PERSPECTIVES: PHOTOEMISSION SPECTROSCOPY

Gaps, Pseudogaps, and Occam's Razor

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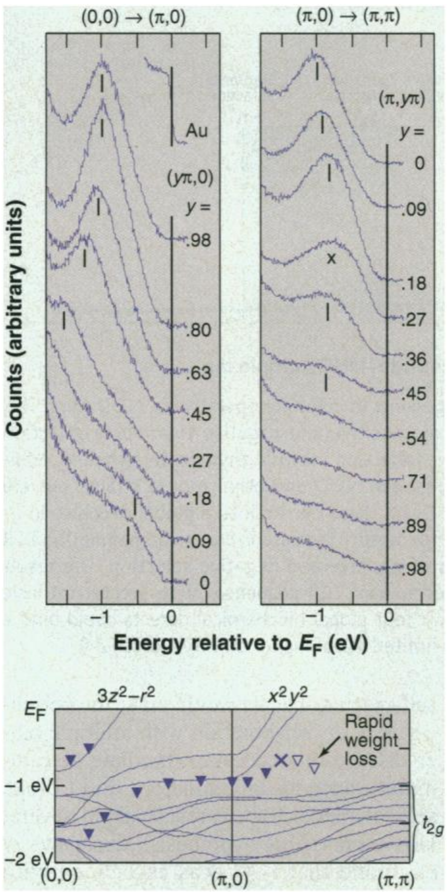
Great strides have been made in recent years in the preparation of excellent single crystals of novel materials [such as high—superconducting transition temperature (T_c) superconductors, colossal magnetoresistant (CMR) materials, and quasi–one-dimensional (1D) systems]. Together with advances in the resolution and intensity of experimental techniques such as angle-resolved photoemission (ARPES), this progress has inevitably led to the discovery of new phenomena heretofore hidden by poor samples and inferior resolution. New theories have mushroomed to explain these phenomena. However, the report by Joynt (*1*) on page 777 of this issue suggests that we should not rush to conclusions, because at least some of the apparently new phenomena may result from extrinsic effects. Such effects are not attributable to the fundamental nature of the material's electronic structure but rather to classical physics artifacts of the photoemission process itself, not heretofore considered or observed.

ARPES is a powerful technique, perhaps the only one that allows direct observation of occupied electron states in a material. From the kinetic energy position of peaks in the ARPES spectrum, one can deduce the binding energy of allowed electron states in the solid, while the photoelectron direction yields the momentum (*2*). At different momenta, or equivalently different directions of the outgoing electrons from the single-crystal sample, the energy position of these peaks shifts with momentum (that is, electrons exist as band states) until at some angle they may coincide with and even cross the Fermi energy (in a metal) and disappear above it into empty states that are not observable by photoemission.

Many recent ARPES investigations in lower dimensional systems report a lack of spectral intensity at the Fermi energy (*3*), as if the bands never reach or cross the Fermi energy (implying that there exists a gap in the energy versus momentum spectrum) in spite of the fact that the materials conduct current and often even undergo a superconducting transition. This is peculiar because only the electrons directly at the Fermi energy are allowed to conduct current. Furthermore, band theoretical calculations of the electron energy spectra for these materials do not predict a gap. For example, band theoretical calculations predict layered $La_{1.2}Sr_{1.8}Mn_2O_7$ to be a (poor) metal, but ARPES band features or peaks never approach the Fermi energy any closer than about 0.5 eV for any momentum (see the figure).



Explaining the gap. ARPES spectra (**top**) for different directions (or momenta) in $La_{1.2}Sr_{1.8}Mn_2O_7$. The symbol π effectively denotes the unit cell boundary in momentum space. Note that the features never come closer than 0.5 eV to the Fermi energy E_F (zero of energy), despite the fact that according to band structure calculations these features should cross the Fermi energy. $3z^2 - r^2$, $x^2 - y^2$ and t_{2g} denote specific types of energy bands (**bottom**). Triangles in the bottom panel mark experimental energy position of spectral peaks in the top panels relative to calculations (solid lines). In the top left panel, a spectrum for Au is shown for reference. [Reproduced from (*3*)]

These observations may be the result of new physics, or they may be attributable to extrinsic artifacts. Joynt (*1*) addresses one such artifact, namely that of ohmic energy losses of photoelectrons emitted from the surface of a solid that is poorly conducting because of either low carrier density or low mobility. As a result, the outgoing electron, which leaves behind a surface image charge, loses energy to the image charge and appears at a kinetic energy smaller than the normal photon energetics would dictate. Thus, the photoelectron appears to come from a higher binding energy. With ohmic losses, photoelectrons whose initial binding energy in the metal coincided with the Fermi energy yield ARPES peaks at a kinetic energy a few tens of millielectron volts lower than their initial binding energy would dictate. Thus, for all practical purposes, an energy gap (or pseudogap) would appear at the Fermi energy.

The observations referred to above for layered $La_{1.2}Sr_{1.8}Mn_2O_7$ and other materials are remarkably similar to the predictions of Joynt for poorly conducting solids. In most materials, the gaps are smaller than that shown in the figure and thus unobservable with poor resolution.

The situation is somewhat complicated by the fact that many 1D and 2D systems (analogs of high-T_c superconductors) often display true gaps at the Fermi energy owing to the emergence of a charge density wave (CDW), that is, a periodic buildup of charge not necessarily correlated with the crystalline periodicity. This is instrumental in creating forbidden electron states or gaps. These gaps are well understood and do not constitute new physics. Instead, the focus here is on non-CDW low-dimensional systems such as CMRs, high-T_c superconductors, or quasi-1D materials. All these materials are characterized by poor metallic conductivity (*4*), the very condition for which Joynt's theory applies. Gaps at the Fermi energy have often been observed in these materials and been attributed to a variety of physical phenomena. The gap in CMRs is postulated to result from polarons (*3*). In high T_c's [where the gap is referred to as a pseudogap (*5*), meaning that some electron states remain at the Fermi energy], antiferromagnetism is often invoked as the origin. 1D systems reflect the greatest flurry of activity because a gap in these systems was actually predicted nearly two decades ago by Haldane (*6*). Although some nuclear magnetic resonance data have been interpreted in terms of a Haldane gap, it has not yet been directly observed in an ARPES measurement. It would be highly desirable to find a quasi-1D non-CDW system, but, even if one were found, we would still have to consider ohmic losses in these poor con-

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ductors. Thus, there are no truly "clean" systems for investigation.

Joynt has been careful not to overstate his theory. He specifically eliminates high-T_c materials from consideration of the ohmic loss phenomenon, concentrating instead on CMR materials for which poor conductivity is not in question. However, it is not clear that he needed to do so. Indeed, early data on high-T_c materials with poor sample stoichiometry yielded a much lower carrier concentration at the Fermi energy. These early ARPES spectra appear remarkably similar to current CMR data, showing no intensity at the Fermi energy even in high-resolution single-crystal spectra.

Of course, one cannot exclude other mechanisms. Experiments with vastly improved crystals showed that metallic-like band crossings of the Fermi energy occur (*7*) in high-T_c materials, although the above-mentioned pseudogaps that deviate strongly from a typical metal still appeared in certain regions of momentum space. Currently, momentum-dependent gaps cannot be explained by Joynt's theory, which is constructed to be momentum independent. Very recent data (*8*), however, show that even better momentum resolution and the use of different photon energies result in a complete elimination of these gaps and that $Bi_2Sr_2CaCu_2O_8$ displays very normal metallic behavior at some photon energies. Perhaps a refinement of Joynt's theory, which, to first order, should also not be photon energy dependent, can resolve this issue.

There is thus good reason to examine the possibility that gaps and pseudogaps observed in CMR data and at least the early high-T_c data can be explained by ohmic losses. Indeed, it might be prudent to scrutinize all reports of gaps with respect to the Joynt theory, including the quasi-1D systems, where even better crystals and resolution than are presently available are required to resolve the issue.

The Joynt report should serve as a warning that one should consider all possibilities to avoid overinterpretation of data. Experience has shown that the simplest explanation is most often the correct one, as postulated in Occam's razor.

References and Notes

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RETROSPECTIVE

Sir Alan Hodgkin (1914–1998)

Peter B. Detwiler

Every now and then giants come along, raise the bar, and lift us all; Alan Hodgkin was one of them. He never worked for a Ph.D.; didn't have a research supervisor; and built, borrowed, or begged equipment to ask and answer his own questions. Yet despite—or because of—what might be viewed today as these initial "handicaps," as a second-year undergraduate, Hodgkin began an active research career that spanned more than 50 years. His studies resulted in landmark discoveries that rewrote textbooks, established the keystones of modern physiology, and set new standards for experimental neuroscience.

He is most recognized for his work on nerves. As a 20-year-old undergraduate at Trinity College, Cambridge, Hodgkin established that the action potential is propagated electrically by currents spreading passively in a local circuit. Later, with Andrew Huxley, he made the first intracellular recordings from squid axon and discovered unexpectedly that the action potential overshot zero by many tens of millivolts. This demonstrated that the action potential was generated by selective changes in the electrical properties of the surface membrane and did not involve proteins in the axoplasm as many thought. Their excitement was cut short 3 weeks later when Hitler's army marched into Poland and England was plunged into war.

Hodgkin was assigned to research on radar and spent the next 5 years working as a physicist, an unusual assignment for a biologist who was self-taught in mathematics and physics, but he was an excellent choice. Hodgkin was a quick study, creative, with penetrating intelligence and common honesty.

"Alan, what was the most important thing you learned at school?" "To read widely and work on my own." "Yes, but what did you like the best about school?" "The holidays." [A. L. Hodgkin, *Chance and Design*, 1992].

Boyhood holidays were spent exploring the outdoors, which was the original source of Hodgkin's enthusiasm for natural history. It was through a keen interest in bird watching that he first recognized the essential relationship between observation (research) and learning.

The war ended, and Hodgkin and Huxley returned to their work on the giant axon. Using a feedback circuit to clamp membrane voltage at fixed levels they dissected the ionic basis of the action potential, and discovered voltage-gated sodium and potassium conductance changes, showing how their properties could account for the excitation and propagation of the nerve impulse. The Nobel Prize in Physiology or Medicine recognized their work in 1963.

Hodgkin became president of the Royal Society in 1970 and switched to research on vision, the focus of his experimental work for the rest of his career. He began working with M. G. F. Fuortes at Woods Hole on the photoreceptors of the horseshoe crab, *Limulus*. They investigated the long delay that preceded the electrical response evoked by a light flash and attributed it to the time taken for a signal to pass through a cascade of chemical reactions. They recognized that stages of chemical amplification may underlie the generation of the photoresponse and that feedback mechanisms were likely to be responsible for the reciprocal changes in response sensitivity and time resolution that occur when the receptor is light- or dark-adapted.

Rarely working with more than one person at a time, Hodgkin undertook research on retinal cones and rods that lasted 17 years and through elegant experimentation and imaginative quantitative analysis established many tenets of retinal photoreceptor physiology. As with his work on the electrical properties of nerve, Hodgkin's research on vision redefined the landscape, expanded the vocabulary, and focused attention on the next set of crucial questions.

Alan Hodgkin was a tall man, with a quiet disposition, a good sense of humor, and lively eyes that could express a full range of emotions. He was modest despite his achievements. He did not put his name on any work that he did not fully participate in. He had no interest in having a large research group and felt that one collaborator at a time was best, two were awkward, and more than that impossible. He was fun to work with. Experiments were rarely planned ahead of time, as there was the unexpressed sense that this would somehow ruin the chase by quenching the feeling of exploration and discovery that was, after all, the point of the process—the chance in *Chance and Design*.

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