Jamal Berakdar

Concepts of Highly Excited Electronic Systems

WILEY-VCH GmbH & Co. KGaA

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for Gize & Sebastian

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Preface

The understanding of elementary excitations in electronic systems is of a basic importance, both from a practical as well as from a fundamental point of view. For example, optical properties and electrical transport in materials are primarily governed by excitation processes. On the other hand, our main source of knowledge on the dynamics of elementary electronic systems, such as isolated atoms, ions or molecules, is their response to an external probing field, that excites the system. Generally, the corresponding quantum mechanical description in terms of excitation amplitudes, entails a thorough understanding of the relevant excitation spectrum of the system under study. For this purpose, efficient theoretical and calculational techniques have been developed, and their implementations have rendered possible a detailed insight into the nature and the dynamics of various electronic states in a variety of materials. This progress is driven, to a large extent, by recent breakthroughs in the experimental fabrication, characterization and spectroscopic techniques which, in addition to providing stringent tests of various aspects of current theoretical approaches, have also pointed out open questions to be addressed by theory. Particularly remarkable is the diversity of the electronic materials studied experimentally, ranging from isolated atoms to clusters and surfaces. It is this aspect which is emphasized in this presentation of some of the theoretical tools for the description of excited states of finite and extended electronic systems. The main goal is to highlight common features and differences in the theoretical concepts that have been employed for the understanding of electronic excitations and collisions in finite few-body (atomic) systems and large, extended systems, such as molecules, metal clusters and surfaces.

The complete work is divided in two parts. The first part, which is this present book, deals with the foundations and with the main features of the theoretical methods for the treatment of few-body correlated states and correlated excitations in electronic systems. The forthcoming second volume includes corresponding applications and the analysis of the outcome of theory as contrasted to experimental findings.

A seen from a quick glance at the table of contents, the book starts by reviewing the main aspects of the two-body Coulomb problem, which sets the frame and the notations for the treatment of few-body systems. Subsequently, we sketch a practical scheme for the solution of two-body problems involving an arbitrary non-local potential. Furthermore, an overview is given on the mainstream concepts for finding the ground state of many-body systems. Symmetry properties and universalities of direct and resonant excitation processes are then addressed. Starting from low-lying two-particle excitations, the complexity is increased to the level of dealing with the N-particle fragmentation in finite Coulomb systems. Having in mind the theoretical treatment of excitations in extended and in systems with a large number of active electrons, we introduce the Green's function theory in its first and second quantization versions and outline how this theory is utilized for the description of the ground-state and of many-particle excitations in electronic materials.

The topics in this book are treated differently in depth. Subjects of a supplementary or an introductory nature are outlined briefly, whereas the main focus is put on general schemes for the treatment of correlated, many-particle excitations. In particular, details of those theoretical tools are discussed that are employed in the second forthcoming part of this work.

Due to the broad range of systems, physical processes and theoretical approaches relevant to the present study, only a restricted number of topics is covered in this book, and many important related results and techniques are not included. In particular, in recent years, numerical and computational methods have undergone major advances in developments and implementations, which are not discussed here, even though the foundations of some of these techniques are mentioned. Despite these restrictions, it is nevertheless hoped that the present work will provide and initiate some interesting points of view on excitations and collisions in correlated electronic systems.

The work is purely theoretical. It should be of interest, primarily for researchers working in the field of theoretical few-body electronic systems. Nonetheless, the selected topics and their presentations are hoped to be interesting and comprehensible to curious experimentalists with some pre-knowledge of quantum mechanics.

The results of a number of collaborations with various friends and colleagues can be found in this book. I would like to take this opportunity to thank few of them. I am particularly indebted to M. Brauner, J. S. Briggs, J. Broad and H. Klar for numerous collaborations, discussions and advice on charged few-particle problems. I would also like to thank P. Bruno, A. Ernst, R. Feder, N. Fominykh, H. Gollisch, J. Henk, O. Kidun, and K. Kouzakov for fruitful collaborations, encouragements and valuable discussions on the theoretical aspects of electronic excitations and correlations in condensed matter. Furthermore, I am grateful to L. Avaldi, I. Bray, R. Dörner, A. Dorn, R. Dreizler, J. Feagin, A. Kheifets, J. Kirschner, A. Lahmam-Bennani, J. Lower, H. J. Lüdde, J. Macek, J. H. McGuire, D. Madison, S. Mazevet, R. Moshammer, Yu. V. Popov, A.R.P. Rau, J.-M.Rost, S. N. Samarin, H. Schmidt-Böcking, A. T. Stelbovics, E. Weigold and J. Ullrich for many insightful and stimulating discussions we had over the years on various topics of this book. Communications, discussions and consultations with E. O. Alt, V. Drchal, T. Gonis, J. Kudrnovský, M. Lieber and P. Ziesche are gratefully acknowledged.

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Jamal Berakdar

Halle, January 2003

1 The two-body Kepler problem: A classical treatment

This chapter provides a brief summary of the theoretical treatment of non-relativistic two-body Coulomb systems. An extensive account can be found in standard textbooks, e. g. [1]. The purpose here is to introduce the basic ideas and notations utilized in the quantum theory of interacting charged particles. Particular attention is given to the approach pioneered by W. Pauli [4] which utilizes the existence of an additional integral of motion due to the dynamical symmetry of Coulomb-type potentials, namely the Laplace-Runge-Lenz vector [2]. Let us consider a system consisting of two interacting particles with charges z_1 and z_2 and masses m_1 and m_2. In the center-of-mass system, the two-particle motion is described by a one-body Hamiltonian H_0 that depends on the relative coordinates of the two particles. Its explicit form is [1]

$$H_0 = \frac{1}{2\mu}\mathbf{p}_0^2 - \frac{z_{12}}{r_0}, \tag{1.1}$$

where $z_{12} = -z_1 z_2$ and the reduced mass is denoted by $\mu = m_1 m_2/(m_1 + m_2)$. The vectors $\mathbf{r}_0$ and $\mathbf{p}_0$ are respectively the two-particle relative coordinate and its conjugate momentum. In addition to the total energy E, the angular momentum $\mathbf{L}_0 = \mathbf{r}_0 \times \mathbf{p}_0$ is a conserved quantity due to the invariance of Eq. (1.1) under spatial rotations. Furthermore, the so-called Laplace-Runge-Lenz vector [2]

$$\mathbf{A} = \hat{\mathbf{r}}_0 + \frac{1}{\mu z_{12}}\mathbf{L}_0 \times \mathbf{p}_0 \tag{1.2}$$

is as well a constant of motion. This is readily deduced by noting that

$$\partial_t \mathbf{p}_0 = -z_{12}\hat{\mathbf{r}}_0/r_0^2$$

---

[1] Unless otherwise specified, atomic units are used throughout this book.

and therefore the time derivative of $\mathbf{A}$ vanishes, i.e.

$$\begin{aligned}\partial_t \mathbf{A} &= \partial_t \hat{\mathbf{r}}_0 + \frac{1}{\mu z_{12}} \mathbf{L}_0 \times (\partial_t \mathbf{p}_0) \\ &= \frac{\partial_t \mathbf{r}_0}{r_0} - \frac{[\mathbf{r}_0 \cdot (\partial_t \mathbf{r}_0)]\mathbf{r}_0}{r_0^3} - \frac{1}{r_0^3}\, [\mathbf{r}_0 \times (\partial_t \mathbf{r}_0)] \times \mathbf{r}_0 = 0.\end{aligned} \tag{1.3}$$

For the derivation of the classical trajectories it is instructive to introduce the dimensionless quantities

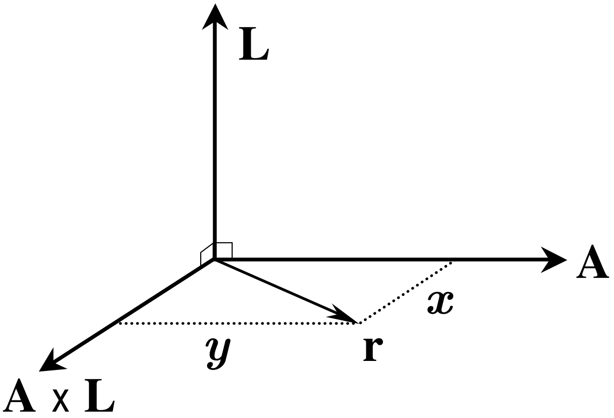

Figure 1.1: The motion of two particles interacting via a Coulomb-type potential takes place in the plane spanned by the vectors $\mathbf{A}$ and $\mathbf{A} \times \mathbf{L}$.

$$\mathbf{r} = z_{12}\, \mathbf{r}_0/a,\ \mathbf{p} = \mathbf{p}_0\, a/(z_{12}\hbar), \ \text{ and }\ \mathbf{L} = \mathbf{L}_0/\hbar,$$

where the length scale is given by $a = \hbar^2/(\mu e^2)$ (for clarity, the electron charge e and $\hbar$ are displayed here). The Hamiltonian (1.1) transforms into $H = 2a/(z_{12}^2 e^2) H_0$, whereas in the scaled coordinates, the Laplace-Runge-Lenz vector ($\mathbf{A}$) has the form

$$\mathbf{A} = \hat{\mathbf{r}} + \mathbf{L} \times \mathbf{p}. \tag{1.4}$$

Thus, the Hamiltonian H_0 (1.1) measured in the energy units $\epsilon = (z_{12}^2 e^2)/(2a)$ is

$$H = H_0/\epsilon = p^2 - 2/r. \tag{1.5}$$

Since $\partial_t \mathbf{A} = 0 = \partial_t \mathbf{L}$ and $\mathbf{A} \cdot \mathbf{L} = 0$ we deduce that the relative motion of the two particles is restricted to a plane $\mathcal{P}$ defined by $\mathbf{A}$ and $\mathbf{L} \times \mathbf{A}$, as illustrated in Fig. 1.1. The relative position vector **r** in the plane $\mathcal{P}$ is uniquely specified by the components [see Fig. 1.1]

$$x = \mathbf{r}\cdot(\mathbf{L}\times\mathbf{A}), \text{ and } y = \mathbf{r}\cdot\mathbf{A}.$$

The components x and y can be written in the form

$$y = r - L^2, \; x = -L^2(\mathbf{r}\cdot\mathbf{p}). \tag{1.6}$$

Furthermore we conclude that since

$$L^2 = r^2p^2 - (\mathbf{r}\cdot\mathbf{p})^2, \quad \text{the relation} \quad x^2/L^4 = r^2p^2 - L^2 \tag{1.7}$$

applies.

Thus, for a given total (scaled) energy $E = p^2 - 2/r$ the components x and y of the position vector **r** are determined by the equation

$$\left[y\,E + (L^2E+1)\right]^2 - \frac{E}{L^4}\,x^2 = L^2E + 1. \tag{1.8}$$

Further straightforward algebraic manipulations lead to

$$A^2 = L^2E + 1 \geq 0.$$

Relation (1.8) is the defining equation for conic sections in the normal form:

- For $E < 0$ the motion proceeds along an *elliptical closed orbit* with **A** being along the main axis. The excentricity of the orbit is determined by $|\mathbf{A}|$.
- For $E > 0$ Eq. (1.8) defines a *hyperbola*.
- If $E = 0$ (and hence $p^2 = 2/r$) we conclude from Eq. (1.7) and from $r = y + L^2$ that

  $$y = x^2/(2L^4) - L^2/2.$$

  This equation describes a *parabola* with a curvature L^{-4}. If in addition $L \ll 1$ the parabola degenerates to an almost *straight line* along **A** starting from the origin [see Fig. 1.1].

2 Quantum mechanics of two-body Coulomb systems

2.1 Historical background

In a seminal work [4] W. Pauli applied the correspondence principle to introduce the hermitian Laplace-Runge-Lenz operator $\mathbf{A}$ and showed that $\mathbf{A}$ commutes with the total Hamiltonian H, i. e. $[H, \mathbf{A}] = 0$. Using group theory he utilized this fact for the derivation of the bound spectrum of the Kepler problem. Later on, V. A. Fock [5] argued that the degeneracy of the levels, having the same principle quantum numbers, is due to a "hidden" dynamical symmetry. I. e. in addition to the symmetry with respect to the (spatial) rotation group $O(3)$, the Kepler problem with bound spectrum possesses a symmetry with respect to a wider (compact) group $O(4)$ (rotation in a four-dimensional space). Shortly after that V. Bargmann [6] showed how the separability of the (bound) two-body Coulomb problem in parabolic coordinates is linked to the existence of the conserved quantity $\mathbf{A}$. J. Schwinger [7] utilized the rotational invariance with respect to $O(4)$ for the derivation of the Coulomb Green's function. It is this line of development which we will follow in the following compact presentation of this topic. A detailed discussion of the Coulomb Green's function in connection with the $O(4)$ symmetry is deferred to section 11.3.

The dynamical symmetry is related to the form of the Coulomb potential and persists in the n dimensional space. In fact, S. P. Alliluev [8] showed that the Hamiltonian of the n-dimensional (attractive) Kepler problem possesses a hidden symmetry with respect to the $O(n+1)$ group. For $n = 3$ (e.g. the hydrogen atom) Fock showed [5] that the spectrum is described by the irreducible representations of $O(4)$. Those are finite dimensional since $O(4)$ is a compact group, i. e. a continuous group with finite volume. For the description of the discrete *and* the continuous spectrum one has to utilize the non-compact analog of $O(4)$, namely the Lorenz group (for more details and further references see Ref. [9]).

2.2 Group theoretical approach to the two-body problem

The classical vector (1.4) can not be translated directly into quantum mechanics as the Laplace-Runge-Lenz vector operator $\mathbf{A}$ because it would be non-hermitian. An acceptable definition for the (polar) vector operator $\mathbf{A}$ that satisfies $\mathbf{A} = \mathbf{A}^\dagger$, is [1]

$$\mathbf{A} = \hat{\mathbf{r}} + \frac{1}{2}\left(\mathbf{L} \times \mathbf{p} - \mathbf{p} \times \mathbf{L}\right). \tag{2.1}$$

Since for any vector operator, such as $\mathbf{p}$ the relation $\mathbf{L} \times \mathbf{p} - \mathbf{p} \times \mathbf{L} = i[\mathbf{L}^2, \mathbf{p}]$ applies, we can write $\mathbf{A}$ in the form

$$\mathbf{A} = \hat{\mathbf{r}} + \frac{i}{2}[\mathbf{L}^2, \mathbf{p}]. \tag{2.2}$$

With this definition of $\mathbf{A}$ one verifies the following commutation relations between the operators $\mathbf{L}$, $\mathbf{A}$ and H

$$\begin{aligned} \mathbf{L} \times \mathbf{L} &= i\mathbf{L}, & (2.3)\\ \mathbf{A} \times \mathbf{A} &= -iH\,\mathbf{L}, & (2.4)\\ \mathbf{L} \times \mathbf{A} + \mathbf{A} \times \mathbf{L} &= i2\mathbf{A}, & (2.5)\\ [H, \mathbf{L}] &= 0 = [H, \mathbf{A}], & (2.6)\\ \mathbf{A} \cdot \mathbf{L} &= 0 = \mathbf{L} \cdot \mathbf{A}. & (2.7) \end{aligned}$$

Furthermore, using Eq. (2.2) it is readily shown that

$$\mathbf{A}^2 = 1 + H(\mathbf{L}^2 + 1). \tag{2.8}$$

Eqs. (2.6, 2.7) state that $\mathbf{L}$ and $\mathbf{A}$ (and H) are conserved while Eq. (2.8) serves to derive Bohr's formula of the energy level scheme, as shown below. Introducing the normalized Laplace-Runge-Lenz operators as

$$\mathbf{N} = \mathbf{A}/h, \;\; h = \begin{cases} 1/\sqrt{-H} & \forall E < 0, \\ 1/\sqrt{H} & \forall E > 0, \\ 1 & E = 0, \end{cases} \tag{2.9}$$

---

[1] Hereafter we use the shorthand notation $\sum_{ij}[\mathbf{A}_i, \mathbf{B}_j]\epsilon_{ijk} = (\mathbf{A} \times \mathbf{B})_k$ where $\mathbf{A}$ and $\mathbf{B}$ are vector operators. A vector operator satisfies the relation $\mathbf{L} \times \mathbf{A} + \mathbf{A} \times \mathbf{L} = 2i\mathbf{A}$ (same applies for $\mathbf{B}$ or any vector operator).

the Hamiltonain H is scaled out of Eqs. (2.4–2.7) which then simplify to

$$\begin{aligned}
\mathbf{L}\times\mathbf{L} &= i\mathbf{L}\,, && (2.10)\\
\mathbf{N}\times\mathbf{N} &= \kappa\, i\mathbf{L}\,, && (2.11)\\
\mathbf{N}\cdot\mathbf{L} &= 0=\mathbf{L}\cdot\mathbf{N}\,, && (2.12)\\
\mathbf{L}\times\mathbf{N}+\mathbf{N}\times\mathbf{L} &= 2\, i\mathbf{N}. && (2.13)
\end{aligned}$$

Here we adopt the definition $\kappa = \mathrm{sgn}(-E)$ and $\kappa = 0$ for $E = 0$. Eq. (2.8) becomes

$$-\kappa H\mathbf{N}^2 = 1 + H(\mathbf{L}^2 + 1), \quad \text{if} \quad E \neq 0, \qquad (2.14)$$

$$\mathbf{N}^2 = 1 + H(\mathbf{L}^2 + 1), \quad \text{if} \quad E = 0. \qquad (2.15)$$

The relations (2.10–2.13) coincide with the commutation relations between the generators of the homogeneous Lorenz group describing rotations and translations. For $E = 0$ (i. e. $\kappa = 0$) the Lorenz group (2.10–2.13) degenerates to the Galilean group. For a given positive energy $E > 0$ the continuum wave functions are the irreducible representations of the Lorenz group. This representation is infinite dimensional and unitary because the values of the orbital angular momentum l are not restricted for a fixed positive energy ($E > 0$). Furthermore, $\mathbf{L}$ and $\mathbf{N}$, the generators of the group, are hermitian for $H > 0$. In contrast, for the bound spectrum ($E < 0$) a finite number of (orbital angular momentum) states corresponding to a given principal quantum number n provides a finite dimensional, non-unitary representation. The non-unitarity is a consequence of the fact that the generators $\mathbf{N}$ are antihermitian for $H < 0$.

2.2.1 The bound spectrum

As well known, for $E < 0$ there is a one-to-one correspondence between the representations of the Lorenz group and the compact $O(4)$ group that have the six generators $(\mathbf{L}, \mathbf{N})$. On the other hand a reduction of the $O(4)$ algebra into two $O(3)$ algebras can be achieved upon introducing the operators

$$\begin{aligned}
\mathbf{J}_{(\mathbf{1})} &= \frac{1}{2}(\mathbf{L}+\mathbf{N})\,, && (2.16)\\
\mathbf{J}_{(\mathbf{2})} &= \frac{1}{2}(\mathbf{L}-\mathbf{N})\,. && (2.17)
\end{aligned}$$

These satisfy the commutation relations of two independent angular momentum operators, namely

$$
\begin{aligned}
\mathbf{J}_{(\mathbf{1})} \times \mathbf{J}_{(\mathbf{1})} &= i\mathbf{J}_{(\mathbf{1})}, & (2.18)\\
\mathbf{J}_{(\mathbf{2})} \times \mathbf{J}_{(\mathbf{2})} &= i\mathbf{J}_{(\mathbf{2})}, & (2.19)\\
[\mathbf{J}_{(\mathbf{2})_\nu} \times \mathbf{J}_{(\mathbf{2})_\nu}] &= 0, \quad \forall\ \nu = 1,2,3. & (2.20)
\end{aligned}
$$

Thus, each of $\mathbf{J}_{(\mathbf{1})}$ and $\mathbf{J}_{(\mathbf{2})}$ can be regarded as the generators of rotations in three dimensions. From a group theory point of view the three components of $\mathbf{J}_{(\mathbf{1})}$ and of $\mathbf{J}_{(\mathbf{2})}$ are the members of two independent Lie algebras $SO_1(3)$ and $SO_2(3)$ [9]. As noticed by O. Klein [10], the Lie algebra implied by Eqs. (2.18–2.20) is then $SO_1(3) \times SO_2(3) = SO(4)$ which describes rotations in a four dimensional space. The representations of the Lie group $SO(4)$ are thus labelled by the two angular momenta $j_1 = 0, 1/2, 1, 3/2 \cdots$ and $j_2 = 0, 1/2, 1, 3/2 \cdots$. The eigenvalues of the Casimir operators $\mathbf{J}^2(1)$and $\mathbf{J}^2(2)$ of the groups $SO_1(3)$ and $SO_2(3)$ are respectively $j_1(j_1+1)$ and $j_2(j_2+1)$. Due to the restriction (2.7) we deduce from (2.16, 2.17) that

$$
\mathbf{J}^2_{(\mathbf{1})} = \mathbf{J}^2_{(\mathbf{2})} = \frac{1}{4}\left(\mathbf{L}^2 + \mathbf{N}^2\right), \tag{2.21}
$$

i. e. $j_1 = j_2$. Furthermore, from Eq. (2.14) follows

$$
H = -(\mathbf{N}^2 + \mathbf{L}^2 + 1)^{-1} = -(4\,\mathbf{J}^2_{(\mathbf{1})} + 1)^{-1}.
$$

This means, employing the $|j_1 m_1\rangle \otimes |j_2 m_2\rangle$ representation, and taking into account the condition $j_1 = j_2 = j$, the energy eigenvalues E are $(2j+1)^2$-fold degenerated and are given by

$$
\begin{aligned}
E &= -\frac{1}{4j(j+1)+1} = -\frac{1}{(2j+1)^2}, \quad j = 0, \frac{1}{2}, 1, \cdots,\\
E &= -\frac{1}{n^2}, \quad n := (2j+1) = 1, 2, 3 \cdots. & (2.22)
\end{aligned}
$$

2.2.2 Eigenstates of two charged-particle systems

The states $|\Psi_{nlm}\rangle$ that form the representations of $SO(4)$ are obtained as follows. Since $|j_1 m_1\rangle$ and $|j_2 m_2\rangle$ are eigenvectors of angular momentum operators they can be regarded as spherical tensors (see appendix A.1 for definitions and notations of spherical tensors) of rank

j with components $m = -j \cdots j$ [note $j = j_1 = j_2 = (n-1)/2$, see Eq. (2.22)]. From $SO(4) = SO_1(3) \times SO_2(3)$ we deduce that $|\Psi_{nlm}\rangle$ is obtained via the tensor product[2]

$$|\Psi_{nlm}\rangle = \sum_{m_1 m_2} \left\langle \frac{n-1}{2} m_1 \; \frac{n-1}{2} m_2 \middle| lm \right\rangle \left| j = \frac{n-1}{2} \; m_1 \right\rangle \otimes \left| j = \frac{n-1}{2} \; m_2 \right\rangle . \quad (2.23)$$

Noting that $\mathbf{L} = \mathbf{J}_{(1)} + \mathbf{J}_{(2)}$ and $\mathbf{N} = \mathbf{J}_{(1)} - \mathbf{J}_{(2)}$ [cf. Eqs. (2.16, 2.17)] we can rewrite Eq. (2.23) in terms of the eigenvalues m and q of the components $\mathbf{L}_z$ and $\mathbf{N}_z$ with respect to an appropriately chosen axis z. Since $m = m_1 + m_2$ and $q = m_1 - m_2$ the state vector $|\Psi_{nlm}\rangle$ is readily expressed in terms of the common eigenstates $|\phi_{nqm}\rangle$ of the operators $\mathbf{L}_z$, $\mathbf{N}_z$ and H in which case Eq. (2.23) takes on the form

$$|\Psi_{nlm}\rangle = \sum_{q} \left\langle \frac{n-1}{2} \; \frac{m+q}{2} \; \frac{n-1}{2} \; \frac{m-q}{2} \middle| lm \right\rangle |\phi_{nqm}\rangle . \quad (2.24)$$

The explicit forms of the wave functions $\Psi_{nlm}(\mathbf{r})$ and $\phi_{nqm}(\mathbf{r})$ are given in the next section.

2.3 The two-body Coulomb wave functions

The quantum mechanical two-body Coulomb problem is exactly solvable in only four coordinate systems [3]:

1. In *spherical coordinates* the two-particle relative position $\mathbf{r}$ is specified by $\mathbf{r} = r(\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta)$ where $\theta \in [0,\pi]$ and $\varphi \in [0, 2\pi]$ are the polar and the azimuthal angles. The chosen set of commuting observables is $\{H, \mathbf{L}^2, \mathbf{L}_z\}$.

2. In the *spheroconic coordinates* the coordinate $\mathbf{r}$ is given by $\mathbf{r} = r(\mathrm{sn}\alpha\,\mathrm{dn}\beta, \mathrm{cn}\alpha\,\mathrm{cn}\beta, \mathrm{dn}\alpha\,\mathrm{sn}\beta)$, where $r \in [0,\infty[$, $\alpha \in [-K, K]$, and $\beta \in [-2K', 2K']$, here $4K$ $(4iK')$ is the real (imaginary) period of the Jacobi-elliptic functions[3] [238]. The set of commuting observables that are diagonalized simultaneously is $\{H, \mathbf{L}^2, \mathbf{L}_x^2 + k'\mathbf{L}_y^2\}$.

---

[2] The tensor product of two spherical tensors $T_{q_1 m_1}$ and $T_{q_2 m_2}$ with ranks q_1 and q_2 and components $m_1 = -q_1, \cdots, q_1$ and $m_2 = -q_2, \cdots, q_2$ is the spherical tensor P_{km} where $P_{km} = \sum_{m_1 m_2} \langle q_1 m_1\, q_2 m_2 | km\rangle\, T_{q_1 m_1} T_{q_2 m_2}$. For more details see appendix A.1.

[3] The Jacobi elliptic integrals are defined as $u = \int_0^{\varphi} \frac{d\theta}{\sqrt{1-k^2\sin^2\theta}}$. $\mathrm{sn}(u) = \sin\varphi$, $\mathrm{cn}(u) = \cos\varphi$ and $\mathrm{dn}(u) = (1-k^2\sin^2\varphi)^{1/2}$. For the definition of the spheroconic coordinates k [k'] is deduced from the modulus of $\mathrm{sn}(\alpha)$ and $\mathrm{cn}(\alpha)$ [$\mathrm{sn}(\beta)$, $\mathrm{cn}(\beta)$ and $\mathrm{dn}(\beta)$].

3. In *spheroidal coordinates* the relative coordinate $\mathbf{r}$ is defined as $\mathbf{r} = \frac{R}{2}\left(\sqrt{(\xi^2-1)(1-\eta^2)}\cos\varphi, \sqrt{(\xi^2-1)(1-\eta^2)}\sin\varphi, \xi\eta+1\right)$ where R is a real positive constant and $\xi \in [1,\infty[$, $\eta \in [-1,+1]$, and $\varphi \in [0, 2\pi[$. In this case the chosen set of commuting operators is $\{H, \mathbf{L}^2 - 2R\mathbf{N}_z, \mathbf{L}_z\}$. For $R \to 0$ the spheroidal coordinates degenerates to the spherical coordinates whereas for $R \to \infty$ they coincide with the parabolic coordinates.

4. In the *parabolic coordinates* the preferred set of commuting operators is $\{H, \mathbf{L}_z, \mathbf{N}_z\}$. It is this coordinate system which will be discussed below and will be utilized in the next chapters of this book for the treatment of the few-body problem.

2.3.1 Spherical coordinates

The derivation of the normalized wave functions $\Psi_{nlm}(\mathbf{r})$ in spherical coordinates can be found in standard books on quantum mechanics [1]. Here we only give the final expression

$$\Psi_{nlm}(\mathbf{r}) = R_{nl}(r)Y_{lm}(\hat{\mathbf{r}}), \tag{2.25}$$

$$R_{nl}(r) = \frac{2}{n^2(n+1)!}\left[\frac{(n-l-1)!}{(n+l)!}\right]^{1/2}\left(\frac{2r}{n}\right)^l e^{-\frac{r}{n}}\, L_{n+l}^{2l+1}\left(\frac{2r}{n}\right). \tag{2.26}$$

The angular motion is described by the spherical harmonics $Y_{lm}(\hat{\mathbf{r}})$ whereas the radial part Eq. (2.26) is given in terms of the associated Laguerre polynomials[4] $L_b^a(x)$ [12, 99].

2.3.2 Parabolic coordinates

As mentioned above, as an alternative set of three commuting operators for the description of the two-body Coulomb problem one may choose $\{H, \mathbf{L}_z, \mathbf{A}_z\}$. The corresponding coordinate system in which the Schrödinger equation separates is the parabolic coordinates. Those are given in terms of the defining parameters of two systems of paraboloids with the focus at the origin and an azimuthal angle φ in the (x, y) plane. The relation between these coordinates

---

[4] The Laguerre polynomials are obtained according to the formula $L_n(z) = e^z \frac{d^n}{dz^n}\left[e^{-z} z^n\right]$. The associated Laguerre polynomials are given by $L_n^m(z) = \frac{d^m}{dz^m} L_n(z)$ and satisfy the differential equation

$$\left[z\partial_z^2 + (m+1-z)\partial_z + (n-m)\right] L_n^m(z) = 0. \tag{2.27}$$

and the cartesian coordinates (in which the position vector $\mathbf{r}$ is given by $\mathbf{r} = (x, y, z)$) is

$$\begin{aligned} x &= \sqrt{\xi\eta}\cos\varphi, & \xi &= r + \mathbf{r}\cdot\hat{\mathbf{z}}, \\ y &= \sqrt{\xi\eta}\sin\varphi, & \eta &= r - \mathbf{r}\cdot\hat{\mathbf{z}}, \\ z &= \tfrac{1}{2}(\xi - \eta), & \tan\varphi &= \tfrac{y}{x}\,; \end{aligned} \tag{2.28}$$

$$\xi \in [0, \infty[,\ \eta \in [0, \infty[,\ \varphi \in [0, 2\pi].$$

The Laplacian Δ expressed in parabolic coordinates reads

$$\Delta = \frac{4}{\xi+\eta}\left(\partial_\xi \xi \partial_\xi + \partial_\eta \eta \partial_\eta\right) + \frac{1}{\eta\xi}\partial^2_\varphi. \tag{2.29}$$

Thus, the Schrödinger equation for an electron in the field of an ion with a charge $Z = 1$ a.u. is

$$\begin{aligned} (H - \bar{E})\phi &= 0, \\ \left(\mathbf{p}^2 - \frac{2}{r} - E\right)\phi &= 0, \end{aligned} \tag{2.30}$$

where $E = 2\bar{E}$. In parabolic coordinates Eq. (2.30) has the following form

$$\left\{\frac{4}{\xi+\eta}\left[\partial_\xi \xi \partial_\xi + \partial_\eta \eta \partial_\eta + 1\right] + \frac{1}{\eta\xi}\partial^2_\varphi + E\right\}\phi = 0. \tag{2.31}$$

Multiplying this equation by $(\xi + \eta)/4$ and upon inserting in (2.31) the ansatz

$$\phi = N_E\, e^{\pm i\, m\varphi}\, u_1(\xi) u_2(\eta), \tag{2.32}$$

$$\text{where} \qquad m \geq 0, \text{ and } N_E \text{ is an energy dependent normalization constant,} \tag{2.33}$$

we obtain the two determining equations for functions $u_1(\xi)$ and $u_2(\eta)$ as

$$\partial_\xi(\xi\partial_\xi u_1) + \frac{E}{4}\xi u_1 - \frac{m^2}{4\xi}u_1 + c_1 u_1 = 0, \tag{2.34}$$

$$\partial_\eta(\eta\partial_\xi u_2) + \frac{E}{4}\eta u_2 - \frac{m^2}{4\eta}u_2 + c_2 u_2 = 0. \tag{2.35}$$

Here c_1 and c_2 are integration constants satisfying

$$c_1 + c_2 = 1. \tag{2.36}$$

Since the function u_1 have the limiting behaviour

$$\lim_{\xi\to 0} u_1 \to \xi^{m/2} \text{ and } \lim_{\xi\to\infty} u_1 \to \exp(-\sqrt{-E}\,\xi/2) \tag{2.37}$$

it is advantageous to write down u_1 in the form

$$u_1 = \xi^{m/2}\exp(-\sqrt{-E}\,\xi/2) g_1(\xi). \tag{2.38}$$

From Eq. (2.34) one deduces for the unknown function g_1 the determining equation

$$\left[x\partial_x^2 + (m+1-x)\partial_x + \left(\frac{c_1}{\sqrt{-E}} - \frac{m+1}{2}\right)\right] g_1 = 0, \tag{2.39}$$

where $x = \xi\sqrt{-E}$. The solution of the differential equation Eq. (2.39) is the associated Laguerre polynomials $L_n^m(z)$, as readily verified upon a comparison with Eq. (2.27), i. e.

$$\begin{aligned} g_1(x) &= L^m_{n_1+m}(x), & (2.40)\\ n_1 &= \frac{c_1}{\sqrt{-E}} - \frac{(m+1)}{2} = 0, 1, 2, \cdots . & (2.41) \end{aligned}$$

In an analogous way one expresses the function u_2 in terms of associated Laguerre polynomials as

$$\begin{aligned} u_2 &= \eta^{m/2} \exp\left(-\sqrt{-E}\,\eta/2\right) L^m_{n_2+m}(\eta\sqrt{-E}), & (2.42)\\ n_2 &= c_2/\sqrt{-E} - (m+1)/2 = 0, 1, 2, \cdots . & (2.43) \end{aligned}$$

With this formula we conclude that the function, defined by Eq. (2.32), has the final form

$$\begin{aligned} \phi &= N_E\, e^{\pm i\, m\varphi} u_1 u_2, \\ &= N_E\, e^{\pm i\, m\varphi} \times \\ &\quad \times \xi^{m/2} \exp\left(-\sqrt{-E}\,\xi/2\right) L^m_{n_1+m}(\xi\sqrt{-E}) \\ &\quad \times \eta^{m/2} \exp\left(-\sqrt{-E}\,\eta/2\right) L^m_{n_2+m}(\eta\sqrt{-E}). & (2.44) \end{aligned}$$

Since $c_1 + c_2 = 1$ we conclude from Eqs. (2.41, 2.43) that

$$\frac{1}{\sqrt{-E}} = n = \frac{1}{\sqrt{-2\bar{E}}},$$

where the integer number n is identified as the principle quantum number and is related to n_1 and n_2 via

$$n := n_1 + n_2 + m + 1 = 0, 1, 2, \cdots, \quad \text{i.e.} \quad E = -\frac{1}{n^2}.$$

The connection between the separability sketched above and the Laplace-Runge-Lenz vector becomes apparent when the component $\mathbf{N}_z$ ($\mathbf{L}_z$) of $\mathbf{N}$ ($\mathbf{L}$), along a chosen quantization axis, is expressed in parabolic coordinates. This has been done by V. Bargmann [6] who showed that the states $|n_1 n_2 m\rangle$ are eigenvectors of $\mathbf{N}_z$, $\mathbf{L}_z$ and H.

The operator $\mathbf{N}$ is a polar vector (odd under parity operation). In contrast $\mathbf{L}$ is an axial vector and as such is even under parity. Therefore, as far as parity is concerned, the states

$|n_1 n_2 m\rangle$ are mixed, i.e. they have no well-defined parity. This is as well clear from the definition of the parabolic coordinates (2.28) that gives preference to the z direction (and therefore the parabolic eigenstates derived above are symmetrical with respect to the plane $z = 0$).

The presence of a preferential space direction in the definition of the parabolic variables makes this coordinate system predestinate for formulating problems that involve a direction determined by physical measurements, such as an external electric field or the asymptotic momentum vector of a continuum electron. A well-known demonstration of this statement is the separability in parabolic coordinates of the two-body Hamiltonian in the presence of an electric field $\mathcal{E}$ (the Stark effect). In this case one chooses the z axis to be along the field and writes down the Schrödinger equation as

$$(H - \mathcal{E}\, z - E)\, \phi = 0.$$

Expressing this relation in the coordinate (2.28) and making the ansatz (2.32) one obtains two separate, one-dimensional differential equations for the determination of u_1 and u_2, namely

$$\left[\partial_\xi \xi \partial_\xi + \frac{E}{4}\xi - \frac{m^2}{4\xi} + \frac{\mathcal{E}}{2}\xi^2 + c_1\right] u_1(\xi) \quad = \quad 0, \tag{2.45}$$

$$\left[\partial_\eta \eta \partial_\eta + \frac{E}{4}\eta - \frac{m^2}{4\eta} - \frac{\mathcal{E}}{2}\eta^2 + c_2\right] u_2(\eta) \quad = \quad 0. \tag{2.46}$$

These relations make evident the complete separability of the Stark effect in parabolic coordinates.

2.3.3 Analytical continuation of the two-body Coulomb wave functions

Another example involving a physically defined direction in space occurs in ionization problems. There, the wave vector $\mathbf{k}$ of the continuum electron is specified experimentally. Thus, a suitable choice for the space direction $\hat{\mathbf{z}}$, that enters the definition of the parabolic coordinates, is $\hat{\mathbf{z}} \equiv \hat{\mathbf{k}}$. In this case the parabolic coordinates are

$$\xi \quad = \quad r + \mathbf{r} \cdot \hat{\mathbf{k}}, \tag{2.47}$$

$$\eta \quad = \quad r - \mathbf{r} \cdot \hat{\mathbf{k}}, \tag{2.48}$$

$$\varphi \quad = \quad \arctan(y/x). \tag{2.49}$$

Since we are dealing in case of $\bar{E} > 0$ with continuum problems one may wonder whether it is possible to utilize the wave function (2.32) (with the asymptotically decaying behaviour (2.37)) to describe the two-particle continuum, i.e. whether Eq. (2.32) can be continued analytically across the fragmentation threshold. To answer this question we note that the associated Laguerre polynomials can be written in terms of the confluent hypergeometric functions[5] ${}_1F_1(a,b,z)$ [11,12] as

$$L_n^m(z) = \frac{(m+n)!}{m!n!}\;{}_1F_1(-n,m+1,z). \tag{2.52}$$

Defining the (generally) complex wave vector $k = \sqrt{2\bar{E}}$ and choosing the phase convention for Eqs. (2.44) such that

$$\phi = N_E\, e^{\pm i\, m\varphi} u_1^* u_2 \tag{2.53}$$

we deduce the general solution of Schrödinger equation for one electron in the field of a residual ion with a unit positive charge (i.e. Eq. (2.32)) as (we recall the assumption that the electron-ion reduced mass is unity)

$$\begin{aligned}\phi \;=\;& N_{k,m}\, e^{\pm i\, m\varphi}\; \xi^{m/2}\eta^{m/2}\; e^{i\mathbf{k}\cdot\mathbf{r}}\\ & {}_1F_1(-i\frac{c_1}{k} + \frac{1-m}{2}, 1+m, -ik\xi)\\ & {}_1F_1(i\frac{c_2}{k} + \frac{1-m}{2}, 1+m, ik\eta),\end{aligned} \tag{2.54}$$

where $\quad m \geq 0,\; N_{k,m} = N(k, \pm m),\; c_1 + c_2 = 1,\; k \in \mathbb{C}.$

Since ${}_1F_1(a,b,z)$ is analytic for all values of the complex arguments a, b, z, except for negative integer values of b one can use Eq. (2.54) for the description of the all bound and continuum states. Outgoing continuum waves characterized by the wave vector $\mathbf{k}$ are obtained from (2.54) upon the substitution $m \to 0,\; c_1 \to -ik/2$ in which case (2.54) reduces to

$$\phi_{out} \;=\; N_k^+ e^{i\mathbf{k}\cdot\mathbf{r}}\;{}_1F_1(-i\alpha_k, 1, ik(r - \hat{\mathbf{k}}\cdot\mathbf{r})\,). \tag{2.55}$$

---

[5] The confluent hypergeometric function ${}_1F_1(a,b,z)$ is the solution of the confluent Kummer-Laplace differential equation [11,12]

$$z\,u'' + (b-z)u' - a\,u = 0. \tag{2.50}$$

${}_1F_1(a,b,z)$ is also called Kummer's function of the first kind. The confluent hypergeometric function has the series representation [11,12]

$${}_1F_1(a,b,z) = 1 + \frac{a}{b}z + \frac{a(a+1)}{b(b+1)}\frac{z^2}{2!} + \cdots = \sum_{j=0}^{\infty}\frac{(a)_j}{(b)_j}\frac{z^j}{j!}, \tag{2.51}$$

where $(a)_j$ denotes the Pochhammer symbols; its form is inferred from (2.51). The power series representing the function ${}_1F_1(a,b,z)$ is convergent for all finite $z \in \mathbb{C}$. If a and b are integers, $a < 0$, and either $b > 0$ or $b < a$, then the series yields a polynomial with a finite number of terms. Except for the case $b \leq 0,\; b \in \mathbb{N}$, the function ${}_1F_1(a,b,z)$ is an entire function of z.