swiss physical society

Nr. 67, Mai 2022

SPG Mitteilungen
Communications de la SSP

Auszug - Extrait

Progress in Physics (91)

“Doing less, does it faster” - Using Compressive Sensing and Parallel Spectroscopy for Fast Quantum Materials Discovery

Jens Oppliger and Fabian Donat Natterer
Department of Physics, University of Zürich, Winterthurerstrasse 190, CH-8057 Zürich

Progress in Physics (91)

“Doing less, does it faster” - Using Compressive Sensing and Parallel Spectroscopy for Fast Quantum Materials Discovery

Jens Oppliger and Fabian Donat Natterer
Department of Physics, University of Zürich, Winterthurerstrasse 190, CH-8057 Zürich

In our modern world, we accumulate, process, and store huge volumes of data that are produced by a multitude of sensors, cameras, and monitoring equipment. Interestingly, the actual amount of meaningful information from this data-deluge can be quite small (sparse information content) and it would lead to cluttering of long-term memory without intensive data processing. This deficiency motivates the development of compression algorithms that *a-posteriori* reduce the data size to render it manageable with limited long-term mass storage.

Efficient compression algorithms rely on the fact that a signal may be described in a transformed base by a small number of non-zero coefficients. For instance, the tone of a sine wave has only two components in Fourier space, whereas its proper description in the time-domain requires a sample rate of at least twice the signal bandwidth, as described by the Nyquist–Shannon sampling criterion. The Fourier base clearly describes this tone more concisely. Similarly, image-compression algorithms work because few coefficients can again express the dominant information content, such as in the popular image compression algorithm underlying JPEG that is based on a discrete cosine transform.

However, the compression algorithms do not curtail the data production or relieve the temporary data storage requirements prior to the compression of the incoming data stream. This means that all in-flowing data needs to be stored and processed for compression.

We may then ask ourselves if data could be recorded directly in compressed form, in other words: *Can a sensor record only the useful or meaningful information of a signal?* Curiously, the answer to that is yes! The seminal works by Candès, Romberg and Tao [1] and Donoho [2] proved mathematically that as long as the signal of interest is compressible (or sparse) in some representation space, it may be (perfectly) reconstructed from a small set of incoherent measurements. This revolutionary concept, coined Sparse Sampling, Compressed Sampling or Compressive Sensing (CS), has started to fundamentally influence many fields of research, most notably magnetic resonance imaging [3], where it led to significantly speeding-up of the data taking, with immediate benefits to patient comfort.

The notion of faster measurements that may be accelerated through the implementation of CS sampling concepts is highly appealing also for condensed matter research. Reflecting about the typical data structure in connection with the requirements for CS, fields of application emerge. We expect to make the biggest strides for data having a highly sparse representation space and whose measurements are time-consuming, such as serial mapping tasks in which one property is measured against one or several external parameters. For the sake of the present discussion, we turn our attention to large-scale mapping experiments using the notoriously slow scanning tunneling microscope (STM) [5].

An especially suitable example is Fourier-transform STM (FT-STM) [6], also referred to as quasiparticle interference imaging (QPI). FT-STM provides insight into the band-structure of two-dimensional quantum materials from the thorough mapping of the local density of states (LDOS) in a large-field-of-view (FOV). Discontinuities in the surface, such as step edges or defects, lead to the elastic scattering of electron waves that create standing wave patterns in the LDOS [7], revealing the momentum transfer $\Delta q = k_i - k_f$ between the initial and final states of its underlying band-structure. The energy dependent LDOS mapping of those standing waves reveals the dispersion relationship of the scattering vectors from which band-structure information can be derived. Similar to the example of a sine wave tone, mentioned above, the standing waves have a sparse representation in Fourier space [8, 9]. The few non-zero coefficients in the QPI images are an excellent foundation for CS sampling concepts. To further appreciate the impact of CS for QPI imaging, let us consider its conundrum. To achieve the best QPI momentum resolution, the size L of the FOV should be large because $\Delta q = 2\pi/L$. On the other hand, access to high-momentum transfer states requires a dense sampling of n spectra per linear dimension in the FOV and the number of required point spectra grows as n^2 with L. Each of those n^2 LDOS measurements takes t_{spc} per spectrum leading to a total QPI mapping time of $t = p \cdot n^2 \cdot t_{spc} + t_{ctr} + t_{travel}$. The travel and control times are related to the motion of the tip across the FOV and overhead related to the hardware of the STM controller. Importantly, the factor $p \in (0,1]$ describes the subsampling parameter, which is $p = 1$ in conventional grid QPI. The conventional QPI mapping time for an assumed $n = 1024$ grid taking 1 s per spectrum is more than 291 hours, far longer than the typical hold-times of a wet cryostat. Such a QPI experiment would be virtually impossible.

Fortunately, the above relationship shows two efficient means of how-to speed-up QPI imaging. Firstly, by subsampling at $p \ll 1$ and secondly by reducing t_{spc}. We achieve the former by sparsely sampling the LDOS [9] and the latter by a faster single-point spectroscopy method [10, 11]. As one CS prescription is the incoherent measurement, we select a small random subset of LDOS coordinates in our FOV for which we follow a near-optimal traveling salesperson path [12] for efficient routing of the tip-motion; also reducing t_{travel}. With the knowledge of sparsity in the QPI representation in mind [8, 9], we solve the compressive sensing problem using a basis pursuit denoising (BPDN) program as implemented with SPGL1 [9, 11, 13]. The sparsely sampled LDOS can be either measured conventionally or via parallel spectroscopy [11]. The latter works by exploiting nonlinearities in the current-voltage (IV) characteristics of the tunneling junction. Instead of applying a small bias modulation, as in

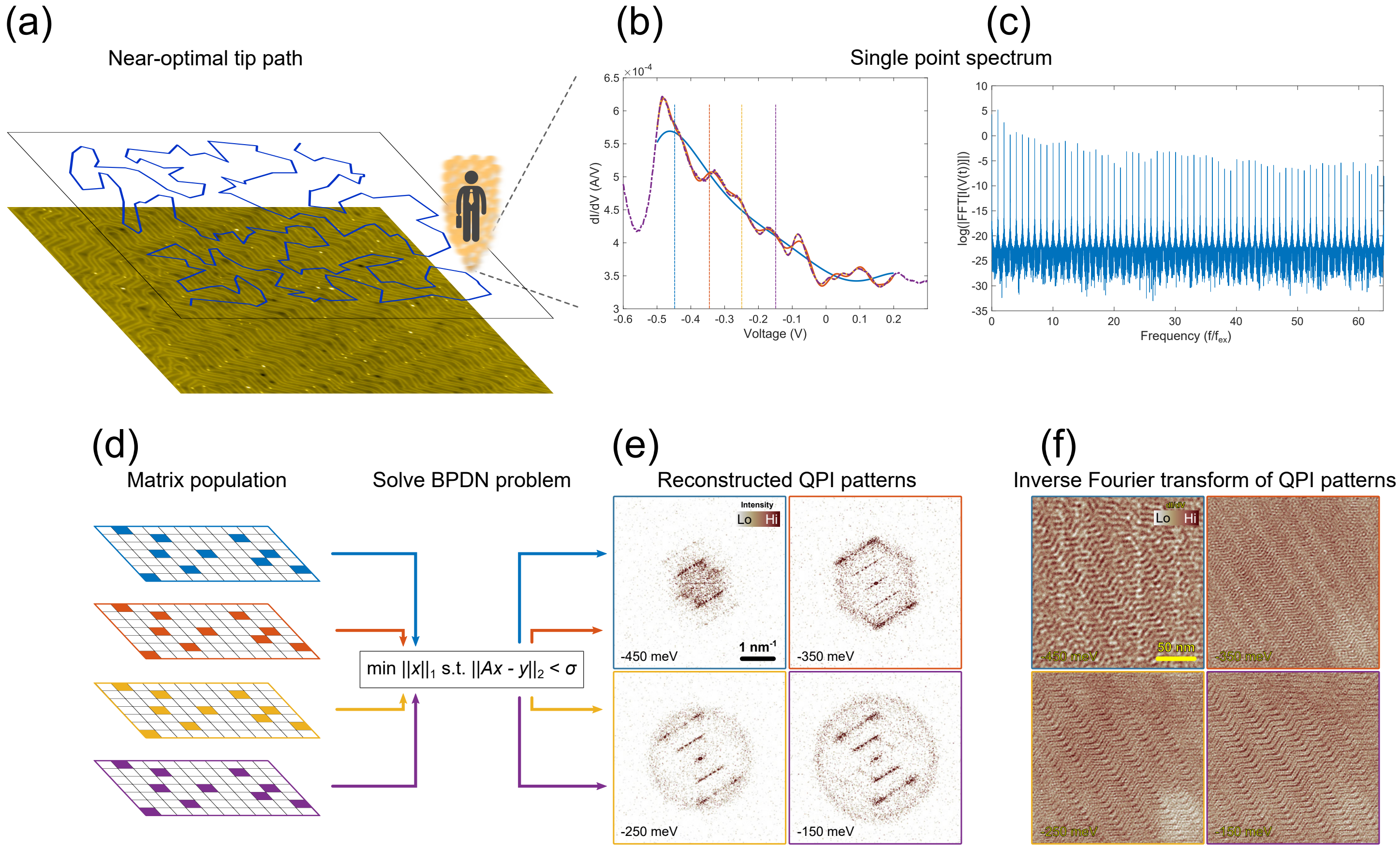

Figure 1: Implementation of compressive sensing (CS) and parallel spectroscopy for fast quasiparticle interference imaging. (a) We subsample the local density of states (LDOS) at a small subset of random coordinates that are visited via a traveling salesperson route. (b) The LDOS is either measured conventionally or via parallel spectroscopy, which uses a large modulation voltage to promote the generation of (c) high-order harmonics from which the current-voltage characteristics can be reconstructed. (d) The sparsely sampled LDOS measurements are fed into the compressive sensing solver that tries to find the sparsest solution in Fourier space, leading to (e) the energy dependent QPI images. (f) The full LDOS can then be obtained from an inverse Fourier transform of the CS reconstructed QPI patterns. Figure adapted from Zengin et al (2021).

conventional tunneling spectroscopy, we apply a large modulation whose amplitude covers the entire energy range. We thereby deliberately generate higher harmonics that we demodulate to the 31st order using a multifrequency lock-in amplifier. From the simultaneous measurement of many harmonics, we can reconstruct the original *IV* characteristics via an inverse Fourier transform [10, 11] at a fraction of the conventional t_{spc}.

Our demonstration [11] shows how we can move from the concept of fast QPI imaging using CS [9] to the actual experimental implementation for quantum materials discovery. We show that both, CS and parallel spectroscopy, independently work to speed-up QPI using the model system of Au(111). For CS, we use subsampling rates between 3 and 7 % and our time per spectrum is reduced to 20 ms using parallel spectroscopy. Most importantly, these two speed-factors also work in combination, enabling up to 1000-fold faster QPI imaging; a weeklong measurement can be achieved within minutes.

Further work for fast QPI imaging will introduce adaptive sparse sampling strategies [14] that enable open-ended measurement tasks without prior insight into the degree of signal sparsity. In addition, a better understanding of piezo-electric positioners will increase the accuracy of the LDOS assignment, improving momentum resolution.

Looking ahead, the fast QPI mapping will enable novel mapping schemes because an experimenter can finally trade measurement time, for instance for better momentum or energy resolution, instead of making compromises constraint by the maximally available measurement-time. Fast QPI imaging invites the exploration of a large parameter space in which the QPI information is measured against one or several external degrees of freedom, such as temperature, magnetic field, chemical/electrostatic doping, or strain. This will become particularly important as a complement to band-structure investigations using angle resolved photoemission spectroscopy that are limited in difficult environments. As we shift our focus away from silicon-based technology, the control of novel quantum materials will become transformative, and their behavior needs to be investigated in extreme environments to find the tuning knobs that steer their functionality.

In summary, the potential of compressive sensing to substantially speed-up measurements invites a reflection of one's experiment to critically assess how it can be enhanced. It also stimulates the introduction of novel measurement schemes that pair well with CS to further boost data throughput.

Bibliography

[1] E. J. Candès, J. K. Romberg, Tao, Terrence, Stable signal recovery from incomplete and inaccurate measurements. *Commun. Pure Appl. Math.* **59**, 1207–1223 (2006).
[2] D. L. Donoho, Compressed sensing. *IEEE Trans. Inf. Theory*. **52**, 1289–1306 (2006).

[3] M. Lustig, D. Donoho, J. M. Pauly, Sparse MRI: The application of compressed sensing for rapid MR imaging - Lustig - 2007 - Magnetic Resonance in Medicine - Wiley Online Library. *Magn. Reson. Med.* **58**, 1182–1195 (2007).

[4] R. Taylor, Compressed Sensing in Python, (available at *http://www.pyrunner.com/weblog/B/*).

[5] G. Binnig, H. Rohrer, Scanning tunneling microscopy-from birth to adolescence. *Rev. Mod. Phys.* **59**, 615 (1987).

[6] L. Petersen, Ph. Hofmann, E. W. Plummer, F. Besenbacher, Fourier Transform–STM: determining the surface Fermi contour. *J. Electron Spectrosc. Relat. Phenom.* **109**, 97–115 (2000).

[7] M. F. Crommie, C. P. Lutz, D. M. Eigler, Imaging standing waves in a two-dimensional electron gas. *Nature* **363**, 524–527 (1993).

[8] Y. Nakanishi-Ohno, M. Haze, Y. Yoshida, K. Hukushima, Y. Hasegawa, M. Okada, Compressed Sensing in Scanning Tunneling Microscopy/Spectroscopy for Observation of Quasi-Particle Interference. *J. Phys. Soc. Jpn.* **85**, 093702 (2016).

[9] J. Oppliger, F. D. Natterer, Sparse sampling for fast quasiparticle-interference mapping. *Phys. Rev. Res.* **2**, 023117 (2020).

[10] R. Borgani, M. Gilzad Kohan, A. Vomiero, D. B. Haviland, Fast Multifrequency Measurement of Nonlinear Conductance. *Phys. Rev. Appl.* **11**, 044062 (2019).

[11] B. Zengin, J. Oppliger, D. Liu, L. Niggli, T. Kurosawa, F. D. Natterer, Fast spectroscopic mapping of two-dimensional quantum materials. *Phys. Rev. Res.* **3**, L042025 (2021).

[12] J. Kirk, Open Traveling Salesman Problem - Genetic Algorithm. *Find. -Optim. Solut. Open Var. TSP Using Genet. Algorithm* (2014), (available at *https://www.mathworks.com/matlabcentral/fileexchange/21196*).

[13] E. van den Berg, M. P. Friedlander, Probing the Pareto frontier for basis pursuit solutions. *SIAM J. Sci. Comput.* **31**, 890–912 (2008).

[14] J. Oppliger, B. Zengin, D. Liu, K. Hauser, C. Witteveen, F. von Rohr, F. D. Natterer, Adaptive Sparse Sampling for Quasiparticle Interference Imaging. *ArXiv220404475 Cond-Mat* (2022) (available at *http://arxiv.org/abs/2204.04475*).

Jens Oppliger is currently pursuing a master's degree in physics at the University of Zurich in the research group of Prof. Fabian Natterer. During his studies he was mainly working with scanning tunneling microscopy to speed-up quasiparticle interference mapping experiments. His main interests are the integration of novel computational methods into scientific research and to develop digital tools to reduce the workload of various experimental techniques in condensed matter physics. This includes novel AI-based concepts surrounding machine/deep learning as well as signal processing theories such as compressive sensing.

Fabian Donat Natterer is an SNSF Professor at the University of Zurich. His group focuses on quantum sensing and quantum materials discovery using scanning probe microscopy. To enhance and enable those activities, his team develops novel SPM measurement schemes, such as compressive sensing and parallel spectroscopy enhanced quasiparticle interference and time-resolved techniques for electron-spin resonance.