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Richard M. Martin, Lucia Reining and David M. Ceperley
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INTERACTING ELECTRONS

Theory and Computational Approaches

Recent progress in the theory and computation of electronic structure is bringing an unprecedented level of capability for research. Many-body methods are becoming essential tools vital for quantitative calculations and understanding materials phenomena in physics, chemistry, materials science, and other fields. This book provides a unified exposition of the most-used tools: many-body perturbation theory, dynamical mean-field theory, and quantum Monte Carlo simulations.

Each topic is introduced with a less technical overview for a broad readership, followed by in-depth descriptions and mathematical formulation. Practical guidelines, illustrations, and exercises are chosen to enable readers to appreciate the complementary approaches, their relationships, and the advantages and disadvantages of each method. This book is designed for graduate students and researchers who want to use and understand these advanced computational tools, get a broad overview, and acquire a basis for participating in new developments.

RICHARD M. MARTIN is Emeritus Professor at the University of Illinois at Urbana-Champaign and Consulting Professor at Stanford University. He has made extensive contributions to the field of modern electronic structure methods and the theory of interacting electron systems and he is the author of the companion book, *Electronic Structure: Basic Theory and Methods*.

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Theory and Computational Approaches

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To our families

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Part V Appendices

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Preface

Recent progress in the theory and computation of electronic structure is bringing an unprecedented level of capability for research. It is now possible to make quantitative calculations and provide novel understanding of natural and man-made materials and phenomena vital to physics, chemistry, materials science, as well as many other fields. Electronic structure is indeed an active, growing field with enormous impact, as illustrated by the more than 10,000 papers per year.

Much of our understanding is based on mean-field models of independent electrons, such as Hartree–Fock and other approximations, or density functional theory. The latter is designed to treat ground-state properties of the interacting-electron system, but it is often also used to describe excited states in an independent-electron interpretation. Such approaches can only go so far; many of the most interesting properties of materials are a result of interaction between electrons that cannot be explained by independent-electron descriptions. Calculations for interacting electrons are much more challenging than those of independent electrons. However, thanks to developments in theory and methods based on fundamental equations, and thanks to improved computational hardware, many-body methods are increasingly essential tools for a broad range of applications. With the present book, we aim to explain the many-body concepts and computational methods that are needed for the reader to enter the field, understand the methods, and gain a broad perspective that will enable him or her to participate in new developments.

What sets this book apart from others in the field? Which criteria determine the topics included? We want the description to be broad and general, in order to reflect the richness of the field, the generality of the underlying theories, and the wide range of potential applications. The aim is to describe matter all the way from isolated molecules to extended systems. The methods must be capable of computing a wide range of properties of diverse materials, and have promise for exciting future applications. Finally, practical computational methods are an important focus for this book.

Choices have to be made since the number of different approaches, their variations, and applications is immense, and the book is meant to be more than an overview. We therefore cannot focus on such important areas as quantum chemistry methods, e.g. coupled cluster theory and configuration interaction methods, nor do we cover all of the developments in lattice models, or explore the vast field of superconductivity. Rather, we concentrate on three methods: many-body perturbation theory, dynamical mean-field

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theory, and stochastic quantum Monte Carlo methods. Our goals are to present each of these widely used methods with its strengths and weaknesses, to bring out their relationships, and to illuminate paths for combining these and other methods in order to create more powerful approaches. We believe that it is a unique feature of this book to have all three methods addressed in a coherent way: the conceptual structure, the actual methods, and selected applications.

The book is written so that a reader interested in many-body theory and methods should not have to go through the details of density functional theory and methods for independent-particle calculations. Summaries of pertinent material are given in this book, and extensive exposition can be found in the companion book by one of us (R. M. Martin, *Electronic Structure: Basic theory and methods*, Cambridge University Press, Cambridge, 2004, reprinted 2005 and 2008). The two books are complementary and can be read independently.

The organization of the book follows naturally: Part I (Chapters 1–4) contains background material including history, experimental motivations, and some classic concepts and models referred to throughout the book. Part II (Chapters 5–8) discusses theoretical foundations useful in all many-body treatments: mean-field theories, correlation functions and Green's functions, many-body wavefunctions, the concepts of quasi-particles, and functionals used in Green's function methods. Part III contains two distinct but related ways to use Green's functions, namely many-body perturbation theory including GW and the Bethe–Salpeter equation (Chapters 9–15), and dynamical mean-field theory (Chapters 16–21). Finally, Part IV (Chapters 22–26) discusses stochastic (quantum Monte Carlo) methods. The descriptions of these three approaches are written so that each can be read independently. Altogether, we try to clarify concepts, differences, and points of contact between the various methods, and possibilities for combining the methods as a basis for future progress in understanding and predicting properties of interacting electron systems.

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Notation

Abbreviations

w.r.t.	with respect to
+c.c.	add complex conjugate of preceding quantity
Re, Im	real and imaginary parts
BZ	first Brillouin zone
1D	one dimension or one-dimensional (similar for 2D and 3D)

Acronyms most used

BSE	Bethe–Salpeter equation
DFT	density functional theory
DMFA	various approximations in DMFT
DMFT	dynamical mean-field theory
EXX	exact exchange in DFT
GGA	generalized gradient approximation
GWA	GW approximation
HF	Hartree–Fock
HFA	Hartree–Fock approximation
KS	Kohn–Sham
LDA	local density approximation
MBPT	many-body perturbation theory
QMC	quantum Monte Carlo
RHF	restricted Hartree–Fock
RPA	random phase approximation
TDDFT	time-dependent density functional theory
UHF	unrestricted Hartree–Fock

General physical quantities

E	energy
μ	chemical potential
E_F	Fermi energy (chemical potential at $T = 0$)
T	temperature (also computer time)
β	inverse temperature, $1/k_B T$
Z	partition function; same notation for canonical and grand canonical (also renormalization factor for spectral weight)
S or A	action

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S	entropy
F	Helmholz free energy
G	Gibbs free energy (when identified), otherwise G denotes a Green's function
Ω	grand potential

Time and frequency

t	time
τ	imaginary time
$\Delta\tau$	imaginary time step
ω	frequency (real or complex as specified or as clear from context)
z	frequency defined in complex plane
ω_n	Matsubara frequencies
z_n	position of ω_n in complex plane, $z_n = \mu + i\omega_n$

Coordinates and operators

$\mathbf{r}$	electron position
σ	electron spin
x	combined space/spin coordinates $(\mathbf{r}, \sigma)$
1	combined space/spin/time coordinates (x_1, t_1)
$\bar{1}$	variable to be integrated
R	N-electron coordinates $R = \{\mathbf{r}_1 \ldots \mathbf{r}_N\}$
N	number of electrons
$\mathbf{R}_I$	position of ion I
Z_I	charge of ion I
$\hat{O}$	general operator in Schrödinger picture
$\langle\hat{O}\rangle$	expectation value
$\hat{O}_H(t)$	operator in Heisenberg picture, for static $\hat{H}$, $\hat{O}_H = e^{i\hat{H}t}\hat{O}e^{-i\hat{H}t}$
$c^\dagger$ and c	creation and annihilation operators for fermions
$\hat{\psi}^\dagger$, $\hat{\psi}$ and $\hat{\psi}^\dagger(t)$, $\hat{\psi}(t)$	field operators for fermions; time argument denotes Heisenberg picture, for static $\hat{H}$, $\hat{\psi}^\dagger(t) = e^{i\hat{H}t}\hat{\psi}^\dagger e^{-i\hat{H}t}$, $\hat{\psi}(t) = e^{i\hat{H}t}\hat{\psi}e^{-i\hat{H}t}$
$b^\dagger$ and b	creation and annihilation operators for bosons
$\hat{n}$	particle number operator
$\hat{\mathbf{S}}$, $\mathbf{m}$	atomic moments or spin, $\mathbf{m} = \langle\hat{\mathbf{S}}\rangle$
T	time-ordering operator
T_τ	time ordering in imaginary time τ
$\hat{\mathcal{A}}$	antisymmetrization operator
Tr	trace
$\mathfrak{Tr}$	$\mathfrak{Tr}F = -\frac{i}{2\pi}\lim_{\eta\to 0^+}\mathrm{Tr}\int_{-\infty}^{\infty} d\omega\, e^{i\eta\omega}F(\omega)$ for $T = 0$ $\mathfrak{Tr}F = \mathrm{Tr}\,\beta^{-1}\sum_n F(i\omega_n)$ for $T \neq 0$ for a general function F

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Hamiltonian and eigenstates

$\hat{H}$	many-body hamiltonian
$\hat{V}_{ee}$	electron–electron interaction
$v_c(\|\mathbf{r}_i - \mathbf{r}_j\|)$	Coulomb interaction
E_α	energy of many-body state labeled α
E_0	ground-state energy
$\Psi_\alpha(R)$ or $\Phi_\alpha(R)$	many-body wavefunction (R denotes $\mathbf{r}_i,\ i = 1$); often subscript α is omitted
$V(R)$	many-body potential energy function
$\Psi_T(R)$ or $\Psi(R)$	trial wavefunction
$U(R)$	N-electron Jastrow factor
$u(r_{ij})$ or $u(\mathbf{r}_i, \mathbf{r}_j)$	Jastrow factor for a pair of electrons
$\Theta(R)$	N-electron phase of the trial wavefunction
$E_L(R\|\Psi)$	local energy of a trial function
E_V	variational energy of a trial function
σ^2	variance of the local energy of a trial function
$\mathcal{O}$	overlap of trial function with exact wavefunction
$\hat{H}_0$	independent-particle hamiltonian
$\chi_m(\mathbf{r})$	single-particle basis function, $m = 1, \ldots, N_{\text{basis}}$
$h_{m,m'}$ or $h^0_{m,m'}$	matrix element of independent-particle hamiltonian
$v(\mathbf{r})$	single-particle potential
$v_H(\mathbf{r})$	Hartree potential
$\psi_i(\mathbf{r})$	single-particle wavefunction, $i = 1, \ldots, N_{\text{states}}$, also orbitals in a Slater determinant
ε_i	independent-particle eigenvalue, $i = 1, \ldots, N_{\text{states}}$
$f(\varepsilon)$	Fermi function

Parameters of model hamiltonians

t, t'	hopping matrix elements
U	on-site interaction in Hubbard-type models
J	intra-atomic exchange interaction, also interatomic Heisenberg exchange constant

Correlation functions, Green's functions, response functions, self-energy, etc.

$C_{AB}(t)$	correlation function for quantities A and B
$n(\mathbf{r})$	density (also spin-resolved $n(\mathbf{r}, \sigma)$)
$n_0(\mathbf{r})$	ground-state density (also $n_0(\mathbf{r}, \sigma)$)
$\rho(\mathbf{k})$	momentum distribution (also $\rho(\mathbf{k}, \sigma)$)
$\rho(\mathbf{r}, \mathbf{r}')$	one-electron density matrix (also $\rho(\mathbf{r}, \sigma; \mathbf{r}', \sigma')$)

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$n(\mathbf{r}, \mathbf{r}')$	pair distribution function (also $n(\mathbf{r}, \sigma; \mathbf{r}', \sigma')$)
$g(\mathbf{r}, \mathbf{r}')$	normalized pair distribution (also $g(\mathbf{r}, \sigma; \mathbf{r}', \sigma')$)
$S(\mathbf{q}, \mathbf{q}')$, $S(\mathbf{k})$	structure factor (also $S(\mathbf{q}, \sigma; \mathbf{q}', \sigma')$ or $S^{\sigma\sigma'}_{\mathbf{k}\mathbf{k}'}$)
$S(\omega)$	dynamic structure factor with similar notation for momenta and spin
G	one-body Green's function expressed as a function of arguments, e.g., $\mathbf{r}, \mathbf{r}'$, σ, t, τ, ω, z or as a matrix in a basis, $G_{m,m'}$
G^0 or G_0	independent-particle Green's function
A	spectral function
Σ	self-energy (irreducible)
Γ	vertex function
Z	renormalization factor of spectral weight (also partition function)
$\mathcal{G}$	Green's function for embedded site or cell
$\mathcal{G}_0$	embedding Green's function for embedded site or cell
Δ	hybridization function for impurity, embedded site or cell
G_2	two-particle Green's function
L	two-particle correlation function, $L = -G_2 + GG$
χ	general linear response function, susceptibility
χ_0	general linear response function for independent particles
ϵ	dielectric function
W	screened interaction
P	polarizability (irreducible)

Functionals

$F[f]$	general functional of the function f
$\mathcal{D}$	domain of a functional
$E_{\rm xc}[n]$	exchange–correlation energy in Kohn–Sham theory
$\Phi[G]$	interaction functional of Green's function G
$F[\Sigma]$	Legendre transform of $\Phi[G]$
$\Psi[G, W]$	interaction functional of G and screened interaction W
$\mathcal{J}(1, 1')$	external probe field – non-local in space and time
$\Omega[\mathcal{J}]$	grand-potential functional of $\mathcal{J}$
$\Gamma[Q]$	effective action functional, Legendre transform of $\Omega[\mathcal{J}]$

Notation for crystals

Ω	volume of cell (primitive cell or supercell)
$\mathbf{T}$	lattice translations

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$\mathbf{G}$	reciprocal lattice vectors
$\mathbf{k}$ or $\mathbf{q}$	wavevector in first Brillouin zone $\mathbf{k}$ for electrons; $\mathbf{q}$ for interactions, susceptibilities
$\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u_{\mathbf{k}}(\mathbf{r})$	Bloch function in crystal, with $u_{\mathbf{k}}(\mathbf{r})$ periodic
$\varepsilon_{\mathbf{k}}$	eigenvalues that define bands as a function of $\mathbf{k}$
$G_{\mathbf{k}}$, $\Sigma_{\mathbf{k}}$	Green's function and self-energy as functions of $\mathbf{k}$
$\chi_{\mathbf{q}}$ or $\chi(\mathbf{q})$	general susceptibility as a function of $\mathbf{q}$
G_{ii} or G_{00}	on-site Green's function at site i
$\mathbf{L}_i$	primitive vector of supercell $i = \{1, 2, 3\}$
$\mathbf{K}$	total wavevector for many-body wavefunction
$\hat{H}(\mathbf{K})$	$\mathbf{K}$-dependent hamiltonian with periodic eigenvectors $u_{\mathbf{K}}(R)$, $R = \{\mathbf{r}_1 \ldots \mathbf{r}_N\}$
Δ_{cf}	crystal field splitting
e_g and t_{2g}	crystal field states in cubic symmetry

Notation for stochastic methods

$\mathcal{S}$, s, R	state vector, i.e., variables describing the instantaneous state of a random walk
$R^{(n)}$, $s^{(n)}$	the nth many-body configuration in a random walk
$\Psi^{(n)}$ or Ψ_τ	projected trial wavefunction after n iterations or imaginary time τ
$\Pi(s)$	many-body distribution function to be sampled
$\langle \tilde{O} \rangle_\Pi$	average of $\tilde{O}$ over distribution Π
$P(s \to s')$, $P_{s's}$	transition probability random walk
$T(s \to s')$	trial transition probability
$A(s \to s')$	acceptance probability
$\tilde{O}$	estimator for property O
$\bar{O}$	estimated mean value of property O
ν_O	variance of property O
σ_O	standard error of $\bar{O}$
κ_O	autocorrelation time for property O in a random walk
$\Delta\tau$	time step in VMC, DMC, or PIMC
$\mathcal{P}$	electron permutation
$G(R, R')$, $\hat{G}$	many-body projector
$\mathcal{G}(R \leftarrow R')$	importance-sampled projector
$\Psi_G(R)$	guiding function for importance sampling
$\rho(R, R'; \beta)$	many-body density matrix

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