

$$\langle a_{a_1}^\dagger a_{a_2}^\dagger a_{a_3} a_{a_4} \rangle \cong \langle a_{a_1}^\dagger a_{a_4} \rangle \langle a_{a_2}^\dagger a_{a_3} \rangle - \langle a_{a_1}^\dagger a_{a_3} \rangle \langle a_{a_2}^\dagger a_{a_4} \rangle, \quad (3.3)$$

and the neglecting of term (A5) of I. We can, in fact, claim that the effects neglected will give a contribution to the integral in Eq. (3.2) not larger than one part in  $10^4$ . It must, however, be mentioned that if one wants to calculate the Pauli or spin paramagnetic susceptibility using the same Green's-function decoupling method used in I, not

only must one take into account term (A5) of I, but one also has to improve upon the Hartree-Fock decoupling (3.3); in the contrary case one finds for the spin susceptibility the Hartree-Fock result, which implies<sup>4</sup> a ferromagnetic instability in the electron gas at  $r_s \approx 6$  which has never been observed.

#### ACKNOWLEDGMENTS

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†Permanent address: Instituto di Fisica, Università di Padova, Italy.

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## X-Ray Edge Problem with Finite Hole Mass\*

G. Yuval†

*Joseph Henry Laboratories, † Princeton University, Princeton, New Jersey 08540*

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The methods used by Schotte and Schotte to study Mahan's x-ray edge problem are extended to the case of finite hole mass. The singular behavior is expected to continue down to a distance  $\Delta\omega \propto 1/M\delta$  above the absorption edge for attractive electron-hole interactions.

### I. INTRODUCTION

When an infinitely heavy hole interacts with an electron gas, the absorption and emission spectra due, respectively, to the creation and annihilation of the hole change their shape. In the absence of electron-hole interactions, the spectra have the usual threshold edge  $\theta(\omega - \omega_0)$ , but in the presence of this interaction, the threshold acquires a  $(\omega - \omega_0)^{-\epsilon}$  singularity (see Fig. 1).

This behavior was first surmised by Mahan,<sup>1</sup> and can be calculated exactly using the path-integral approach due to Nozières and De Dominicis,<sup>2</sup> or that due to Schotte and Schotte.<sup>3</sup>

If the hole mass is now allowed to be finite, the problem becomes more complicated, and it no longer seems possible to use the methods of Ref. 2. See Refs. 4-6 for some approaches to the problem.

In this article we shall extend the method of Ref. 3 to the case of finite hole mass. In this method, the electron Fermi gas is replaced by the Bose gas of its density oscillations; this allows us to use the path-integral theory of a system inter-

acting with an ensemble of independent harmonic oscillators. In the one-dimensional gas of  $S$  electrons (the only ones that can interact with a stationary hole via a Dirac's  $\delta$  function interaction), Schotte and Schotte, following Tomonaga,<sup>7</sup> define density-wave operators

$$\rho_{\mathbf{k}} = \sum_{\mathbf{k}_1 - \mathbf{k}_2 = \mathbf{k}} \frac{1}{\sqrt{N}} a_{\mathbf{k}_1}^\dagger a_{\mathbf{k}_2},$$

$$E(k_1) - E(k_2) = kv_F,$$

where  $N$  is the number of electrons and  $k_0$  is the momentum at the top of the conduction band. To within a good approximation (see Tomonaga), the  $\rho_{\mathbf{k}}$  obey boson commutation relations, and have the dispersion law

$$E_{\mathbf{k}} = kv_F,$$

where  $v_F$  is the Fermi velocity.

Schotte and Schotte also transform the electron creation and annihilation operators appearing in the problem into boson operators. If an electron is created at the origin at time  $t=0$ , and annihilated there at time  $t_0$ , these two fermion operators can

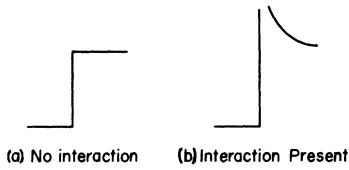


FIG. 1. Absorption threshold behavior.

be replaced by a potential at the origin that acts on the Bose gas between time 0 and  $t_0$  [see their Eq. (24)]. In proving this, the  $E$ -vs- $k$  relation of the electron gas is not used; the equivalence of Fermi operators to a potential acting on the Bose gas is thus independent of the  $E$ - $k$  relation. Once the problem has been transformed into a Bose-gas one, we have the heavy hole interacting with a large number of independent harmonic oscillators. We now follow Feynman<sup>8</sup> and eliminate the harmonic oscillators; these are replaced by a noninstantaneous self-interaction of the hole with itself. To find the behavior of the hole under such a noninstantaneous interaction, we have to use path integrals and integrate over the amplitudes of all possible histories of the hole. This is feasible here, because the only possible history is the creation of the hole and its subsequent annihilation, and only the times at which these occur can be varied.

The amplitude of each path is  $e^{-a}$ , where  $a$  is a bilinear form in the disturbance applied to the Bose gas.<sup>9</sup> For an infinite hole mass, Schotte and Schotte find  $a \propto \ln t$ , where  $t$  is the time during which the hole exists. The amplitude of the path is then  $t^{-1-\epsilon}$ , which gives the singular spectrum of Fig. 1. (The spectrum is found<sup>2</sup> by Fourier transforming the time distribution of the path amplitudes.)

In Sec. II, we shall extend the methods described to the case of finite hole mass.

II. FINITE-MASS CASE

If the hole mass is finite, it is no longer possible to deal only with  $S$  states, since the hole can move. We can still transform the Fermi gas into a Bose gas, i. e. ,

$$\rho_{k,E} \propto \sum_{\substack{\mathbf{k}_1 - \mathbf{k}_2 = \mathbf{k} \\ E_1 - E_2 = E}} a_{\mathbf{k}_1, E_1}^\dagger a_{\mathbf{k}_2, E_2}$$

This gas will not have a unique energy-momentum relation as was the case in Sec. I it will have  $E$  and  $k$  spread over a four-dimensional distribution, but as we nowhere need a unique  $E - k$  relation in the path-integral calculation, this nonuniqueness does not matter: The amplitude of a path still has the form  $e^{-a}$ , with an  $a$  bilinear form in the perturbation acting on the boson. That is,

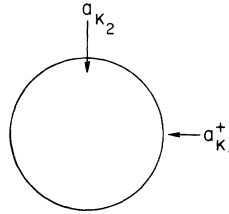


FIG. 2. Typical excitation.

$$a = \int F(\mathbf{r}, t) k(\mathbf{r} - \mathbf{r}', t, t') F(\mathbf{r}', t') d^3\mathbf{r} d^3\mathbf{r}' dt dt',$$

where  $F(\mathbf{r}, t)$  is the perturbation due to the heavy hole (we shall consider the form of  $F$  later).

The kernel  $k(\mathbf{r}, t)$  can be obtained by Fourier transforming its behavior in  $E - \vec{k}$  space, which in turn can be found from the boson spectrum. This approach is expected to be straightforward but tedious. However, we can use the following short-cut approach.

The x-ray edge problem is an infrared-divergence one, due to a large number of bosons of very low energy. A low-energy boson is constructed as in Fig. 2 with the electron and hole in it very close to the Fermi sphere. Therefore, for the purpose of computing the boson's momentum, we can project the two fermions onto the Fermi sphere as in Fig. 3 and the error involved will be very small; this is because, if we create an electron of momentum  $k_F + \epsilon_1$  and annihilate one of momentum  $k_F - \epsilon_2$  with the two momenta forming an angle  $\alpha$ , the system's momentum will be changed by  $2k_F \sin \frac{1}{2} \alpha + O(\epsilon_1 + \epsilon_2)$ .

If we perform this projection, which corresponds to assuming  $V_F = \infty$  and changing the  $E - \vec{k}$  spectrum as in Fig. 3, we find that the spectrum of the Fermions in  $E - \vec{k}$  space decomposes into a direct product  $f(E)g(\vec{k})$ , where  $f(E) = \text{const}$ ,  $g(\vec{k}) = \delta(|\vec{k}| - k_F)$ . The spectra of the empty states and of the occupied states decompose in the same way, with  $f(E) \propto \theta(E)$  and  $f(E)$ , respectively. Since this decomposition property is preserved under convolutions and Fourier transforms,  $k(\mathbf{r}, t)$  has this property too, that is  $k(\mathbf{r}, t) = q(\mathbf{r}) s(t)$ .

Now Schotte and Schotte have already found  $s(t)$ , because it also appears in the infinite-mass case. They find  $s(t)$  behaves like  $1/(1+t^2) - \pi\delta(t)$ , which corresponds to the Fourier transform of  $|E|$ .<sup>10</sup>

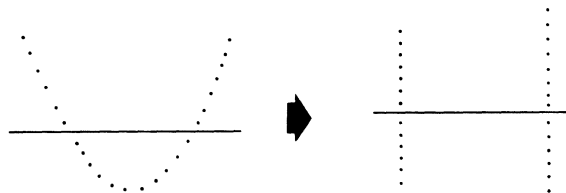
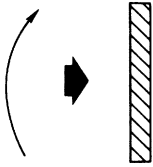


FIG. 3. Changing the  $E - k$  spectrum.

HOLE DOES NOT MOVE



HOLE MOVES

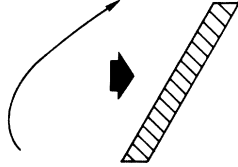


FIG. 4. Behavior of the potential.

For a square-wave disturbance, we have  $a \propto \ln t$  by double integration. We can see that this is the correct form; the energy spectra of the electrons created and of those annihilated are both step-functions. The energy spectrum of the gains is the convolution of these two spectra, and thus behaves like  $E \operatorname{sgn}(E)$ , with a sharp corner at  $E=0$ .  $s(t)$  is obtained by summing up contributions from the oscillators corresponding to all these gains, and this amounts to a Fourier transform; because of the sharp corner at  $E=0$ , we find a  $t^{-2}$  behavior for large times.

The three-space function  $q(r)$  is the Fourier transform of the momentum spectrum of the bosons, which in turn is the convolution of the momentum spectra of the electron and of the holes. But both these spectra are assumed to be on the Fermi surface (this is the  $v_F = \infty$  approximation), and thus we find

$$q(r) \propto (\sin^2 k_F r)/r^2.$$

The other result of Schotte and Schotte which we want to extend to the finite-mass case is their transformation turning the fermion creation and annihilation operators into boson operators. This result depends only on the commutation relation between the fermi operators and  $k$ , and the Hamiltonian nowhere appears in its derivation. Therefore, to extend it from a pair of operators at the origin—for which Schotte and Schotte have already shown the equivalence—to the general case we only need a Gallilean transformation. Following such a transformation (so as to make both operators act at the same place), we replace the fermion operators by boson operators as in Ref. 3, and transform back to the original co-ordinate system. The potential that replaces the pair of Fermi operators is on the straight line in  $E-\vec{k}$  space between these operators in one frame, and it is therefore on this straight line in the other Gallilean frame also (see Fig. 4).

The finite-mass x-ray edge problem has at this point been reduced to a path-integral problem for a hole moving through a Bose gas, through which a

potential due to the creation and annihilation operators moves uniformly in a straight line (see Fig. 5). If the scattering phase shift of the hole is  $\delta$ , the disturbance acting on the Bose gas at the hole site will be proportional to  $\delta$ . The disturbance along the straight line  $CA$  will be independent of  $\delta$ ; it will remain even when  $\delta=0$ , when the amplitude of the path will be the Green's function for a hole and electron moving independently.

In the sum of those two disturbances in the Bose gas  $a$  is bilinear. If  $\delta$  is small, we shall ignore the term which contains  $\delta$  in second order,<sup>11</sup> and make  $a(\delta) = a_0 + a_1 \delta$ . Under this approximation, the heavy hole does not interact with its own motion any longer; it only interacts with the potential on the straight-line segment  $CA$ . If we once assume this, we find that, for a given segment  $CA$ , the path-integral problem becomes equivalent to a time-dependent Schrödinger equation for the heavy hole in a potential due to the force moving along  $CA$ . This potential is found by taking this latter force and convoluting with  $k(r, t)$ . We find that the heavy hole moves in a potential of the form  $(\sin^2 k_F r)/r^2$ , the strength of which varies as  $1/(t-t_1) + 1/(t_2-t)$  where  $t_1$  and  $t_2$  are the times of creation ( $C$ ) and annihilation ( $A$ ), respectively. If  $\delta < 0$  (an attractive electron-hole interaction), this potential is attractive.

If the hole mass is  $M$ , it will be tightly bound by the potential due to  $CA$  for a time proportional to  $M\delta$  at the beginning and end of its path.<sup>12</sup> Therefore, for times up to a certain limit which is proportional to  $M\delta$ , the path-integral will behave as in the infinite-mass case (but  $\delta$  will be renormalized). If the time interval between  $C$  and  $A$  is larger, the potential on the hole will no longer affect it strongly (at least to first order in  $\delta$ ), and we are back to an independent-particle problem. Performing a Fourier transform, we then expect the spectrum to maintain its singular behavior down to a frequency  $\Delta\omega \propto 1/M\delta$  above the threshold, and then revert to a simple step-function behavior below this frequency.

If the electron-hole interaction is repulsive, so will the interaction be between the line  $CA$  and the hole path. In this case, the singular behavior will already disappear for very-short-time intervals.



FIG. 5. Relevant paths.

The method used here does not assume independence between successive recoils of the hole; that

assumption does seem to appear in the methods of Müller-Hartmann *et al.*<sup>13</sup> and of Doniach.<sup>5</sup>

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<sup>†</sup>Present address: Theoretical Physics Department, The Hebrew University, Jerusalem, Israel.

<sup>‡</sup>Work performed in part at Battelle Memorial Institute, Columbus, Ohio.

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<sup>10</sup>We write  $1/(1+t^2) - \pi\delta(t)$ , instead of just  $1/t^2$ , in order to get the correct Fourier coefficients at zero frequency ( $E=0$ ).

<sup>11</sup>Which, among other things, means neglecting the finite hole lifetime due to the creation of electron-hole pairs.

<sup>12</sup>A  $[(\sin^2 kr)/r^2]$  potential always has bound states (like those of an inverse-square potential) but these become very weakly bound for a weak potential, and need not concern us.

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## Photoemission Studies of Indium<sup>†</sup>

R. Y. Koyama\* and W. E. Spicer  
Stanford University, Stanford, California 94305  
(Received 28 June 1971)

Measurements of the electron energy distributions of photoemitted electrons from crystalline and bulk liquid samples of indium show structure which can be related to the occupied density of states. The distributions from the crystalline sample show two major peaks: a strong one just below the Fermi level and a weaker one about 4.5 eV below the Fermi level. Similar structure in the distributions from the liquid sample suggest that electron energy levels for indium are determined primarily from short-range interactions. Two model calculations based on direct transitions and nondirect transitions can each predict the observed structure with reasonable accuracy. In either calculation, structure in the energy distributions can be traced to similar structure in the density of valence states.

### I. INTRODUCTION

The initial motivation of this work was to investigate the importance of long-range order in a nearly free-electron metal by studying photoemission from crystalline and amorphous indium. Although we did not anticipate it at the onset of the work, it has become evident that the photoemission from crystalline indium is itself not unambiguously explained in terms of a single simple model. Rather, it has proved necessary to investigate direct<sup>1</sup> and non-direct<sup>2</sup> optical excitation models and to consider the possibility of surface excitation of plasmon effects.<sup>3</sup> However, it appears that independent of the detailed model, it is possible to associate structure in the photoemission energy distribution curves (EDC) from crystalline indium with structure in the density of states. This allows for rather direct

comparison between the photoemission results from crystalline and liquid indium.

As one might expect, we find that indium has an electronic structure that is relatively free-electron-like. Its optical properties<sup>4</sup> are quite similar to those of aluminum. The measurements we present here indicate that the energy bands of indium are distorted somewhat more than those of aluminum from the "pure" free-electron case. Structure in the electron energy distributions suggest stronger interaction of the electron with the lattice potential.

### II. EXPERIMENTAL METHODS

#### A. Measurements

The two experimental quantities of interest are the quantum yield and the photoelectron energy distribution. The quantum yield is defined as the