Diffusion Tensor Magnetic Resonance Tomography and Cerebral White Matter Tractography

Walter Schempp

Lehrstuhl fuer Mathematik I
University of Siegen
57068 Siegen, Germany

schempp@mathematik.uni-siegen.de

Abstract
The technique of diffusion tensor imaging provides two unique insights into tissue microstructure: It quantifies non–invasively diffusion anisotropy of proton motion, which is a useful signum of cerebral white matter integrity, and provides an estimate of the principal direction of axon fibers, which enables white matter tractography.

The paper presents a novel approach to the magnetic resonance modality of diffusion tensor imaging which is based on the Lévy-Khintchin integral representation of the expectation value of Lévy processes thought of as random walks in continuous time, that is they are stochastic processes with independent and stationary increments. The proof is based on nilpotent harmonic analysis, contact geometry and the symbolic calculus of quantum field theory.

Diffusion tensor imaging provides indirect insights into the brain microstructural characteristics of patients suffering of different forms of dementias, improving the comprehension of the underlying pathophysiological processes that result in macroscopic brain tissue loss over time.

Keywords : Harmonic analysis on the Heisenberg unipotent Lie group, clinical magnetic resonance tomography, diffusion tensor imaging, DTI white matter tractography, Lévy stochastic processes, Lévy–Hinčin spectral formula for the expectation operator E, matter–waves

"There are three stages in the history of every medical discovery. When it is first announced, people say that it is not true. Then, a little later, when its truth has been borne in on them, so that it can no longer be denied, they say it is not important. After that, if its importance becomes sufficiently obvious, they say that anyhow it is not new."

- Sir James Mackenzie

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"Long ago, Paul Lévy invented a strange family of random walks - where each segment has a very broad probability distribution. These flights, when they are observed on a macroscopic scale, do not follow the standard Gaussian statistics. When I was a student, Lévy's idea appeared to me as (a) amusing, (b) simple - all the statistics can be handled via Fourier transforms - and (c) somewhat baroque: where would it apply? As often happens with new mathematical ideas, the fruits came later."

- Pierre–Gilles de Gennes

"Diffusion MRT *has tremendous potential in elucidating brain structure and cicuitry in health and disease, but the approach is fraught with methodological and interpretational challenges."*

- David C. van Essen

"The sciences do not try to explain, they hardly even try to interpret, they mainly make models. By a model is meant a mathematical construct which, with the addition of certain verbal interpretations, describes observed phenomena. The justification of such a mathematical construct is solely and precisely that it is expected to work."

- John von Neumann

1 Introductory Remarks

Seeing deeply inside a test object is an invaluable aid to understanding it, so true three–dimensional subsurface imaging is a pressing objective in areas ranging from molecular and cell biology to investigations of the electronic and structural properties of materials. The challenge is made more difficult by the desire to see the test object without affecting it in the *in vivo* visualization process. This requires a delicate touch, involving as weak an interaction as possible with the object. But such an approach often conflicts with the need for the high spatial resolution that makes fine detail visible for the observer under avoidance of radiation damage.

The modality of nuclear magnetic resonance (NMR) is arguably one of the most versatile and sophisticated experimental methods in chemistry, physics and biology, providing non–invasive insight into the structure and dynamics of matter at the molecular scale. The second–generation imaging variant of NMR, magnetic resonance tomography (MRT), offers an impressive scenario of three–dimensional pictures. Year after year, MRT protocols reveal surprising insights into morphology, function, and metabolism. In addition, MRT protocols provide a unique window to quantify the diffusional characteristics of a wide range of biological specimens. Rather than measuring how energetic particles interact with these test objects to receive an image at the molecular scale, the technique of MRT uses pulse trains of radio waves whose energy is less than a billionth of that of X–rays used for the diffraction studies of computer tomography (CT) or the electrons used in an electron microscope ([2], [5]).

Fortunately, the anatomy that has been demonstrated with MRT studies is well integrated into the knowledge that has been achieved through the X–ray CT modality. However, the contrast mechanisms for the two imaging modalities are completely different. CT relies on differential attenuation of an X–ray beam, whereas MRT relies on the synchronized interaction of the *phase response* of tissues to applied electromagnetic fields. The representation theory of the three–dimensional real Heisenberg unipotent Lie group $\mathcal{N}$ allows to implement the phase response. The bimodal *coadjoint orbit* picture of the unitary dual $\hat{\mathcal{N}}$ in the vector space dual Lie$(\mathcal{N})^*$ of the real Heisenberg nilpotent Lie algebra Lie$(\mathcal{N})$ provides a visualization of $\hat{\mathcal{N}}$ which consists of the equivalence classes of irreducible unitary linear representations of $\mathcal{N}$.

The MRT scanner manufacturers are in a never–ending battle to upstage each other with the strength of their linear gradient control packages. What this translates to for the practicing radiologist is shorter time T_E to spin echo acquisition, smaller fields of view, faster scanning protocols, and higher contrast resolution. The community of radiologists encourages these battles with their demands for image quality, but pay through one of their apertures for the scanners' costs.

2 Quantum Engineering and Visualization

Anisotropic diffusion of water molecules in neural fibers such as nerve, white matter in spinal cord, or white matter in human brain forms the basis for the utilization of diffusion tensor imaging, sometimes referred to as DTI, to track fiber pathways. The fact that molecular water diffusion within confining cellular structures is sensitive to the underlying tissue microstructure provides a unique technique of measuring the orientation and integrity of these neural fibers which may be useful for assessing a variety of neurological disorders and monitoring the course of these diseases.

Diffusion in the context of diffusion–weighted MRT refers to the processes of stochastic thermal motion and random collisions of molecules or atoms in fluids and gases, a phenomenon also known as linear Brownian random motion. The Brownian random displacements of molecules in biological tissues results in phase shifts that are widely dispersed and therefore the phase dispersion can be used as an internal signum of contrast. The molecular displacements are over distances comparable with the cell's dimensions and reflect the geometry and spatial organization of tissue compartments. Anisotropic diffusion allows to gather functional insight concerning exchanges between these compartments in various normal physiological or pathophysiological states ([2], [4]).

The stochastic wave functions emitted by pulse stimulated nuclear ^{1}H *spin tagged* water molecules provide a *quantum field* theoretic description of anisotropic quantum diffusion processes which is similar to a classical random walk. Indeed, between two photon emissions, the quantum wave functions obey a phase coherent *deterministic* evolution, just as a Brownian particle obeys a free flight between any two collisions. The quantum phenomenon of photon emission is considered in linear gradient controlled directions inside the coherent magnetic field which is externally driven by the MRT scanner, just as the collisions experienced by a Brownian particle. In the

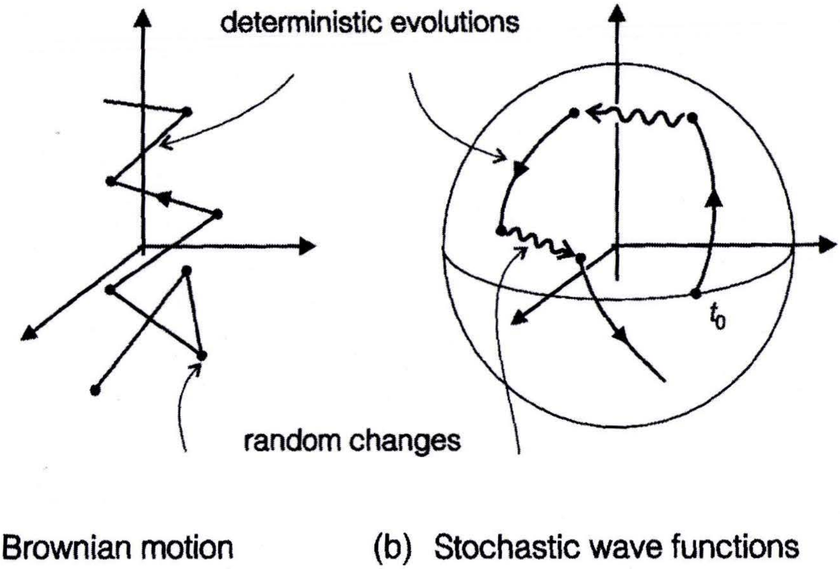

Figure 1: Random flight protocols: (a) A classical particle under the influence of collisions with gas molecules interrupting free flights. (b) Feynman diagram of a stochastic wave function under the influence of stimulated photon emissions. The stochastic wave function is normalized and therefore the random flight with waiting periods or relaxation times is on the two–dimensional Bloch sphere $\mathbb{S}_2$ embedded into the three–dimensional real projective space $\mathbb{P}_3(\mathbb{R})$.

pioneering work of Felix Bloch (1905 to 1983) and Edward Mills Purcell (1912 to 1997) on NMR in bulk matter, Bloch's experimental design was couched in more dynamical terms, which can be seen as deriving the nuclear $\mathbf{Spin}(3, \mathbb{R})$ choreography from the two–dimensional Bloch sphere $\mathbb{S}_2$ in the three–dimensional real projective space $\mathbb{P}_3(\mathbb{R})$. Its north pole represents the spin–up state $\uparrow$, its south pole the spin–down state $\downarrow$. In terms of the *photon echo* polarization concept of bimodal wave optics, the north pole represents circularly right polarized light, and the south pole circularly left polarized light. The points on the equator represent linearly polarized light.

Reorienting nuclear magnetic moments was the conceptual image that influenced Bloch's experimental design in his discovery of the NMR phenomenon. Quantum field theory, spin factors, and Feynman diagrams visualizing the interaction between vectors and spinors were still not available in the fall of 1945 when NMR in bulk matter was a reality. However, unbeknownst to each other at that time, the experimental achievements of Bloch and Purcell opened up a very active area of physical research and contributed to the theoretical development which inspired all the subsequent research studies on these matters until today ([6], [8]).

In clinical MRT studies, stochastic molecular motion can be observed through the phenomenon of signal attenuation caused by the phase dispersion. This fact was first recognized in the seminal spin–echo experiment performed by the NMR pioneer Erwin Louis Hahn in 1950, long before the invention of magnetic resonance as a non–invasive imaging modality for the *in vivo* visualization of soft tissue. Hahn explained the reduction of signal intensity of the spin–echo in terms the dephasing of nuclear spin populations caused by translational diffusion within an inhomogeneous magnetic field and proposed that one could measure the diffusion coefficient of a solution containing nuclear spin–labeled molecules. A few years later, Hermann Y. Carr and Edward Mills Purcell refined Hahn's spin–echo experiment by describing diffusion–weighted NMR experiments ([7]). However, without the inclusion of the excitations by spin–echo carrier π pulse sequences into the nuclear $\mathbf{Spin}(3, \mathbb{R})$ choreography, the recently accomplished *quantum entanglement* transfer between macroscopicically separated mechanical oscillators and their nuclear spin motion could not be successfully realized.

In the experiment formerly considered by Carr and Purcell, a constant magnetic field gradient is applied through the entire Hahn spin–echo experiment. As a result of the Larmor precession at the magnetic field superimposed by the constant gradient, the protons undergo a phase shift in the clockwise direction on the plane perpendicular to the direction of the main magnetic field. Therefore the net phase shift that influences the NMR signal at the echo time $\mathrm{T_E}$ is related via spinorial resonance to the motional history of the water molecules in the ensembles. By exploiting this resonance phenomenon, the NMR spin–echo gets sensitive to the effects of diffusion within the underlying tissue microstructure. This elevated NMR as a gold standard for measuring molecular diffusion. Quantum field theory leads via the Bargmann–Fock representation of the three–dimensional real Heisenberg unipotent Lie group $\mathcal{N}$ to the fundamental spinorial version of the Lévy–Hinčin representation associated with the real vector space duality $(\mathrm{Lie}(\mathcal{N}), \mathrm{Lie}(\mathcal{N})^*)$ and its canonical $\mathbb{R}$–bilinear form of linear gradient control

$$\mathrm{Lie}(\mathcal{N}) \times \mathrm{Lie}(\mathcal{N})^* \ni (v, \ell) \mapsto \ell(v) \in \mathbb{R}$$

In the control by means of superpositions of linear gradients on the main magnetic field, the dual vector space $\mathrm{Lie}(\mathcal{N})^*$ is assumed to be transversally fibered under the bimodal coadjoint action $\mathrm{CoAd} = {}^t\mathrm{Ad}^{-1}$ of the Heisenberg unipotent Lie group $\mathcal{N}$.

This action provides $\mathrm{Lie}(\mathcal{N})^*$ with a *bipartite* principal $\mathcal{N}$ fibration of transversal planes and gives rise to the tautologous Hopf fibration $\mathbb{S}_1 \hookrightarrow \mathbb{S}_3$ over the Bloch sphere $\mathbb{S}_2 \cong \mathbb{P}_1(\mathbb{C})$ with the third homotopy group $\pi_3(\mathbb{S}_2) \cong \mathbb{Z}$ of nuclear $\mathbf{Spin}(3, \mathbb{R})$ choreography.

Actually nilpotent harmonic analysis, Lie sphere geometry and the *symbolic calculus* of quantum field theory reveal to form the natural framework for establishing the spinorial version of the Lévy–Hinčin formula for the expectation operator

$$\mathbb{E}(\mathbf{e}(\ell(X_t)), \mu) = \exp\Big(-t\,(\frac{1}{2}Q(\ell) + i\gamma(\ell) + \int_{\mathrm{Lie}(\mathcal{N})} (1 - \mathbf{e}(\ell(v)) + i\ell(v)\mathbf{1}_{\mathcal{B}}(v))\,\mathrm{d}\lambda(v))\Big)$$

of the Lévy process $(X_t)_{t\in\mathbb{R}_+}$ with respect to the infinitely divisible spectral measure μ uniquely determined by the Lévy measure λ on $\mathrm{Lie}(\mathcal{N})$, the positive semi–definite quadratic form Q derived from the projection onto the Bargmann–Fock representation of $\mathcal{N}$, the drift coefficient γ, and the open unit ball $\mathcal{B} \subset \mathrm{Lie}(\mathcal{N})$. As usual, $\mathbf{e}(\theta) = e^{i\theta}$ for the phase angle $\theta \in \mathbb{R}$ describes the phase circle $\mathbb{S}_1 \cong \mathbb{T}$ within the symplectic plane $\mathbb{R} \oplus \mathbb{R} \cong \mathbb{C}$. It forms the prototypical fiber of the tautologous Hopf fibration $\mathbb{S}_1 \hookrightarrow \mathbb{S}_3 \longrightarrow \mathbb{S}_2$ over the Bloch sphere in $\mathbb{P}_3(\mathbb{R})$.

To switch from first–generation NMR to third–generation diffusion–weighted MRT imaging methods, there are at least three reasons why DTI forms an important *in vivo* visualization modality. First, macroscopic morphological MRT based on the signatures of relaxation times cannot reveal detailed anatomy of the white matter. The second reason is that, even after decades of intensive anatomical studies of the human brain, the understanding of its connectivity is far from complete. There are many pathophysiological conditions in which abnormalities in specific connections are suspected, but are difficult to delineate. It is anticipated that DTI tractography may provide new information about human brain connectivity. Third, DTI is a non–invasive imaging modality which admits high spatial resolution for the *in vivo* visualization ([9]).

On diffusion–weighted MRT images, structures with unrestricted diffusion such as cerebrospinal fluid are dark, while structures with restricted diffusion are bright. In the living human brain, gray matter diffusion is isotropic. White matter diffusion is variable and dependent on the relative orientation of the myelin sheats along the axonal tracts. The myelin sheats are able to restrict free diffusion. This can be used to advantage. By applying the magnetic field gradient in one direction the pulse sequence is sensitized for diffusion in that direction. Fiber tracts parallel to this direction will show maximal signal loss, whereas the effect is minimal if the linear gradient is perpendicular to the fiber tracts. By application of diffusion gradients in three directions the anisotropy of the white matter can be visualized in studying, for example, myelination progress; to use the values of diffusion in different directions and ensemble average the values to cancel the anisotropy and obtain so–called trace maps, for example for the diagnosis of infarctions and infections; or to maximize the anisotropy information by using multiple gradients to obtain diffusion tensor measurements, which allow the display of fiber tracts in the Cerebrum.

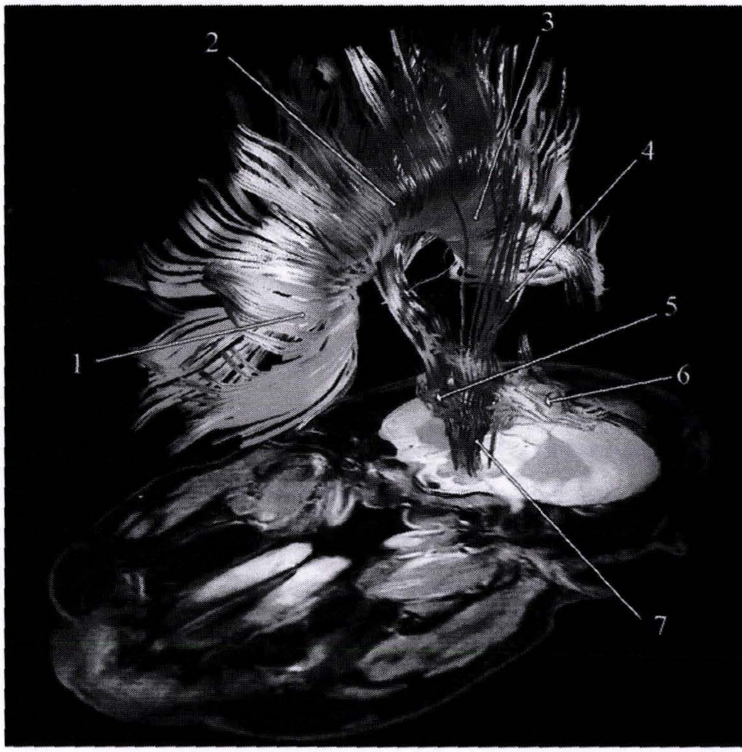

Figure 2: Three–dimensional fiber–tracking diffusion tensor MRT of the Corpus callosum: transversal seed region (1 = Genu corporis callosi, 2 = Truncus corporis callosi, 3 = Splenium corporis callosi, 4 = Tractus pyramidalis, 5 = Pedunculus cerebellaris medius, 6 = Pedunculus cerebellaris superior, 7 = Tractus frontopontinus). The thin horizontal tomographic slice through the cerebral anatomy is performed by the morphological MRT modality.

Close inspection of the main diffusion directions suggests that the macroscopic shape of white matter tracts can be reconstructed by connecting several diffusion orientations. By choosing a starting point within a *seed region* and following the main diffusion direction, trajectories can be constructed that visualize the fiber tracts of white matter. A typical example arises when a seed region was placed within the corpus callosum, the guiding structure of cerebral anatomy, and all fibers through the seed region were reconstructed at macroscopic resolution. The colour

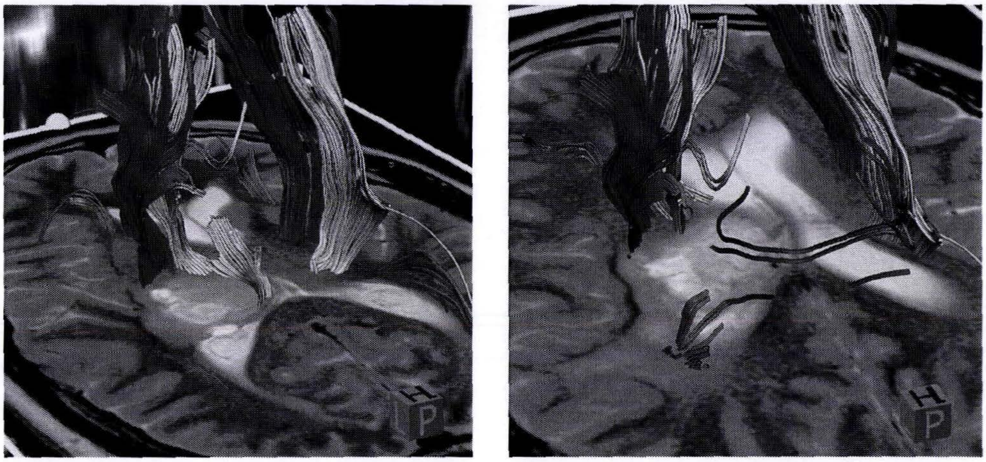

Figure 3: DTI tractography visualizes radial displacement of white matter by a left thalamic Glioblastoma multiforme. The optic radiations of the left hemisphere are displaced inferolaterally, and the transthalamic white matter tracts are displaced radially at the rostral margin of the brain tumor with abrupt termination. The longitudinal fiber tracts remain intact under the anterior deviation within the transversal seed plane.

encoding indicates the orientation of the various fiber pathways, and the three–dimensional reconstructions demonstrate the clear discrimination of white and gray matter structures in the living human brain. Although the gray matter primarily contains neurons and their processes, the white matter is composed predominantly of myelinated bundles of axons. A discrimination of white and gray matter is of great value for the clinical diagnosis of multiple sclerosis where the number of nerve fibers is significantly decreased to demyelinating lesions ([10]).

3 Visualization and Stochastic Processes

The probabilistic aspects of DTI are formed by the concept of Lévy process with drift. The flights of Lévy processes can be thought of as random flights in *continuous* time scale, that is they are stochastic processes with spatially homogeneous or stationary independent increments. The Weierstraß random walk is a one–dimensional example of a Lévy flight. Such Lévy flights attracted new interest in their application to the quantum optical techniques of laser cooling to bring atoms to rest, and risk evaluation in financial mathematics. Lévy processes can be thought of as a unification of Brownian random motion and Poisson process. On first encounter, these two types of stochastic processes would seem to be considerably different from one another. Firstly, Brownian motion has continuous paths whereas a Poisson process does not. Secondly, a Poisson process is a non–decreasing stochastic process and thus has trajectories of bounded variation over finite time horizons whereas a Brownian random motion does not have monotone paths and in fact its paths are of unbounded variation over finite time horizons. As prototypes of Markov processes, Lévy processes involve many aspects of probability theory and its applications. The property of spatial homogeneity of Lévy processes provides significant simplifications of the theory of Markov processes.

According to the Lévy–Itô decomposition, a Lévy process can be uniquely represented as the decomposition into three independent Lévy processes, the first component being a linear transform of a linear Brownian random motion with drift, the second component being a compound Poisson process with jumps of size at least 1, and finally the third component being a pure–jump martingale with jumps of size less than 1 ([1]). The drift is controlled by incorporating additionally bipolar gradients within a spin–echo sequence, referred to as diffusion gradients or Stejskal–Tanner gradients in order to measure the stochastic molecular motion via the signal attenuation profile. Orginally, these were two identical gradients on both sides of the refocusing π pulse of a spin–echo pulse sequence. The pulsed gradient spin–echo (PGSE) sequence replaced the constant magnetic field proposed by Carr and Purcell with sequenes of short duration gradient pulses.

Today, diffusion–weighted MRT imaging of the brain is almost exclusively performed with single–shot echo planar imaging (EPI) sequences with spin–echo excitation in the parallel imaging mode. The diffusion preparation of these pulse sequences is the same as in the standard spin–echo sequences, but instead of acquiring a single spin–echo after each pulse stimulation, the full symplectic seed plane can be read. The advantages of spin–echo EPI sequences are a very short acquisition time of less than 200 ms per tomographic slice and its insensitivity to non–diffusion–related signal losses due to voluntary patient motions such as breathing and swallowing, and involuntary motions which include cerebrospinal fluid pulsations and the bulk motions of the cardiac cycle. Higher magnetic field densities of 3 Tesla and above enable DTI at higher contrast resolution and shorter acquisition time. However, susceptibility artifacts in areas such as the skull base and the posterior fossa increase markedly at higher magnetic field densities.

It is well known that any *infinitely divisible* probabilistic spectral diffusion measure μ on $\mathbb{R}^3 \hookrightarrow \mathbb{P}_3(\mathbb{R})$ can be viewed as the distribution of a Lévy process evaluated at time $t_0 = 1$. The converse is obvious. The proof provides an explicit construction of this Lévy process, and sheds a probabilistic light on the linear gradient controlled spinorial Lévy–Hinčin representation. In particular, the Lévy–Hinčin spectral formula reflects the rich mathematical structure of Lévy flights. Because it is quadratic at the level of the Heisenberg nilpotent Lie algebra Lie($\mathcal{N}$), the quantum field theoretic version of the Siegel theory of quadratic forms ([12]) and the Lie sphere geometry can be applied to establish a Fourier transform version of the underlying stochastic processes which offer an *imaging fusion* of DTI tractography and MRT modality.

Fiber tractography based on the modality of DTI reveals macroscopic white matter connectivity of the human brain. The mathematical approach to non–invasive cerebral white matter tractography is based on the transition from harmonic analysis on the real three–dimensional real Heisenberg unipotent Lie group to stochastic harmonic analysis of infinitely divisible probabilistic spectral diffusion measures μ. It consists in the cross–sectional implementation of the spinorial Lévy–Hinčin representation of the underlying Poisson point process in terms of the compact Heisenberg nilmanifold $\mathcal{N}^0$. The stochastic point process on this principal circular fiber bundle over the two–dimensional compact flat torus $\mathbb{T}^2$ describes the evolution process of a single nuclear ^{1}H spin tagged water molecule as a stochastic evolution consisting of a train of coherent evolution periods separated by quantum jumps consisting of pulse stimulated emission processes. The contact geometric implementation of streamline tractography by a DTI Task Card is performed by the Kepplerian symplectic sampling technique of sweeping over the cross–sectional nuclear spin trajectories.

The DTI modality also provides indirect insights into the brain microstructural characteristics of patients suffering of different forms of dementias, improving the comprehension of the underlying pathophysiological processes that result in macroscopic brain tissue loss over time. It has also been successfully used to provide specific markers which are able to support the diagnosis of different forms of dementias in the early stages and to monitor the course of disease. There is, however, still a long distance for an efficient model of the Alzheimer disease ([10]).

4 Quantum Engineering Matter–Waves

The magnetic field density ≥ 1.5 Tesla of clinical MRT scanners in which the patient is placed is created by coils cooled to liquid ^{4}He temperatures and exhibiting superconductivity, a fundamentally quantum effect. When trapped bosonic atoms are laser cooled down to very low temperatures, their de Broglie wavelength increases until it becomes of the order of the mean interatomic distance. At this point, the quantum system undergoes a phase transition, with a sizeable fraction of atoms condensing into the trap lowest energy state. Eventually, when the temperature is lowered to still smaller values using evaporative cooling, the condensed phase extends to the whole ultra–cold sample. The realization of this very special form in the laboratory seventy years later after its prediction in 1925 has been one of the landmarks of the quantum century.

In trapped Bose–Einstein ccndensates the atoms all belong to a global wave function. They are quanta in this giant matter–wave, in the same way as photons are quanta of the radiation field of a clinical MRT scanner during examination. In this new form of matter, the wave–particle dualism first introduced through the work of Louis–Victor Pierre Raymond duc de Broglie (1892 to 1987), has come full circle. In the quantum synthesis, the particle aspect appears as a classical attribute of matter and a quantum property of radiation. In duality, waviness is a classical feature for light, a quantum one for matter. This profound difference boils down to the fact that the radiation field is made of gregarious photonic bosons which naturally behave as collective waves, while matter is, deep down, a collection of fermions, spontaneously behaving as discrete entities.

The aspect of waviness becomes an essential feature of matter when it is made of atoms in which fermions are bound together in even number. The *pairing* of fermions in composite bosons is essential to understand phase coherence of matter–waves via the bimodal coadjoint orbit picture $\mathrm{Lie}(\mathcal{N})^*/\mathrm{CoAd}(\mathcal{N})$ of the unitary dual $\hat{\mathcal{N}}$ of the three–dimensional real Heisenberg unipotent Lie group $\mathcal{N}$ in the projective space $\mathbb{P}_3(\mathbb{R})$. Actually, the phase coherence of Bose–Einstein condensates is one of the most surprising manifestations of the quantum superposition principle which justifies the treatment of quantum engineering matter–waves by harmonic analysis on the Heisenberg Lie group $\mathcal{N}$, akin to the quantum phenomenon of superconductivity.

Exploring the phase coherence of bosonic matter–waves at the lowest temperatures encountered in nature has become a very attractive field of experimental and theoretical research. Among the new fields of research, atom optics in $\mathbb{P}_3(\mathbb{R})$ stands as an especially promising area of investigations. The bimodal coadjoint orbit picture $\mathrm{Lie}(\mathcal{N})^*/\mathrm{CoAd}(\mathcal{N})$ of the unitary dual $\hat{\mathcal{N}}$ of the three–dimensional real Heisenberg unipotent Lie group $\mathcal{N}$ provides a model that is useful for quantum engineering phase coherent matter–waves.

5 Concluding Remarks

Due to the *contact geometry* of the Heisenberg unipotent Lie group $\mathcal{N}$, the fourth–generation MRT modality, namely the technique of magnetic resonance force microscopy (MRFM), permits to pushing MRT to the nanoscale by measuring magnetic forces at the sub–attonewton scale. The powerful molecular imaging modality of MRFM can perform non–destructively three–dimensional images of biological specimens such as the tobacco mosaic virus particles. Therefore it is of particular interest to structural biologists trying to unravel the structure and interactions of proteins, especially for those proteins that cannot be crystallized for X–ray analysis.

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