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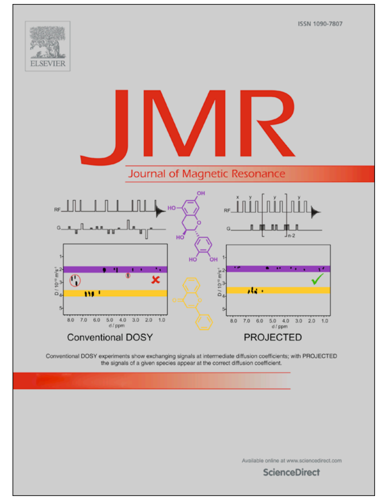

Spectral Diffusion and Dynamic Nuclear Polarization: beyond the High Temperature Approximation

W.Th. Wenckebach

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Spectral Diffusion and Dynamic Nuclear Polarization: beyond the High Temperature Approximation

W.Th. Wenckebach

Paul Scherrer Institute, CH-5232 Villigen, Switzerland

Abstract

Dynamic Nuclear Polarization (DNP) has proven itself most powerful for the orientation of nuclear spins in polarized targets and for hyperpolarization in magnetic resonance imaging (MRI). Unfortunately, the theoretical description of some of the processes involved in DNP invokes the high temperature approximation, in which Boltzmann factors are expanded up to first order, while the high electron and nuclear spin polarization required for many applications do not justify such an approximation. A previous article extended the description of one of the mechanisms of DNP—thermal mixing—beyond the high temperature approximation [1]. But that extension is still limited: it assumes that fast spectral diffusion creates a local equilibrium in the electron spin system.

Provotorov's theory of cross-relaxation enables a consistent further extension to slower spectral diffusion, but also invokes the high temperature approximation. The present article extends the theory of cross-relaxation to low temperature and applies it to spectral diffusion in glasses doped with paramagnetic centres with anisotropic g-tensors. The formalism is used to describe DNP via the mechanism of the cross effect. In the limit of fast spectral diffusion the results converge to those obtained in [1] for thermal mixing. In the limit of slow spectral spectral diffusion a hole is burnt in the electron spin resonance (ESR) signal, just as predicted by more simple models. The theory is applied to DNP of proton and ^{13}C spins in samples doped with the radical TEMPO.

Keywords: dynamic nuclear polarization, hyperpolarization, thermal mixing, cross effect, spectral diffusion, low spin temperature

1. Introduction

Dynamic Nuclear Polarization (DNP) is a powerful tool to obtain high nuclear spin polarization. During several decades the main drive for its development was the study of the role of spin in nuclear and particle physics—for a review see [2]. Then its potential to enhance Nuclear Magnetic Resonance

Email address: tom.wenckebach@psi.ch (W.Th. Wenckebach)