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A Practical Method for Automated Shimming with Normal Spectrometer Hardware

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Shimming, the iterative adjustment of the currents passed through correction coils placed around the active volume of an NMR magnet in order to maximize the homogeneity of the magnetic field, wastes thousands of hours of spectrometer and operator time each year. It is a tedious and at times a frustrating task, and few instrument operators would hesitate to delegate it to an automatic system were such a system to be efficient, general, and reliable. This Communication describes what may prove to be just such a system: information from spin-echo experiments on the solvent deuterium resonance using pulsed shim coil currents is used to calculate iterative shim current corrections, giving rapid convergence to excellent field homogeneity. Although the present experiments have been restricted to optimization of the most important set of shims, those acting along the long (z) axis of the sample, in principle the method can be extended to shim all gradients.

The classical method for correcting static magnetic field inhomogeneities in magnetic resonance is by the use of shaped magnetic fields generated by ''shim'' or ''Golay'' coils (*1*). For many years, the only ways to find the optimum combination of currents through the different coils was by trial and error, using either the spectrum itself or the strength of the deuterium field-frequency lock signal as a criterion of field quality, and a variety of strategies for this have been proposed [see, for example, Ref. (*2*)]. Most existing automatic methods for field homogeneity adjustment in high-resolution spectrometers rely on ''blind'' strategies such as simplex optimization, which can perform adequately in favorable circumstances but converges slowly and is easily diverted by local optima. It is relatively well known that the application of field gradients in high-resolution NMR spectroscopy can be used to provide information on the spatial dependence of field inhomogeneity, and hence could be used as the basis of directed automated shimming methods [see, for example, a recent review of ''profile shimming'' in Ref. (*3*)].

Magnetic resonance imaging systems, in which three-dimensional signal localization is routine and large signals are available, have made use of directed automatic shimming methods for some time, with early methods based on direct frequency measurements and more recent work using phase maps obtained from time-shifted spin echoes (*4*). Similar principles have recently been applied with impressive success in ''gradient shimming'' methods for high-resolution NMR. These methods use strong pulsed field gradients to encode information on field inhomogeneity into proton gradient echoes from H_2O samples (*5, 6*). This allows iterative shimming with rapid convergence and excellent final results. The principal disadvantages of the methods published to date are that they require special pulsed field gradient hardware (gradient driver amplifier, actively shielded gradient probe), that they are applicable only to samples with an extremely strong dominant resonance such as H_2O (although some success has been reported using solvent deuterium), and that a separate calibration is needed for every probe used. The use of shim coil gradient pulses, shaped to minimize eddy-current effects, in proton field mapping for automatic shimming has been described recently (*7*); the present work takes a different approach, using deuterium Carr–Purcell echoes and much weaker gradients.

The use of H_2O signals for such ''gradient shimming'' experiments is a natural development from the use of water signals for automated shimming in magnetic resonance imaging (*4*), but a more natural choice for high-resolution NMR spectroscopy would be to use the deuterium resonance of the sample solvent. Almost all samples have such a resonance available, and almost all probes are capable of deuterium observation using the lock channel. The principal problem is the limited signal-to-noise ratio of deuterium NMR, compounded by the relatively inefficient coupling to the spins afforded by the lock channels of most probes. The success of gradient shimming relies on accurate measurements of phase shifts as a function of frequency, which in turn requires good signal-to-noise ratio. The key here is to choose the gradient strength to achieve the right compromise between signal-to-noise ratio and signal dispersion; fortunately, for deuterium (and indeed for many experiments using protons and other nuclei), the gradient requirements are

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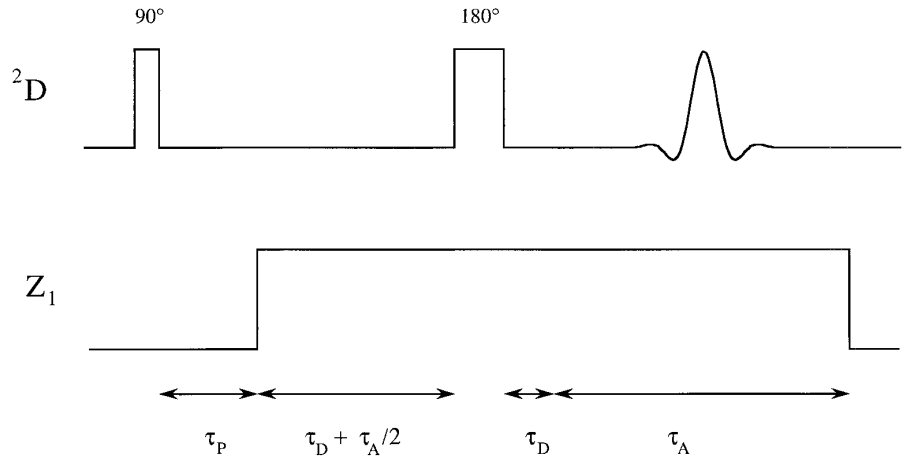

FIG. 1. Pulse sequence for gradient shimming using shim coil gradients only; EXORCYCLE phase cycling was used (*9*). The pulsed field gradient shown was provided through the *z*1 shim using the homospoil facility. The introduction of a delay τ_D (typically 10–20 ms) allows time for unwanted signals elicited by the 180° pulse to decay and hence reduces the need for phase cycling, allowing single-transient experiments to be used where signal-to-noise ratio suffices.

sufficiently modest that they can easily be met by typical shim power supplies. In the experiments described here, the requisite gradient pulses were provided by the instrument ''homospoil'' facilities, requiring little or no instrument modification.

Figure 1 shows a Carr–Purcell method A spin-echo sequence modified to encode information on field homogeneity into a signal profile. If necessary the transmitter can be offset from the midpoint of the signal profile in order to remove the influence of time-domain dc errors, and the spectrum shifted back to the center of the spectral window before processing. The spin echo generated at the midpoint of the acquisition time τ_A can be Fourier transformed to give an absolute value display of the signal strength as a function of frequency; if the field gradient (here assumed to lie along the z axis) applied during the latter part of the experiment is large compared to the other (static) gradients acting, then the spectrum obtained is a simple profile of the signal intensity as a function of z. If the field gradient is linear then the z axis scale of the profile will be linear, but this is not a requirement of the method; it suffices that the field change along the sample with the gradient applied be monotonic as a function of z.

The phase of the signal as a function of frequency (or z) will be a complex function of the field gradient, the offset from resonance, and the radiofrequency field strength distribution of the pulses. If, however, the sequence is repeated twice with different values of the delay τ_P, then the effect of the signal precession during τ_P will be to ensure that the difference in phase between the signals at corresponding points in the signal profiles for the two different delays will simply be proportional to the frequency offset at that position z during τ_P. Hence the phase differences can be used to calculate a frequency profile as a function of z which maps out the imperfections in the sample z shimming [see, for example, Refs. (*4, 5*)]. The use of a Carr–Purcell echo rather than a gradient echo removes the need to change the sign of the applied field gradient, allowing the instrument homospoil facility to be used; because the gradients used are modest, the gradient can remain on during the refocusing 180° pulse.

Given the ability to map frequency as a function of position, automated shimming reduces to the measurement of a basis set of the frequency profiles produced by each of the n_z shim coils available for the z axis (requiring $n_z + 1$ pairs of experiments), followed by iterative cycles of alternate measurement of the unwanted gradients in the sample and calculation of the changes in shim coil current required to correct the measured frequency profile. In an ideal experiment, a single cycle would suffice; in practice, the limitations imposed by finite signal-to-noise ratio and the impurities in the basis set of profiles caused by the applied gradients perturbing the signal distribution in the profiles mean that several cycles are needed where the shimming errors are large, but the method is rapidly convergent.

The choice of experimental parameters is critical, particularly the gradient strength, the difference $\Delta\tau_P$ between the precession delays used, and the changes in shim coil settings used to obtain the basis set of shim coil frequency profiles. The overriding requirement is that sufficient signal-to-noise ratio be obtainable to allow efficient and rapid shimming. For a finite amount of magnetization available, this limits the maximum gradient strength usable. The minimum gradient strength is dictated by the need for the applied gradient to dominate the errors in shimming, and for the gradient to be sufficient to allow the echo to be well sampled within the time frame of the deuterium T_2^*.

The signal-to-noise ratio of the shim coil frequency profiles is determined by the fixed uncertainty in phase introduced by the finite signal-to-noise ratio of the signal

amplitude profile. If the signal-to-noise ratio of the signal amplitude profile, conventionally defined as the signal amplitude divided by twice the root-mean-square noise amplitude, is S, then the rms uncertainty in the phase calculated from the phase difference between two profiles will be $1/(S\sqrt{2})$ radians. It is therefore important to maximize the phase excursion in the profiles, subject to the requirement that the phase remain unambiguous. The latter condition depends on the quality of the anti-aliasing algorithm used (*8*) to determine the phase where it passes a $\pm 180°$ boundary, and on the signal-to-noise ratio. On the other hand, the shim offsets used should be sufficiently small that they do not significantly perturb the signal amplitude profile, i.e., that the gradients used remain small compared to the gradient imposed during the spin echo. The choice of delay difference $\Delta\tau_P$ is dictated partly by the need to avoid phase ambiguities, and partly by the need to maximize the signal-to-noise ratio of the phase profile. Increasing $\Delta\tau_P$ increases the phase excursion, but decreases the signal amplitude through transverse relaxation and through signal dephasing due to gradients orthogonal to the applied gradient. If both sources of signal loss can be characterized by a simple time constant T_2^*, then in most cases the optimum value of $\Delta\tau_P$ will be on the order of T_2^*.

The shimming procedure outlined above was implemented on a Varian Associates INOVA 300 spectrometer using a Sparc 4 host computer. The only hardware modifications used were the use of a programmable switching line (sp1) and a double pole–double throw coaxial relay to switch automatically between gradient shimming and normal operation, and the addition of extra capacitance (11 μF in parallel with C41 of schematic 01-902295-00 sheet 3) to defeat the homospoil duration protection circuit. It should be emphasized that while this modification had no ill effect on the 14-channel shim supply on the instrument used, it may not be safe on other instruments, and great care should be taken not to overload either the shim power supply or the shim coils themselves. A more satisfactory long-term solution would be to allow software control of the homospoil amplitude, and to incorporate a safety cutoff to limit gradient system power dissipation (both peak and average). The software used was a very minor modification of that supplied as standard (revision 5.2F) with the INOVA instrument for gradient shimming using the pulsed field gradient accessory.

The shim profile basis set illustrated in Fig. 2 for the 5 z channels (nominally $z1c$, $z2c$, $z3$, $z4$, and $z5$) of the 14-channel shim set was obtained using the sequence of Fig. 1 applied to the standard degassed lineshape test sample of 5% chloroform in acetone-d_6. Four transients were used per experiment, with a recycle delay of 7.5 s and a delay τ_D of 20 ms; the deuterium 90° pulse width using the lock channel of the dual 5 mm $^{13}C/^{1}H$ probe (probe A) was 60 μs. One hundred twenty-eight complex data points were acquired per transient at a spectral width of 1 kHz, giving an acquisition time of 0.128 s; only the central 35% of the spectral window was used in the construction of the field maps. Delays τ_P of 0 and 0.1 s were used, with τ_D set to 100 μs since phase cycling was in use. Both z and transverse shims were optimized manually by conventional means before commencing mapping. The profile map can be quite informative; there is, for example, a clear first-order component in the profile for $z3$, which accords with the commonplace observation of a $z1/z3$ interaction in manual shimming on this instrument. The establishment of the shim profile basis set required approximately 8 min; this would be considerably reduced for

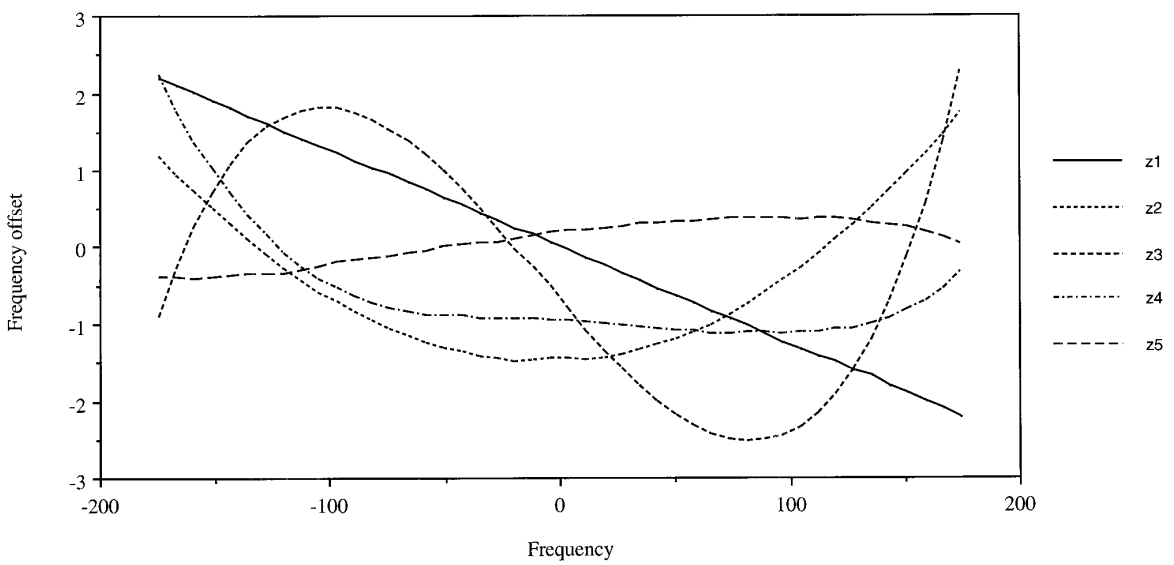

FIG. 2. Basis set of frequency profiles for the five z shims. Changes in shim coil settings were adjusted to give approximately comparable maximum frequency excursions for each shim.

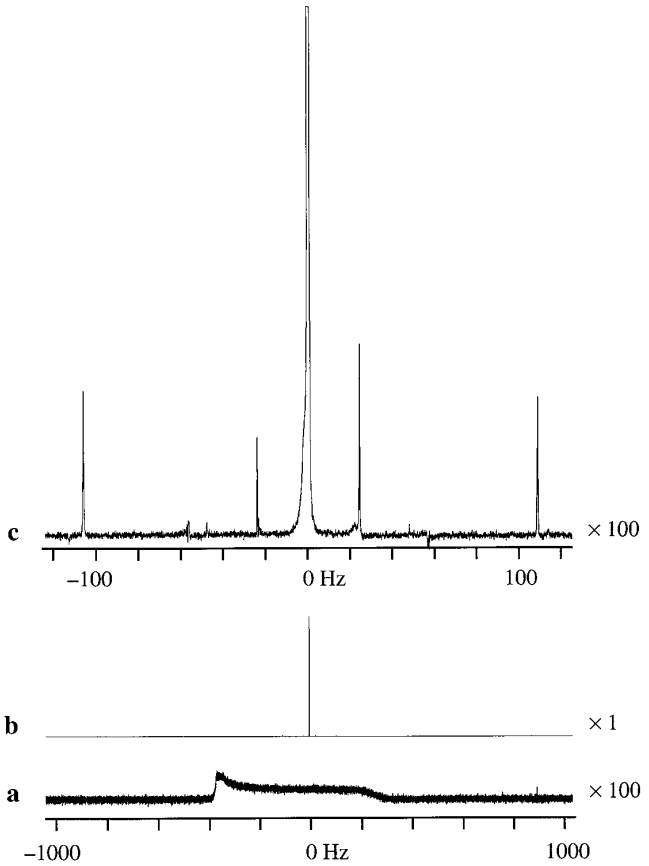

FIG. 3. The 300 MHz proton spectra of the chloroform resonance of a 5% solution of chloroform in acetone-d_6 measured in a new dual $^{13}C/^{1}H$ 5 mm probe (a) with all z shims set to zero; (b) after automatic z shimming; and (c) spectrum (b) expanded. Mild Gaussian multiplication with a time constant of 10 s was used.

a solvent with a shorter deuterium spin–lattice relaxation time. Usable maps can be obtained in as little as 1 min in favorable cases.

Figure 3 shows the application of the shimming method to a reasonably challenging problem. The shim settings used for the basis set measurement were taken and all the z shims set to zero, giving the spectrum of Fig. 3a. The sequence of Fig. 1 was then used to perform iterative correction of the z shim settings using the same experimental parameters as before, converging in 5 cycles in a total time of 2 min (approximately 40 s of acquisition and 80 s of processing). The optimization was then repeated with $\Delta\tau_P$ set to 0.3 s, again converging in five cycles in 2 min. The resultant spectrum, shown in Figs. 3b and 3c, shows a linewidth of about 0.25 Hz and comfortably exceeds the manufacturer's lineshape specification.

Figure 4 illustrates the advantages of a method which uses a single calibration for all probes, since the basis set used is determined entirely by the shim set. Probe A was exchanged for probe B, and the sample replaced by the standard sensitivity test sample of 0.1% ethylbenzene and 0.01% tetramethylsilane in deuteriochloroform. Probe B, originally manufactured as a 400 MHz 5 mm broadband probe, is particularly troublesome to shim manually. After suffering a blown tuning capacitor, it was stolen from a service engineer and dumped in the Bridgewater Canal. After recovery from the canal, it was washed in distilled water, dried, and adapted to operation at 300 MHz. Figure 4a shows the test spectrum obtained with the shim settings used for probe A; Fig. 4b shows the spectrum, with a TMS linewidth of 0.3 Hz, obtained after automatic z shimming (a total of 5 cycles in 6 min, two with a $\Delta\tau_P$ of 50 ms, and three with 300 ms). The longer shimming time was caused by the need to use 16 transients per measurement because of the much weaker signal of deuteriochloroform. The two probes used were of similar construction and had similarly positioned coil centers; some modifications to the existing software would be needed to allow the same shim basis maps to be used for probes with different coil centers, and of course any shim map used should cover the active volume of the probe. It should be noted that the treatment experienced by probe B is not essential to the success of the method.

The method described allows excellent shimming to be obtained in a short time with a bare minimum of operator intervention. The examples shown were deliberately chosen to be extreme; in practice, most samples show smaller shimming errors and convergence should be correspondingly quicker. Initial experience suggests that routine shimming typically takes a few tens of seconds, with convergence in one or two cycles. The software used makes extensive use of high-level (Vnmr macro) programming, and could be speeded up significantly. The INOVA 300 homospoil facility was used here to generate a z field gradient of about 0.48 G cm^{-1}; this figure is probably rather larger than is ideal, and a factor of 2 or 4 reduction should improve performance. Similar experiments were carried out, with similar results, on a Varian Associates Unity 500 spectrometer, this time without the need for hardware modification; here the homospoil gradient was 0.09 G cm^{-1}. Successful experiments were also performed on the 10 mm diameter broadband probe of an INOVA 400 spectrometer; the carbon-13 resolution obtained (0.13 Hz) using deuterium gradient shimming via the lock coil was significantly better than that obtainable with manual shimming.

Gradient shimming methods using normal shim coils rather than actively shielded gradient coils, and deuterium solvent signals rather than H_2O, appear likely to prove adequate even in their present form for the great majority of shimming tasks, and there is considerable scope for further improvement. More efficient programming should increase speed quite significantly. The already rapid convergence of the method could be improved further if the precession delay difference $\Delta\tau_P$ were chosen adaptively during the course of optimization, and if the purity of the initial shim coil basis mapping were improved by introducing compensation for the distortions caused by the finite $z1$ gradient strength used.

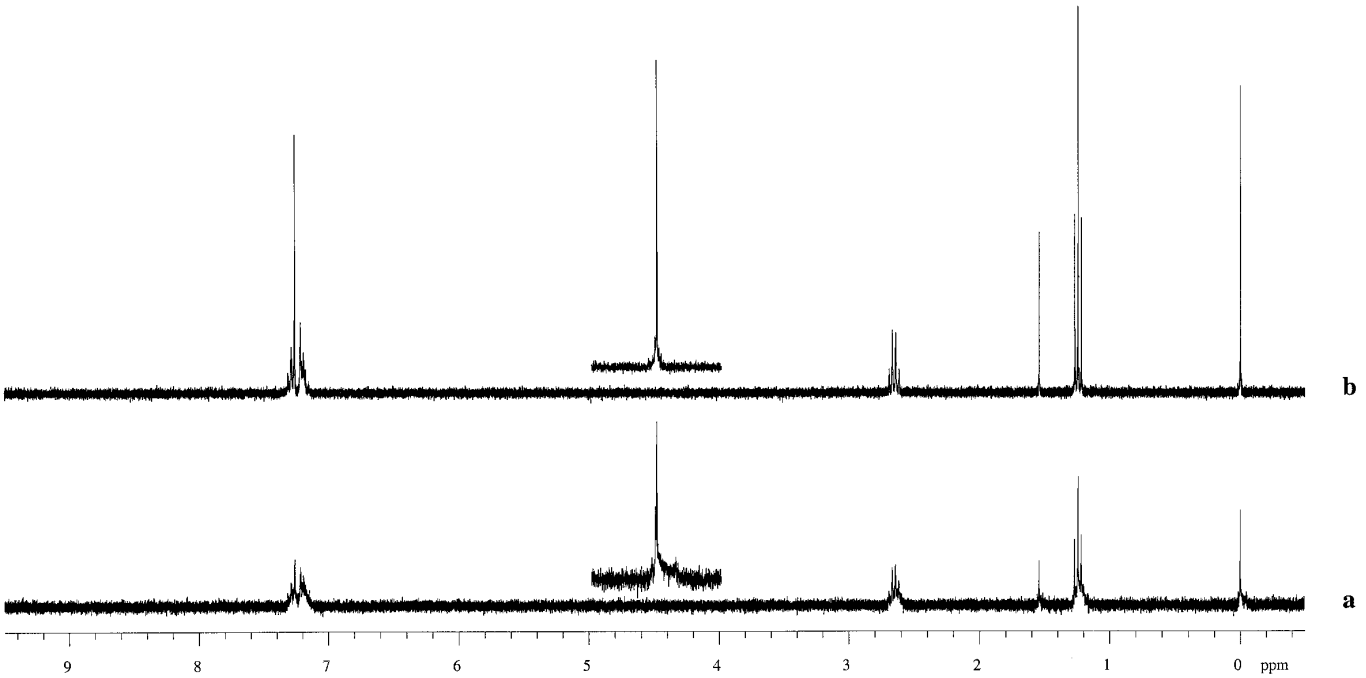

FIG. 4. The 300 MHz proton spectra of the standard sensitivity test sample of 0.1% ethylbenzene and 0.01% tetramethylsilane in deuteriochloroform, measured in probe B (a) using the shims for probe A used in acquiring the spectrum of Figs. 3b/3c and (b) after automatic *z* shimming. Insets show a 100 Hz region about the TMS resonance for each spectrum. Four transients were acquired with an acquisition time of 8.192 s and a spectral width of 4 kHz, zero-filled twice, and Fourier transformed without time-domain weighting.

Problems may be encountered in using particularly complex signals (e.g., those of toluene-d_8) for automated shimming, but if so they should be susceptible to deconvolution methods; good results have been obtained using the signals of methanol-d_4 without the need for any changes in the method. If a shim map measured on one probe were to be used on a second probe with a significantly different coil position, it would be necessary to ensure that the same frequency scales were used, rather than simply assuming that the center of the spectrum corresponded to the same position in both cases, and of course any shim map used would have to cover the active volume of the probe.

The present algorithm performs a least-squares fit of the available shim coil correction functions to the observed frequency errors for a defined spectral window; different choices for optimization function could be used to optimize different aspects of lineshape, for example, shimming for optimum linewidth at half-height at the expense of the base of the lineshape. It should be possible to use similar shim coil gradient automated shimming methods, using deuterium or proton signals, for the transverse as well as the *z* shimming of static samples, and for the ''cold'' shimming of all gradients in a newly installed probe.

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