Knotek notes that their theory is not in disagreement with that of Redhead, Menzel and Gomer. The latter model applies to valence-level electrons whereas the former model applies to core-type excitations. Clear examples of each process are emerging.

Last year, Knotek, Vernon O. Jones (Naval Weapons Center, China Lake, California) and Victor Rehn (China Lake and Stanford Synchrotron Radiation Lab) showed[2] experimentally that photons also can cause desorption by the core-hole Auger-decay mechanism. By reacting a TiO_2 surface with water, they obtained a high density of OH^+ and H on the surface. Then, using photons from the Stanford Synchrotron Radiation Laboratory 8-deg beam line, they observed photon-stimulated desorption of the H^+ and OH^+ ions. Knotek told us that photodesorption occurred at the identical threshold (although much sharper) as for ESD and that the ions per core hole created were the same for both PSD and ESD within a factor of two.

In the same year, a Bell Labs group, including Phil Woodruff, Mort Traum, Neville Smith and Helen Farrell and their collaborators, working at the University of Wisconsin Synchrotron Radiation Facility, observed[3] photon-stimulated desorption of O^+ and other ions from the metal surface W(100). Both the Sandia–China Lake[2] and Bell Labs groups[3] reported showing that photons of specific energies selectively knock inner-shell electrons from surface atoms, causing ion desorption, in accordance with the theory of Knotek and Feibelman. Also in 1979 R. Fanchey and Menzel (Technical University of Munich) observed photon-stimulated desorption of O^+ and CO^+ from CO on tungsten.

The recent NBS–IBM experiment[4] combined the angle-resolved electron-stimulated desorption technique with a two-dimensional display-type spectrometer originally designed by Dean E. Eastman (IBM) primarily for angle-resolved photoemission measurements. The collaboration, consisting of Madey and Roger Stockbauer (NBS), J. F. van der Veen (IBM) and Eastman, used the University of Wisconsin Synchroton Radiation Facility at Stoughton for photons (8–120 eV). Earlier, Madey and his collaborators had found, with ESD, that the adsorbed layers of oxygen on tungsten single crystals produced three separated ion beams. The NBS–IBM group used the same conditions on a W(111) surface and found that photon stimulation also produced three ion beams with angular distributions at all photon energies essentially identical to those found with electron (500-eV) stimulation. The NBS–IBM group finds that the direction the atoms or molecules move when released from a surface by photon stimulation is directly related to the angle of the surface bonds being broken.

In the NBS—IBM experiment, using the two-dimensional detector, desorbing positive ions are reflected and focused by an electrostatic ellipsoidal "mirror," and the signal is amplified by an image intensifier and displayed. From the spot positions, one determines the ion trajectories and thus the angle at which the atoms had been bonded to the surface.

Significance. Other surface-structure measurement techniques such as low-energy electron diffraction generally require long-range order. But both ESD and PSD are sensitive to the local geometry—to the excitation of adsorbed atoms and molecules in individual bonding sites. Both provide electronic structure information on atomic sites on the outermost layer of the surface to which specific adsorbates are bonded. Angle-resolved ESD and PSD promise to give the location and angle of surface bonds directly, with little calculation, even for specimens without long-range order.

Angle-resolved PSD is expected to be useful in the chemical and structural analysis of the surfaces of metal-oxide catalysts. Madey has demonstrated the specific sensitivity of angle-resolved ESD to surface steps and defect sites, which may be of importance in catalysis.

A feature of PSD and ESD with both positive and negative aspects is that ion yields depend sensitively on the nature of chemical bonding and vary enormously for different species, Eastman told us.

Knotek says ESD is one of the most sensitive techniques available for detecting hydrogen, which is of extreme importance in catalysis. However, until calibration studies have been done, Knotek notes that one cannot tell how many hydrogen atoms are present.

Other groups doing PSD include Joachim Stohr and Rolf Jaeger at the Stanford Synchrotron Radiation Lab, David Shirley and collaborators at Lawrence Berkeley Lab and Stockbauer and Madey at the NBS synchroton, SURF II. Both the SSRL and Sandia groups are trying to do surface EXAFS with PSD.

Yates, Sylvia Ceyer and Madey at NBS are now coupling angle-resolved ESD with electron-energy loss spectroscopy in the same apparatus to study the structure of surface molecules. —GBL

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21-term series yields critical indices

Discoveries in physics often hinge on a disagreement between theory and experiment of a percent or less. Because of such a discrepancy, many workers in statistical mechanics have been concerned about the complete validity of the scaling and renormalization-group theories of critical phenomena. For the three-dimensional Ising model, the experimentally derived values for the critical exponents in fluids have agreed to three significant figures with those predicted by the renormalization group. However, the predictions disagreed by a couple of percent with exponents calculated by series expansions, and the claimed accuracy of these expansion estimates was much less than a percent.

Unfortunately theorists have a finite lifetime; so until this year the best high-temperature series expansion used to determine critical indices had 15 terms, still a backbreaking calculation. Adding even one extra term to the series would have required more than twice as much computer time as calculating all the previous terms.

Now Bernhard Nickel of the University of Guelph (Ontario, Canada) has found a clever way of extending the series to 21 terms, and the discrepancy between the series result and renormalization-group theory seems to have disappeared. (Nickel reported his results at the Cargese Summer Institute in July and the Statphys 14 meeting at Edmonton, Alberta in August.) The general reaction among statistical mechanicians is a collective sigh of relief that the renormalization group-scaling theory is still a beautiful, correct picture of critical phenomena.

Scaling and renormalization group. The magnetic susceptibility, for example, diverges at the critical point as $(T-T_c)^{-\gamma}$, where T_c is the critical temperature and γ is the critical index of the magnetic susceptibility. Other thermodynamic and correlation parameters, such as specific heat and correlation length, each have a singularity at a critical point, all of which can be described by power laws with different critical indices.

Since the pioneering work on scaling

done by Benjamin Widom (Cornell University), Leo Kadanoff (now at the University of Chicago), A. Z. Patashinski and V. L. Pokrovski (Novosibirsk) and others, it was generally believed that the critical indices are not all independent of each other but are related by scaling laws. For example, one scaling law relates the critical index for specific heat, α, with the critical index for correlation length, ν.

$$d\nu = 2 - \alpha \quad (1)$$

where d is the dimensionality of the system. Another scaling law is

$$d\nu = \alpha + 2\beta \quad (2)$$

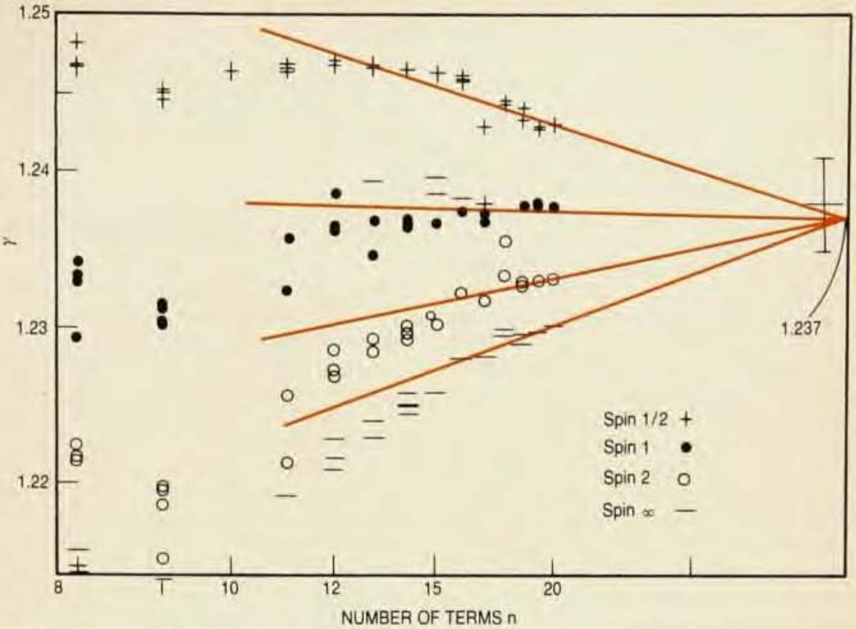
where β is the critical index for the order parameter.

Building on Kadanoff's concept of universality—the effect of scale transformations on Hamiltonians near the critical point, in 1971 Kenneth Wilson (Cornell) and others developed the renormalization-group approach. This theory provides a framework for the scaling laws and allows one to obtain explicit values for the independent critical indices. Although renormalization-group calculations are only approximate, they generally were in good agreement with experiment and consistent with one another.

Because the accuracy of experiments is limited, another approach for determining critical exponents is used—high order perturbation theory. For the susceptibility, one can do a series expansion in powers of exchange energy divided by temperature. The infinite number of terms in the series determines the susceptibility and the value of γ exactly.

Because one must terminate the series after n terms, various methods must be used to estimate the value of γ, such as ratio tests and Padé approximants. In the late 1960's, such series expansions were taken to 12 terms—by a group at Kings College, London, including Cyril Domb, Martin F. Sykes, John Essam and Douglas Hunter, by Michael Fisher and R. J. Burford (then both at Kings) and by Michael Wortis, Michael Moore, Marty Ferer and David Jasnow (all then at the University of Illinois). These calculations showed values for $\gamma = 1.250$, $\nu = 0.637$ to 0.643, $\beta = 0.3125$ and $\alpha = 0.125$. Plugging these calculated values into the scaling laws showed a disagreement with scaling that could not be accounted for by the estimated errors.

In 1970 Fisher suggested that perhaps the original scaling postulates were too strong. Although scaling predictions for critical exponents involving thermodynamic quantities agreed well with series results, those involving spatial dimensions did not. He referred to those scaling relations involving both kinds of parameters as "hyperscaling," and suggested that hyperscaling might not apply.



Padé estimates of γ, the critical index of the magnetic susceptibility, based on n terms in the series for the body-centered cubic lattice calculated by Bernhard Nickel (University of Guelph, Ontario). The model discussed in the story is the spin-½ Ising model, in which each spin can be ± 1, that is, up or down. The spin 1, 2 and ∞ labels refer to other models that are expected to lie in the same universality class. The straight lines are a guide to the eye indicating a possible trend with n to the universal value $\gamma = 1.237$.

One of the best recent series expansion calculations, involving Padé approximants, has been done by George Baker (Los Alamos), who told us that although dimensional dependence or hyperscaling is satisfied in one and two dimensions, he, like previous theorists, found a small failure in hyperscaling predictions.

Despite this small, nagging discrepancy, renormalization-group theory enjoyed one success after another, particularly after the ε expansion approach was developed by Fisher and Wilson (PHYSICS TODAY, March 1972, page 17). High-precision calculations were started about 1975 by Nickel, Baker, Daniel Meiron (then at MIT) and the late Melville Green (Temple University) and by a group at Saclay—Jean Zinn-Justin, Jean-Claude LeGuillou and Edouard Brézin. The Saclay group developed a method, effectively incorporating hyperscaling, for analyzing asymptotic higher-order terms to estimate critical exponents. These more accurate renormalization-group calculations disagreed with the series expansions, too. For γ, for example, their value was 1.240 instead of 1.250. The discrepancy between the series and renormalization group calculations has been troubling for the last decade (PHYSICS TODAY, December 1977, page 42), but during this entire period most statistical physicists probably would have agreed that the renormalization group theory looked right.

Nickel's new work builds on the calculation scheme developed by Wortis in the late 1960's. For the three-dimensional Ising model of spins on a lattice, in the series expansion, you use for the first term, the interaction between nearest-neighbor spins, and for the second term, two interactions—once between the spin and its neighbor and then between this neighbor and its neighbor. In the third term, you have three interactions with four spins. So as you go to higher order, you must calculate terms involving more and more spins and also sample more and more of the lattice.

Nickel explained to us, to do a brute-force calculation with the Wortis method, you fix one spin at the origin and look at its effect on distant spins. Then you have to sum over all possible spin locations in three dimensions.

For the body-centered cubic lattice, however, Nickel had the following insight, quite obvious once you know about it: He could do all sums on a line in one dimension and then cube the answer. Previously, theorists had tried only general methods that worked for all lattices.

With this simplification, Nickel was able to extend the series for the susceptibility and correlation length to 21 terms. Earlier series calculations had only been done to 15 and 12 terms respectively. Nickel stopped at 21 terms because that appeared to be a reasonable amount of computer time—20 or 30 hours on an Amdahl V5. Without his simplifying approach, Nickel says the 21-term brute-force calculation would probably have taken several years.

Once he had the series, he "had to play extrapolation games" to estimate the critical exponents. He made a series of estimates, keeping more and more terms, and found that a plot of estimates *vs.* number of terms is very flat up until 12 or 15 terms. If you had stopped calculating there, as previous theorists had done, you would assume that $\gamma = 1.250$ was close to the right answer.

This change can plausibly be interpreted, Nickel told us, as the result of competition between the leading divergence, $(T - T_c)^{-\gamma}$, and a weaker but still divergent term also near T_c, which is expected to be there. The effect of this weaker divergence on the estimates of γ will not be negligible unless you have calculated enough terms.

But are 21 terms enough? At present, Nickel finds $\gamma = 1.238 \pm 0.003$ and $\nu = 0.631 \pm 0.003$, in good agreement with the renormalization-group calculations. One recently quoted 12-term series estimate for γ was 1.250 ± 0.003, a 1% difference in result. Thus Nickel's work suggests that previous error estimates in series calculations were a factor of three or four too low.

The new error estimates made by Nickel may also not be realistic, he told us. So now he is collaborating with John Rehr (University of Washington) in analyzing the 21-term series by methods that explicitly account for the weaker divergent terms.

Although Nickel has only done such a long series expansion for the bcc lattice, according to the universality principle, the critical exponents are identical for whole classes of systems. So Nickel believes his bcc results can be applied to other lattice geometries because they are all in the same universality class. He says, "The good news is that at present the evidence from high-temperature series is consistent with the renormalization-group picture of the critical point. The bad news is that we have learned how easy it is to be misled by the apparent convergence of estimates from short series and that to exclude, with reasonable confidence, the possibility of a violation of hyperscaling or universality or the complicated critical region behavior as envisaged by Baker and John M. Kincaid [earlier this year] will require much more effort in deriving longer series."

Baker, although enthusiastic about Nickel's new series terms, says he doesn't believe Nickel has shown his extrapolation procedures to be better than either traditional methods or variational procedures. Concerning his old speculation that hyperscaling does not hold, Fisher says, "I'm sitting on the fence."

Kadanoff is convinced that Nickel has shown that the left- and right-hand sides of equation (2) are consistent. "We have other extremely good reasons for believing that the scaling phenomenology and renormalization-group theory are right. Nickel has weakened the strength of the apparent discrepancy. Now we can return to our theoretical prejudices." —GBL

Great undersea waves may be solitons

Peculiar striations more than a hundred kilometers long, visible on satellite pictures of the surface of the Andaman and Sulu Seas in the Far East, appear to be of interest in fields as far removed from oceanogaphy as quantum field theory. A recent report[1] of underwater current and temperature variations associated with such surface phenomena in the Andaman Sea, by Alfred Osborne, a physicist at Exxon Production Research (Houston), and Terrence Burch, an oceanographer with EG&G Environmental Consultants (Waltham, Mass.), suggests that these striations mark the propagation of "solitons," exotic solutions of nonlinear wave equations that have captured the interest of mathematical physicists studying a broad range of phenomena spanning 22 orders of magnitude in size.

The surface striations seen in the satellite pictures are interpreted as secondary phenomena that accompany the passage of "internal solitons," solitary wavelike distortions of the boundary between the warm upper layer of sea water and the cold lower depths. These internal solitons are traveling ridges of warm water extending downward hundreds of meters below this thermal boundary. Carrying enormous energies, these presumed solitons appear to be the cause of the usually strong underwater currents periodically experienced by Exxon's deep-sea drilling rigs between Sumatra and the Malay Peninsula in the Andaman Sea. They have even been implicated in the mysterious disappearances of several submarines. If one wants to continue deep-sea drilling for oil in areas where solitons occur, one will have to build drilling and production facilities that can withstand the large horizontal forces they generate.

John Apel and James Holbrook of the Pacific Marine Environmental Laboratory (Seattle) will report the results of their recent studies in the Sulu Sea, between Borneo and the Philippines, at the December meeting of the American Geophysical Union in San Francisco. Noting that these great internal waves usually appear in groups of up to ten, they prefer to describe them as damped "cnoidal" wave trains, a nonlinear hydrodynamic phenomenon closely related to solitons, and sharing most of their bizarre properties.

The history of solitons has its colorful beginning with a fortuitous observation in 1834 by the Naval architect John Scott Russell, while riding on horseback alongside a Scottish canal. "I was observing the motion of a boat... which suddenly stopped—not so the mass of the water in the channel which it had put in motion... Suddenly leaving it behind, (it) rolled forward with great velocity, assuming the form of a great solitary... well defined heap of water, which continued along the channel apparently without change of form or diminution of speed. I followed it on horseback ... still rolling on at... eight or nine miles an hour, preserving its original figure. Its height gradually diminished, and after a chase of one or two miles I lost it in the windings of the channel."

Standard linear dispersive wave theory does not permit such solitary waves of constant shape, even in the limit of a frictionless fluid. A "well defined heap of water" would rapidly lose its shape by frequency or amplitude dispersion. Not until D. J. Kortewegs and Hendrick de Vries wrote down the appropriate nonlinear wave equation in 1895 was it seen that localized nondispersive solitary waves could exist. In their (K–de V)equation, as in other nonlinear wave equations that admit of soliton solutions, the shape-preserving solitary waves result from a cancellation of the dispersive term by the nonlinear term. Unlike ordinary dispersive linear waves, the solitons have only crests, unaccompanied by troughs (with respect to the equilibrium surface).

It was another 70 years before Martin Kruskal (Princeton) and Norman Zabusky (now at the University of Pittsburgh) discovered the peculiar property of these solitary-wave solutions that led them to the name "soliton"—a coinage suggestive of a particle. From computer-generated numerical solutions of the K–de V equation, they discovered in 1965 that the solitary waves preserve their shape and velocity even when they pass through one another. We have then highly localized entities that preserve their identities as they propagate—and even when they "collide." Small wonder that quantum field theorists speculate that solitons may describe as-yet-undiscovered elementary particles—in particular, magnetic monopoles.