic fashion. The corresponding Rayleigh–Schrödinger expansions are also considered since it has been known for many years that they form the basis of a valid many-body theory (in the post-Brueckner sense). The many-body problem in atoms and molecules is discussed in Chapter 3. The properties of a valid many-body theory are elaborated and common approaches to the electron correlation problem are considered in some detail. The linked diagram theorem of many-body perturbation theory is described and the perturbative approach to the correlation problem considered alongside the configuration interaction and cluster expansion ansatz.

In Chapter 4, the application of Brillouin–Wigner methods to many-body systems is described in some detail. This chapter deals with the central purpose of this monograph – the development of many-body Brillouin–Wigner methods in particular for applications to the problem of describing molecular electronic structure using ab initio methods – methods which start from first principles and can be systematically refined. (Semi-empirical methods and density functional theory, which in practice involves parametrization, will not be considered.) The application of Brillouin–Wigner theory to the configuration interaction and cluster expansion techniques is described as well as perturbation theory based methods. The use of Brillouin–Wigner
methods in obtaining many-body corrections to theoretical approaches which are not valid many-body theories, such as limited configuration interaction, is addressed. Finally, Chapter 5 contains a summary and considers the prospects for future progress in the application of Brillouin–Wigner methods to the correlation problem in atoms and molecules and elsewhere.

A number of colleagues have participated in the development of many-body Brillouin–Wigner methods over recent years. Without their dedicated efforts this work would not have been possible. We single out the late J. Mášik who contributed substantially to the recent development of Brillouin–Wigner methods in electronic structure theory before his untimely death at the age of only 33. We would also like to mention (in alphabetical order): P. Babinec, P. Čársky, P. Mach, P. Neogrády, P. Papp, J. Pittner, M. Polášek, H.M. Quiney and J. Urban. We are most grateful for their enthusiasm and their friendship.

We are grateful to our wives for their encouragement and support during the writing of this book, without which this book would not have been completed. We thank Mr Radovan Javorčík, Chargé d’Affaires at the Embassy of the Slovak Republic, for facilitating many of our meetings in London. We thank Mrs Kathryn Wilson who undertook the labour of reading the whole book and corrected many careless slips and helped us with points of style. Nevertheless any errors in the present volume are ours alone and we would be grateful to any reader who takes the trouble to write to us on such matters. We have established a webpage at

quantumsystems.googlepages.com/brillouin–wigner

where we can both collect errors in the present volume and details of further developments in Brillouin–Wigner many-body theory.


IH acknowledges support from the VEGA Grant agency, Slovakia, under project number 1/3040/06 and support by the Grant Agency of the Czech Republic under project number MSM 4781305903. SW is a senior academic visitor in the Physical and Theoretical Chemistry Laboratory, University of Oxford, and is grateful to the hospitality extended to him there.

Bratislava and Oxford,  
July, 2009  

Ivan Hubač  
Stephen Wilson
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We present a summary of the nomenclature employed in this volume.

\( \mathcal{H} \)  hamiltonian operator
\( \mathcal{H}_0 \)  zero order hamiltonian operator
\( \mathcal{H}_1 \)  perturbation operator
\( \Psi \)  exact wave function
\( \Psi_0 \)  exact ground state wave function
\( \Psi_\alpha \)  exact wave function for the state \( \alpha \)
\( \mathcal{E} \)  exact energy
\( \mathcal{E}_0 \)  exact ground state energy
\( \mathcal{E}_\alpha \)  exact energy for state \( \alpha \)
\( \Phi \)  zero order wave function
\( \Phi_0 \)  zero order ground state wave function
\( \Phi_\alpha \)  zero order wave function for state \( \alpha \)
\( \Phi_m \)  model space
\( \Psi_\alpha^p \)  model function
\( \mathcal{E} \)  energy of the reference system
\( \mathcal{E}_0 \)  ground state energy of the reference system
\( \mathcal{E}_\alpha \)  energy of the state \( \alpha \) of the reference system
\( \lambda \)  perturbation parameter
\( \mathcal{E}_0^{(p)} \)  pth order energy coefficient for the ground state
\( \mathcal{E}_\alpha^{(p)} \)  pth order energy coefficient for the state \( \alpha \)
\( \Omega \)  wave operator
\( \Omega_0 \)  wave operator for the ground state
\( \Omega_\alpha \)  wave operator for the state \( \alpha \)
\( \mathcal{V} \)  reaction operator
Nomenclature

$V_0$ reaction operator for the ground state
$V_\alpha$ reaction operator for the state $\alpha$
$\chi_p$ basis function
$\chi^{(p)}_0$ $p$th order wave function for the ground state
$\chi^{(p)}_\alpha$ $p$th order wave function for the state $\alpha$
$\mathcal{G}$ general resolvent
$\mathcal{R}$ resolvent for Rayleigh–Schrödinger theory
$\mathcal{R}_0$ resolvent for Rayleigh–Schrödinger theory
$\mathcal{B}$ resolvent for Brillouin–Wigner theory
$\mathcal{B}_0$ resolvent for Brillouin–Wigner theory
$\mathcal{B}_\alpha$ resolvent for Brillouin–Wigner theory
$\mathcal{B}_g$ resolvent for generalized Brillouin–Wigner theory
$\mathcal{P}$ reference or model space
$\mathcal{Q}$ orthogonal or complementary space
$P$ projector onto the reference space $\mathcal{P}$
$Q$ projector onto the orthogonal or complementary space $\mathcal{Q}$
$\mathcal{H}_{\text{effective}}$ effective hamiltonian operator
$X^+_i$ creation operator in the particle formalism
$X_i$ annihilation operator in the particle formalism
$\delta_{pq}$ Kronecker delta
$[A, B]$ commutator $AB - BA$
$[A, B]_+$ anticommutator $AB + BA$
n$[...]$ normal product in the particle formalism
$Y^+_i$ creation operator in the particle–hole formalism
$Y_i$ annihilation operator in the particle–hole formalism
$N[...]$ normal product in the particle–hole formalism
$T$ cluster operator
$T_1$ single excitation cluster operator
$T_2$ single excitation cluster operator
$T_3$ triple excitation cluster operator
$T_4$ quadruple excitation cluster operator
$T_p$ p-fold excitation cluster operator
ABBREVIATIONS

We present here a definition of the abbreviations used in this volume.

CI  configuration interaction
BW  Brillouin–Wigner
RS  Rayleigh–Schrödinger
CC  coupled cluster
PT  perturbation theory
MR  multi-reference
FCI  full configuration interaction
CISD  single-reference configuration interaction with single and double replacements
MR-CI  multi-reference configuration interaction
BWPT  Brillouin–Wigner perturbation theory
RSPT  Rayleigh–Schrödinger perturbation theory
MBPT  many-body perturbation theory
MPPT  Møller–Plesset perturbation theory
MR-BWPT  multi-reference Brillouin–Wigner perturbation theory
MR-RSPT  multi-reference Rayleigh–Schrödinger perturbation theory
MR-MBPT  multi-reference many-body perturbation theory
MR-MPPT  multi-reference Møller–Plesset perturbation theory
CCSD  single-reference coupled cluster with single and double replacements
CCSD(T)  single-reference coupled cluster with single and double replacements plus a perturbative estimate of the triple replacement component
<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>CCSDT</td>
<td>single-reference coupled cluster with single, double and triple replacements</td>
</tr>
<tr>
<td>MR-CCSD</td>
<td>multi-reference coupled cluster with single and double replacements</td>
</tr>
<tr>
<td>MR-CCSD(T)</td>
<td>multi-reference coupled cluster with single and double replacements plus a perturbative estimate of the triple replacement component</td>
</tr>
<tr>
<td>MR-CCSDT</td>
<td>multi-reference coupled cluster with single, double and triple replacements</td>
</tr>
<tr>
<td>BWCC</td>
<td>Brillouin–Wigner coupled cluster</td>
</tr>
<tr>
<td>BWCCSD</td>
<td>Brillouin–Wigner single-reference coupled cluster with single and double replacements</td>
</tr>
<tr>
<td>BWCCSD(T)</td>
<td>Brillouin–Wigner single-reference coupled cluster with single and double replacements plus a perturbative estimate of the triple replacement component</td>
</tr>
<tr>
<td>MR-BWCC</td>
<td>multi-reference Brillouin–Wigner coupled cluster</td>
</tr>
<tr>
<td>MR-BWCCSD</td>
<td>multi-reference Brillouin–Wigner coupled cluster with single and double replacements</td>
</tr>
<tr>
<td>MR-BWCCSD(T)</td>
<td>multi-reference Brillouin–Wigner coupled cluster with single and double replacements plus a perturbative estimate of the triple replacement component</td>
</tr>
<tr>
<td>CPA</td>
<td>coupled-pair approximation</td>
</tr>
<tr>
<td>CPMET</td>
<td>coupled-pair many-electron theory</td>
</tr>
</tbody>
</table>
Atomic units are employed throughout this volume. In Table 1, we give the experimentally determined values of the basic atomic units.

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Symbol</th>
<th>Value</th>
<th>S.I. Units</th>
<th>Relative uncertainty (ppm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Planck’s constant</td>
<td>ℏ</td>
<td>$\frac{h}{2\pi}$</td>
<td>Js</td>
<td>0.60</td>
</tr>
<tr>
<td>Elementary charge</td>
<td>e</td>
<td>$1.60217733 \times 10^{-19}$</td>
<td>C</td>
<td>0.30</td>
</tr>
<tr>
<td>Electron mass</td>
<td>$m_e$</td>
<td>$9.1093897 \times 10^{-31}$</td>
<td>kg</td>
<td>0.59</td>
</tr>
</tbody>
</table>

The atomic unit of length is the first Bohr radius

$$a_0 = \frac{\hbar^2}{m_e e^2}$$

The unit of energy is the Hartree

$$E_H = \frac{e^2}{a_0}$$

In Table 2, we give numerical values of these atomic units together with various other derived atomic units.
<table>
<thead>
<tr>
<th>Quantity</th>
<th>Value</th>
<th>S.I. Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bohr radius, $a_0$</td>
<td>$5.2917726 \times 10^{-11}$</td>
<td>m</td>
</tr>
<tr>
<td>Energy, $E_H$</td>
<td>$4.3598 \times 10^{-18}$</td>
<td>J</td>
</tr>
<tr>
<td>Time</td>
<td>$2.4189 \times 10^{-17}$</td>
<td>s</td>
</tr>
<tr>
<td>Electric dipole moment</td>
<td>$8.4784 \times 10^{-30}$</td>
<td>Cm</td>
</tr>
<tr>
<td>Electric quadrupole moment</td>
<td>$4.4866 \times 10^{-40}$</td>
<td>Cm$^2$</td>
</tr>
<tr>
<td>Electric octopole moment</td>
<td>$2.3742 \times 10^{-50}$</td>
<td>Cm$^3$</td>
</tr>
<tr>
<td>Electric field</td>
<td>$5.1423 \times 10^{11}$</td>
<td>Vm$^{-1}$</td>
</tr>
<tr>
<td>Electric field gradient</td>
<td>$9.7174 \times 10^{21}$</td>
<td>Vm$^{-2}$</td>
</tr>
<tr>
<td>Polarizability (dipole)</td>
<td>$1.6488 \times 10^{41}$</td>
<td>C$^2$m$^2$J$^{-1}$</td>
</tr>
<tr>
<td>Hyperpolarizability</td>
<td>$3.2063 \times 10^{-53}$</td>
<td>C$^3$m$^3$J$^{-2}$</td>
</tr>
<tr>
<td>Magnetic moment</td>
<td>$1.8548 \times 10^{-23}$</td>
<td>JT$^{-1}$</td>
</tr>
<tr>
<td>Magnetizability</td>
<td>$7.8910 \times 10^{-29}$</td>
<td>JT$^{-2}$</td>
</tr>
<tr>
<td>Magnetic vector potential</td>
<td>$1.2439 \times 10^{-5}$</td>
<td>mT</td>
</tr>
<tr>
<td>Force constant (harmonic)</td>
<td>$1.5569 \times 10^{3}$</td>
<td>Jm$^{-2}$</td>
</tr>
<tr>
<td>Force constant (cubic)</td>
<td>$2.9421 \times 10^{13}$</td>
<td>Jm$^{-3}$</td>
</tr>
<tr>
<td>Force constant (quartic)</td>
<td>$5.5598 \times 10^{23}$</td>
<td>Jm$^{-4}$</td>
</tr>
<tr>
<td>Probability density</td>
<td>$6.7483 \times 10^{30}$</td>
<td>m$^{-3}$</td>
</tr>
</tbody>
</table>