Electronic Supplementary Material for PCCP

Supporting materials to the article "**Para-Hydrogen Induced Polarization in Multi-spin Systems Studied at Variable Magnetic Field**" by *S. E. Korchak, K. L. Ivanov, A. V. Yurkovskaya, H.-M. Vieth*.

In these supporting materials we will present the details of magnetic field variation, which was used in our field-cycling experiments on Para-Hydrogen Induced Polarization (PHIP) to transport the polarized spin system from polarization field, B_p, to the NMR detection field, B_0. As has been pointed out in the text of the article, consideration of the real $B(t)$ profile is necessary for simulating the experimental PHIP spectra.

In our experimental setup[1, 2] field variation was carried out by moving mechanically the whole NMR probe in the fringe field of the NMR magnet and in the field of additional coils used for controlling the magnetic field below 0.1 Tesla. The magnetic field dependence on the position, z, along the bore axis of the cryomagnet is shown in Figure 1. The fields have been measured precisely by a Hall probe. The coordinate z=0 corresponds to the lowest position of the NMR probe in our experiments, which is characterized by the lowest external magnetic field. The largest coordinate, z_0, corresponds to the NMR probe located at the position, where the magnetic field is maximal (B=B_0=7 Tesla) the NMR spectrum is recorded. The distance dependence of the magnetic field is an S-shaped curve with rather small field gradients at $z\approx 0$ and $z\approx z_0$ and a steep step in between. The field gradient is largest for z between 400 and 500 mm.

The NMR probe was moved and precisely positioned along the cryomagnet bore axis by using a digitally controlled step motor. The step motor can move the probe with a selected acceleration/deceleration a_z. Once the velocity of the probe, v_z, has reached v_{max}=2.7 m/s the probe moves with this maximal velocity until deceleration is introduced. To transport the probe with the polarized sample we move the probe from the selected position z_p (corresponding to the polarization field B_p, at which non-thermally polarized spin system is formed) to the detection field (z=z_0), thus the whole travel distance is equal to $z_0 - z_p$. At z=z_p acceleration stage of the probe starts with zero initial velocity, then (1) a_z=a_0=const>0 and v_z grows linearly; (2) if v_z reaches v_{max} at $z < (z_0 - z_p)/2$ (which happens if $a_0 \tau_{fv}/2 > v_{\max}$) the velocity stays constant before deceleration starts; (3) the probe is decelerated so that a_z= $-a_0$ and the velocity linearly decreases and the probe reaches the detection field at t=τ_{fv} with zero velocity. If $a_0 \tau_{fv}/2 < v_{\max}$ the motional phase with constant velocity equal to v_{max} is skipped. Both regimes of probe motion are shown in Figure 2 for two different starting positions z_p. For small z_p values (large total distance, $z_0 - z_p$, Fig.2a) and sufficiently high a_0 value all phases of motion (acceleration-constant velocity-deceleration) are present; if the total distance becomes smaller only the acceleration and deceleration stages are present (Fig.2b).

Thus, in the case $a_0\tau_{fv}/2 > v_{\max}$ (Fig.2a) there are all three motional phases present and the maximal velocity is achieved during the probe transport. In the case $a_0\tau_{fv}/2 < v_{\max}$ (Fig.2b) the maximal velocity is not achieved and there are only the acceleration and deceleration phases present.

Knowing the position dependence of the magnetic field and the kinematics of the probe motion (i.e., summarizing up the data presented in Figure 1 and 2) we can determine the field variation profiles, $B(t)$, used in our experiments. These profiles are shown in Figure 3 for three different polarization fields B_p. As it is seen clearly the magnetic field changes non-linearly during the switching and maximal field variation speed is reached between approximately 1 and 6 Tesla where (a) the field gradient is the largest and also (b) the probe velocity is high. The low field region (where the spin system is coupled strongly) below 1 Tesla, which is characterized by moderate field gradients) is passed at a much lower speed. Because of this it is crucial to take into account the real field variation profile and not to restrict oneself to model cases of purely adiabatic or sudden field switching. It is also clear that the assumption of linear field variation is rather unrealistic and often in contradiction with the actual $B(t)$ profile.

References

1 S. Grosse, F. Gubaydullin, H. Scheelken, H.-M. Vieth and A. V. Yurkovskaya, *Applied Magnetic Resonance*, 1999, **17**, 211-225.

2 S. Grosse, A. V. Yurkovskaya, J. Lopez and H.-M. Vieth, *Journal of Physical Chemistry A*, 2001, **105**, 6311-6319.

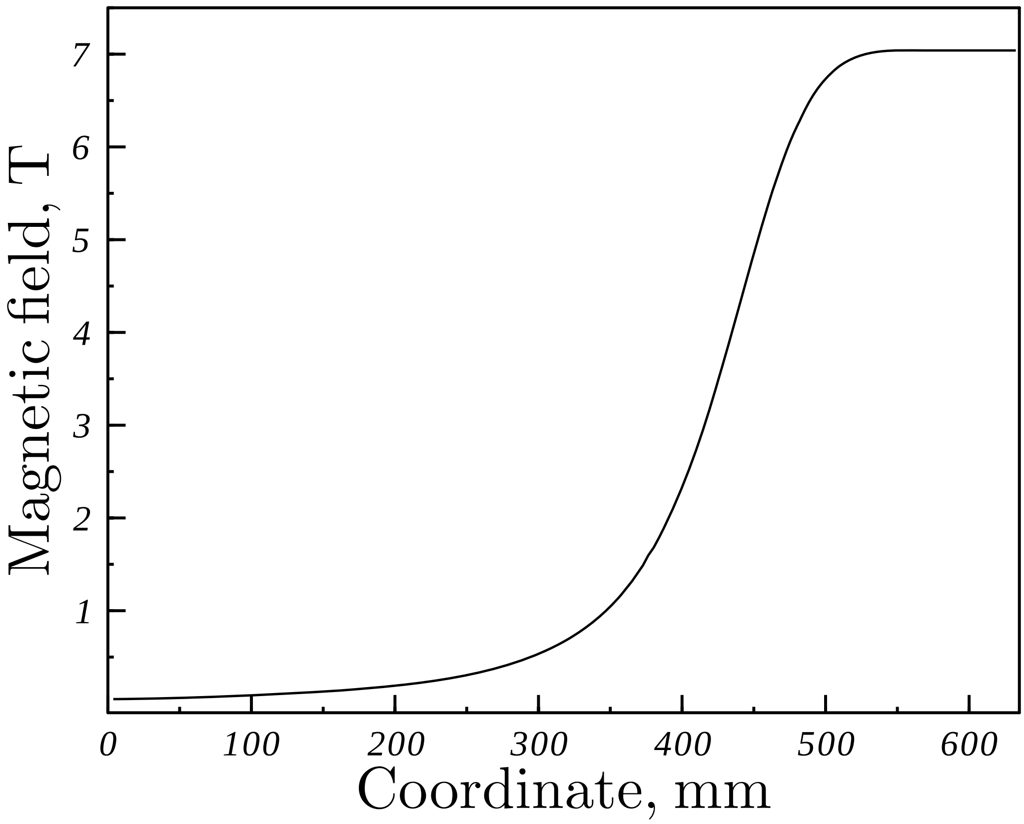

Figure S1. Distance dependence of the magnetic field strength.

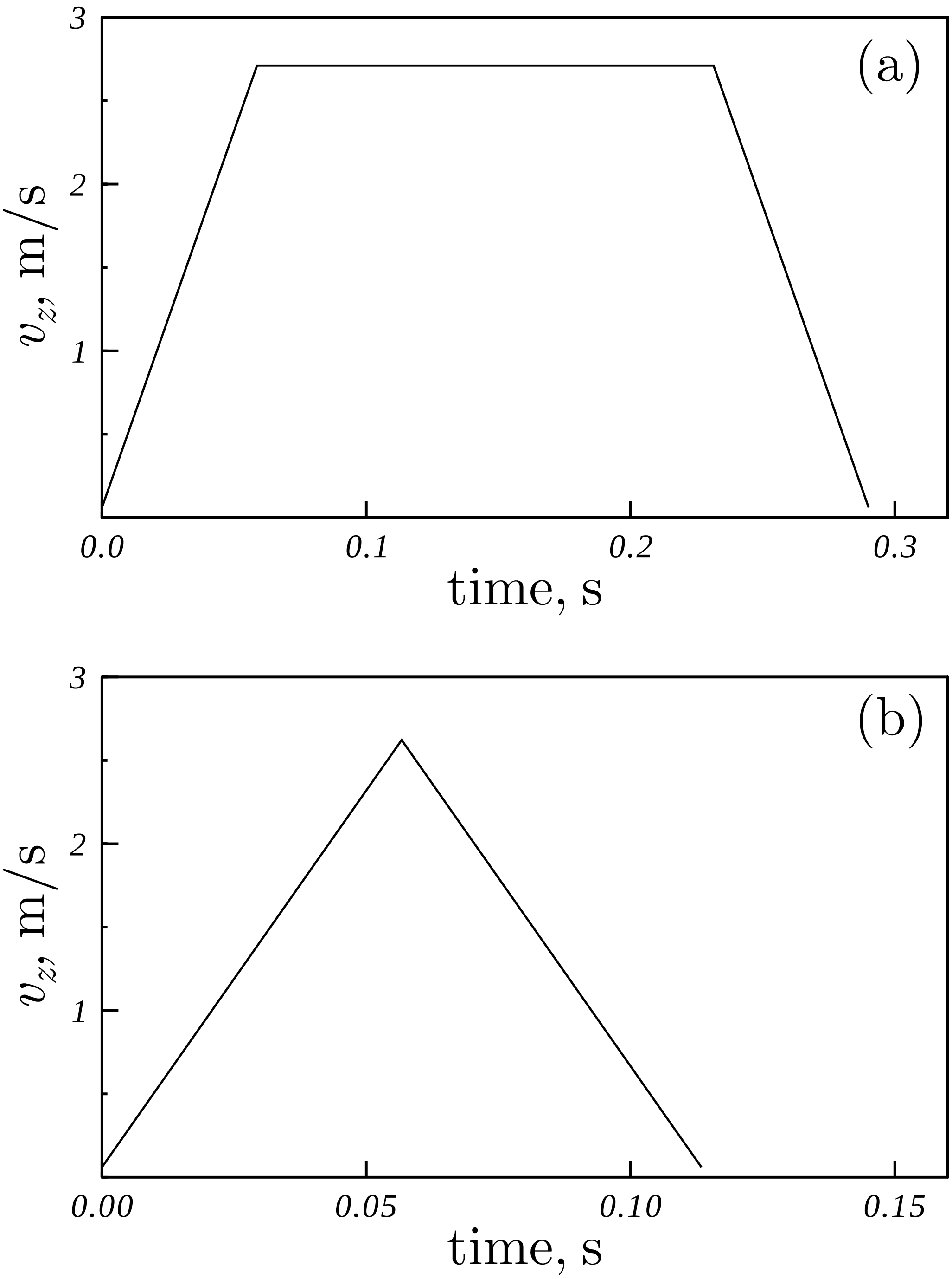

Figure S2. Probe velocity profiles during probe shuttling from positions z_p=26 mm (subplot a, corresponding to B_p=50 mT) and z_p=350 mm (subplot b, corresponding to B_p=1 T). Here a_0=45.2 m/s^2, v_{max}=2.7 m/s.

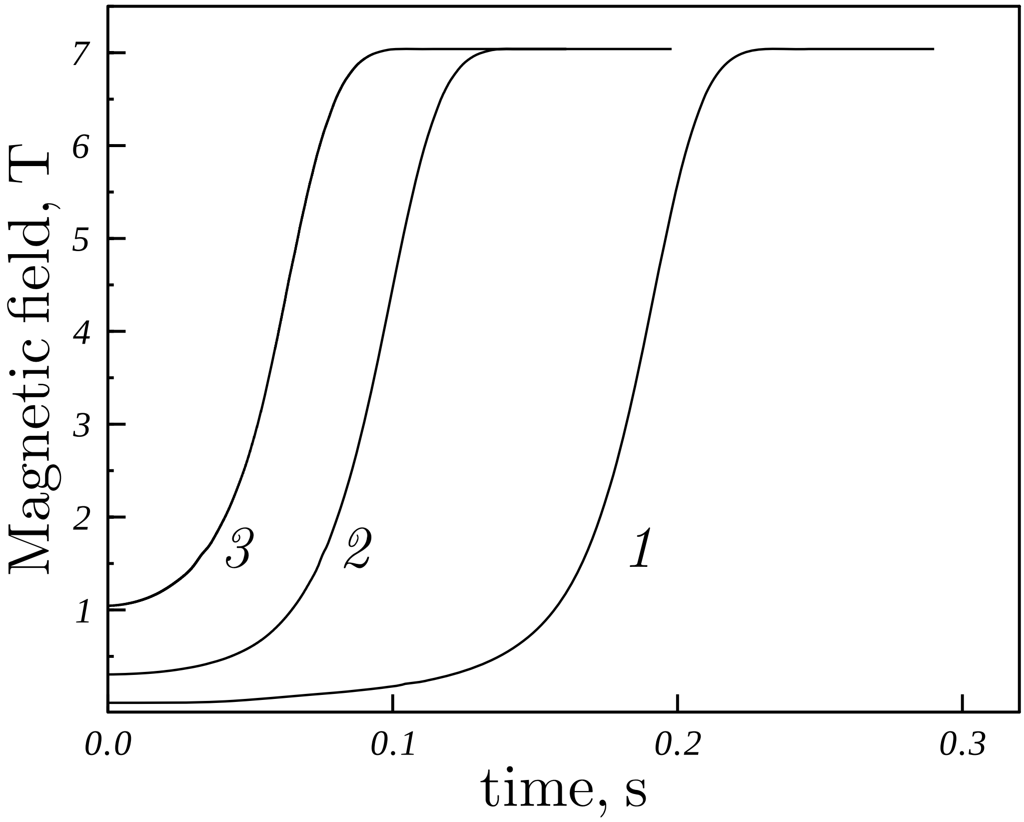

Figure S3. Magnetic field variation profiles for different polarization fields B_p of 0.1 mT (curve 1); 0.3 T (curve 2); 1 T (curve 3).