

Final-state potential in x-ray spectra

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An examination is made of the one-electron theory of x-ray transitions in metals. A question is raised whether the one-electron theory should be calculated using the potential of the central atomic core which does, or does not, include the screened core hole. It is suggested that one should use the potential of the final state, which has the core hole in absorption and not in emission. This suggestion agrees with emission data, as well as Mahan-Nozières-De Dominicis theory which is solved numerically for a square-well potential.

I. INTRODUCTION

A great deal of attention has been given to the edge singularities in the x-ray emission and absorption of simple metals.¹⁻¹¹ In this paper we wish to discuss the other parts of the spectra. The edge singularities, even when they exist, occupy only a narrow energy range of 0.5–1.0 eV near threshold, so another theory is needed for the other parts of the spectra. It is often assumed or asserted that these remaining parts of the spectra can be described by a one-electron theory. We will assume that this is the case, and then address ourselves to the issue of *which* one-electron theory is suitable. One must perform many-body theory in order to answer this simple question.

In either absorption or emission, one-electron theory has the rate of transition as the square of a matrix element and, summed over all initial and final states consistent with energy conservation,

$$A(\omega), E(\omega) = \sum_{if} |M_{if}|^2 \delta(\omega + E_i - E_f), \quad (1)$$

$$M_{if} = \int d^3r \psi_h(\mathbf{r})^* \vec{p} \cdot \vec{A} \psi_c(\mathbf{r}). \quad (2)$$

The matrix element is an integral between initial and final one-electron states, with a standard $\vec{p} \cdot \vec{A}$ kernel, where \vec{A} is the vector potential. The core wave functions ψ_c are fairly well understood, and the only question is the continuum wave function $\psi_h(\mathbf{r})$ for particle states in the conduction band of the metal. In a one-electron theory, this continuum wave function is a solution to a one-particle Schrödinger equation,

$$[-\nabla^2 + V(\mathbf{r}) - k^2] \psi_h(\mathbf{r}) = 0.$$

The only remaining question is which potential $V(\mathbf{r})$ to use in this equation. That is the subject we wish to discuss.

There are several potentials that one might

choose. The first one that comes to mind is the ordinary ground state of the metal. This presumably is a regular lattice of ions of charge Z , with nearly-free-electron states in the conduction band. The ground-state potential has all atomic core states filled and is the potential one uses to find the Bloch states of the solid. This potential we call $V_g(\mathbf{r})$.

The x-ray absorption removes an electron from the core state of an atom. This atom, which we call the central atom, will have a potential which is now different from the others, since it appears as an ion of charge $Z+1$. The potential of this core of $Z+1$ could also be used in the one-particle Schrödinger equation. Another feature that has been discussed several times is the nature of the screening of this extra positive charge on the ion. The simplest model assumes that the electron screening is infinitely fast, so that one should use the statically screened potential, which we call $V_h(\mathbf{r})$.

A more realistic calculation would include the dynamic nature of the screening. Minnhagen¹¹ has demonstrated this to be an important feature of x-ray-photoemission (XPS) spectra, and presumably it plays some role in x-ray spectra. This is certainly obvious for energetic transitions in absorption but is less obvious nearer to the absorption or emission edges, say within half of a plasmon energy. Any treatment of this effect is certainly not a one-particle calculation. The calculations we report here do not include the response time of the screening but instead take the core hole potential to be switched on fully screened. Further work is required to see whether this approximation has any validity and, if so, over what frequency range.

In emission spectra, another important question is the degree of relaxation. After the core hole is created, the electronic system relaxes around the core hole to form the screening charge and to dissipate the transients associated with absorption.

The question is whether these transients have died away, and the electronic system become fully relaxed, before the average x-ray emission event occurs. Examples have been found where the phonon system is not fully relaxed before the emission event, and partial relaxation effects were predicted and confirmed experimentally.¹²⁻¹⁴ However, the electronic system is expected to relax more quickly than the phonon system, roughly in the ratio of the plasma frequency to the Debye frequency. For the outer shell core holes of simple metals, whose lifetime is roughly $\tau \sim \hbar/(0.04 \text{ eV})$, one finds that $\omega_p \tau \gg 1$, so that the electronic system is expected to be fully relaxed before the average emission event. We shall follow custom and assume this to be the case.

In absorption, the initial state of the system is described by the potential V_g and the final state by V_h . From the relaxed state, the emission is from the initial state V_h to the final state V_g . These assignments are summarized in Table I. A major point is the following observation: a consistent selection of potential for both emission and absorption calculations would be to use either the initial-state potential in both cases or the final-state potential in both cases. The conclusion of this paper is that one should use the final-state potential for both emission and absorption. This is the choice V_h for absorption and V_g for emission.

This conclusion, although fairly simple, is not in accordance with the conventional method of calculation, which is to take one potential, usually V_g , and use it to calculate both an emission and absorption spectra. We argue that this calculation is satisfactory for emission but not for absorption.

The choice of final state potential is supported by the calculations which we are reporting. We solve the *s*-wave part of the Mahan-*Nozières-De Dominicis* (MND) equations numerically for a hole potential which is approximated as a square well. The solutions, of course, show edge singularities, but further from the edge the emission and absorption potential can be described as one-electron spectra with a final-state potential— V_h in absorption and V_g in emission. A new feature, which emerges from the numerical solution, is

that the emission spectra is uniformly enhanced over that simply calculated with V_g . That is, the one-electron spectra is multiplied everywhere by a constant, which we call λ , which typically has values between 1.5 and 2. This enhancement factor is a consequence of the sum rules that apply to the emission spectra. These state that the area under the emission curve must be that of the initial-state potential. Since the spectra of the final-state potential V_g has a smaller area than this, the total theoretical emission spectra is uniformly multiplied by the constant λ . This appears to be a new prediction which has emerged from our computations. It is probably difficult to detect experimentally, since experimentalists never measure the absolute emission rate from a solid.

Before describing our calculations, we wish to note that there is an abundant amount of other evidence to support the choice of final-state potential. The evidence is both theoretical and experimental. The first theoretical evidence is the observation of *Nozières and De Dominicis*³ that the long-time asymptotic limits of their theory go to that of the final-state potential. This is not as strong a conclusion as the one we are proposing, which is that one can use the final-state potential about 1 eV from the edge. However, their asymptotic results provided us with our first clue to the nature of the answer. Another theoretical clue was in the recent numerical calculations of *Grebennikov et al.*⁷ They solved the MND equations for a narrow band and a separable potential. The many results they report are entirely consistent with the choice of final-state potential. The present calculations do not use the separable potential model, but, in fact, retain all off-diagonal matrix elements. There have been other numerical solutions to the MND equations.⁸⁻⁹

The experimental evidence favors the choice of emission spectra as calculated using V_g . This became apparent after calculations were done for emission spectra using the other potential V_h . These have been of three types: mean spherical model,¹⁵ atoms in jellium,⁵ and periodic cluster calculations.⁹ There is a common feature to all of these calculations. The screened core hole potential V_h describes a system with a screening charge of electrons close to the central core hole. The extra electron amplitude near the core hole raises the low-frequency transition rate. It makes a low-energy resonance in the theoretical spectra of the $L_{2,3}$ emission of Na, Mg, and Al which is totally lacking in the experimental spectra. The conclusion is rather obvious that one should not calculate the one-particle emission spectra using V_h but instead by using V_g . The attempt to provide a theoretical justification for this choice was the

TABLE I.

	Absorption	Emission
Initial state	V_g	V_h
Final state	V_h	V_g

motivation for the present research. The conclusion is further reinforced by the important observation of von Barth and Grossman⁹ that the satellite spectra—a transition from $Z+2$ to $Z+1$ ion states—is also described well by the final-state potential with $Z+1$. In this case it is V_h , the potential with a single core hole. Thus, the available emission data, when compared with these theories, strongly favors the choice of final-state potential. von Barth and Grossman have also deduced the need of the final-state rule in emission from their one-particle calculations.

II. ABSORPTION AND EMISSION THEORY

In the MND theory,¹⁻³ the only perturbation is from the conduction electrons interacting with the transient potential of the control core hole. This transient is assumed to switch on infinitely fast. The theory of the x-ray transition is a study in how the free-particle system responds to the potential suddenly switched on in the core of the atom. In absorption, the sudden switching is of the screened core hole. In emission, where the relaxed state has the core hole and the electron system fully adjusted to it, the sudden switching is of a negative hole. That is, the core hole is switched off. There are two Hamiltonians in the problem. They correspond to the one-particle Hamiltonians of the system with, and without, the core hole. Alternately, they are the one-particle Hamiltonians for the potentials V_g and V_h , respectively. We call these one-particle Hamiltonians H_g and H_h .

$$H_g = E_{\text{kin}} + V_g = \sum_{\vec{k}} \xi_{\vec{k}} C_{\vec{k}}^\dagger C_{\vec{k}}, \quad (3)$$

$$H_h = E_{\text{kin}} + V_h = \sum_{\lambda} \xi_{\lambda} C_{\lambda}^\dagger C_{\lambda}. \quad (4)$$

Each may be solved exactly for the static potentials. The eigenstates of H_g are denoted with the subscript \vec{k} for energy $\xi_{\vec{k}}$, operators $C_{\vec{k}}$ etc. Similarly, the eigenstates of H_h are denoted with the subscript λ .

In the theory of absorption, one begins by expanding all operators in the initial-state basis. This is because the 10^{23} particles in the conduction band are eigenstates of this Hamiltonian H_g before the occurrence of the x-ray transition. The current operator \mathcal{J} , which is used in describing the optical absorption rate, is also expanded in this initial-state basis. From the Kubo formula, the optical transition is described by the theoretical formulas

$$A(t) = \langle \mathcal{J}(t) \mathcal{J}(0) \rangle = \langle e^{iH_g t} \mathcal{J} e^{-iH_g t} \mathcal{J} \rangle,$$

$$\mathcal{J} = \sum_{\vec{k}} M_{\vec{k}} (C_{\vec{k}} d + d^\dagger C_{\vec{k}}^\dagger), \quad (5)$$

$$M_{\vec{k}} = \int d^3r \psi_{\vec{k}}(r) \vec{p} \cdot \vec{A} \psi_c(r).$$

Since we will limit our numerical solution to s-wave final states, it is possible to specify that all wave functions $\psi_{\vec{k}}$ and matrix elements $M_{\vec{k}}$ are real. The operators d^\dagger and d are for a core hole, whose one-particle wave function is given by $\psi_c(r)$. The matrix element $M_{\vec{k}}$ is the same as mentioned earlier in Eq. (2). As shown by Nozières and De Dominicis,³ the correlation function for absorption may be reduced to the time correlation function

$$A(t) = e^{-i\omega_T t} \sum_{\vec{k}\vec{k}' > k_F} M_{\vec{k}} M_{\vec{k}'} \langle e^{iH_g t} C_{\vec{k}} e^{-iH_h t} C_{\vec{k}'}^\dagger \rangle. \quad (6)$$

As shown by Combescot and Nozières (CN),⁴ this correlation function is given exactly by

$$A(t) = \rho(t) \sum_{\vec{k}\vec{k}' > k_F} M_{\vec{k}} \left(\phi_{\vec{k}\vec{k}'}(t) - \sum_{\vec{p}\vec{p}' < k_F} \phi_{\vec{k}\vec{p}} \phi_{\vec{p}\vec{p}'}^{-1} \phi_{\vec{p}'\vec{k}'} \right) M_{\vec{k}'}, \quad (7)$$

$$\phi_{\vec{k}\vec{k}'} = \langle \vec{k} | e^{-iH_h t} | \vec{k}' \rangle, \quad (8)$$

$$\rho(t) = e^{iE_g t} \det[\phi_{\vec{p}\vec{p}'}(t)] = \det(\langle \vec{p} | e^{iH_g t} e^{-iH_h t} | \vec{p}' \rangle). \quad (9)$$

The term $\rho(t)$ contains the Anderson renormalization catastrophe, while the other factors are the one-particle processes plus the excitonic enhancements. Although (7) appears more complicated than (6), in fact it is far simpler. This is because (6) is a many-particle equation and $|\rangle$ is a many-particle wave function, while (7) is basically a one-particle equation. One may evaluate (7) by simply evaluating the matrix elements

$$\phi_{\vec{k}\vec{k}'}(t) = \sum_{\lambda} \langle \vec{k} | \lambda \rangle \langle \lambda | \vec{k}' \rangle e^{-i\xi_{\lambda} t} \quad (10)$$

and then inverting the matrix $\phi_{\vec{p}\vec{p}'}(t)$ to obtain the final function of time in (7). At finite times, the off-diagonal matrix elements $\phi_{\vec{k}\vec{k}'}(t)$ exist because the one-particle states $|\vec{k}\rangle$ are not eigenstates of H_h but rather H_g . These off-diagonal matrix elements were evaluated numerically using (10) in order to do the absorption calculation. Another important feature of (7) is that the inverse matrix is only taken over the set of states which are occupied in the ground state of the system—this is the ground state before the perturbation of the core hole is switched on. The determinant $\rho(t)$ is evaluated over the same set of states.

The MND theory of emission proceeds along similar lines. The problem is initially solved in the basis states of the initial-state potential—in

this case the states λ of the potential V_h . For example, the current operator is

$$J = \sum_{\lambda} M_{\lambda} (dC_{\lambda} + C_{\lambda}^{\dagger} d^{\dagger}).$$

The emission spectra can be shown to be described by the time correlation function

$$E(t) = \sum_{\lambda\lambda'} M_{\lambda} M_{\lambda'} \langle g | e^{iH_h t} C_{\lambda}^{\dagger} e^{-iH_g t} C_{\lambda'} | g \rangle, \quad (11)$$

which has the exact solution of CN,

$$E(t) = \rho'(t) \sum_{\lambda\lambda' < k_F} M_{\lambda} M_{\lambda'} \Lambda_{\lambda\lambda'}^{-1}, \quad (12)$$

$$\Lambda_{\lambda\lambda'}(t) = \langle \lambda | e^{-iH_g t} | \lambda' \rangle = \sum_k \langle \lambda | k \rangle \langle k | \lambda' \rangle e^{-i\epsilon_k t}, \quad (13)$$

$$\rho'(t) = e^{iE_h t} \det | \Lambda_{\lambda\lambda'}(t) |.$$

The Fourier transform of time is obtained by a matrix inversion of $\Lambda_{\lambda\lambda'}$ over the occupied states ($\lambda, \lambda' < k_F$).

The emission formula (12) of CN has a different form than the absorption spectra (7), since one contains two terms while the other contains one term. The two formulas can be made to resemble each other by the following procedures. First, we view the absorption theory as an emission process. This is done by viewing the unoccupied states of the conduction band as being due to holes. This is a conventional picture in a semiconductor or a band of finite width—indeed it is used for the core hole. Now we use the hole picture for the conduction states, and the picture is valid whether or not the conduction band has a finite width. This is shown pictorially in Fig. 1. The absorption process puts an additional electron in the conduction band with energy $\xi > 0$. This is the same as removing a hole state, so that it corresponds to the emission of a hole. The hole energy is measured with the opposite sign as the

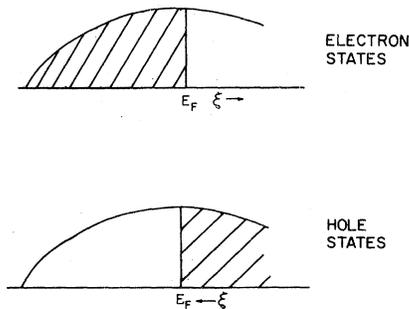


FIG. 1. The top figure is the conventional view of the conduction band, where the shaded region is the band of occupied electrons. The bottom figure is the same band in the hole picture, where the shaded region is the band of occupied holes.

particle energy. With this in mind, the rate of “hole emission” is given by

$$A(t) = \bar{\rho}(t) \sum_{k, k' > k_F} M_k M_{k'} \bar{\phi}_{kk'}^{-1}, \quad (14)$$

$$\bar{\phi}_{kk'} = \langle k | e^{iH_h t} | k' \rangle.$$

$$\bar{\rho}(t) = e^{-iE_g t} \det | \bar{\phi}_{kk'} | = \det (\langle k | e^{iH_h t} e^{-iH_g t} | k' \rangle). \quad (15)$$

This result can be derived in complete analogy with (12) and (13). The absorption formula (14) is identical to Eq. (7): the two formulas are shown below to be equal. The notation in (14) means that the matrix $\bar{\phi}_{kk'}(t)$ is found over the occupied set of hole states ($k, k' > k_F$) and then the inverse is taken over this occupied set of states. The inverse is not taken over the complete set of k states, since that leads to the trivial result $\bar{\phi}^{-1} = e^{-iH_h t}$. The determinant $\bar{\rho}(t)$ is taken over the occupied hole states. One can derive a simple relationship between this determinant and the previous one in (9).

In a similar way, the conduction-band-hole picture can be used to describe the usual emission theory as “hole absorption.” Thus the emission formula (12) can be written as

$$E(t) = \bar{\rho}(t) \sum_{\lambda\lambda' < k_F} M_{\lambda} M_{\lambda'} \left(\bar{\phi}_{\lambda\lambda'}(t) - \sum_{m, m' > k_F} \bar{\phi}_{\lambda m} \bar{\phi}_{m m'}^{-1} \bar{\phi}_{m' \lambda'} \right), \quad (16)$$

$$\bar{\rho}(t) = \det | \bar{\phi}_{\lambda\lambda'}(t) | e^{-iE_h t},$$

$$\bar{\phi}_{\lambda\lambda'}(t) = \langle \lambda | e^{iH_g t} | \lambda' \rangle. \quad (17)$$

These formulas demonstrate that emission and absorption can be written in a symmetrical fashion.

The new formulas derived from the conduction-band-hole picture are numerically less useful for systems with free-electron behavior. This is because the matrices $\bar{\phi}$ and $\tilde{\phi}$ must be inverted over the semi-infinite set of states ($k, k' > k_F$) or ($\lambda, \lambda' > k_F$). Of course, the fall off of M_k at large k makes the higher states less important for the absorption or emission process.

The derivation of these formulas is by using an identity for certain determinants. First, let A be a matrix of dimension N , and A^{-1} is its inverse

$$A \bar{A}^{-1} = 1,$$

$$\det(A) \det(\bar{A}^{-1}) = 1.$$

Let $\det(A)_n$ denote the determinant of A over any n -by- n subset of its rows and columns. The theorem is

$$\det(A)_n = \det(A^{-1})_{N-n} \det(A)_N.$$

This is used to derive Eqs. (14)–(17).

First let us review how CN derived their ab-

sorption formula (7). It is the determinant of a matrix of order $L+1$, where L is the number of particles in the ground-state Fermi sea. The matrix has elements $\phi_{pp'}$ where the indices p, p' run over the L ground states and one excited state ($p=k, p'=k'$). An evaluation of this determinant leads to (7). We call this the $n=L+1$ determinant A in the theorem, and $N-n$ are the remaining elements. The inverse of $A = \phi = e^{-iH_h t}$ is just $A^{-1} = e^{iH_h t} \equiv \bar{\phi}$. This gives

$$\det(\phi_{pp'})_n = \det(\bar{\phi}_{pp'})_{N-n} \det(\phi)_N,$$

or

$$\rho(t) \left(\phi_{kk'}(t) - \sum_{pp' < k_F} \phi_{kp} \phi_{pp'}^{-1} \phi_{p'k'} \right) = \bar{\rho}(t) \bar{\phi}_{kk'}^{-1} \det(\phi)_N.$$

The theorem can be used in the same way to relate the ground-state determinants of the particle and hole states

$$\rho(t) = \bar{\rho}(t) \det(\phi)_N,$$

which proves that $(\vec{k}, \vec{k}' > k_F)$

$$\phi_{kk'}(t) - \sum_{pp' < k_F} \phi_{kp} \phi_{pp'}^{-1} \phi_{p'k'} = \bar{\phi}_{kk'}^{-1},$$

where $\phi_{kk'} = \langle k | e^{-iH_h t} | k' \rangle$, and $\phi_{pp'}^{-1}$ is its inverse over the occupied ground states, and $\bar{\phi}_{kk'} = \langle k | e^{iH_h t} | k' \rangle$, and $\bar{\phi}_{kk'}^{-1}$ is its inverse over the unoccupied ground states. For a full band, the determinant over the band is just a phase factor.

$$\det(\phi)_N = \exp[-iNtV(0)].$$

This theorem establishes the relationship between the two absorption formulas (7) and (14). Similar steps provide a link between the emission formulas (12) and (16).

III. SUM RULES AND λ

The emission spectra does not go into the one-particle spectra of the final state potential. Instead, it goes into a multiple λ of this one-particle spectra. This multiplication by λ is a consequence of the sum rules. These sum rules had been shown earlier by Grebennikov *et al.*,⁷ although they did not deduce the necessity of λ . The sum rules state that the total area under the emission curve is not altered by the many-body effects—the switching on of the core hole.

$$\int d\omega E(\omega) = E(t=0) = \sum_{\lambda < \lambda_F} M_\lambda^2. \quad (18)$$

The total area of the emission spectra is given by the area under the curve of the one-particle spectra using the initial-state potential. But if we now say that the shape of the emission curve (except for the edge singularities) is given by the one-particle spectra of the final-state potential,

the area in this spectra is

$$\sum_{k < k_F} M_k^2. \quad (19)$$

There is no reason why the values of (18) and (19) are equal. In fact, (18) is larger, so that the shape of the emission spectra must be multiplied by λ . To summarize this effect, the area under the emission curve is given by one potential while the shape is given by another. At the moment, we do not have a method of calculating λ , except by solving the MND equations numerically and then empirically fitting the computed spectra.

IV. NUMERICAL METHODS

At first the numerical procedures sound straightforward. We are going to evaluate the single-particle matrix elements (10) and (13) and invert them over a grid of points in the Fermi sea of occupied states. This produces, in (7) and (12), functions of time which are Fourier transformed. Each of these steps is a standard computer operation, so that the calculation looks easy. It is actually difficult because of the singular nature of the edge singularities. These introduce long-time behaviors in the correlation functions which are slowly converging. This makes the numerical computation difficult, since other round off errors make it impossible to go to very long times. Thus we shall discuss the numerical methods at greater length than usual, as the techniques employed were unusual.

The calculations were only done for the s -wave channel of the final state. Since the MND theory factors into orbital components, the sum rules and other features all pertain to each l component as well. The potential V_s was taken to be zero, while V_h was an attractive square well. Its radius a was taken to be $ak_F = 1$, while the square-well depth was taken to be $V = -vE_F$, where $v = 1.0, 1.5$, or 2.0 . The case $v = 1.0$ is relatively weak, since $2\delta/\pi = 0.22$ and the Anderson parameter $\alpha = 0.025$, which is small. The case $v = 1.5$ is more like a metal, since it has $2\delta/\pi = 0.37$ and $\alpha = 0.07$.

The single-particle matrix elements in (10) and (13) were done by integrating over the set of states which are indicated. More explicitly, the matrix element $\phi_{kk'}$ is

$$\begin{aligned} \phi_{kk'}(t) &= (\pi/2) \delta(k - k') e^{i\epsilon_k t} + [h(k, k') - h(k', k)] \\ &\quad \times P/(k^2 - k'^2), \\ h(k, k') &= \cos \delta_r \langle k' | V | R_k \rangle e^{i\epsilon_k t} + \frac{2}{\pi} \int_0^\infty dp e^{i\delta^2 t} \langle k | V | R_p \rangle \\ &\quad \times \langle k' | V | R_p \rangle P/(p^2 - k^2), \end{aligned} \quad (20)$$

where $\langle k | V | R_p \rangle$ is normalized so that $R_p \rightarrow$

$\sin(pr + \delta_p)$ as $pr \rightarrow \infty$. These were evaluated over a grid of thirty points from zero to k_F , so that the matrix inversion was 30×30 . The function $M(r) = \exp(-r/b)$ with $b = \frac{1}{2}a = \frac{1}{2}k_F^{-1}$ was used for the s -wave part of the optical matrix elements, $M_\lambda = \int dr M(r) R_\lambda(r)$. The wave functions $R_p(r)$ for the square-well potential are easily found to use in the matrix element M_λ and the matrix $\langle k | V | R_p \rangle$ in (20).

In the emission calculation, some of the transients were eliminated by writing (12) as

$$E(t) = \sum_\lambda g_\lambda(t) e^{it(\epsilon_\lambda + \Delta)},$$

$$g_\lambda(t) = \rho'(t) e^{-i(\epsilon_\lambda + \Delta)t} M_\lambda \sum_{\lambda'} M_{\lambda'} \Lambda_{\lambda\lambda'}^{-1}, \quad (21)$$

$$\Delta = -\frac{\hbar}{m} \sum_{\lambda'} \delta_\lambda k_{\lambda'}.$$

This choice makes $g_\lambda(t)$ a slowly varying function of time. The Fourier transform was taken of this quantity, for each λ value, and the final spectra is obtained from a summation over

$$E(\omega) = 2 \operatorname{Re} \sum_\lambda \bar{g}_\lambda(\omega - \epsilon_\lambda - \Delta),$$

$$\bar{g}_\lambda(\omega) = \int_0^\infty dt e^{-i\omega t} g_\lambda(t).$$

The time integrals do not converge rapidly, since $g_\lambda(t)$ is not oscillatory but has long-time asymptotic behavior associated with the edge singularities. Therefore one always has to truncate the time integrals, which we typically did at $tE_F = 10$ or $tE_F = 15$. Since the complex function $g_\lambda(t)$ is not zero at this maximum time t_M , we actually Fourier transformed the quantity $g_\lambda(t) - g_\lambda(t_M)$ and assumed that the function $g_\lambda(t)$ had the value of $g_\lambda(t_M)$ from t_M to infinity. With this assumption, we obtain the formula

$$E(\omega) = 2 \operatorname{Re} \sum_\lambda \{ h_\lambda(\omega - \epsilon_\lambda - \Delta) + g_\lambda(t_M) \times [\pi \delta(\omega - \epsilon_\lambda - \Delta) - iP(\omega - \epsilon_\lambda - \Delta)^{-1}] \}$$

$$h_\lambda(\omega) = \int_0^\infty dt e^{-i\omega t} [g_\lambda(t) - g_\lambda(t_M)]. \quad (22)$$

This was integrated to various t_M , and the maximum value selected which was consistent with having a minimum of round off errors in the time integrations. Since the time integrals were not carried to infinity, we obtain a rounded edge singularity and some "noise" in the computed spectrum.

The factor Δ in (21) is from Fumi's theorem¹⁶ for the ground-state energy of the core hole. This arises from the Anderson term, which at large

time has the approximate asymptotic behavior

$$\lim_{t \rightarrow \infty} \rho(t) = \exp[i\Delta t - \alpha \ln(itE_F)].$$

The oscillatory behavior $\exp(i\Delta t)$ is eliminated from $g_\lambda(t)$ by the multiplication by $\exp(-it\Delta)$, as is indicated in (21). Since all our results are plotted with the energy zero as the bottom of the band, we have renormalized Δ out of the figures. We also have computed the spectra both with and without the factor $\rho(t)$. This is to demonstrate that the final-state potential arises from the exciton term, rather than from the Anderson term.

Before doing the absorption calculation, (7) is manipulated into a slightly different form. The summations over the complete set of states \bar{k} and \bar{k}' are eliminated and replaced by summations over the complete sets λ and λ' . To this end, the matrix element $M_{\bar{k}}$ is written as $\int dr M(r) \psi_{\bar{k}}$, so that we have for the first term in (7)

$$\sum_{\bar{k}\bar{k}'} M_{\bar{k}} \phi_{\bar{k}\bar{k}'} M_{\bar{k}'} = \sum_{\lambda\lambda'} M_\lambda \langle \lambda | e^{-iH_{\bar{h}}t} | \lambda' \rangle M_{\lambda'},$$

$$M_\lambda = \int dr M(r) | \lambda \rangle.$$

Since the states $|\lambda\rangle$ and $|\lambda'\rangle$ are eigenstates of $H_{\bar{h}}$, this first term may be replaced by

$$\sum_\lambda M_\lambda^2 e^{-i\epsilon_\lambda t},$$

which is just the one-particle spectra for the final state basis. Similar manipulations on the other term in (7) bring us to the alternate equation

$$A(t) = \rho(t) \sum_{\lambda\lambda'} \left(M_\lambda^2 e^{-i\epsilon_\lambda t} \delta_{\lambda\lambda'} - \sum_{p' < k_F} M_\lambda \langle \lambda | p' \rangle \times \phi_{p'p'}^{-1} \langle p' | \lambda' \rangle M_{\lambda'} e^{it(\epsilon_\lambda + \epsilon_{\lambda'})} \right).$$

The first term is just the one-particle spectra in the final-state basis. This is trivial to calculate, so that only the second term causes difficulties. This was treated like the emission term in (22). This second term has interesting characteristics. Since the absorption is zero for $\omega < E_F$ it exactly cancels the first term of $\omega < E_F$. For $\omega > E_F$ it gives the edge singularities and then dies away slowly at higher frequencies.

V. RESULTS

The absorption and emission curves for $v = 1.0, 1.5,$ and 2.0 are shown in Figs. 2–4. The main conclusions are drawn from the emission spectra. This is because with our choice of core hole potential parameters the various one-particle absorption spectra are asymptotically similar. Thus

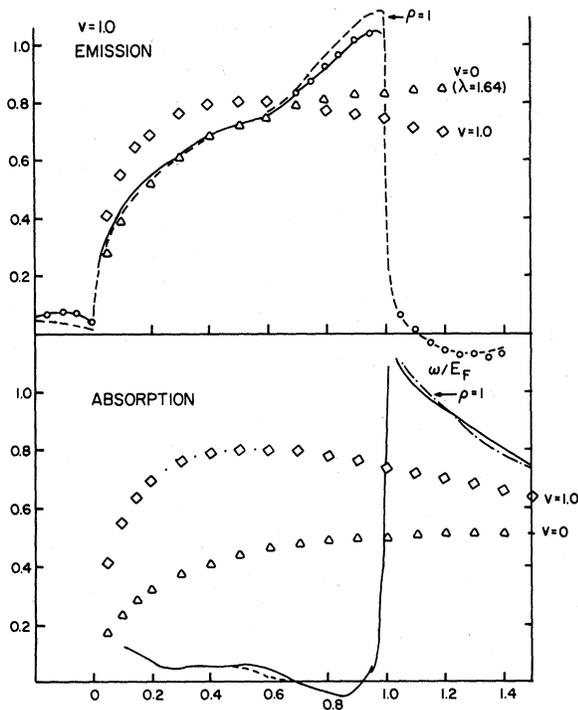


FIG. 2. The theoretical emission and absorption spectra for a square well of depth $v = 1.0 E_F$ and width $1.0 k_F^{-1}$. The top part is emission. The solid curve is the theoretical spectra. The dashed curve marked $\rho = 1$ is the theoretical curve without the Anderson renormalization factor and with only the exciton term. The effect of the Anderson term is mostly to reduce the magnitude of the edge singularity. The points marked with diamond ($v = 1.0$) are the one-particle spectra calculated for the initial state potential. The curve marked with triangles ($v = 0, \lambda = 1.64$) is the one-particle spectra calculated with the final-state potential and multiplied by the factor 1.64. This fits the full theoretical curve (solid line) except in the edge singularity. The bottom curve is absorption, and the points are marked as in emission. The effects of numerical round off are evident in the emission for $\omega > E_F$ and absorption for $\omega < E_F$.

it is hard to decide which one-particle spectra is resembled by our MND spectra, since the one-particle spectra are similar. One could formally decide the issue by using a repulsive core hole potential, which would make the various absorption spectra different. However, since we have shown that the absorption and emission theories are formally identical, then any conclusion drawn from emission must also apply to absorption. Thus we concentrate on the emission spectra.

In the top part of Fig. 2, the solid line shows the MND spectra found from (12). The dashed line is the spectra found from (12) with $\rho = 1$ so that the Anderson term is absent. The two curves are very similar except in the edge region, where the

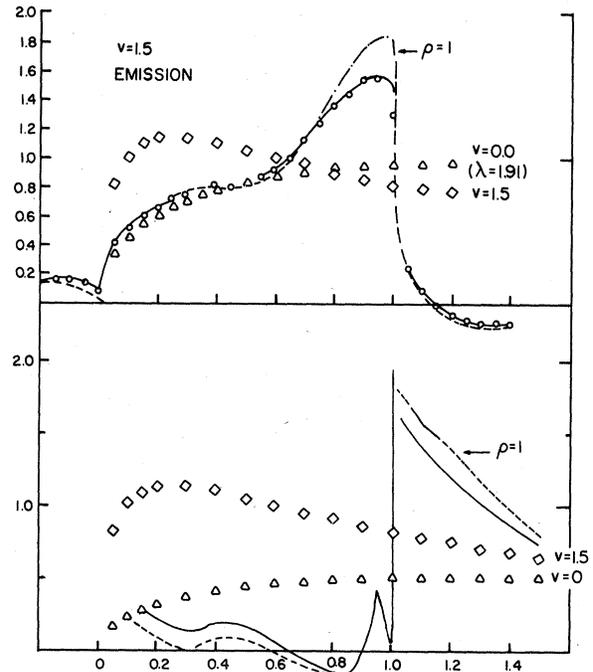


FIG. 3. The theoretical emission and absorption spectra for a square well of depth $v = 1.5 E_F$ and width $1.0 k_F^{-1}$. The top part is emission. The solid curve is the theoretical spectra. The dashed curve marked $\rho = 1$ is the theoretical curve without the Anderson renormalization factor and with only the exciton term. The effect of the Anderson term is mostly to reduce the magnitude of the edge singularity. The points marked with diamond ($v = 1.5$) are the one-particle spectra calculated for the initial state potential. The curve marked with triangles ($v = 0, \lambda = 1.91$) is the one-particle spectra calculated with the final-state potential, and multiplied by the factor 1.91. This fits the full theoretical curve (solid line) except in the edge singularity. The bottom curve is absorption, and the points are marked as in emission. The effects of numerical round off are evident in the emission for $\omega > E_F$ and absorption for $\omega < E_F$.

solid line is lower because the Anderson term causes the expected reduction of the edge singularity. Our edges are not singular, as mentioned earlier, which we ascribe to the Fourier transforms being truncated at finite times. The Anderson term also introduces a uniform shift of the spectra by Δ , which we have omitted in the figures. Also shown, for comparison, are the one-particle spectra calculated with the core hole—this is the curve labeled “ $v = 1.0$ ” and shown by diamonds \diamond . This does not resemble the MND spectra in any way. The curve marked by triangles Δ is the final-state spectra (no core hole) multiplied by the empirical parameter $\lambda = 1.64$. This is an excellent fit to the MND spectra except in the region of edge singularities. It is this rather good agreement

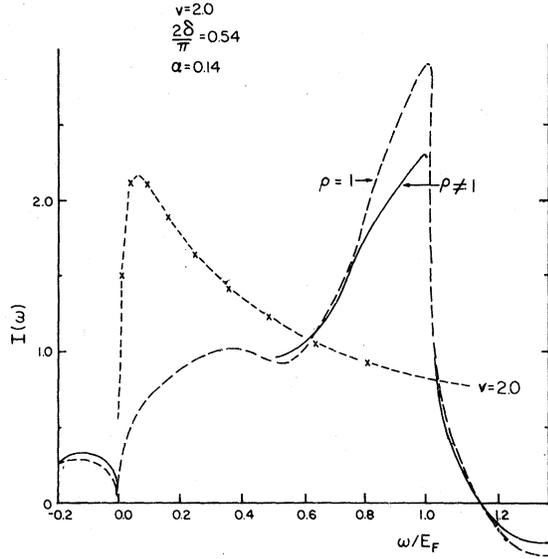


FIG. 4. The theoretical emission spectra for a square well of depth $v = 2.0 E_F$ and width $1.0 k_F^{-1}$. The solid curve is the full theoretical spectra. The dashed curve marked $\rho = 1$ is the theoretical curve without the Anderson renormalization factor but with the exciton term. The other curve labeled $v = 2.0$ is the one-particle spectra calculated for the initial-state potential. This is quite different from the theoretical curve.

which causes us to deduce that the MND spectra, away from the edge singularities, is well described by the final-state spectra multiplied by λ . The emission spectra shows emission for $\omega > E_F$, and this is due to round off error. Similarly, the emission spectra with $\rho = 1$ for $\omega < 0$ is also due to round off error. The Anderson term $\rho(t)$ introduces some spectral weight in this area, due to electron-hole emission. Fig. 3 shows the same kind of result calculated for $v = 1.5$. The conclusions are similar: the spectra away from the edge singularities is better described by the $v = 0$ curve multiplied by $\lambda = 1.91$ than by the $v = 1.5$ one-particle curve.

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APPENDIX: SCATTERING THEORY

In this Appendix the CN equations are derived by scattering theory. The correlation function for absorption in (6) is solved by directly expanding the S matrix, deducing the n th term, and then resumming the series. The same result (7) is obtained as was found by CN. The present derivation is longer than theirs and only of academic interest. It can be used to prove the "conduction-band-hole" results.

The correlation function in (6) is written in terms of an S matrix

$$\begin{aligned} F_{kk'}(t) &= \langle | e^{iH_g t} C_k e^{-iH_h t} C_{k'}^\dagger | \rangle, \\ F_{kk'}(t) &= \langle | TC_k(t)S(t)C_{k'}^\dagger(0) | \rangle, \\ S(t) &= T \exp \left(-i \int_0^t dt_1 V(t_1) \right), \end{aligned} \quad (A1)$$

$$V = \sum_{kk'} V_h(k, k') C_k^\dagger C_{k'},$$

which is expanded and evaluated term by term. The first several terms in this expansion are

$$\begin{aligned} F_{kk'}(t) &= e^{-it\xi_k t} \left(\delta_{kk'}(1-n) + (-i)V_h(k, k')(1-n)(1-n') \int_0^t dt_1 e^{it_1(\xi_k - \xi')} \right. \\ &\quad + (-i)^2(1-n)(1-n') \sum_{k_1} V_h(k, k_1)V_h(k_1, k') \int_0^{t_1} dt_1 e^{it_1(\xi_k - \xi_1)} \\ &\quad \times \int_0^{t_1} dt_2 e^{it_2(\xi_1 - \xi')} [\Theta(t_1 - t_2) - n_1] + (-i)^3(1-n)(1-n') \\ &\quad \times \sum_{k_1 k_2} V_h(k, k_1)V_h(k_1, k_2)V_h(k_2, k') \int_0^t dt_1 e^{it_1(\xi_k - \xi_1)} \int_0^{t_1} dt_2 e^{it_2(\xi_1 - \xi_2)} \\ &\quad \times [\Theta(t_1 - t_2) - n_1] \int_0^{t_2} dt_3 e^{it_3(\xi_2 - \xi')} [\Theta(t_2 - t_3) - n_2] + \dots \left. \right), \end{aligned} \quad (A2)$$

where $n = n_k$, $n' = n_{k'}$, $n_j = n_{k_j}$, $\xi = \xi_k$, $\xi' = \xi_{k'}$, $\xi_j = \xi_{k_j}$, etc.

Beginning with the third term in the series, the kernel of the time integral contains the Green function $G_j(t) = e^{-it} [\Theta(t) - n_j]$. We have kept only the exciton terms in this expansion and have ignored the terms which make electron-hole pairs in the electron gas, and hence lead to the Anderson renormalization catastrophe. The series of terms are exactly summed with the following integral equation:

$$F_{kk'}(t) = e^{it}(1-n) \left(\delta_{kk'} - i(1-n') \int_0^t dt_1 \mathcal{F}_{kk'}(t_1; t) \right), \quad (\text{A3})$$

$$\begin{aligned} \mathcal{F}_{kk'}(t_1; t) = & V_h(k, k') e^{it_1(t-t')} - i \int_0^t dt_2 \sum_{k_1} e^{it_1(t-t_2)} \\ & \times V_h(k, k_1) \mathcal{F}_{k_1 k'}(t_2; t) [\Theta(t_1 - t_2) - n_1]. \end{aligned} \quad (\text{A4})$$

We need to determine the function $\mathcal{F}_{kk'}(t; t)$. It is expressed in terms of an integral over another function $\Psi_k(r; t_1, t)$:

$$\mathcal{F}_{kk'}(t_1; t) = e^{it_1 t} \int d^3r \phi_k^*(r) V_h(r) \Psi_k(r, t_1, t), \quad (\text{A5})$$

$$\begin{aligned} \Psi_k(r, t_1, t) = & \phi_k(r) e^{-it_1 t} - i \sum_{k_1} \phi_{k_1}(r) e^{-it_1 t_1} \\ & \times \int_0^t dt_2 \mathcal{F}_{k_1 k}(t_2; t) [\Theta(t_1 - t_2) - n_1]. \end{aligned} \quad (\text{A6})$$

We have written the equation for $\Psi_k(r; t; t_1)$, which is deduced from (A4). We evaluate the function Ψ_k by operating upon it with $(i\partial/\partial t_1 - H_g)$. The eigenfunctions ϕ_k are eigenstates of H_g and thus give zero with this operation. This yields

$$\begin{aligned} \left(i \frac{\partial}{\partial t_1} - H_g \right) \Psi_k(r; t; t_1) = & -i \sum_{k_1} \phi_{k_1}(r) e^{-it_1 t_1} \\ & \times \int_0^t dt_2 \delta(t_1 - t_2) \mathcal{F}_{k_1 k}(t_2; t) \\ = & \sum_{k_1} \phi_{k_1}(r) e^{-it_1 t_1} \mathcal{F}_{k_1 k}(t_1; t). \end{aligned}$$

$$\begin{aligned} \left(i \frac{\partial}{\partial t_1} - H_g \right) \Psi_k(r, t, t_1) = & V_h(r) \Psi_k(r, t_1, t), \\ \left(i \frac{\partial}{\partial t_1} - H_h \right) \Psi_k(r, t_1, t) = & 0. \end{aligned} \quad (\text{A7})$$

Thus the function Ψ_k is an eigenstate of the final state potential H_h . We define $\phi_\lambda(r)$ as the set of eigenfunctions of H_h , $H_h \phi_\lambda = \epsilon_\lambda \phi_\lambda$, and expand Ψ_k in terms of these eigenfunctions.

$$\Psi_k(r, t_1, t) = \sum_\lambda \phi_\lambda(r) e^{-it_1 \epsilon_\lambda} \alpha_\lambda(k, t), \quad (\text{A8})$$

$$\mathcal{F}_{kk'}(t_1, t) = \sum_\lambda \langle k | V | \lambda \rangle e^{it_1(\epsilon_k - \epsilon_\lambda)} \alpha_\lambda(k, t). \quad (\text{A9})$$

The equation for \mathcal{F} is deduced from the definition

of Ψ_k in (A5). The expansion coefficient $\alpha_\lambda(k, t)$ now needs to be determined. It is a function of t but not t_1 , so we may choose any value of t_1 in order to find α_λ . Choose $t_1 = 0$. From our other equation (A6) for Ψ_k we have

$$\begin{aligned} \Psi_k(r, 0, t) = & \phi_k(r) + \sum_{k_1} \phi_{k_1}(r) n_1 \mathcal{Q}_{k_1 k}(t), \\ \mathcal{Q}_{k_1 k}(t) = & i \int_0^t dt_2 \mathcal{F}_{k_1 k}(t_2, t). \end{aligned} \quad (\text{A10})$$

The next step is to do the integral over t_2 , for which we define the special symbol $\mathcal{Q}_{k_1 k}(t)$. This uses the equation for $\mathcal{F}_{k_1 k}$ in (A9)

$$\begin{aligned} \mathcal{Q}_{k_1 k}(t) = & i \sum_\lambda \langle k_1 | V | \lambda \rangle \alpha_\lambda(k, t) \int_0^t dt_2 e^{it_2(\epsilon_{k_1} - \epsilon_\lambda)}, \\ = & \sum_\lambda \frac{\langle k_1 | V | \lambda \rangle}{\epsilon_{k_1} - \epsilon_\lambda} \alpha_\lambda(k, t) (e^{it(\epsilon_{k_1} - \epsilon_\lambda)} - 1). \end{aligned}$$

From the definition of the equation for the wave function for ϕ_λ one can deduce that value of $\langle k | V | \lambda \rangle / (\epsilon_k - \epsilon_\lambda)$

$$\begin{aligned} \phi_\lambda = & \phi_k + \sum_{k'} \phi_{k'} \frac{\langle k' | V | \lambda \rangle}{\epsilon_\lambda - \epsilon_{k'} + i\delta}, \\ \langle \lambda | k \rangle = & \delta_{\lambda, k} + \frac{\langle k | V | \lambda \rangle}{\epsilon_\lambda - \epsilon_k + i\delta}, \\ \mathcal{Q}_{k_1 k}(t) = & \sum_\lambda \langle k_1 | \lambda \rangle \alpha_\lambda(k, t) (1 - e^{it(\epsilon_{k_1} - \epsilon_\lambda)}), \end{aligned} \quad (\text{A11})$$

from which it follows that

$$\begin{aligned} \Psi_k(r, 0, t) = & \phi_k(r) + \sum_{k_1, \lambda} \phi_{k_1}(r) n_1 \langle k_1 | \lambda \rangle \\ & \times \alpha_\lambda(k, t) (1 - e^{it(\epsilon_{k_1} - \epsilon_\lambda)}), \\ \Psi_k(r, 0, t) = & \sum_\lambda \phi_\lambda(r) \alpha_\lambda(k, t). \end{aligned}$$

We have written above the two equations for $\Psi_k(r, 0, t)$ which are deduced from (A8) and (A10). We multiply them both by $\int \phi_\lambda^*$, equate the results, and finally derive the equation for the coefficient α_λ :

$$\begin{aligned} \alpha_\lambda(k, t) = & \langle \lambda | k \rangle + \sum_{k_1, \lambda'} \langle \lambda | k_1 \rangle n_1 \langle k_1 | \lambda' \rangle \\ & \times \alpha_{\lambda'}(k, t) (1 - e^{it(\epsilon_{k_1} - \epsilon_{\lambda'})}). \end{aligned}$$

This may be written in a shorthand notation by defining two operators

$$\begin{aligned} P = & \sum_{k_1} |k_1\rangle n_1 \langle k_1|, \\ \Phi = & e^{itH_g} e^{-itH_h}. \end{aligned}$$

The first is the projection operator on the ground state of the system described by the initial state Hamiltonian H_g . The second is an exponential

operator in the form of an S matrix. Together, they permit the equation for α_λ to be rewritten as

$$\alpha_\lambda(k, t) = \langle \lambda | k \rangle + \sum_{\lambda'} \langle k | P(1 - \Phi) | \lambda' \rangle \alpha_{\lambda'}(k, t).$$

We now iterate this equation and obtain the series of terms

$$\alpha_\lambda(k, t) = \langle \lambda | \{ 1 + P(1 - \Phi) + [P(1 - \Phi)]^2 + [P(1 - \Phi)]^3 + \dots \} | k \rangle.$$

They may be summed to the desired result by using the property of projection operators $P^2 = P$, to prove that

$$[P(1 - \Phi)]^n = (1 - P\Phi)^{n-1}P(1 - \Phi),$$

$$\alpha_\lambda = \left\langle \lambda \left| \left(1 + \sum_{n=0}^{\infty} (1 - P\Phi)^n P(1 - \Phi) \right) \right| k \right\rangle,$$

$$\alpha_\lambda = \left\langle \lambda \left| \left(1 + \frac{1}{1 - (1 - P\Phi)} P(1 - \Phi) \right) \right| k \right\rangle,$$

so that

$$\alpha_\lambda(k, t) = \left\langle \lambda \left| \left(1 + \frac{1}{P\Phi(t)} P[1 - \Phi(t)] \right) \right| k \right\rangle.$$

The term $(1/P\Phi)P$ gives zero since it acts on a state $|k\rangle$ which has $k > k_F$. Therefore we finally prove that

$$\alpha_\lambda(k, t) = \left\langle \lambda \left| \left(1 - \frac{1}{P\Phi(t)} P\Phi(t) \right) \right| k \right\rangle. \quad (\text{A12})$$

At first it looks as if the numerator and denominator in the last term are equal and should cancel. This is not the case. The inverse operator $1/P\Phi$ is not the full inverse of Φ but only an inverse over those states $P < k_F$ beneath the Fermi surface. This is the role of the projection operator, which is also in the denominator—perhaps this would be clearer if we wrote it in the equivalent manner $(P\Phi P)^{-1}P\Phi$. The numerator is evaluated to the right on the state $|k\rangle$, which is not in the set of inverse states, since $k > k_F$. Thus the product of these operators $(1/P\Phi)P\Phi$ gives unity if acting upon the occupied states but not if acting upon the unoccupied states. This point was also shown by CN.

The result for $\alpha_\lambda(k, t)$ permits us to evaluate the various quantities we have defined along the way. Comparing (A3), (A10), (A11), and (A12) gives

$$\begin{aligned} F_{kk'}(t) = e^{i\bar{\xi}_k \bar{n}_k} \left[\delta_{kk'} - i\bar{n}_{k'} \left(V_h(k, k') \int_0^t dt_1 e^{it_1(\bar{\xi}_1 - \bar{\xi})} + i \sum_{k_1} V_h(k, k_1) V_h(k_1, k') \int_0^t dt_1 e^{it_1(\bar{\xi}_1 - \bar{\xi})} \int_0^t dt_2 e^{it_2(\bar{\xi}' - \bar{\xi}_1)} \right. \right. \\ \times [\Theta(t_2 - t_1) - \bar{n}_1] + (i)^2 \sum_{k_1 k_2} V_h(k, k_1) V_h(k_1, k_2) V_h(k_2, k_1) \\ \left. \left. \times \int_0^t dt_1 e^{it_1(\bar{\xi}_1 - \bar{\xi})} \int_0^t dt_2 e^{it_2(\bar{\xi}_2 - \bar{\xi}_1)} \int_0^t dt_3 e^{it_3(\bar{\xi}' - \bar{\xi}_2)} [\Theta(t_2 - t_1) - \bar{n}_1][\Theta(t_3 - t_2) - \bar{n}_2] + \dots \right) \right]. \end{aligned}$$

$$F_{kk'}(t) = e^{-i\bar{\xi}_k t(1 - n_k)} [\delta_{kk'} - i(1 - n_{k'}) \mathcal{G}_{kk'}(t)],$$

$$\begin{aligned} \mathcal{G}_{kk'}(t) &= \sum_{\lambda} \langle k | (1 - \Phi) | \lambda \rangle \alpha_\lambda(k', t), \\ &= \sum_{\lambda} \langle k | [1 - \Phi(t)] | \lambda \rangle \left\langle \lambda \left| \left(1 - \frac{1}{P\Phi} P\Phi \right) \right| k' \right\rangle. \end{aligned}$$

The intermediate summation $\sum |\lambda\rangle\langle\lambda|$ can be eliminated, and gives

$$\begin{aligned} \mathcal{G}_{kk'}(t) &= \left\langle k \left| (1 - \Phi) \left(1 - \frac{1}{P\Phi} P\Phi \right) \right| k' \right\rangle, \\ F_{kk'}(t) &= \left\langle k \left| e^{-iH_k(1 - P)} \right. \right. \\ &\quad \times \left. \left. \left[1 - (1 - \Phi) \left(1 - \frac{1}{P\Phi} P\Phi \right) (1 - P) \right] \right| k' \right\rangle. \end{aligned} \quad (\text{A13})$$

Most of the various factors in $F_{kk'}(t)$ cancel or give zero. For example, terms such as

$$(1 - P)(1/(P\Phi)P\Phi) = 0$$

give zero because they are effectively the combination $(1 - P)P = 0$. This leaves us with the remaining combination

$$(1 - P)\Phi[1 - (1/P\Phi)P\Phi](1 - P).$$

The factors $(1 - P)$ on each end are unnecessary because the center part in brackets vanishes for states $k < k_F$. Thus we have the final result

$$F_{kk'}(t) = \langle k | e^{-iH_k \Phi(t)} [1 - (1/P\Phi)P\Phi] | k' \rangle.$$

This is just the CN result which was given earlier in (7). We have derived the term in brackets, since $\phi = \exp(-iH_k)\Phi(t)$. This is multiplied by the matrix elements and the Anderson renormalization factor to give the final absorption spectra. Thus we have shown that the CN result, obtained from matrix arguments, can also be found by expanding the S matrix.

The next logical step would be to show that the CN emission formula also can be derived from scattering theory. This we will do, but for a special case. Since we also wish to prove the electron-hole symmetry, whereby absorption into electron states can also be viewed as emission from conduction-band-hole states, we will evaluate emission from conduction-band-hole states. Thus we define the hole occupation number $\bar{n}_k = 1 - n_k$ and the hole energy as $\bar{\xi}_k = -\xi_k$. The absorption correlation function $F_{kk'}(t)$ in (A2) can be rewritten in these hole variables

The argument of each Green's function has been rewritten as

$$\Theta(t_1 - t_2) - n_1 = -[\Theta(t_2 - t_1) - \bar{n}_1].$$

The formulas can be made more familiar by re-labeling each of the dummy time variables t_1, t_2, t_3 , etc., in the inverse order t_3, t_2, t_1 . Then it is easy to see that we have the integral equation for this series of

$$F_{kk'}(t) = e^{it_1 \bar{H}_k} \bar{n}_k \left(\delta_{kk'} - i\bar{n}_{k'} \int_0^t dt_1 \bar{F}_{k'k}(t_1, t) \right),$$

$$\bar{F}_{k'k}(t_1, t) = V_h(k', k) e^{it_1(\bar{E}' - \bar{E})} + i \sum_{k_1} e^{it_1(\bar{E}' - \bar{E}_1)}$$

$$\times V_h(k', k_1) \int_0^t dt_1 \bar{F}_{k_1 k}$$

$$\times (t_2, t) [\Theta(t_1 - t_2) - \bar{n}_1].$$

This integral equation is solved by the same basic techniques as before with only slight differences. Again one defines a type of wave function $\bar{\Psi}$ which obeys an equation

$$\bar{F}_{k'k}(t_1, t) = e^{it_1 \bar{E}'} \int d^3r \phi_{k'}^*(r) V_h(r) \bar{\Psi}_k(\bar{r}, t_1, t),$$

$$\bar{\Psi}_k(r, t_1, t) = \phi_k(r) e^{-it_1 \bar{E}} + i \sum_{k_1} \phi_{k_1}(r) e^{-it_1 \bar{E}_1}$$

$$\times \int_0^t dt_2 \bar{F}_{k_1 k}(t_2, t) [\Theta(t_1 - t_2) - \bar{n}_1],$$

$$\left(i \frac{\partial}{\partial t_1} - \bar{H}_g \right) \bar{\Psi}_k = i^2 \sum_{k_1} \phi_{k_1}(r) e^{-it_1 \bar{E}_1} \bar{F}_{k_1 k}(t_1, t)$$

$$= -V_h(r) \bar{\Psi}_k,$$

$$\left(i \frac{\partial}{\partial t_1} - \bar{H}_h \right) \bar{\Psi}_k = 0,$$

$$\bar{H}_h = \bar{H}_g - V_h.$$

The hole potential is subtracted from \bar{H}_g since in

the emission process the hole vanishes. The function $\bar{\Psi}_k$ can be expanded in the complete set of states ϕ_λ which are eigenstates of \bar{H}_h , with coefficient $\bar{\alpha}_\lambda$. Then an equation is derived for this coefficient $\bar{\alpha}_\lambda$, which is solved again by iteration.

$$\bar{\Psi}_k(r, t_1, t) = \sum_\lambda \bar{\alpha}_\lambda(k, t) \phi_\lambda(r) e^{-it_1 \bar{E}_\lambda},$$

$$\bar{\alpha}_\lambda = \langle \lambda | k \rangle + \sum_{k'} \langle \lambda | k' \rangle n_{k'} \langle k' | (1 - \Phi) | \lambda' \rangle \bar{\alpha}_\lambda(k', t),$$

$$\bar{\Psi} = e^{it_1 \bar{H}_g} e^{-it_1 \bar{H}_h},$$

$$\bar{\alpha}_\lambda(k, t) = \left\langle \lambda \left| \sum_{l=0}^{\infty} [\bar{P}(1 - \Phi)]^l \right| k \right\rangle,$$

$$\bar{\alpha}_\lambda(k, t) = \langle \lambda | [1 + (1/\bar{P}\Phi)\bar{P}(1 - \Phi)] | k \rangle.$$

By following the same steps used to derive (A13), one gets to the similar equation

$$F_{kk'}(t) = \langle k | e^{it_1 \bar{H}_g} \bar{P} [1 + (1 - \Phi)]$$

$$\times [1 + (1/\bar{P}\Phi)\bar{P}(1 - \Phi)] \bar{P} | k' \rangle,$$

which can be shortened by eliminating the combinations which vanish. This finally produces the desired result

$$F_{kk'}(t) = \langle k | e^{it_1 \bar{H}_g} \bar{P} [1/\bar{P}\Phi(t)] \bar{P} | k' \rangle.$$

This is the same result which is expressed in (14), where $\exp(it_1 \bar{H}_g) \Phi^{-1} = \bar{\Phi}^{-1}$. One takes the inverse of this operator over the range of occupied hole states $(k, k') > k_F$ and then evaluates the indicated matrix elements. This is precisely the CN prescription for the emission spectra. Thus we have shown that the CN emission equations can be derived from scattering theory, and also that the absorption into electron states is mathematically equivalent to the emission from hole states in the conduction band. The same symmetry applies to the other process, and the emission from the electron states is equivalent to absorption into the hole states of the conduction band.

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