A firmware-defined digital direct-sampling NMR spectrometer for
condensed matter physics

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We report on the design and implementation of a new digital, broad-band nuclear magnetic resonance (NMR) spectrometer suitable for probing condensed matter. The spectrometer uses direct sampling in both transmission and reception. It relies on a single, commercially-available signal processing device with a user-accessible field-programmable gate array (FPGA). Its functions are defined exclusively by the FPGA firmware and the application software. Besides allowing for fast replication, flexibility, and extensibility, our software-based solution preserves the option to reuse the components for other projects. The device operates up to 400 MHz without, and up to 800 MHz with undersampling, respectively. Digital down-conversion with ±10 MHz passband is provided on the receiver side. The system supports high repetition rates and has virtually no intrinsic dead time. We describe briefly how the spectrometer integrates into the experimental setup and present test data which demonstrates that its performance is competitive with that of conventional designs. © 2014 AIP Publishing LLC.

I. INTRODUCTION

A spectrometer is the key component of any pulsed magnetic-resonance experiment, including nuclear magnetic resonance (NMR), nuclear quadrupole resonance (NQR), or ferromagnetic resonance (FMR). Below, we use the term NMR for any of these variants. Resonant or close-to-resonance radio-frequency (RF) pulses, centered at the so-called reference frequency, are used to excite the nuclear spins into a superposition of non-degenerate eigenstates. The subsequent time evolution of the nuclear spins produces a time-varying macroscopic magnetic moment, which is detected inductively. Usually, multiple transients are averaged in order to improve the signal to noise ratio (SNR). In addition, phase cycling1,2 suppresses various undesired contributions. This requires a well defined phase relation between the excitation pulses and the recorded signal. Hence, phase-coherent pulsing and data acquisition are the two primary functions of an NMR spectrometer.

Traditionally, NMR spectrometers were assembled from basic building blocks, involving lumped analog circuit elements, quadrature hybrids, and discrete digital logic chips.3 These usually rather complicated designs tended to be time-consuming to implement and difficult to maintain. Therefore, more recent spectrometer designs rely on commercially-available analog signal processing blocks.4 Although easier to maintain and upgrade, their construction still involves a substantial amount of analog and digital signal routing [cf. Fig. 1(a)], introducing many potential points of failure.

As the spectral width of the received signal is typically much smaller than the resonance frequency of the investigated nuclear transition, it is convenient to down-convert the response of the nuclear spin system such that its frequency spectrum is approximately centered around zero. The resulting low-frequency baseband signal can then be sampled more easily and the amount of output data is significantly reduced. In addition, quadrature detection is employed in order to distinguish spectral components above and below the spectrometer reference frequency.5

Most spectrometers rely on analog mixers for down-conversion and quadrature detection. It has been proposed that the same could in principle be achieved in the digital domain, provided the received signal can be sampled at a sufficiently high rate.6 A typical laboratory NMR spectrometer is expected to handle frequencies up to about 500 MHz. Although undersampling7 may be adequate for standard experiments, it seems less suited when searching for signals in the presence of unknown spurious response and environmental noise. Hence, according to the Cardinal Theorem of Interpolation Theory (also known as the Sampling Theorem),8 the sampling rate for an all-digital NMR spectrometer is required to be of the order of 1 GS/s (1 GS = 10^9 samples). For a typical width of 2 bytes per sample, this yields data rates of about 2 GB/s. The need for fast digitizers as well as the substantial amount of data to be processed are probably the main reasons why the all-digital approach to spectrometer design has rarely been chosen in the past.

There are various reports on magnetic-resonance instrumentation involving digital signal processing.9–19 However, most of these focus on either the transmitter11,16 or the receiver9,14,15,19 only. Other spectrometers can only be used in ultra-low magnetic fields,13 or rely on external mixers for down-converting the signals to lower intermediate frequencies.12,15 Other designs described in the literature either lack physical implementations,17 or use dedicated integrated circuits providing direct-digital synthesis (DDS) for signal generation, digital down-conversion (DDC) for reception, or digital signal processors (DSP) for pulse

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programming. All solutions able to operate as full-fledged NMR spectrometers known to us require purpose-built hardware. Also, none of them supports frequencies exceeding 50 MHz without using undersampling or external mixers. Moreover, the data interfaces (mostly USB) are rather slow, which can be a limitation in the presence of fast relaxation rates, unless some means of on-device averaging are provided.

In this work, we report on the development, the realization, and the performance of a fully soft- and firmware defined, direct-sampling digital NMR spectrometer. The spectrometer was implemented and tested using a single commercially-available radio-processor board [Fig. 1(b)], equipped with high-performance digital-to-analog and analog-to-digital converters (DACs and ADCs), as well as a field-programmable gate array (FPGA). Such hardware is available from various manufacturers and the implementation described here can easily be adapted to a different device. In the following, we present a complete, operational, and easy to replicate spectrometer suitable for NMR experiments in condensed matter physics.

II. DESIGN

Before describing the design in detail, we show how the spectrometer integrates into the NMR setup (Fig. 2). To this end, one can consider the spectrometer as a black box with three ports: (i) signal input (RX), (ii) signal output (TX), and (iii) amplifier unblank (TTL). A power amplifier is required to produce sufficiently strong excitation pulses. In order to reduce the noise, the unblank signal is used to shut off the amplifier during idle periods. Modern NMR probes use a single coil for excitation and reception. Therefore, an additional routing device called duplexer is needed. The duplexer ensures that the strong excitation signals from the amplifier reach the NMR probehead without overloading the sensitive receive path. At the same time, the weak response originating from the sample is allowed to pass to the receiver. Signal levels in condensed matter experiments can be as low as $-100$ to $-85$ dBm. Therefore, one or more wide-band pre-amplifiers are inserted into the receive path of the NMR setup. Computer-controlled attenuators are placed between the spectrometer and the power amplifier, as well as between the preamplifier and the spectrometer. They allow for the scaling of the input signals to make the most effective use of the receiver’s dynamic range, as well as for the adjustment of the excitation-pulse amplitude.

In our case, the spectrometer is based on a radio-processor board (SDR14, Signal Processing Devices AB, Sweden, Fig. 1) with two input and two output channels, sampled with 16-bit and 14-bit resolution, at 0.8 GS/s and 1.6 GS/s, respectively. In addition, there are several general-purpose input/output (GPIO) TTL signaling lines available.

FIG. 2. Hardware components of the NMR setup (see text for details). Firmware and software components are marked in red. Lines and arrows indicate signal and information flow; high-frequency analog signals are highlighted using thick blue lines.

<table>
<thead>
<tr>
<th>Component</th>
<th>Characteristics</th>
</tr>
</thead>
<tbody>
<tr>
<td>RF in</td>
<td>2 channels, 16-bit resolution, 0.8 GS/s, 512 Mb DRAM</td>
</tr>
<tr>
<td>RF out</td>
<td>2 channels, 14-bit resolution, 1.6 GS/s, 512 Mb DRAM</td>
</tr>
<tr>
<td>GPIO</td>
<td>5 channels, TTL, 200 MS/s</td>
</tr>
<tr>
<td>FPGA</td>
<td>Xilinx Virtex-6</td>
</tr>
<tr>
<td>Interface</td>
<td>PCI Express</td>
</tr>
</tbody>
</table>
LX240T Virtex-6 FPGA\textsuperscript{22} which offers the possibility to implement additional on-device logic.

The main advantages of FPGAs are (i) parallel data processing, (ii) portability, and (iii) the possibility to simulate and test the design prior to implementation. Typical FPGAs contain generic logic units, providing combinatorial logic gates and memory elements (flip-flops), grouped into so-called logic slices, as well as additional specialized circuits such as multipliers. These elements are linked by programmable interconnects, the configuration of which is described by a binary file. These configuration data are referred to as the firmware and can be replaced at will, enabling the use of the same device for different applications without any hardware changes. Logic circuits implemented on modern FPGAs can be far more complex than what can be realized by assembling individual discrete elements on printed circuit boards. An important difference to most software-based approaches, including DSPs, is that FPGAs support true hardware parallelism with disjoint logic networks switching independently of one another. Hence, even complicated data manipulations such as DDC and filtering can be performed in real-time. Instead of explicitly routing individual signals using graphical schematics, as in small-scale circuit design, and graphical programming languages like National Instruments’ LabVIEW, the connectivity of the circuits is defined in abstract terms using high-level hardware description languages (HDLs). The task of finding the most efficient realization of a circuit using the resources provided by a given FPGA is then delegated entirely to the software tools provided by the FPGA manufacturer. This approach is capable of handling very complex designs. Moreover, since HDLs like VHDL and Verilog are standardized, they enable source-code portability across different FPGA devices, even when produced by different manufacturers. Sub-circuits can be combined into modules with well-defined interfaces. This simplifies the documentation and improves the code reusability. In addition, libraries providing highly-optimized implementations of commonly-used circuits are available. Finally, many development tools also include a simulator, which enables the testing of individual modules before actually realizing them inside the FPGA.

The layout of the FPGA logic used to implement the digital spectrometer is shown in Fig. 3. Its individual sub-components are described in Subsections II A–II E.

A. Interface, software, and pulse programming

The radio-processor board used in this work provides a PCI express (PCIe) interface, enabling fast data transfers to and from the host computer. Drivers for Windows and Linux operating systems, an application programming interface (API) for the C programming language, and an FPGA development kit built around the Xilinx ISE FPGA development package are supplied by the manufacturer. Hardware initialization, data acquisition, and data transfers are handled by the manufacturer’s firmware and drivers. A set of user-programmable registers is provided to communicate with the user-defined logic. These registers can be accessed at rates of over 80,000 reads/writes per second and are used to program, reset, and trigger the NMR experiments.

On the software side, our solution is based on a C++ shared library which controls the NMR user logic on the FPGA and handles the acquired data. The library provides a high-level interface for performing NMR experiments. Currently, MathWorks MATLAB is used to both control and monitor the execution of the experiments, as well as to perform the data analysis.

Timing relies on a 48-bit timer counting the number of clock cycles elapsed since the start of the NMR pulse sequence. Given the 200 MHz clock frequency of the firmware, this yields a time granularity of 5 ns and a maximum sequence duration of about 16 days, which is sufficient for our purposes. The pulser units employ program tables stored in the FPGA memory to determine during which time intervals their outputs should be asserted (i.e., set to logical “1”). Currently, we use three such pulsers: Receiver (RX) gate, transmitter (TX) gate, and amplifier unblank.

B. Data transfer and averaging

Broad spectra and small probed sample masses are not uncommon in condensed matter magnetic-resonance

FIG. 3. FPGA firmware block diagram of the digital spectrometer (see text for details). External and internal I/O refer to input/output connections to hardware outside and inside the measurement computer, respectively (cf. Fig. 2). Lines and arrows indicate information propagation; the flow of waveform data towards and from the radio-frequency front-end is highlighted using thick blue lines.
experiments. As a result, signals can be weak and a substantial number of scans needs to be averaged for obtaining a sufficient SNR. As spin-lattice NMR relaxation rates may be very high, the spectrometer should be able to support high repetition rates.

The recorded signals are down-converted in real-time. Therefore, the memory required for storing the complex baseband data (two channels at 25 MS/s, 2 bytes per sample, records of typically 1 ms duration) is small and many records can be stored in the 512 MiB (1 MiB = 2^20 bytes) receiver DRAM (dynamic random-access memory) of the radio-processor device. Typical data transfer rates for our hardware are of the order of 100 to 400 MiB/s, which is of the order of the output data rate and therefore may represent a significant overhead. Our solution is to divide the receiver DRAM into segments and to implement an on-device looping feature within our NMR logic (cf. scanner block in Fig. 3). One memory segment can be read out while the other segment is being written to. This interleaved read-out process enables a simultaneous measurement and data transfer, such that the repetition rate of the NMR experiment is solely limited by the relaxation time of the studied nuclei.

On-device averaging requires simultaneous read and write access to the receiver DRAM, which is not supported by our hardware. Instead, we use the interleaved read-out technique and perform averaging in software. The employed data types are 16-bit signed integer for the raw data, 32-bit integer for the average (1st moment), and 64-bit integer for a variance estimate (2nd moment). Tests have shown that the averaging speed is solely limited by the memory bandwidth of the host computer, most of which is required for loading and updating the aggregated data (sums and sums of squares). Therefore, we divide the sequence of acquired records into chunks of several records. Each record is split into pages to improve the locality of reference and hence make better use of the fast processor cache. Different pages are then averaged in parallel. This optimized implementation can average over 2 GS/s on our test system (Intel Xeon E3-1240 with dual-channel DDR3-1333 memory), which is by far sufficient even for raw-data acquisition without DDC.23 The performance could be improved even further by optimizing chunk and page sizes, upgrading the host computer hardware, or delegating the task to a suitable GPU device. Finally, if required, on-device averaging of short waveforms can be implemented by using the memory cells available within the FPGA.

C. Transmitter

The transmitter section of the spectrometer uses direct-digital synthesis (DDS), hence eliminating the need for the external signal synthesizers often encountered in conventional NMR setups. Due to the FPGA clock frequency of 200 MHz, eight phase-offset complex DDS cores are used in parallel in order to generate data at the DAC sampling rate of 1.6 GS/s. These data also serve as a local oscillator (LO) signal for the receiver section described below. A quadrature phase-shift keying (QPSK) modulator is used to change the phase of the generated signal in steps of 90°, before forwarding it to the DAC. The 32-bit width of the phase accumulator results in a frequency resolution of less than 0.5 Hz, enough for our application. The phase-switching delay of the present transmitter is only limited by the output bandwidth. A low-latency frequency switching capability, or even additional DDS units, could be added with little effort. The latter is especially interesting for spin-lattice relaxation experiments using different nuclear transitions for excitation and detection.25 If required, soft pulses and arbitrary waveform generation could be included as well.

Most conventional spectrometers require image rejection filters to suppress unwanted mixing products. These filters often have to be adjusted depending on the operating frequency of the spectrometer. By contrast, DDS only requires a fixed analog reconstruction filter to constrain the output signal to the desired Nyquist zone (0 to 0.8 GHz in our case).

D. Receiver

Our solution features what is known as a direct-digital receiver.9 The incoming signal is sampled right after amplification, without any further analog processing. The data are then subjected to DDC. The DDC unit consists of two main components: a complex multiplier acting as a digital quadrature mixer that shifts the spectrum of the acquired signal towards zero intermediate frequency (IF), and a digital low-pass filter which removes the mixing image and reduces the data rate from 800 MS/s to 25 MS/s per quadrature. Due to the powerful FPGA on our radio-processor board, a rather complex filter chain consisting of five half-band finite impulse response (FIR) decimation filters can be incorporated. The filter coefficients were obtained using the MathWorks MATLAB DSP System Toolbox. Some of the filters require parallel processing, which prevented the use of automatic code-generation tools. For example, the first filter stage transforms a 4-parallel complex data stream (800 MS/s) into a 2-parallel complex data stream (400 MS/s). The internal data processing is performed with 24-bit precision. Whenever truncation is required, convergent rounding to even (unbiased rounding) with saturation is used.

Each filter stage reduces the data rate by a factor of two. Therefore, for a given sampling rate \( f_s \) before the filter, spectral components in a frequency interval \( \left[ \frac{f_s}{4} - v, \frac{f_s}{4} \right] \), will give rise to aliases in the range \([0, v]\). Our filters are designed for a 10 MHz bandwidth. The filter parameters have been chosen such that aliases within this band are suppressed by at least 70 dB. The passband ripple is less than 0.01 dB for the combined filter chain. These values are sufficient for our application. Yet, since there are still FPGA resources available, they can easily be improved if required.

Although any clock jitter will in general affect the measured spectra,29 such effects are not relevant for this work because the linewidths encountered in condensed matter NMR experiments tend to be rather large. Moreover, such problems can be mitigated with little effort by using an external clock source. Likewise, an external clock reference may be used whenever a higher frequency accuracy is required.

Finally, we included an option to bypass the mixer, which is useful for experiments at very low frequencies (below about...
TABLE I. Overview of the resources used by the spectrometer logic and the manufacturer’s firmware, as well as the total resources available on the FPGA chip. We distinguish logic slices, block random-access memory (BRAM), and 48-bit multipliers (DSP48).

<table>
<thead>
<tr>
<th></th>
<th>NMR logic</th>
<th>Manufacturer’s logic</th>
<th>Available</th>
</tr>
</thead>
<tbody>
<tr>
<td>Slices</td>
<td>2862</td>
<td>16457</td>
<td>37680</td>
</tr>
<tr>
<td>BRAM</td>
<td>44</td>
<td>277</td>
<td>416</td>
</tr>
<tr>
<td>DSP48</td>
<td>69</td>
<td>151</td>
<td>768</td>
</tr>
</tbody>
</table>

7 MHz), where the mixer images are no longer rejected by the decimation filters. In order to ensure phase-coherent averaging, the DDS phase accumulators are reset before every single scan.

E. Implementation

The FPGA logic modules have been implemented in Verilog. Most of the modules use an AXI4-stream interface to ensure robust data-flow management. Due to the large amount of data processed per clock cycle, register slices had to be added in order to ensure timing closure. The resource usage of the final design is summarized in Table I. Given the total resources available, the requirements of the NMR-specific logic are very reasonable and leave plenty of room for future extensions.

III. TESTING

A. Synthetic tests

To demonstrate the performance of the digital receiver, we applied a fixed-frequency test signal to the receiver. In Fig. 4, we plot the power of the strongest spectral component in the recorded signal as a function of the spectrometer reference frequency, excluding frequencies outside the ±10 MHz passband of the digital quadrature detector. The results are in very good agreement with the simulated filter response. Additional measurements served to characterize the RF properties of the hardware. An important parameter is the spurious-free dynamic range (SFDR), defined as the intensity ratio (in dB) between the strongest spurious signal and a given signal. The SFDR of both, the inputs and the outputs of our device, was determined experimentally. The results are summarized in Fig. 5. The hardware used in this work employs interleaved sampling using four ADCs per input channel. Small variations in the characteristics of the components give rise to alias frequencies in the recorded data, which adversely affect the SFDR. The manufacturer firmware uses a proprietary technique to reduce the impact of these imperfections. The algorithms are configured to work in the first Nyquist band, which explains the deterioration of the otherwise excellent input SFDR upon approaching 400 MHz. Harmonic distortion, known to originate from the test-signal source, has been excluded in the data analysis. Since the noise floor of the radio-processor board is lower than the one of our oscilloscope, we use a loopback measurement to characterize the output-signal quality. Therefore, the output SFDR values above 390 MHz are upper bounds only. Finally, the combined gain of output and input (cf. inset of Fig. 5) is found to be reasonably flat up to 800 MHz.

B. Magnetic resonance experiments

Several NMR experiments were made to assess the performance of the new spectrometer. The results are compared with data obtained using a conventional spectrometer under the same experimental conditions (magnet, probe, and sample). All measurements were carried out at room temperature. Figure 6 shows the resonance spectrum of $^2$H in heavy water in a magnetic field of 7 T. The spectrum was obtained by averaging two free-induction decay signals following a $\pi/2$ pulse. The linewidth of 0.7 kHz (FWHM) is due to the imperfect shimming of our magnet. The reference frequencies of both spectrometers were set to 46.155 MHz. The signals
measured with both spectrometers are in good agreement. In addition, the comparison also illustrates two advantages of the direct-sampling approach. First, the low-frequency analog output signals, often called video signals, of the conventional NMR spectrometer are particularly prone to contamination by the ubiquitous low-frequency noise. The resulting artifact is clearly visible in Fig. 6. Second, the analog quadrature demodulators used in most conventional spectrometers are never perfectly balanced. For the type of conventional spectrometer used in this work, a resonance at frequency \( v \) will in general give rise to a spurious spectral component at \( 2ν_0 − v \), where \( ν_0 \) denotes the reference frequency of the spectrometer. These spurious signals are commonly called “ghosts,” and they are indeed observed in the data displayed in Fig. 6. By contrast, both effects are absent in the data recorded using the digital receiver.

As a test case complementary to the slowly-relaxing, narrow-band deuterium resonance, NMR measurements were made on \(^{59}\text{Co}\) in ferromagnetic cobalt powder in zero external magnetic field. The internal magnetic field gives rise to a rather broad spectrum spanning the range of 210–225 MHz, with two dominant peaks originating from different crystallographic phases.\(^{32, 33}\) Because both, the detected signal as well as the driving RF field, are dramatically enhanced due to magnetic order,\(^{34}\) very short pulses can be used, which increases the excitation bandwidth. Figure 7 shows the \(^{59}\text{Co}\) spectrum recorded with the digital spectrometer using a spin-echo sequence with 50 ns pulse duration and 20 \( \mu \text{s} \) pulse separation. The gray trace was obtained by varying the frequency in steps of 1 MHz and combining the individual spectra.\(^{35}\) The shaded curve instead was recorded at a fixed reference frequency of 216.123 MHz. After correcting for the finite spectral width of the refocussing RF pulse,\(^{36}\) the two spectra are in good agreement. Although such short pulses are rather exceptional in NMR, the data confirm the broad bandwidth of the new spectrometer.

**IV. DISCUSSION**

Currently, high-performance radio-processor devices with user-programmable FPGAs, as well as fast data processing equipment are available, rendering an all-digital approach to NMR feasible. Following this idea, we present a complete digital solution for NMR instrumentation adapted to the needs of condensed matter physics experiments. The setup relies on standard, general-purpose, commercially-available components. The spectrometer is based exclusively on the FPGA firmware and the application software.

This firmware-defined approach has multiple advantages. It reduces application-specific hardware development to a minimum and makes the replication of an experimental setup extremely simple once the code has been developed. Due to their intrinsic parallelism, FPGAs are ideally suited for real-time data-stream processing. Additional functions can be implemented and tested without risk, since previous “known-to-work” configurations can be quickly restored at any time. The acquisition of the components may turn out as a cost-effective investment because they can be used for non-NMR purposes as well. Maintenance efforts are also reduced, since hardware development and repairs are taken care of by the equipment manufacturer. On the programming side, we use Verilog and C++, which both are industry-standard and device-independent. Therefore, this approach can be adapted to different hardware. As a side effect, the spectrometer is very compact and hence can in principle be easily transported.

The use of direct sampling in both transmitter and receiver, results in an SFDR which is superior to that of many conventional spectrometers (Sec. III A). The channels of the digital quadrature detector are perfectly balanced and hence free of spurious signals (Sec. III B). The passband of the digital down-conversion filter is 20 MHz wide and extremely flat. A comparable filter based on analog components would be difficult to realize. The flexible digital architecture allows for the accommodation of additional features, such as soft pulses,\(^{37}\) signal emphasis,\(^{38}\) or even stochastic NMR.\(^{39, 40}\) In addition, the large raw bandwidth of the device may also be interesting for complex multi-resonance experiments.

NMR nuclei can be divided into two groups according to their gyromagnetic ratio: low-frequency nuclei, up to and including \(^{31}\text{P}\), and the high-frequency nuclei: \(^{203, 205}\text{Tl}\), \(^{3}\text{He}\), \(^{19}\text{F}\), and \(^{1.9}\text{H}\). The Nyquist frequency of the reported spectrometer corresponds to a magnetic field of over 23 T for the low-frequency nuclei, which are the ones most commonly studied.
in condensed matter physics. This is comparable to the maximum fields of the best superconducting laboratory magnets available at the time of this writing. Moreover, as shown in Sec. III A, performance in undersampling mode is good up to 800 MHz, which may be useful for measuring, e.g., $^1$H in high magnetic fields.

To our knowledge, the present work is the first successful implementation of an exclusively soft- and firmware based direct-sampling NMR spectrometer covering the range of NMR frequencies accessible in mid-size physics laboratories. The spectrometer supports fast repetition rates and its dead-time is solely limited by the recovery time of the external components shown in Fig. 2. Besides presenting and discussing synthetic benchmarks, we have shown that the spectrometer performs flawlessly in typical laboratory NMR experiments. Moreover, we have demonstrated that such a setup can compete with and even outperform good conventional spectrometers.

ACKNOWLEDGMENTS

We thank SP Devices for providing the radio-processor board initially used for this work, as well as for their rapid response to technical issues encountered during development and testing. This work was financially supported in part by the Schweizerische Nationalfonds zur Förderung der Wissenschaftlichen Forschung (SNF) and the NCCR research pool MaNEP of the SNF.

8E. T. Whittaker, Proc. R. Soc. Edinb. 35, 181 (1915). Similar results have been obtained by other authors, including C. E. Shannon, H. Nyquist, V. A. Kotel’nikov, H. Raabe, and I. Someya.
2065 dB gain with up to 60 dBm output in our case.
23According to the manufacturer, the updated version of the radio-processor device is capable of transferring data at a rate of up to 3 GiB/s.
28We call a data stream consisting of n samples per clock cycle n-parallel.
33Instead of the originally predicted shape, for short pulses, we observe a linear relation between pulse width and signal amplitude.