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Dispersion relation approach to the x-ray edge problem

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We present a dispersion relation formulation of the open-line amplitude for the x-ray edge problem within the contact potential model. Using both multiple-scattering and determinant techniques, we find that to a very good approximation the many-body effects can be described within a single-particle transition-rate expression using a renormalized matrix element. This renormalized matrix element may be expressed exactly in terms of a frequency integral over the scattering phase shift for the core-hole potential. There are small corrections to the transition rate due to multiple particle-hole-pair final states, and a systematic series expansion for these is presented. This series is summed at threshold to yield an exact expression for the critical amplitude multiplying the power-law singularity. Our analytic results given an exact description at threshold and are shown to be quite accurate away from threshold. Comparison with the asymptotic expression of Nozières and De Dominicis is made.

I. INTRODUCTION

Since the original work of Mahan,[1] there has been considerable interest in many-body effects at x-ray absorption (and emission) thresholds in metals.[2–8] Absorption of an x-ray photon injects an extra electron into the conduction band and simultaneously turns on the core-hole potential. Mahan found in a perturbation theory of this process that the cross section exhibits a power-law singularity at threshold

$$I(\omega)\sim(\Lambda/\omega)^{2g}\,, \tag{1.1}$$

where ω is the photon energy relative to threshold, Λ is an energy of order of the Fermi energy, and g is a measure of the strength of the core-hole potential seen by the conduction electrons. Nozières and De Dominicis[2] subsequently obtained a solution to the problem which is exact asymptotically close to threshold. They found

$$I(\omega)\sim(\Lambda/\omega)^{[2\delta(0)/\pi]-\alpha}\,, \tag{1.2}$$

where $\delta(0)$ is the core-hole potential scattering phase shift at the Fermi level in the final-state angular-momentum channel. The parameter α is given by (ignoring spin)

$$\alpha=\sum_{l=0}^{\infty}(2l+1)\left[\frac{\delta_l(0)}{\pi}\right]^2 \tag{1.3}$$

and arises from the Anderson orthogonality catastrophe.[9] The Mahan, Nozières, and De Dominicis (MND) theory has been applied to experimental studies of x-ray edges[10] and has also been found relevant to the Kondo problem.[11]

One of the difficulties in the analysis of experimental x-ray spectra is that the MND theory is rigorously valid only asymptotically close to threshold. Experimental resolution and core-hole lifetime broadening make this region inaccessible. There has been considerable recent theoretical progress on extending the solution away from threshold using what are essentially exact numerical solutions to the problem,[7,8,12,13] but unfortunately little progress has been made analytically. Pardee and Mahan[14] have presented a dispersion relation expression for the x-ray edge amplitude which takes into account the frequency variation of the scattering phase shift away from threshold. However, there are ambiguities in this approach since one of the required functions cannot be fully determined and the validity of the derivation itself is not self-evident.

Our method is to calculate the transition-rate amplitude using infinite order perturbation theory and working in frequency space rather than to calculate the Green's function in time space as Nozières and De Dominicis did.[2] This difference in procedure results in a much simpler treatment of the problem. An infinite subset of diagrams in the perturbation theory is exactly summed analytically yielding a result which is similar in form to that of Pardee and Mahan but without any of the associated ambiguities. Our central result is that the many-body effects in the open-line amplitude (the amplitude for injecting the extra electron) can be described to a very good approximation with a single-particle transition-rate expression using a renormalized matrix element. This renormalized matrix element may be expressed exactly in terms of a dispersion integral over the scattering phase shift for the core-hole potential. There are corrections to the transition rate due to multiple particle-hole-pair final states and a rapidly convergent expansion for these is presented. An important feature of the present work is that this series is summed at threshold to yield an exact value for the critical amplitude multiplying the power-law singularity in the open-line propagator. Our analytic results which are exact at threshold are shown to be quite accurate away from threshold.

Our main results may be briefly summarized as follows. We obtain for the transition rate to zero-pair final states

$$R(\omega)=2\pi\rho(\omega)\Theta(\omega)\exp\left[\mathrm{Re}\frac{2}{\pi}\int_0^{\Lambda}d\nu\frac{\delta(\nu)}{\nu-\omega}\right] . \tag{1.4}$$

A more complicated (but explicit) expression is obtained for the transition rate to arbitrary final states. The zero-pair approximation to the critical amplitude is $A_0=0.866$, the one-pair contribution is $A_1=-0.11A_0$, while the total value for the critical amplitude is $A=0.788$. In units where the integrated oscillator strength is one-half, the zero-pair term contributes $S_0=0.574$ and the sum of the integrated strength for the zero- and one-pair terms is $S_0+S_1=0.475$.

In Sec. II we discuss the analytic solution for single-particle final states using dispersion relation techniques. In Sec. III the corrections due to multiple particle-hole-pair final states are presented, and Sec. IV discusses an alternative approach to the problem in terms of determinants. Section V presents the numerical results and Sec. VI contains the conclusions.

II. EXACT ANALYTIC RESULTS: NO PAIR FINAL STATES

In the spirit of the MND model we assume a finite conduction band with Fermi level at zero energy and Hamiltonian

$$H_0=\sum_k \epsilon_k c_k^\dagger c_k . \tag{2.1}$$

In the presence of the core hole the conduction electrons experience an attractive contact potential

$$V=U\sum_{pq} c_p^\dagger c_q . \tag{2.2}$$

The optical absorption is determined by the product (in time space) of two correlation functions, the open-line and closed-loops amplitudes.[2] We will deal only with the open-line amplitude $\phi(\omega+i\delta)$ which is the propagator for the extra electron in the presence of the suddenly switched-on core-hole potential. We begin by reviewing the perturbation theory.

The first few terms in the series analyzed by Mahan[1] are represented by the diagrams in Fig. 1. For example, Fig. 1(a) represents simple photoexcitation with no subsequent scattering

$$\phi_a(\omega+i\eta)=\sum_p (1-f_p)\frac{1}{\omega-\epsilon_p+i\eta} , \tag{2.3}$$

where f_p is the Fermi function. Diagrams 1(b) and 1(c), respectively, represent single and double scattering from the core hole

$$\phi_b=U\phi_a^2 , \tag{2.4}$$

$$\phi_c=U^2\phi_a^3 . \tag{2.5}$$

One sees that the subset of diagrams representing direct scattering of the photoexcited electron can be summed as a geometric series

$$\Phi_D=\frac{\phi_a}{1-U\phi_a} . \tag{2.6}$$

In order to illustrate the meaning of this result, assume a constant density of states ρ, and a bandwidth 2Λ centered on the Fermi level at zero. Then

$$\phi_a(\omega+i\eta)=\rho\int_0^{\Lambda}d\Omega\frac{1}{\omega-\Omega+i\eta} , \tag{2.7}$$

$$\phi_a(\omega+i\eta)=\rho\ln\left|\frac{\lambda-\omega}{\omega}\right| -i\pi\rho\Theta(\omega)\Theta(\Lambda-\omega) , \tag{2.8}$$

where Θ is the step function. From (2.6) we see that Φ_D has an isolated pole below the Fermi level (for $U<0$) at

$$\left|\frac{\Lambda-\omega}{\omega}\right|=\exp(-1/\rho U) . \tag{2.9}$$

This bound excitation state is analogous to that in Cooper pairing and results from the fact that the Pauli principle prevents the core hole from scattering the photoelectron into states below the Fermi level. We know, however, that for the same reason a true exciton state cannot be formed below the Fermi level. This error is corrected by considering diagrams of the type shown in Fig. 1(d) in which exchange processes occur. Here the original photoelectron trades places with one of the Fermi sea electrons. The amplitude corresponding to this process is

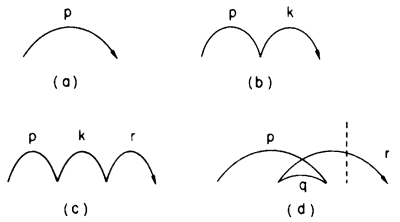

FIG. 1. Diagrams representing the perturbation series for the open-line amplitude. The dotted line in (d) represents a "cut" which implies taking the imaginary part of the cut line.

$$\phi_d = -\sum_{kpq}(1-f_p)f_q(1-f_k)\frac{1}{\omega-\epsilon_p+i\eta}U\frac{1}{\omega-\epsilon_p-\epsilon_k+\epsilon_q+i\eta}U\frac{1}{\omega-\epsilon_k+i\eta}\ . \tag{2.10}$$

Note the minus sign due to exchange.

Matters simplify if one considers only the most singular contribution to the imaginary part of the amplitude. The direct terms yield

$$-\frac{1}{\pi}\mathrm{Im}\Phi_D \sim \rho - 2\rho^2 U \ln\left|\frac{\Lambda-\omega}{\omega}\right| + 3\rho^3U^2\ln^2\left|\frac{\Lambda-\omega}{\omega}\right|\ , \tag{2.11}$$

while evaluation of (2.10) for the exchange terms gives

$$\mathrm{Im}\phi_d \sim -\rho^3U^2\ln^2\left|\frac{\Lambda-\omega}{\omega}\right| \tag{2.12}$$

so that the series is no longer geometric. Consideration of these and higher terms shows that one is instead generating the beginning of an exponential series of the form

$$\mathrm{Im}\phi \sim \rho\exp\left[-2\rho U\ln\left|\frac{\Lambda-\omega}{\omega}\right|\right] = \rho\left|\frac{\Lambda-\omega}{\omega}\right|^{-2\rho U}\ , \tag{2.13}$$

which is Mahan's original result.

We now turn to an exact evaluation of a subset of terms in this perturbation series. The object of primary interest is the spectral density

$$P(\omega) = -2\,\mathrm{Im}\phi(\omega+i\eta)\ . \tag{2.14}$$

The key to our approach is the fact that P can be expressed as a transition rate

$$P(\omega) = 2\pi\sum_f |M_f|^2\delta(\omega-E_f)\ , \tag{2.15}$$

where M_f is an effective matrix element connecting the initital state to some final-state f. This final state will contain one electron plus some n particle-hole pairs. We have found that if the sum is restricted to those final states containing zero pairs, the spectral function may be evaluated *exactly*. This restriction corresponds to taking "cuts" across the diagrams for ϕ which cross only a single line. A typical cut is indicated by the dotted line in Fig. 1(d). The cut signifies taking the imaginary part of the propagator which is cut.

Let the sum of this subset of terms be denoted by $R(\omega)$. One has following (2.15)

$$R(\omega) = 2\pi\sum_k(1-f_k)|M_k(\omega+i\eta)|^2\delta(\omega-\epsilon_k)\ , \tag{2.16}$$

where ϵ_k is the *single-particle* energy, and M_k is the effective matrix element for going to the single-particle final state. Because of the contact nature of the interaction it turns out that R may be expressed as

$$R(\omega) = 2\pi|T(\omega+i\eta)|^2\rho(\omega)\Theta(\omega)\ , \tag{2.17}$$

where

$$\rho(\omega) = \sum_k\delta(\omega-\epsilon_k) \tag{2.18}$$

is the single-particle density of states and T is independent of the wave vector k. The perturbation series for the T matrix is shown diagrammatically in Fig. 2. These terms represent, for example,

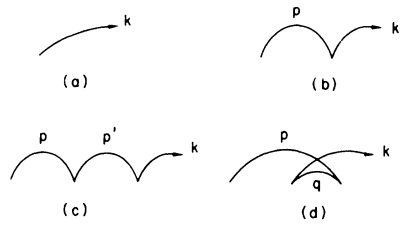

FIG. 2. Digrams representing the perturbation series for the many-body T matrix.

$$T_a = 1 , \tag{2.19}$$

$$T_b = U\sum_p (1-f_p)\frac{1}{\omega-\epsilon_p+i\eta} , \tag{2.20}$$

$$T_c = T_b^2 , \tag{2.21}$$

$$T_d = -U^2\sum_{pq}(1-f_p)f_q\frac{1}{\omega-\epsilon_p+i\eta} \times\frac{1}{\omega-\epsilon_p+\epsilon_q-\epsilon_k+i\eta} . \tag{2.22}$$

Note the minus sign in T_d for exchange. Note also that T_d seems to depend on the final-state wave vector k contrary to the assumption that T is independent of k. However, by making use of the delta function in (2.16), Eq. (2.22) may be rewritten

$$T_d = -U^2\sum_{pq}(1-f_p)f_q\frac{1}{\omega-\epsilon_p+i\eta}\frac{1}{\epsilon_q-\epsilon_p} . \tag{2.23}$$

It is with this crucial step that we drop all contributions to $P(\omega)$ from multipair final states. Thus there is no contribution to the imaginary part of (2.23) from a term containing $\delta(\omega-\epsilon_p+\epsilon_q-\epsilon_k)$ as there is in (2.22). Of course virtual transitions to intermediate states containing multiple pairs are still included properly. A second consequence of the delta function in (2.16) and the momentum independent core-hole potential is that the T matrix is to be evaluated on the mass shell so that forward scattering dispersion relation methods apply.[15]

Direct evaluation of the first few terms in the series for the T matrix verifies that Eq. (2.17) does indeed correctly reproduce the desired subset of contributions to $P(\omega)$ and therefore justifies our procedure. We now solve exactly for $T(\omega+i\delta)$. It turns out to be convenient to consider $\tilde{T}(\tau)$, the Fourier transform of T. We have found that $\tilde{T}(\tau)$ satisfies the following integral equation:

$$\tilde{T}(\tau)=\delta(\tau)+U\Theta(\tau)\int_{-\infty}^{\infty}d\tau'\tilde{T}(\tau')\tilde{g}(\tau-\tau') , \tag{2.24}$$

where $\tilde{g}$ is the time-ordered unperturbed Green's function. It is straightforward to iterate (2.24) and Fourier transform the resulting terms to verify that they correctly reproduce Eqs. (2.19)–(2.23).

For future reference we define the retarded Green's function

$$g^R(\omega+i\eta)\equiv\sum_k\frac{1}{\omega-\epsilon_k+i\eta} . \tag{2.25}$$

Fourier transformation of (2.24) yields

$$T(\omega+i\eta)=1+Ug^R(\omega+i\eta)T(\omega+i\eta) + UZ(\omega) , \tag{2.26}$$

where

$$Z(\omega)\equiv-\sum_q f_q\frac{1}{\omega-\epsilon_q+i\eta}T(\epsilon_q-i\eta) . \tag{2.27}$$

Examination of the first few terms in the series for $T(\omega\pm i\eta)$ shows that $\mathrm{Im}T(\omega\pm i\eta)$ vanishes for negative ω. Using this fact, Eq. (2.26) yields

$$\frac{\mathrm{Im}T(\omega+i\eta)}{\mathrm{Re}T(\omega+i\eta)}=\Theta(\omega)\frac{U\,\mathrm{Im}g^R(\omega+i\eta)}{1-U\,\mathrm{Re}g^R(\omega+i\eta)} . \tag{2.28}$$

Standard scattering theory tells us that the one-body (equilibrium) t matrix for the core-hole potential is given by

$$t(\omega+i\eta)=\frac{U}{1-Ug^R(\omega+i\eta)} . \tag{2.29}$$

The t matrix therefore satisfies

$$\frac{\mathrm{Im}t(\omega+i\eta)}{\mathrm{Re}t(\omega+i\eta)}=\frac{U\,\mathrm{Im}g^R(\omega+i\eta)}{1-U\,\mathrm{Re}g^R(\omega+i\eta)} . \tag{2.30}$$

Combining (2.28) and (2.30) yields

$$\frac{\mathrm{Im}T(\omega+i\eta)}{\mathrm{Re}T(\omega+i\eta)}=\Theta(\omega)\frac{\mathrm{Im}t(\omega+i\eta)}{\mathrm{Re}t(\omega+i\eta)} . \tag{2.31}$$

This very important equation shows that the many-body T matrix has the same phase as the one-body t matrix above threshold. The one-body t matrix satisfies

$$t(\omega+i\eta)=|t(\omega+i\eta)|e^{i\delta(\omega)} , \tag{2.32}$$

where $\delta(\omega)$ is the (S wave) scattering phase shift due to the core-hole potential. Hence we obtain

$$T(\omega+i\eta)=|T(\omega+i\eta)|e^{i\delta(\omega)\Theta(\omega)} , \tag{2.33}$$

and finally

$$\frac{T(\omega+i\eta)}{T(\omega-i\eta)}=e^{2i\delta(\omega)\Theta(\omega)} . \tag{2.34}$$

This very simple result contains all the information needed to solve for the T matrix. The analyticity

of T and its sudden discontinuity in phase at threshold guarantees the existence of a power-law singularity.

We now proceed to solve (2.34) following the standard dispersion relation procedures used by Pardee and Mahan. It is clear that T has a branch cut on the real axis between $\omega=0$ and $\omega=\Lambda$, the upper band edge. Since the exponential is an entire function, T can always be expressed in the form

$$T(z)=\exp[\phi(z)] . \tag{2.35}$$

Consideration of the perturbation series for T shows that for $|z|\to\infty$

$$T(z)\sim 1+O(1/z) , \tag{2.36}$$

and hence

$$\phi(z)\sim 1/z . \tag{2.37}$$

By Cauchy's theorem

$$\phi(z)=\oint_C \frac{dz'}{2\pi i}\frac{\phi(z')}{z'-z} , \tag{2.38}$$

where C is a contour enclosing the point z. Deforming the contour around the branch cut and out to infinity yields

$$\phi(z)=\int_0^\Lambda \frac{d\omega}{2\pi i}\frac{\phi(\omega+i\eta)-\phi(\omega-i\eta)}{\omega-z} . \tag{2.39}$$

From (2.37) it follows that there is no contribution from the contour at infinity. Hence the subtraction procedure of Pardee and Mahan is unnecessary and the associated ambiguity in ϕ does not exist. Furthermore, the branch structure used to derive (2.39) is based on the assumption that the potential does not pull any bound states out of the band. If this is true there is no polynomial ambiguity in ϕ of the form indicated by Pardee and Mahan. Hence solution of (2.39) determines ϕ *exactly*. Minor modifications in the procedure due to the presence of bound states are briefly discussed in Sec. V.

Combining (2.34) and (2.35) yields the discontinuity across the branch cut,

$$\phi(\omega+i\eta)-\phi(\omega-i\eta)=2i\delta(\omega)\Theta(\omega)+n\,2\pi i . \tag{2.40}$$

The arbitrary integer n is fixed by the requirement that in the zero phase-shift limit there must be no branch cut (i.e., no singularity). Hence $n=0$. This is equivalent to Nozières and De Dominicis taking the perturbative solution to their Dyson equation. Equation (2.39) becomes

$$\phi(z)=\frac{1}{\pi}\int_0^\Lambda d\nu\frac{\delta(\nu)}{\nu-z} . \tag{2.41}$$

Knowledge of the scattering phase shift therefore completely determines T. The spectral density for photoabsorption into no-pair final states is thus given exactly by (2.17) with

$$T(\omega+i\eta)=\exp\left[\frac{1}{\pi}\int_0^\Lambda d\nu\frac{\delta(\nu)}{\nu-\omega-i\eta}\right] . \tag{2.42}$$

Using (2.42), Eq. (2.17) may be written in a form which explicitly displays the singularity structure

$$R(\omega)=2\pi\rho(\omega)\Theta(\omega)\left|\frac{\Lambda-\omega}{\omega}\right|^{2\delta(0)/\pi} e^{2f(\omega)} , \tag{2.43}$$

where

$$f(\omega)\equiv \mathrm{Re}\frac{1}{\pi}\int_0^\Lambda d\nu\frac{\delta(\nu)-\delta(0)}{\nu-\omega} \tag{2.44}$$

is finite for small ω. This result is in complete agreement with the Nozières and De Dominicis solution in the asymptotic region and (as will be shown later) is fairly accurate even away from threshold.

The present calculation is essentially a one-body scattering result modified to take into account exchange scattering due to the presence of the Fermi sea. It is instructive to consider the single-particle limit in which exchange is not present and (2.41) may very readily be evaluated. We do this by putting the Fermi level at the bottom of the band so that

$$\phi(z)=\frac{1}{\pi}\int_{-\Lambda}^\Lambda d\nu\frac{\delta(\nu)}{\nu-z} . \tag{2.45}$$

Using (2.32) to express the phase shift as

$$\delta(\nu)=\mathrm{Im}\ln\left[\frac{t(\nu+i\eta)}{U}\right] \tag{2.46}$$

allows (2.45) to be expressed as a contour integral which yields

$$\phi(z)=\ln\left[\frac{t(z)}{U}\right] \tag{2.47}$$

and hence

$$T(z)=\frac{t(z)}{U} . \tag{2.48}$$

Combining (2.29) and (2.48) with (2.17) yields

$$R(\omega) = -2\,\mathrm{Im}G(\omega+i\eta)\ , \tag{2.49}$$

where

$$G(\omega+i\eta) = \frac{g^R(\omega+i\eta)}{1-Ug^R(\omega+i\eta)} \tag{2.50}$$

is the dressed propagator for the final-state potential. This is of course the exact answer (for all frequencies) in the one-body limit.

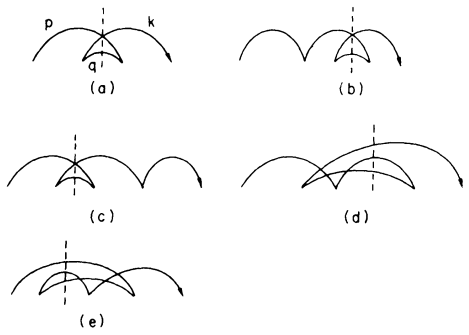

FIG. 3. Cut diagrams representing transitions to final states with one electron plus one particle-hole pair.

III. MULTIPLE-PAIR FINAL STATES

A. General results

The results obtained so far sum all contributions from single-particle, no-pair final states. As noted earlier these correspond to cuts in the Green's-function diagram which cross only a single line as in Fig. 1(d). We now wish to consider more complicated final states. For example, the cut in Fig. 3(a) corresponds to

$$\mathrm{Im}\phi = -\pi\sum_{kpq}(1-f_p)f_q(1-f_k)\frac{1}{\omega-\epsilon_p}U\delta(\omega-\epsilon_p+\epsilon_q-\epsilon_k)U\frac{1}{\omega-\epsilon_k}\ . \tag{3.1}$$

This is the simplest possible diagram leading to a single particle plus one-pair final state. Some typical higher-order diagrams contributing to the same final state are shown in Figs. 3(b)–3(e). In analogy with the previous results it is possible to express the spectral density as a transition rate

$$R_1(\omega) = -2\pi U^2\sum_{kpq}(1-f_k)f_q(1-f_p)T_{kpq}(\omega+i\eta)T^*_{pkq}(\omega+i\eta)\delta(\omega-\epsilon_p+\epsilon_q-\epsilon_k)\ . \tag{3.2}$$

Again note the minus sign due to exchange. The first few terms in the perturbation series for T_{kpq} are shown diagrammatically in Fig. 4. The contribution from the diagram shown in Fig. 4(a) is, for example,

$$T^{(a)}_{kpq}(\omega+i\eta) = \frac{1}{\omega-\epsilon_k+i\eta}\ , \tag{3.3}$$

while the next two terms are

$$T^{(b)}_{kpq} = \sum_{p'}(1-f_{p'})\frac{1}{\omega-\epsilon_{p'}+i\eta}U\frac{1}{\omega-\epsilon_k+i\eta} \tag{3.4}$$

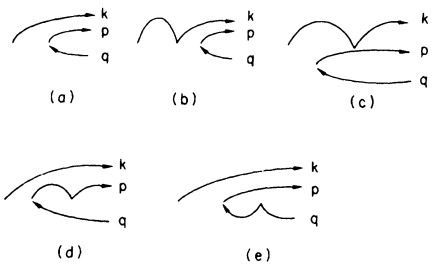

FIG. 4. Diagrams representing the series for the T matrix associated with the diagrams in Fig. 3.

and

$$T^{(c)}_{kpq} = \sum_{p'}(1-f_{p'})\frac{1}{\omega-\epsilon_{p'}+i\eta} \times U\frac{1}{\omega-\epsilon_{p'}+\epsilon_q-\epsilon_p+i\eta}\ . \tag{3.5}$$

Note that substitution of (3.3) into (3.2) yields. (3.1). Note also the arrangement of the momentum labels on the T matrices in (3.2). The combination appearing in (3.2) corresponds to the connected diagram shown in Fig. 5(a). The combination $T_{kpq}T^*_{kpq}$ does not appear because it corresponds to the disconnected diagram shown in Fig. 5(b). These disconnected diagrams contribute to the core-hole self-energy (and the orthogonality catastrophe) but not to the open-line amplitude.[2]

By making use of the delta function in (3.2) when evaluating the higher-order diagrams in the perturbation series for T, it is possible to systematically combine various terms to yield the following very simple *exact* result for T_{kpq}:

FIG. 5. Diagrams representing the product of two T matrices. (a) corresponds to the cut diagram shown in Fig. 3(a). (b) is a disconnected diagram which is discarded.

$$T_{kpq}=\frac{U}{\Delta_{pq}}t^{+}(\epsilon_k)t^{+}(\epsilon_p)t^{-}(\epsilon_q)\ , \tag{3.6}$$

where

$$\Delta_{pq}\equiv\epsilon_p-\epsilon_q\ , \tag{3.7}$$

t^{+} is the many-body T matrix given by (2.42) and t^{-} is given by

$$t^{-}(z)\equiv\exp\left[\frac{1}{\pi}\int_{-\Lambda}^{0}d\nu\frac{\delta(\nu)}{\nu-z}\right]\ . \tag{3.8}$$

The quantity t^{+} describes electron propagation while t^{-} describes hole propagation in the presence of the suddenly switched on core-hole potential.

Equation (3.6) is a suprisingly simple result which says that the effective T matrix for scattering into a final state with two particles and one hole factors into a product of three separate t matrices describing the propagation of each individual particle. This simplicity arises because the core hole is recoilless and so the various scattering events are uncoupled.[2]

The derivation of (3.6) is a lengthy algebraic exercise but we may illustrate the first few steps by rewriting (3.5) as

$$T^{(c)}_{kpq}=U\sum_{p'}(1-f_{p'})\left[\frac{1}{\omega-\epsilon_{p'}+\epsilon_q-\epsilon_p+i\eta}-\frac{1}{\omega-\epsilon_{p'}+i\eta}\right]\frac{1}{\Delta_{pq}}\ . \tag{3.9}$$

Utilizing the delta function in (3.2) yields

$$T^{(c)}_{kpq}=U\sum_{p'}(1-f_{p'})\left[\frac{1}{\epsilon_k-\epsilon_{p'}+i\eta}\frac{1}{\Delta_{pq}}-\frac{1}{\omega-\epsilon_{p'}+i\eta}\frac{1}{\omega-\epsilon_k}\right]\ . \tag{3.10}$$

The second term in (3.10) cancels (3.4) (note $\omega\neq\epsilon_k$). Again using the energy conserving delta function to rewrite (3.3), we have for the sum of the first three terms in the series

$$T_{kpq}=\frac{U}{\Delta_{pq}}\left[1+U\sum_{p'}(1-f_{p'})\frac{1}{\epsilon_k-\epsilon_{p'}+i\eta}\right]\ . \tag{3.11}$$

Comparison with (2.19) and (2.20) suggests that this is the beginning of the series for

$$T_{kpq}=\frac{U}{\Delta_{pq}}t^{+}(\epsilon_k)\ . \tag{3.12}$$

Examination of higher-order terms confirms that this is indeed correct. Contributions from higher-order diagrams such as those shown in Figs. 4(d) and 4(e) in which the particle-hole pair also suffers scattering correct (3.12) to yield the final exact expression (3.6). Substitution of (3.6) into (3.2) yields

$$R_1(\omega)=2\pi U^2\sum_{kpq}(1-f_k)(1-f_p)f_q\frac{|t^{+}(\epsilon_k)t^{+}(\epsilon_p)t^{-}(\epsilon_q)|^2}{\Delta_{kq}\Delta_{qp}}\delta(\omega-\epsilon_k-\Delta_{pq})\ . \tag{3.13}$$

It is possible to generalize (3.13) to the case of an arbitrary final state with one electron plus n particle-hole pairs. The result is

$$\begin{aligned}R_n(\omega)=2\pi U^{2n}\sum_{k,p_1\cdots p_n,q_1\cdots q_n}&(1-f_k)(1-f_{p_1})\cdots(1-f_{p_n})f_{q_1}\cdots f_{q_n}\\&\times\frac{|t^{+}(\epsilon_k)t^{+}(\epsilon_{p_1})\cdots t^{+}(\epsilon_{p_n})t^{-}(\epsilon_{q_1})\cdots t^{-}(\epsilon_{q_n})|^2}{\Delta_{kq_1}\Delta_{q_1p_1}\Delta_{p_1q_2}\Delta_{q_2p_2}\cdots\Delta_{q_np_n}}\\&\times\delta(\omega-\epsilon_k-\Delta_{p_1q_1}\cdots-\Delta_{p_nq_n})\ .\end{aligned} \tag{3.14}$$

The derivation of this (exact) result is similar to that leading to (3.6) and (3.13) and involves a considerable amount of algebra. The manipulations involved may be illustrated by considering Fig. 6 which shows the simplest diagram for some of the $n=2$ terms. It is necessary to consider all $(n+1)!n!$ permutations of the particle and hole momentum labels taking due account of the exchange antisymmetry. As noted earlier, when squaring the T matrix, it is essential to retain only those parts of the product coming from connected diagrams. Making use of the energy conserving delta function allows one to combine various terms and greatly simplify the resulting expression to end up with (3.14).

B. Critical amplitude

The asymptotic expression of Nozières and De Dominicis[2] is

$$R(\omega)=2\pi\rho(\omega)A(\omega)(\Lambda/\omega)^{\epsilon}\,, \tag{3.15}$$

where $\epsilon\equiv 2\delta(0)/\pi$ and $A(\omega)$ is of order unity. This expression is asymptotically exact in the sense that the singularity exponent ϵ is obtained precisely; however, the prefactor A is unknown. It is therefore of interest to attempt to determine this coefficient within the context of the present method. Following the nonmenclature of the critical phenomena literature, we shall refer to $A\equiv A(0)$ as the critical amplitude.

From (2.43) and (2.44) we see that in the no-pair approximation one has for the critical amplitude

$$A_0=\exp\left[\frac{2}{\pi}\int_0^{\Lambda}d\nu\frac{\delta(\nu)-\delta(0)}{\nu}\right]. \tag{3.16}$$

It will be shown later that this is a fairly good approximation but it is not exact. This is because the multipair contributions to the absorption rate all having a leading divergence of the form $(\Lambda/\omega)^{\epsilon}$; hence they contribute to the critical amplitude. For example, Eq. (3.13) may be evaluated at threshold through a change of variables and the use of the asymptotic form of t^{+} and t^{-} to yield the one-pair contribution

$$A_1=-A_0M_{00}\,, \tag{3.17}$$

where

$$M_{nm}=U^2C_+C_-\int_0^1\frac{d\alpha}{\alpha^{\epsilon}}\int_0^1 d\beta\left[\frac{\beta}{1-\beta}\right]^{\epsilon}\times\frac{(1-\alpha)^n(1-\beta)^m}{\alpha+\beta-\alpha\beta}\,, \tag{3.18}$$

and

$$C_{\pm}=\lim_{\omega\to 0}\left|\frac{\omega}{\Lambda}\right|^{\pm\epsilon}|t_{\pm}(\omega)|^2\,. \tag{3.19}$$

Note that the product C_+C_- is equal to the one-body t matrix evaluated at the Fermi level. Using the general expression (3.14) one finds for the higher contributions

$$A_2=A_0\sum_{l=0}^{\infty}M_{0l}M_{l0}\,, \tag{3.20}$$

$$A_3=-A_0\sum_{nm}M_{0n}M_{nm}M_{m0}\,, \tag{3.21}$$

and so forth. This is evidently the beginning of the series for

$$A=A_0(I+M)^{-1}_{00} \tag{3.22}$$

where I is the identity matrix. M is an infinite matrix but its elements converge rapidly to zero as one moves away from the upper left corner. Hence, it is possible to rapidly and accurately evaluate the required inverse using truncated version of the matrix. We thus have a convenient method for determining the exact critical amplitude for the contact model. A specific example will be discussed in Sec. V.

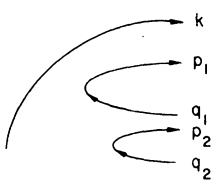

FIG. 6. One of the simplest diagrams in the series for the T matrix associated with transition into two-pair final states.

IV. SOLUTION BY DETERMINANTS

A. General results

Some early work on the x-ray edge problem by Friedel[3] and by Combescot and Nozières[5] (CN) took advantage of the fact that the required overlap matrix elements can be expressed as determinants.

In this section we show that it is possible to obtain the multipair expansion for the open-line amplitude in terms of determinants and we present an exact analytic evaluation of the no-pair term for the contact potential model. The starting point for this calculation is the following expression for the optical-absorption rate[3,5,7,8,12]:

$$R(\omega)=\sum_{\{\lambda\}}2\pi\,|\,\bar{M}(\lambda)\,|^2\delta\left(\omega-\sum_{\lambda}\bar{\epsilon}_\lambda\right), \tag{4.1}$$

where λ refers to an exact single-particle eigenstate of the final-state Hamiltonian with eigenvalue $\bar{\epsilon}_\lambda$ and the sum is over all possible sets of occupied final states. $\bar{M}$ is a matrix element given by

$$\bar{M}(\lambda)=\sum_{k>k_F}M_k\det A_k(\lambda)\,, \tag{4.2}$$

where k_F is the Fermi wave vector, and M_k is the bare optical transition matrix element. The matrix A_k is given by

$$A_k=\begin{matrix}\langle k\,|\,\lambda_1\rangle & \langle k\,|\,\lambda_2\rangle & \langle k\,|\,\lambda_3\rangle & \cdots\\ \langle p_1\,|\,\lambda_1\rangle & \langle p_1\,|\,\lambda_2\rangle & \cdots & \\ \langle p_2\,|\,\lambda_1\rangle & \cdots & & \end{matrix}, \tag{4.3}$$

where $\{p_i\}$ is the set of all wave vectors inside the Fermi surface.

The above formulation leads naturally to an expansion of the absorption rate in terms of the number of excited electron-hole pairs in the final state. Sets $\{\lambda\}$ of occupied final states may be selected which have no pairs, one pair, etc. The no-pair term may be evaluated as follows. The set of states $\{\lambda\}$ consists of the N lowest eigenstates of H denoted by $|\bar{p}_j\rangle$ plus one extra state above the Fermi level and denoted $|\bar{s}\rangle$. We require the determinant of

$$A=\begin{matrix}\langle k\,|\,\bar{s}\rangle & \langle k\,|\,\bar{p}_1\rangle & \langle k\,|\,\bar{p}_2\rangle & \cdots\\ \langle p_1\,|\,\bar{s}\rangle & \langle p_1\,|\,\bar{p}_1\rangle & \cdots & \\ \langle p_2\,|\,\bar{s}\rangle & \cdots & & \end{matrix}. \tag{4.4}$$

This determinant may be exactly evaluated in the contact potential model as discussed below.

B. Contact model

The contact model neglects the finite range of the core-hole potential and approximates it as a delta function. We consider only the S-wave channel and assume for convenience that the core hole is surrounded by a large sphere of radius R ($R\to\infty$ at the end of the calculation). The eigenvalue condition is taken to be the vanishing of the wave function on the surface of the sphere.

The initial radial wave functions are given by

$$\langle r\,|\,n\rangle=\left[\frac{2}{R}\right]^{1/2}\sin\frac{n\pi r}{R} \tag{4.5}$$

where n is an integer. The final-state wave functions are of the form

$$\langle r\,|\,\bar{n}\rangle=e^{i\delta_n}\left[\frac{2}{Rf_n}\right]^{1/2}\times\sin\left[\frac{n\pi r}{R}+\delta_n(1-r/R)\right], \tag{4.6}$$

where δ_n is the scattering phase shift and

$$f_n=1+\sin(2\delta_n)/2(n\pi-\delta_n)\,. \tag{4.7}$$

Direct evaluation of the overlap matrix element yields for $n\neq m$

$$\langle n\,|\,\bar{m}\rangle=\frac{v_n e^{i\delta_m}\sin\delta_m}{R(\epsilon_n-\bar{\epsilon}_m)}\,, \tag{4.8}$$

where $v_n=n\pi/R$. The quantity f has been replaced by unity in the large R limit.

The determinant of the matrix given in (4.4) may now be explicity evaluated. There are common factors of v_n/R in each row and $e^{i\delta_m}\sin\delta_m$ in each column. Taking these out yields

$$\det(A)=\frac{v_k}{R}e^{i\delta_s}\sin\delta_s\prod_{p<k_F}\left[\frac{v_p e^{i\delta_p}\sin\delta_p}{R}\right]\det(F)\,, \tag{4.9}$$

where F is a matrix of energy denominators and has the form

$$F_{ij}=\frac{1}{\epsilon_i-\bar{\epsilon}_j}\,. \tag{4.10}$$

The requireed determinant is readily evaluated[16]

$$\det(F)=\frac{\prod_{i>j}(\epsilon_i-\epsilon_j)\prod_{k>1}(\bar{\epsilon}_k-\bar{\epsilon}_1)}{\prod_{nm}(\epsilon_m-\bar{\epsilon}_n)}\,. \tag{4.11}$$

Separating out from (4.11) the constant Anderson factor representing the overlap of the two ground states, (4.9) may be written as

$$\det(A)=Q\langle k\,|\,\bar{s}\rangle\prod_{p<k_F}\left[\frac{(\epsilon_k-\epsilon_p)(\bar{\epsilon}_s-\bar{\epsilon}_p)}{(\epsilon_k-\bar{\epsilon}_p)(\epsilon_p-\bar{\epsilon}_s)}\right], \tag{4.12}$$

where Q is the Anderson factor. Q is not included in the definition of the open-line amplitude and so we drop it.

There remains the task of evaluating (4.12). We follow the standard method discussed in Gottfried[17] to turn this expression into a dispersion integral. Denoting the infinite product in (4.12) by Z we may write

$$Z=\exp\left\{\sum_{p<k_F}\left[\ln\left[\frac{\epsilon_k-\epsilon_p}{\epsilon_k-\bar{\epsilon}_p}\right]+\ln\left[\frac{\bar{\epsilon}_s-\bar{\epsilon}_p}{\bar{\epsilon}_s-\epsilon_p}\right]\right]\right\}. \tag{4.13}$$

In the large R limit one has

$$Z=\exp\left[\sum_{p<k_F}(\bar{\epsilon}_p-\epsilon_p)\left[\frac{1}{\epsilon_k-\bar{\epsilon}_p}-\frac{1}{\bar{\epsilon}_s-\epsilon_p}\right]\right]. \tag{4.14}$$

Using

$$\bar{\epsilon}_p-\epsilon_p=-v_p\delta_p/R \tag{4.15}$$

and defining (with ϵ_F denoting the Fermi energy)

$$D(\epsilon)\equiv\lim_{R\to\infty}\frac{1}{R}\sum_{p<p_F}\frac{v_p\delta_p}{\epsilon_p-\epsilon}=\frac{1}{\pi}\int_{-\infty}^{\epsilon_F}d\epsilon'\frac{\delta(\epsilon')}{\epsilon'-\epsilon}, \tag{4.16}$$

we obtain

$$\det(A)=\langle k\mid\bar{s}\rangle\exp[D(\epsilon_k)-D(\epsilon_s)]. \tag{4.17}$$

We are now in a position to evaluate the effective matrix element defined by (4.2). In performing the wave-vector summation over $k>k_F$ one must separate the term $k=s$ from those with $k\neq s$ to obtain

$$\bar{M}=M_s\langle s\mid\bar{s}\rangle+\frac{1}{R}\sum_{k>k_F,k\neq s}\frac{v_kM_ke^{D(\epsilon_k)}}{\epsilon_k-\bar{\epsilon}_s}\times e^{i\delta_s}\sin\delta_s e^{-D(\epsilon_s)}. \tag{4.18}$$

A word of caution concerning the overlap $\langle s\mid\bar{s}\rangle$ is required. In this case it is apparently necessary to go to the $R=\infty$ limit *before* evaluating the overlap integral so that one obtains

$$\langle s\mid\bar{s}\rangle=e^{i\delta_s}\cos\delta_s. \tag{4.19}$$

Returning to (4.18) the summation becomes an integral yielding

$$\bar{M}=e^{i\delta_s}\left[M_s\cos\delta_s+\frac{1}{\pi}\sin\delta_s e^{-D(\epsilon_s)}\int_{\epsilon_f}^{\infty}d\epsilon\frac{M(\epsilon)e^{D(\epsilon)}}{\epsilon-\epsilon_s}\right], \tag{4.20}$$

where the principal part is understood. To further reduce this expression we take advantage of an identity derived from the single-particle t matrix

$$e^{i\delta(\epsilon)}\sin\delta(\epsilon)=\pi U\exp[D(\epsilon)+\Delta(\epsilon+i\eta)]. \tag{4.21}$$

where U is the strength of the contact potential and

$$\Delta(z)\equiv\int_{\epsilon_f}^{\infty}d\omega\frac{\delta(\omega)}{\omega-z}. \tag{4.22}$$

It follows that

$$e^{-D(\epsilon_s)}\sin\delta_s=\pi Ue^{p(\epsilon_s)} \tag{4.23}$$

and

$$e^{D(\epsilon)}=\frac{\sin\delta(\epsilon)}{\pi U}e^{-p(\epsilon)}, \tag{4.24}$$

where

$$p(\epsilon)\equiv\mathrm{Re}\Delta(\epsilon+i\eta). \tag{4.25}$$

Equation (4.20) becomes

$$\bar{M}=e^{i\delta_s}\left[M_s\cos\delta_s+\frac{1}{\pi}e^{p(\epsilon_s)}\int_{\epsilon_F}^{\infty}d\epsilon\frac{M(\epsilon)}{\epsilon-\epsilon_s}\sin\delta(\epsilon)e^{-p(\epsilon)}\right]. \tag{4.26}$$

This is identical to an expression considered by Goldberger and Watson.[18] As they point out for the case in which the optical matrix element $M(\epsilon)$ is a constant [$M(\epsilon)=1$], Eq. (4.26) readily reduces to

$$\bar{M}(\epsilon_s)=\exp[\Delta(\epsilon_s+i\eta)] \tag{4.27}$$

which is identical to our previous result (2.42) and equivalent to the Pardee-Mahan expression. This completes the discussion of the intensity for transition to no-pair final states and confirms our previous result for the effective-matrix element.

The required determinant can also be evaluated for the case of single-pair final states. Let the electron final state be labeled $\bar{s}_1$ and $\bar{s}_2$ and the hole be labeled $\bar{p}_1$. In the contact model one obtains

$$\det A(k,s_1,s_2,p_1)=\frac{\langle k\,|\,\bar{s}_1\rangle\langle k\,|\,\bar{s}_2\rangle}{\langle k\,|\,\bar{p}_1\rangle}\frac{(\bar{\epsilon}_{s_1}-\bar{\epsilon}_{s_2})(\epsilon_{p_1}-\bar{\epsilon}_{p_1})}{(\bar{\epsilon}_{s_1}-\bar{\epsilon}_{p_1})(\bar{\epsilon}_{s_2}-\bar{\epsilon}_{p_1})}\exp[\Delta(\epsilon_k)+\Delta(\epsilon_{p_1})-\Delta(\epsilon_{s_1})-\Delta(\epsilon_{s_2})]\ . \tag{4.28}$$

This it is straightforward to obtain the effective matrix elements for this case also, although we have not attempted to carry out the k summation to compare (4.28) with our previous result.

We again emphasize that the determinant method (like the previous one) succeeds because of the simplifications associated with a contact potential (or more generally for an arbitrary separable potential[2]).

V. NUMERICAL RESULTS

As a specific model to which we can apply our method we have chosen the simple flat band model with the (half-filled) density of states

$$\rho(\omega)=\Theta(\omega+\Lambda)\Theta(\Lambda-\omega) \tag{5.1}$$

and bandwidth $\Lambda=\frac{1}{2}$. We take the strength of the contact potential to be that used by Oliveira,[19] $U=-(1/\pi)\tan(\pi/5)$ so that $\delta(0)=\pi/5$. The single-particle Green's function is

$$g(\omega)=\ln\left[\frac{\omega+1/2}{\omega-1/2}\right] \tag{5.2}$$

and the one-body t matrix is

$$t=\frac{U}{1-Ug}\ . \tag{5.3}$$

The scattering phase shift is given by

$$\tan\delta(\omega)=\frac{U\,\mathrm{Im}g(\omega+i\eta)}{1-U\,\mathrm{Re}g(\omega+i\eta)}\ . \tag{5.4}$$

One of the characteristics of this model is that for any nonzero value of U there is a bound state at

$$E_B=\tfrac{1}{2}\coth(1/2U)\ , \tag{5.5}$$

which in the present case is just below the bottom of the band at

$$E_B=-0.513\ . \tag{5.6}$$

Thus the phase shift is π at the bottom of the band and there is an isolated pole in the one-body t matrix at E_B. This is handled with the dispersion integral formalism by extending the domain the integration (Eq. 3.8) to E_B and setting the phase shift equal to π between the band bottom and E_B where it vanishes suddenly. As noted by CN the existence of a bound state leads to a second threshold, but in the present case the associated oscillator strength is quite small because the measure of the delta function in the local density of states is quite small. Defining f_0 by

$$\mathrm{Im}t=\pi f_0\delta(\omega-E_B) \tag{5.7}$$

for $\omega\sim E_B$ we find

$$f_0=E_B^2-\tfrac{1}{4}=0.0136\ . \tag{5.8}$$

This is a measure of the oscillator strength for the empty band case. The value is even smaller for a partially filled band. For convenience we neglect the contribution of this weak second threshold to the oscillator strength calculations described below.

Within this simple model we have calculated the lowest order contributions to the critical amplitude to be

$$A_0=C_+=0.866\ , \tag{5.9a}$$

and

$$A_1=-0.11A_0\ , \tag{5.9b}$$

while the exact critical amplitude given by (3.22) is

$$A=0.910A_0\ . \tag{5.10}$$

As noted in Sec. III, this calculation involves numerically inverting a truncated version of an infinite matrix. Successive inversion of $N\times N$ matrices up to $n=30$ yielded rapid convergence.

It is interesting to compare Oliveira's[19] results with our value of the critical amplitude $A=0.788$. Using a numerical renormalization group scheme Oliveira found $A=0.82$ with an estimated accuracy of a few percent. This value may be improved slightly by extrapolating his results for various mesh sizes to the continuum limit which yields $A=0.80$ in rather good agreement with our result. Actually these two results cannot be directly compared since Oliveira's calculation includes the closed-loops contribution and our does not. However, for the value of the phase shift $\delta(0)=\pi/5$ the orthogonality exponent α is very small ($\alpha=0.04$). It seems likely that inclusion of the closed loops which modifies the singularity exponent by only a small amount will modify the critical amplitude by an even smaller amount.

Equation (5.10) indicates that multipair corrections to the critical amplitude are quite modest, suggesting that the no-pair contribution may dominate the spectrum.[20] This idea was confirmed by evaluating the integrated intensity for the no-pair and one-pair rates. Defining

$$S_n=\frac{1}{2\pi}\int_0^{(2n+1)/2} d\omega\, R_n(\omega)\ , \tag{5.11}$$

we find

$$S_0=0.574 \tag{5.12}$$

and

$$S_0+S_1=0.475\ . \tag{5.13}$$

As noted earlier we have neglected a small contribution to S, due to the second threshold. One estimates that $S_2\sim+S_1^2$ so that the sum

$$\sum_n S_n\rightarrow\tfrac{1}{2} \tag{5.14}$$

is rapidly coverging to the value $\frac{1}{2}$ as required by the oscillator strength sum rule. Note that the zero-pair approximation exceeds the sum-rule limit by only about 14% while the zero- plus one-pair terms fall short by only 5%.

Various calculated transition rates are graphed in Fig. 7. The middle curve shows the quantity $R_0(\omega)/2\pi\rho$ which is proportional to the transition rate into no-pair final states. The lowest curve is $[R_0(\omega)+R_1(\omega)]/2\pi\rho$ which includes zero- and one-pair final states. The upper curve represents $A(\Lambda/\omega)^\epsilon$, the Nozières–De Dominicis (ND) asymptotic form scaled by the exact critical amplitude $A=0.788$.

As noted earlier R_1 is negative due to exchange antisymmetry which means that the spectral density associated with the open-line propagator is negative for $\omega>\Lambda$. This violates the usual rule that the spectral density of an equilibrium Fermion propagator is non-negative. However, the open-line amplitude is not an equilibrium propagator because of the transient nature of the core-hole potential.[2] The complete expression for the transition rate including the closed loops is, of course, non-negative. It is only artifical factorization of the rate into two terms which produces the apparent contradiction.

We should also note that R_1 is smooth and monotone. The apparent discontinuity in the graph of $(R_0+R_1)/2\pi\rho$ at $\omega=0.5$ is an artifact of the sudden vanishing of R_0 at the upper band edge.

It is clear from Fig. 7 that the asymptotic ND form deviates from the more accurate dispersion

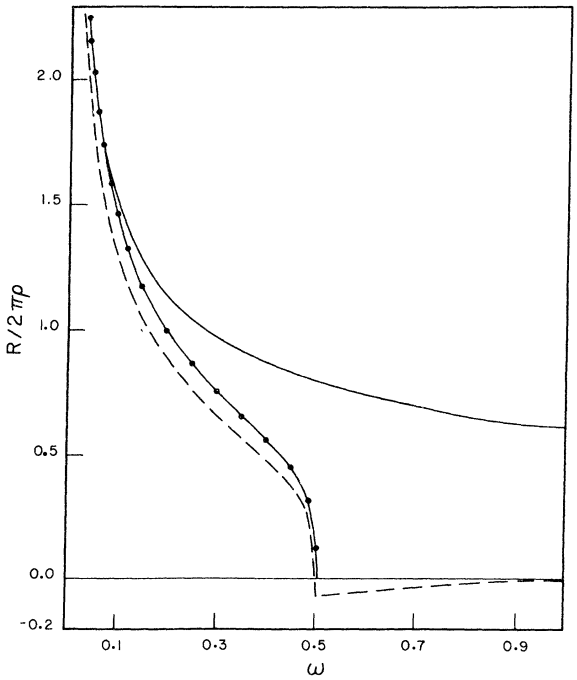

FIG. 7. Calculated transition rates as described in the text. The top curve is the asymptotic ND result. The middle curve is the no-pair result and the bottom curve the zero- plus one-pair result.

relation results even rather close to threshold. This is partly an artifact of this model with its sharp cut off at the upper band edge. The form suggested by perturbation theory

$$R=2\pi\rho A\left[\frac{\Lambda-\omega}{\omega}\right]^\epsilon\Theta(\omega)\Theta(\Lambda-\omega) \tag{5.15}$$

lies much closer to the correct result. Because of the simplicity of the model it is not clear what conclusions one can draw regarding the actual range applicability of the ND asymptotic form to experimental data.

VI. CONCLUSIONS

We have presented a dispersion relation formulation of the open-line amplitude of the MND x-ray edge problem within the contact potential model. Our results put the earlier analysis of Pardee and Mahan on a firmer footing by explicitly establishing which contributions to the total spectral density are included in the dispersion relation expression.

Using both multiple scattering and determinant techniques we have found that to a good approximation, the many-body effects can be described

within a single-particle transition rate expression using a renormalized matrix element. This effective matrix element may be expressed exactly in terms of a simple dispersion integral. There are small corrections to the transition rate due to multiple particle-hole-pair final states and a systematic expansion for these was presented. This series was summed at threshold to yield an exact expression for the critical amplitude multiplying the power-law singularity. Our results give an exact description at threshold (including the prefactor) and were shown to be rather accurate away from threshold.

Note added in proof. We have recently received a preprint from Ulf von Barth and Günter Grossmann in which they obtain the same result as our Eq. (2.42) for the no-pair final-state transition amplitude.

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