New Probe for Unoccupied Bands at Surfaces

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Electrons accelerated by the potential inside a surface emit photons with a probability related by time reversal to excitation of an electron in photoemission. Conservation of energy and momentum in the transition gives information about unfilled bands, of the same kind that angle-resolved photoemission gives for the filled bands. Particularly interesting is the possibility of using the new spin-polarized electron sources to study magnetism with the inverse photoemission technique.

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It is the purpose of this Letter to suggest a new experiment: measurement of the bremsstrahlung-radiation spectrum from electrons, with energies no more than a few tens of electron volts, incident on clean surfaces. The experiment will be sensitive to the surface region because of the finite path length of low-energy electrons and will provide information about the density of unoccupied states into which the incident electron falls. In fact, if the energy and direction of the incident beam are carefully defined and both momentum and energy are conserved in the transition,

$$\vec{k}_f = \vec{k}_i - \vec{Q}, \tag{1}$$

$$E_f = E_i - \hbar\omega, \tag{2}$$

where the subscripts i and f refer to the initial and final electron states and $\vec{Q}$ is the photon momentum, then peaks are expected in the spectrum of emitted light when $E_f(\vec{k}_f)$ corresponds to an energy level in the solid. The low electron and photon energies make this $\vec{k}$ selection feasible, as opposed to bremsstrahlung isochromat spectroscopy,[1] which measures $\vec{k}$-integrated densities of states because of thermal and other broadening in $\vec{k}$.

Such a speculation would not at first carry much weight, except that very closely related experiments have already been performed and can be used to predict the result of the present experiment in a qualitative sense. Angle-resolved photoemission experiments[2] (PE) turn incident photons into emitted electrons. The experiment proposed here is to turn incident electrons into emitted photons. The matrix elements for the two experiments are related by time reversal and for this reason the *photon*-emission experiment will be referred to as inverse photoemission, or IPE for short.

In a separate paper a detailed derivation of the IPE yield will be given, but the following argument gives the essential result with a minimum of effort. Consider two surfaces identical in properties, except that the first surface has a given set of levels occupied by electrons. The PE yield from these levels is J_{el} (= electrons per hartree per steradian per photon). In the second surface these same levels are now empty, e.g., because the Fermi energy is lower. The levels are now accessible to an IPE experiment with yield J_{ph} (= photons per hartree per steradian per electron). State by state the transition probabilities are linked by time reversal and are equal. J_{el} and J_{ph} are not equal because the number of states in a steradian of photons is not the same as in a steradian of electrons. In a steradian of electrons, the number of states is

$$[\Omega/(2\pi)^3]\,|\vec{k}|^2\cos\theta = [\Omega/(2\pi)^3]\,2E\cos\theta, \tag{3}$$

where Ω is the size of a large box containing the system, $\vec{k}$ is the electron momentum, E the electron energy in hartrees, and θ the polar angle of electron emission. In a steradian of photons, the number of states is

$$\frac{\Omega}{(2\pi)^3}\,|\vec{Q}|^2\cos\Xi = \frac{\Omega}{(2\pi)^3}\,\frac{\omega^2}{c^2}\cos\Xi, \tag{4}$$

where $\vec{Q}$ is the photon momentum, ω the photon energy, c (= 137.0) the velocity of light in atomic units, and Ξ the polar angle of photon emission. It follows that

$$J_{ph}/J_{el} = \omega^2\cos\Xi/2Ec^2\cos\theta. \tag{5}$$

A consequence of Eq. (5) is that IPE gives the same information as angle-resolved PE, but for the empty states. Detailed plots of empty bands can be made, unoccupied–surface-state energies mapped as functions of $\vec{k}$, adsorbate levels studied, and all the other information found for the empty bands that is supplied by PE for the occupied bands. The information is complementary.

Photon beams and electron beams can be handled easily, but the key question is whether the photon count rate can be made high enough. Working against the experiment is the large factor of c^2 in the denominator of (5). In favor is the fact that because $\vec{Q}$ is always small, a full 2π sr may be collected without disturbing the $\vec{k}$ conservation of Eq. (1). The count rate can be estimated by taking a typical value for the total yield from the d band of a noble metal, which is about 10^{-2} electrons per photon[3] at $\hbar\omega = 0.4$ hartree, most of which falls in the primary spectrum. This estimate is consistent with calculated values.[4] In the $3d$ series this is distributed over a 0.15-hartree bandwidth, giving an estimate

$$J_{el} \simeq 10^{-2}/2\pi \times 0.15 \simeq 10^{-2}. \quad (6)$$

A typical electron energy *in vacuo* would be 0.15 hartree; hence on setting the angular factors equal to unity,

$$J_{ph} \simeq 0.4^2 \times 10^{-2}/2 \times 0.15 \times (137)^2 \simeq 3 \times 10^{-7}. \quad (7)$$

Suppose that the incident beam has a current of 100 μA ($\simeq 10^{15}$ electrons per second) and that half of the 2π sr of photons is captured; then in a 0.003-hartree (0.1-eV) bandwidth, there are

$$3 \times 10^{-7} \times 10^{15} \times \pi \times 0.003$$

$$\simeq 3 \times 10^{6} \text{ photons/sec}. \quad (8)$$

This is a high count rate even after allowing for possible monochromator inefficiency.

Several points are worth making with regard to the experiments. Provided that the photons are in the near ultraviolet with energies less than the LiF cutoff at 11.6 eV, the experiment should be relatively easy. In the vacuum ultraviolet, the problems are worse largely because of the limited acceptance angle of most monochromators operating in this region. At higher still photon energies, IPE rapidly gains over PE experiments (though they both become harder), the reason being that 2π sr of photons contain more states at higher energy. This improvement continues up to values of ω where it is necessary to restrict the range of $\vec{Q}$ accepted by the detector to maintain good resolution in $\vec{k}$ selection. The intrinsic $\vec{k}$ resolution of the PE/IPE process is set by the electron inelastic scattering length to about 0.1 a.u. and only when $|\vec{Q}|$ is of this order is it necessary to restrict the angular acceptance for photons:

$$\omega = c|\vec{Q}| = c \times 0.1/2 = 137/20 \text{ hartree}, \quad (9)$$

or about 150 eV. Above this energy PE and IPE experiments at optimum resolution sample equal areas of $\vec{k}$ and $\vec{Q}$ space and therefore the photon/electron and electron/photon yields into the detectors are equal. The IPE experiment retains the advantage because electron beams are generally far cheaper and more intense than photon beams.

There are other techniques available at present for the study of empty states but most are subject to restrictions which make them less powerful than IPE. They fall into two categories according to whether bands below the vacuum level can be studied. Of those applicable below $E = 0$, such as appearance-potential, x-ray–absorption, or bremsstrahlung isochromat spectroscopies, none has a $\vec{k}$ selection rule and so information is given only about the density of states, not the detailed band-by-band mapping that angle-resolved PE gives for the occupied states. Some techniques operating above the vacuum level do give $\vec{k}$ information, such as low-energy electron diffraction (LEED) and angle-resolved photoemission. Firstly, it must be said that most of the interest lies between E_F and the vacuum level, and even for the states accessible to LEED and PE, both techniques suffer defects. LEED is more responsive to band gaps than to bands and is not useful for plotting dispersion relationships. Angle-resolved PE is a powerful technique when used in the final-state spectroscopy mode, but does assume a knowledge of the initial state of the electron: of both $\vec{k}$ and E.

It is now possible to make spin-polarized electron beams relatively cheaply[5] with currents up to 100 μA and with good angular and energy resolution. On the other hand, detection of spin-polarized electrons involves use of a Mott detector, which is inefficient and expensive. The magnetism in d-band materials can as well be regarded as due to spin polarization of the holes in the d band, opening the possibility for studies of magnetism by spin-polarized inverse photoemission (SPIPE), analogous to the pioneering studies of spin-polarized PE currently being made.[6,7] The completion of parallel SPIPE and SPPE studies would provide invaluable complementary information about the hole and electron states in ferromagnetic materials.

The ideal experiment to test for IPE would combine ease of adaptation to current apparatus with high photon yield. To keep the signal in the near ultraviolet, very low electron energies should be used. Tungsten is a good material for the experi-

ment because it has several desirable qualities. The mean free path of the incident electron is larger than in most other materials [at least for the (100) and (111) surfaces] giving more opportunity for photon emission. The top part of the *d* bands is unoccupied giving a range of high density of states to which the electron can make a transition, and providing a rich band structure on which to test whether direct transitions are observed. Tungsten also has a strong potential which increases the electron-photon interaction.

In conclusion, theoretical estimates all point to inverse photoemission being an easy experiment with plenty of signal. Experimental confirmation is essential for further progress.

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General Relation of Correlation Exponents and Spectral Properties of One-Dimensional Fermi Systems: Application to the Anisotropic $S = \frac{1}{2}$ Heisenberg Chain

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A relation between the spectrum and correlation exponents of the Luttinger model is argued to be a general property of a universality class called "Luttinger liquids." The spinless fermion model equivalent to the $S=\frac{1}{2}$ Heisenberg-Ising-XY chain in a field is argued to belong to this class, allowing for the first time the systematic calculation of its correlation exponents.

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Interacting quantum systems in one dimension (1D) have many distinctive features not present in higher dimensions, and which can be seen in various kinds of soluble models. In this Letter, I develop a new connection between two very different classes of soluble fermion models which in general have been studied by two separate sets of workers. These classes are (i) the Luttinger model,[1] a model with long-range (noncontact) forces, which has a conserved fermion current, and a gapless elementary excitation spectrum of free bosons with a linear spectrum, and (ii) models with contact interactions that can be solved by the Bethe *Ansatz*,[2] and which have a gapless linear excitation spectrum. It is now known that models soluble by the Bethe *Ansatz* have an S matrix that is nontrivial (i.e., their elementary excitations are *not* free particles) but *factorizable*.[3] This property reflects the existence of an infinite set of conserved quantities, but which does *not* include the current.

The idea underlying the result is simple, and is an extension of an idea implicit in the work of Luther and Peschel[4]: This is that the low-energy properties of the Luttinger model are characteristic of a larger universality class of systems, which includes most, and probably all, 1D fermion systems with a gapless linear spectrum. By analogy with the Fermi-gas/Fermi-liquid relation in higher dimensions, where the noninteracting elementary excitation spectrum of the Fermi gas provides the model for the low-energy spectrum of the Fermi liquid, I propose to call such systems "Luttinger liquids." Provided relevant

