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Golden-rule approach to the soft-x-ray-absorption problem

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The cross section of the soft-x-ray absorption is derived based on the Fermi golden rule, by summing the transition probabilities over all possible final states. It is shown that the factor connected with the Anderson orthogonality catastrophe is canceled in the process of summation, and the spectrum is finally expressed by the core-hole propagator times the open-line propagator, as shown by Nozières and De Dominicis. Our results are compared with the results obtained by Mahan and collaborators and are shown to improve over theirs in several respects, expecially in the core-hole propagator. With the use of the new integral kernel, the integral equation for the threshold region is treated and the exact form of the edge anomaly, including the analytical form of the prefactor of the power-law spectrum of Nozières and De Dominicis, is obtained.

I. INTRODUCTION

After the work of Mahan[1] and Nozières and coworkers,[2,3] which explained successfully the threshold anomaly of the soft-x-ray absorption or emission spectrum, much attention has been paid to clarifying the extent in the frequency range for which the solution of Nozières and De Dominicis[3] (ND), exact near the threshold, has its practical applicability. In the frequency range where the solution of Mahan and ND does not work, many authors have tried to find a better description of the phenomena. For this purpose, calculating the absorption or emission cross section in terms of Slater determinants of a many-electron system has been a very powerful tool, because the ND model Hamiltonian is a simple one-body Hamiltonian that enables us to write down straightforwardly the initial and final states of the optical transition. As a matter of fact, the matrix inversion method introduced by Combescot and Nozières[4] (CN) enabled them to deduce detailed edge anomalies for a core-hole potential sufficiently strong to give rise to a bound state. Their method, based on the calculation of determinants and inverse matrices, is quite suitable for numerical calculations and has lead to exact information on the validity and the limitation of the ND solution.[5-7] Furthermore, a series of analytical treatments of Mahan and co-workers[8-11] showed that, by rewriting the core-hole propagator $G(t)$ and the open-line propagator $L(t)$ in terms of the Slater determinants and decomposing them into sums of the contributions from various final states, one can obtain an expression of the spectrum having a wider range of validity.

The matrix formulation of the x-ray absorption and emission problem has been initiated by the remarks of Friedel.[12] He demonstrated usefulness of the Fermi golden rule by showing that the characteristics of the edge anomaly manifest themselves already in the lowest-order transition probabilities that were calculated using initial- and final-state Slater determinants.

If we start from the Fermi golden rule, we need only sum the transition probabilities between the ground state of the initial-state Hamiltonian H_I and all possible states of the final-state Hamiltonian H_F. Owing to the scattering by the core-hole potential in the final state, however, two complications occur in the derivation: One is the need to project the many-body final state Ψ_F onto the initial ground state Φ_I for calculating the matrix element, because the one-particle wave functions of H_I and H_F are not orthogonal in general. When Ψ_F is the ground state of H_F, however, the projection $\langle \Psi_F \mid \Phi_I \rangle$ becomes vanishingly small as the number of electrons in the system tends to infinity. This orthogonality, known as Anderson's orthogonality catastrophe[13] (AOC), occurs not only when Ψ_F is the ground state but also when it is an excited state. The other complication is thus that we must carry out a precise calculation in order to obtain a finite result by summing an infinitely large number of vanishingly small quantities.

It seems that this is the reason why there has been no complete formulation based on the golden rule. In fact, in their formalism, CN tacitly avoided the calculation of the transition probabilities by representing $G(t)$ and $L(t)$ in terms of initial-state one-particle wave functions.[4] Also, the formulation of Mahan and co-workers[8-11] starts from the definitions of $G(t)$ and $L(t)$, which are, of course, both finite. This means that they also avoided the derivation from the golden rule of the exact form $G(t)L(t)$ of the spectrum, which appears to be one of the most difficult steps because of the AOC.

In this paper we straightforwardly follow the line proposed by Friedel. We classify the final states according to the number of excited electrons above the Fermi level and calculate the transition probabilities. We show that a factor connected with the AOC is exactly canceled when the summation is carried out over all possible final states and that the result of the summation—the total transition probability—is expressed in a closed form. Since the matrix elements in the golden rule incorporate only the wave functions of the initial and final states, the closed form obtained is free from the complicated nature of the core-hole potential. In addition, the validity of our closed form is not limited to the threshold region.

Since the series of papers by Mahan and co-workers are

the most important in the literature along the line pursued in this paper, let us briefly review their findings and see in what respects our results improve upon theirs. For the special model of a contact or separable core-hole potential, Penn, Girvin, and Mahan[10] and Mahan[11] decomposed $G(t)$ and $L(t)$ into the superposed contributions that are classified according to the number of excited electron-hole pairs in the final states. They attempted to resum the series thus obtained. As for $L(t)$, the resummation was in fact accomplished for that special core-hole potential.[10] The resummation of the series for $G(t)$ was not complete, however.[11] In the linked-cluster expansion of $G(t)$, therefore, only a few leading terms were given.

In this paper we show that the resummation can be carried out, leading to closed expressions for both $L(t)$ and $G(t)$, which are valid for an arbitrary form of the core-hole potential. Of course, in the case of the contact core-hole potential the present formulas reproduce all the results that have been obtained by Mahan and co-workers. For details see Sec. IV.

As for the threshold behavior, we demonstrate that our formulas reproduce, both for $G(t)$ and $L(t)$, the exact results obtained by ND. In addition, we present the analytical form of the prefactor of the power-law spectrum, which is called the critical amplitude and is obtained numerically in Ref. 10. The agreement of our formula with the numerical value is quite good, showing that our approach in this respect improves upon the ND solution of the threshold behavior.

In Sec. II, we classify the final states, calculate the matrix elements, and show that the resummation can be carried out to yield the closed form of the total transition probability. In Sec. III, various quantities necessary for deriving the spectrum are calculated for a contact potential. In Sec. IV, we discuss the relationship between our results and those of Mahan and co-workers. In Sec. V, the result of ND is seen to be reproduced by our formula, and the critical amplitude is derived. Section VI ends the paper with a brief summary. In this paper, the formulation is given only for the absorption case.

II. FORMULATION BASED ON THE FERMI GOLDEN RULE

We consider the optical absorption process of $N+1$ electrons. In the initial state, the system is in the ground state composed of N band electrons and one core-state electron. In the final state all of the $N+1$ electrons are in the band states, which are perturbed by the scattering potential of the core hole left behind. The possibility of the existence of a bound state in the final state is not considered in this paper. Let the initial and final band states φ_k and ψ_κ be determined by the one-body Hamiltonian h_I and h_F, respectively. The Hamiltonian h_F is h_I plus the core-hole potential. Owing to the completeness relation, ψ_κ is resolved into a superposition of $\{\varphi_k\}$:

$$\psi_\kappa=\sum_k a_{k\kappa}\varphi_k \ , \tag{2.1}$$

where

$$a_{\kappa k}=a_{k\kappa}^*=\langle \psi_\kappa \mid \varphi_k \rangle \tag{2.2}$$

is the overlap integral. We use Greek (Latin) letters for the indices that specify the final (initial) band states.

The Slater determinants of the N lowest eigenstates of h_I and h_F are denoted by

$$\begin{aligned}\Phi_I^0&=\mid \varphi_1,\varphi_2,\ldots,\varphi_N \mid \ ,\\ \Psi_F^0&=\mid \psi_1,\psi_2,\ldots,\psi_N \mid \ .\end{aligned} \tag{2.3}$$

These two states represent the ground states of N band electrons in the initial and final states, respectively. Let their energies be E_I^0 and E_F^0, which are the sums of the N lowest eigenvalues of h_I and h_F. The difference, or the ground-state energy shift due to the core-hole potential, is denoted as ΔE^0:

$$\Delta E^0=E_F^0-E_I^0 \ . \tag{2.4}$$

From Fumi's theorem,[14] ΔE^0 is expressed as a sum of the phase shifts, but we do not need an explicit form of ΔE^0. The overlap integral between Φ_I^0 and Ψ_F^0 is an important quantity in what follows. We denote it as Δ:

$$\begin{aligned}\Delta&=\langle \Psi_F^0 \mid \Phi_I^0 \rangle\\ &=\det \underline{A}\end{aligned} \tag{2.5}$$

with an $N\times N$ matrix $\underline{A}$ defined by

$$(\underline{A})_{\mu m}=a_{\mu m} \ . \tag{2.6}$$

Together with Δ, the overlap integrals of Φ_I^0 with an excited final state of N band electrons are equally important. For an excited state Ψ_F, obtained from Ψ_F^0 by replacing the orbitals $\mu_1<\mu_2<\cdots<\mu_n$ in Eq. (2.3) with a set of n new orbitals above the Fermi energy $\gamma_1<\gamma_2<\cdots<\gamma_n$, respectively, we denote the overlap $\langle \Psi_F \mid \Phi_I^0 \rangle$ as

$$\Delta(\bar{\mu}_1,\bar{\mu}_2,\ldots,\bar{\mu}_n;\gamma_1,\gamma_2,\ldots,\gamma_n) \ .$$

For example, we set

$$\Delta(\bar{\mu};\gamma)=\det \begin{vmatrix} a_{11} & \cdots & a_{1N} \\ \vdots & & \vdots \\ a_{\gamma 1} & \cdots & a_{\gamma N} \\ \vdots & & \vdots \\ a_{N1} & \cdots & a_{NN} \end{vmatrix}_{<\mu} \ , \tag{2.7}$$

where the μth row $(a_{\mu 1},a_{\mu 2},\ldots,a_{\mu N})$ in Δ has been replaced by $(a_{\gamma 1},a_{\gamma 2},\ldots,a_{\gamma N})$. We use the bar on the symbol μ to emphasize that the state μ is empty. Expanding $\Delta(\bar{\mu};\gamma)$ with respect to the μth row, we have

$$\frac{\Delta(\bar{\mu};\gamma)}{\Delta}=\sum_{m(<)} a_{\gamma m}(\underline{A}^{-1})_{m\mu} \ , \tag{2.8}$$

where the summation is over the states (of h_I, as indicated by the Latin symbol m) below the Fermi energy [symbolized by $(<)$ index] and $\underline{A}^{-1}$ is an inverse matrix of $\underline{A}$ defined by Eq. (2.6). According to AOC,[13] the ground-state overlap Δ vanishes in the limit of large N. Likewise, the new overlap integrals $\Delta(\bar{\mu};\gamma)$, $\Delta(\bar{\mu}_1,\bar{\mu}_2;\gamma_1,\gamma_2)$, etc., vanish in the same limit, as shown later.

In the optical absorption, the system jumps from the initial state

$$\Phi_I = |\varphi_1,\varphi_2,\ldots,\varphi_N,\varphi_c| \ , \tag{2.9}$$

φ_c being the core state, to the ground or excited state of the final state of $N+1$ band electrons. We classify the final states in terms of the number of electrons excited above the Fermi level. Let $\Psi_f^{(n)}$ be the final state, having n electrons above the Fermi energy. Since one of the n electrons comes from the core state, $\Psi_f^{(n)}$ has $n-1$ holes. The subscript f specifies collectively the hole and electron states. The state $\Psi_f^{(2)}$ with $f=(\bar{\mu};\gamma_1,\gamma_2)$, for example, describes the state with one hole at the state μ and two excited electrons at γ_1 and γ_2.

Now the transition from Φ_I to $\Psi_f^{(n)}$ is assumed to be due to the dipole moment W:

$$W=\sum_{i=1}^{N+1} w_i \ . \tag{2.10}$$

Our aim in this section is to obtain the closed expression of the absorption spectrum from the golden-rule formula ($\hbar=1$):

$$\begin{aligned} I(\omega) &= 2\pi \sum_{n,f} |\langle \Psi_f^{(n)} | W | \Phi_I \rangle|^2 \delta(E_f^{(n)}-E_I-\omega) \\ &= 2\,\mathrm{Re} \sum_{n,f} \int_0^\infty dt\, |\langle \Psi_f^{(n)} | W | \Phi_I \rangle|^2 \\ &\qquad \times e^{-i(E_f^{(n)}-E_I-\omega_+)t} \\ &= \sum_n I^{(n)}(\omega) \ . \end{aligned} \tag{2.11}$$

Here $\omega_+=\omega+i\delta$ and the third equality defines the contribution to the spectrum from the final states with n excited electrons. Measuring the one-electron energies from the Fermi energy ($\epsilon_{\mathrm{Fermi}}=0$), we have for

$$f=(\mu_1,\mu_2,\ldots,\mu_{n-1};\gamma_1,\gamma_2,\ldots,\gamma_n)$$

the following:

$$\begin{aligned} E_f^{(n)}-E_I-\omega &= \left[\sum_{i=1}^{n}\epsilon_{\gamma_i}-\sum_{i=1}^{n-1}\epsilon_{\mu_i}+E_F^0\right]-(E_I^0+\epsilon_{\mathrm{core}})-\omega \\ &= \sum_{i=1}^{n}\epsilon_{\gamma_i}-\sum_{i=1}^{n-1}\epsilon_{\mu_i}+\Delta E^0-\epsilon_{\mathrm{core}}-\omega \\ &= \sum_{i=1}^{n}\epsilon_{\gamma_i}-\sum_{i=1}^{n-1}\epsilon_{\mu_i}+\omega_{\mathrm{th}}-\omega \ , \end{aligned} \tag{2.12}$$

where ϵ_{core} is the energy of the core state φ_c ($\epsilon_{\mathrm{core}}<0$), ΔE^0 is the ground-state energy shift of N electrons introduced in Eq. (2.4), and the third equality defines the renormalized threshold energy ω_{th},

$$\omega_{\mathrm{th}}=\Delta E^0-\epsilon_{\mathrm{core}} \ . \tag{2.13}$$

Let us begin with $n=1$ (no hole in the final state). The symbol f now specifies only the state of the excited electron. Let it be γ. Then

$$\langle \Psi_f^{(1)} | W | \Phi_I \rangle = \det \begin{vmatrix} a_{11} & \cdots & a_{1N} & w_{1c} \\ \vdots & & \vdots & \vdots \\ a_{N1} & \cdots & a_{NN} & w_{Nc} \\ a_{\gamma 1} & \cdots & a_{\gamma N} & w_{\gamma c} \end{vmatrix} \ , \tag{2.14}$$

with

$$w_{\gamma c}=\langle \psi_\gamma | w | \varphi_c \rangle \ ,$$

etc. Expanding Eq. (2.14) with respect to the last column, one can see that the cofactors involved have just the form given by Eq. (2.7). Hence

$$\begin{aligned} \langle \Psi_f^{(1)} | W | \Phi_I \rangle &= \Delta \left[w_{\gamma c} - \sum_{\mu(<)} \frac{\Delta(\bar{\mu};\gamma)}{\Delta} w_{\mu c} \right] \\ &\equiv \Delta p(\gamma) \ . \end{aligned} \tag{2.15}$$

The symbol $\mu(<)$ denotes the sum over the perturbed states below the Fermi level. The second term of $p(\gamma)$ expresses the exchange process (replacement transition of Friedel[12]), which can occur due to the nonorthogonality between $\{\psi_\kappa\}$ and $\{\varphi_k\}$. It is important that the matrix element (2.15) is proportional to Δ. The cross section of the one-electron jump thus vanishes by AOC. Let us rewrite $p(\gamma)$ in a slightly different form, making use of the completeness relation of $\{\varphi_k\}$. It holds that

$$p(\gamma)=\sum_{b(>)} \left[a_{\gamma b} - \sum_{\mu(<)} \frac{\Delta(\bar{\mu};\gamma)}{\Delta} a_{\mu b} \right] w \ , \tag{2.16}$$

where $b(>)$ means the sum over the (unperturbed) states above the Fermi level and

$$w=\langle \varphi_b | w | \varphi_c \rangle \ . \tag{2.17}$$

In accordance with ND, the matrix element between the core state φ_c and φ_b is assumed to be independent of b. Now substituting Eq. (2.15) into Eq. (2.11) and using Eq. (2.12) for $n=1$, we have

$$\begin{aligned} I^{(1)}(\omega) &= 2\,\mathrm{Re} \int_0^\infty dt\, e^{i(\omega_+-\omega_{\mathrm{th}})t} |\Delta|^2 \\ &\qquad \times \sum_{\gamma(>)} |p(\gamma)|^2 e^{-i\epsilon_\gamma t} \ , \end{aligned} \tag{2.18}$$

the summation being over the states above the Fermi level.

Next, we turn to $n=2$. The excited state $\Psi_f^{(2)}$ with $f=(\bar{\mu}_1;\gamma_1,\gamma_2)$ ($\gamma_1<\gamma_2$) is now involved. Since

$$\langle \Psi_f^{(2)} | W | \Phi_I \rangle = \det \begin{vmatrix} a_{11} & \cdots & a_{1N} & w_{1c} \\ \vdots & & \vdots & \vdots \\ a_{\gamma_1 1} & \cdots & a_{\gamma_1 N} & w_{\gamma_1 c} \\ \vdots & & \vdots & \vdots \\ a_{N1} & \cdots & a_{NN} & w_{Nc} \\ a_{\gamma_2 1} & \cdots & a_{\gamma_2 N} & w_{\gamma_2 c} \end{vmatrix} <\mu_1 \ , \tag{2.19}$$

the expansion with respect to the $(N+1)$th column yields

$$\begin{aligned} \langle \Psi_f^{(2)} | W | \Phi_I \rangle &= \Delta(\bar{\mu}_1;\gamma_1) w_{\gamma_2 c} - \Delta(\bar{\mu}_1;\gamma_2) w_{\gamma_1 c} \\ &\quad - \sum_{\substack{\mu_2(<) \\ (\mu_2\neq\mu_1)}} \Delta(\bar{\mu}_1,\bar{\mu}_2;\gamma_1,\gamma_2) w_{\mu_2 c} \ . \end{aligned} \tag{2.20a}$$

Now for $\mu_1 \neq \mu_2$ and $\gamma_1 \neq \gamma_2$, we have

$$\Delta(\bar{\mu}_1,\bar{\mu}_2;\gamma_1,\gamma_2)=\Delta \det \begin{vmatrix} \Delta(\bar{\mu}_1;\gamma_1)/\Delta & \Delta(\bar{\mu}_1;\gamma_2)/\Delta \\ \Delta(\bar{\mu}_2;\gamma_1)/\Delta & \Delta(\bar{\mu}_2;\gamma_2)/\Delta \end{vmatrix}, \tag{2.20b}$$

which is the relation known as Jacobi's identity.[15] One can use Eq. (2.20b) in the right-hand side of Eq. (2.20a) without imposing the restriction $\mu_2 \neq \mu_1$, since Eq. (2.20b) vanishes when $\mu_2=\mu_1$. We expand Eq. (2.20b) with respect to the second row, put it into Eq. (2.20a), and compare the result with Eq. (2.15) of the one-electron jump. We then find

$$\langle \Psi_f^{(2)} \mid W \mid \Phi_I \rangle = \Delta(\bar{\mu}_1;\gamma_1)p(\gamma_2)-\Delta(\bar{\mu}_1;\gamma_2)p(\gamma_1) . \tag{2.20c}$$

The restriction $\gamma_1 \neq \gamma_2$ in $f=(\bar{\mu}_1;\gamma_1,\gamma_2)$ can be relaxed in Eq. (2.20c). For $I^{(2)}(\omega)$ of the spectrum, we must take the absolute square of Eq. (2.20c). We find

$$I^{(2)}(\omega)=2\,\mathrm{Re}\int_0^\infty dt\, e^{i(\omega_+-\omega_{\mathrm{th}})t} \mid \Delta \mid^2 \sum_{\gamma_1,\gamma_2(>)} [\mid p(\gamma_1) \mid^2 K(\gamma_2,\gamma_2 \mid t)-p^*(\gamma_1)p(\gamma_2)K(\gamma_1\gamma_2 \mid t)]e^{-i\epsilon_{\gamma_1}t-i\epsilon_{\gamma_2}t}, \tag{2.20d}$$

where

$$K(\gamma_1\gamma_2 \mid t)=\frac{1}{\mid \Delta \mid^2}\sum_{\mu(<)} \Delta(\bar{\mu};\gamma_1)\Delta(\bar{\mu};\gamma_2)^* e^{i\epsilon_\mu t} . \tag{2.21}$$

Note the absence of the restriction $\gamma_1<\gamma_2$ in Eq. (2.20d).

All the necessary procedures for obtaining the matrix element $\langle \Psi_f^{(n)} \mid W \mid \Phi_I \rangle$ are embodied in the case of $n=2$. Instead of treating general n, we write down the main formulas for $\Psi_f^{(3)}$ with $f=(\bar{\mu}_1,\bar{\mu}_2;\gamma_1,\gamma_2,\gamma_3)$:

$$\langle \Psi_f^{(3)} \mid W \mid \Phi_I \rangle = \Delta(\bar{\mu}_1,\bar{\mu}_2;\gamma_1,\gamma_2)w_{\gamma_3 c}-\Delta(\bar{\mu}_1,\bar{\mu}_2;\gamma_3,\gamma_2)w_{\gamma_1 c}-\Delta(\bar{\mu}_1,\bar{\mu}_2;\gamma_1,\gamma_3)w_{\gamma_2 c}-\sum_{\substack{\mu_3(<) \\ (\mu_3\neq\mu_1,\mu_2)}} \Delta(\bar{\mu}_1,\bar{\mu}_2,\bar{\mu}_3;\gamma_1,\gamma_2,\gamma_3)w_{\mu_3 c} , \tag{2.22a}$$

$$\Delta(\bar{\mu}_1,\bar{\mu}_2,\bar{\mu}_3;\gamma_1,\gamma_2,\gamma_3)=\Delta \det \begin{vmatrix} \Delta(\bar{\mu}_1;\gamma_1)/\Delta & \Delta(\bar{\mu}_1;\gamma_2)/\Delta & \cdots \\ \Delta(\bar{\mu}_2;\gamma_1)/\Delta & \cdots & \cdots \\ \Delta(\bar{\mu}_3;\gamma_1)/\Delta & \cdots & \cdots \end{vmatrix} . \tag{2.22b}$$

Combining these two expressions and expanding Eq. (2.22b) with respect to the third row, we have

$$\langle \Psi_f^{(3)} \mid W \mid \Phi_I \rangle = \Delta(\bar{\mu}_1,\bar{\mu}_2;\gamma_1,\gamma_2)p(\gamma_3)-\Delta(\bar{\mu}_1,\bar{\mu}_2;\gamma_3,\gamma_2)p(\gamma_1)-\Delta(\bar{\mu}_1,\bar{\mu}_2;\gamma_1,\gamma_3)p(\gamma_2) . \tag{2.22c}$$

Again, all the restrictions for $\{\mu\}$ and $\{\gamma\}$ may be dropped. To derive $I^{(3)}(\omega)$ from Eq. (2.22c) we must note

$$\frac{1}{2!}\sum_{\mu_1,\mu_2(<)} \Delta(\mu_1,\mu_2;\gamma_1,\gamma_2)[\Delta(\mu_1,\mu_2;\gamma_3,\gamma_4)]^* \exp(i\epsilon_{\mu_1}t+i\epsilon_{\mu_2}t)= \mid \Delta \mid^2 \det \begin{vmatrix} K(\gamma_1,\gamma_3 \mid t) & K(\gamma_1,\gamma_4 \mid t) \\ K(\gamma_2,\gamma_3 \mid t) & K(\gamma_2,\gamma_4 \mid t) \end{vmatrix} . \tag{2.23}$$

The identity is obvious when we note that the right-hand side has a form of Gram's determinant when one uses Eq. (2.21), so that it is decomposed into a linear combination of products of two determinants, as in the form of the left-hand side of Eq. (2.23). Another thing to observe in $I^{(3)}(\omega)$ is that the three terms proportional to $\mid p(\gamma) \mid^2$ are all equal when the sum is taken over $\{\mu\}$ and $\{\gamma\}$, and so are all the contributions of the type $p^*(\gamma_1)p(\gamma_2)$. This fact may be checked by making an appropriate interchange of symbols in the summation over $\{\mu\}$ and $\{\gamma\}$. Thus, from Eq. (2.22c), it follows that

$$\begin{aligned} I^{(3)}(\omega)=2\,\mathrm{Re}\int_0^\infty dt\, e^{i(\omega_+-\omega_{\mathrm{th}})t} & \\ \times \mid \Delta \mid^2 \sum_{\{\gamma(>)\}} \Bigg[& \mid p(\gamma_1) \mid^2 \frac{1}{2!}\det \begin{vmatrix} K(\gamma_2,\gamma_2 \mid t) & K(\gamma_2,\gamma_3 \mid t) \\ K(\gamma_3,\gamma_2 \mid t) & K(\gamma_3,\gamma_3 \mid t) \end{vmatrix} \\ & -p^*(\gamma_1)p(\gamma_2)\det \begin{vmatrix} K(\gamma_1,\gamma_2 \mid t) & K(\gamma_1,\gamma_3 \mid t) \\ K(\gamma_3,\gamma_2 \mid t) & K(\gamma_3,\gamma_3 \mid t) \end{vmatrix} \Bigg] \exp\Big(-\sum_{i=1}^{3}\epsilon_{\gamma_i}t\Big) . \end{aligned} \tag{2.22'}$$

On the one-electron states $\{\gamma\}$, there is no restriction except that they lie above the Fermi energy. The expression of $I^{(n)}(\omega)$ may be obtained similarly.

Our remaining task is to sum $I^{(n)}(\omega)$ over n to derive $I(\omega)$. We have

$$I(\omega)=2\,\mathrm{Re}\int_0^\infty dt\, e^{i(\omega_+-\omega_{\mathrm{th}})t}\,|\Delta|^2\left[\sum_{\gamma(>)}|p(\gamma)|^2 e^{-i\epsilon_\gamma t}D(t)-\sum_{\gamma,\gamma'(>)}p^*(\gamma)p(\gamma')D(\gamma,\gamma'\,|\,t)e^{-i\epsilon_\gamma t-i\epsilon_{\gamma'}t}\right], \tag{2.24}$$

where

$$D(t)=1+\sum_{\gamma_1(>)}K(\gamma_1,\gamma_1\,|\,t)e^{-i\epsilon_{\gamma_1}t}+\frac{1}{2!}\sum_{\gamma_1,\gamma_2(>)}\det\begin{vmatrix}K(\gamma_1,\gamma_1\,|\,t) & K(\gamma_1,\gamma_2\,|\,t)\\ K(\gamma_2,\gamma_1\,|\,t) & K(\gamma_2,\gamma_2\,|\,t)\end{vmatrix}e^{-i(\epsilon_{\gamma_1}+\epsilon_{\gamma_2})t}+\cdots, \tag{2.25}$$

$$D(\gamma,\gamma'\,|\,t)=K(\gamma,\gamma'\,|\,t)+\sum_{\gamma_1(>)}\det\begin{vmatrix}K(\gamma,\gamma'\,|\,t) & K(\gamma,\gamma_1\,|\,t)\\ K(\gamma_1,\gamma'\,|\,t) & K(\gamma_1,\gamma_1\,|\,t)\end{vmatrix}e^{-i\epsilon_{\gamma_1}t}+\cdots. \tag{2.26}$$

It is to be noted that the factor $D(\gamma,\gamma'\,|\,t)$ depends explicitly on γ and γ', the excited one-electron states involved in $p(\gamma)$ and $p(\gamma')$, while $D(t)$ is a quantity determined independently of $p(\gamma)$. For example, when $\omega-\omega_{\mathrm{th}}$ is very large as in x-ray photoelectron spectroscopy (XPS), the factor $D(\gamma,\gamma'\,|\,t)$ will become vanishingly small because of the fact that ϵ_γ and $\epsilon_{\gamma'}$ are then much larger than the Fermi energy [see, e.g., the (γ,γ') dependence of K given by Eqs. (2.21) and (3.21)]. Thus the XPS incorporates only the factor $D(t)$.[16,17] This means that the readjustment of N electrons to a created core hole or the shake-off transition of Friedel[12] will be described by the factor $D(t)$.

To sum the series into a closed form, first observe that $D(t)$ is the Fredholm series[18] of

$$\det|\,\delta_{\gamma_1\gamma_2}+K(\gamma_1,\gamma_2\,|\,t)e^{-i\epsilon_{\gamma_2}t}\,|\,,$$

i.e.,

$$D(t)=\det|\,\underline{\mathbb{1}}+\underline{K}(t)e^{-i\underline{\epsilon}t}\,|\,, \tag{2.27}$$

with

$$[\underline{K}(t)e^{-i\underline{\epsilon}t}]_{\gamma_1\gamma_2}=K(\gamma_1,\gamma_2\,|\,t)e^{-i\epsilon_{\gamma_2}t}. \tag{2.28}$$

Next, consider the following integral equation for the quantity $q(\gamma\,|\,t)$:

$$q(\gamma\,|\,t)+\sum_{\gamma'(>)}K(\gamma,\gamma'\,|\,t)e^{-i\epsilon_{\gamma'}t}q(\gamma'\,|\,t)=p(\gamma). \tag{2.29}$$

Then, by the Fredholm formulas of integral equations,[18] it holds that

$$I(\omega)=2\,\mathrm{Re}\int_0^\infty dt\, e^{i(\omega_+-\omega_{\mathrm{th}})t}\,|\Delta|^2 D(t)I_0(t), \tag{2.30}$$

with

$$I_0(t)=\sum_{\gamma(>)}p^*(\gamma)e^{-i\epsilon_\gamma t}q(\gamma\,|\,t). \tag{2.31}$$

Equation (2.30) is the closed form of the spectrum we have been looking for. $D(t)$ is given by Eq. (2.27) and $q(\gamma\,|\,t)$ is the solution of Eq. (2.29). $K(\gamma,\gamma'\,|\,t)$ defined by Eq. (2.21) is the fundamental quantity for both $D(t)$ and $I_0(t)$.

Since Eq. (2.30) is proportional to $|\Delta|^2$, one may imagine that the quantity $D(t)$ has a factor of $|\Delta|^{-2}$ to give a finite absorption spectrum. In Appendix A, it is indeed shown that

$$D(t)=D(0)\exp\left[\int_0^t d\tau A(\tau)\right], \tag{2.32}$$

with

$$D(0)=|\Delta|^{-2}, \tag{2.33}$$

$$A(\tau)=\mathrm{Tr}\left[\left[\frac{d}{d\tau}\underline{K}(\tau)e^{-i\underline{\epsilon}\tau}\right][\underline{\mathbb{1}}+\underline{K}(\tau)e^{-i\underline{\epsilon}\tau}]^{-1}\right]. \tag{2.34}$$

The symbol Tr stands for the trace of the matrix to follow. Formally, the inverse matrix $[\underline{\mathbb{1}}+\underline{K}(t)e^{-i\underline{\epsilon}t}]^{-1}$ in Eq. (2.34) determines $q(\gamma\,|\,t)$. From Eq. (2.31)

$$I_0(t)=\sum_{\gamma,\gamma'(>)}p^*(\gamma)e^{-i\epsilon_\gamma t}\{[\underline{\mathbb{1}}+\underline{K}(t)e^{-i\underline{\epsilon}t}]^{-1}\}_{\gamma\gamma'}p(\gamma'). \tag{2.35}$$

In summary,

$$I(\omega)=2\,\mathrm{Re}\int_0^\infty dt\, e^{i(\omega_+-\omega_{\mathrm{th}})t}\exp\left[\int_0^t d\tau A(\tau)\right]I_0(t), \tag{2.36}$$

with $A(t)$ and $I_0(t)$ given by (2.34) and (2.35), respectively.

We end this section by comparing the identity of our formulas with the ones obtained by other authors. We find that $(t>0)$

$$\begin{aligned}\frac{D(t)}{D(0)}e^{-i\Delta E^0 t}&=-\mathcal{G}(-t)e^{-i\epsilon_{\mathrm{core}}t}\\&=iG(t)e^{-i\epsilon_{\mathrm{core}}t}\\&=\langle\Phi_I^0\,|\,e^{iH_I t}e^{-iH_F t}\,|\,\Phi_I^0\rangle,\end{aligned} \tag{2.37}$$

where ΔE^0 is the ground-state energy shift in Eq. (2.4), $\mathcal{G}(t)$ is the core-electron propagator used by ND (Ref. 3) and CN (Ref. 4), $G(t)$ is the core-hole propagator of Mahan,[11] and H_I and H_F are N-electron Hamiltonians of the initial and the final states, respectively. For the proof, see Appendix A, where the first equality is shown by transforming $D(t)$ into the form involving the expression of $\mathcal{G}(-t)$ given by CN.[4]

Similarly it is found that

$$I_0(t)=-L(-t), \tag{2.38}$$

where $L(t)$ is the open-line propagator defined by Eq. (29)

of CN.[4] For the equivalence of the Fourier transform of $I_0(t)$ to the quantity used by Mahan and co-workers, see Sec. V.

The approach based on the golden rule thus demonstrates correctly that the spectrum is made up of two disconnected contributions—the deep-hole and the open-line contributions. This fact is easy to understand in terms of the diagrammatic expansion, as shown by ND. In the CN paper, the disconnectedness is neatly demonstrated by rewriting the spectrum using a matrix whose rows and columns are labeled by the unperturbed one-electron states. The present method may be said to be a derivation based on the matrices represented in terms of the perturbed states. As compared with the ND and CN methods, the present derivation is rather complicated because of the careful treatment required to take an exact account of AOC in each overlap integral involving the final states $\Psi_f^{(n)}$. However, we have reached ultimately, say, Eq. (2.34), which is the general form of the linked-cluster expansion of $G(t)$, free from a special model of a core-hole potential.[17]

III. SOME IDENTITIES FOR A CONTACT CORE-HOLE POTENTIAL

The formulation given in Sec. II is now applied to the case of a contact core-hole potential:

$$V_{kk'}=-V\ . \tag{3.1}$$

We sometimes treat the variables, say, k and κ of φ_k and ψ_κ as discrete, although we take finally the continuum limit by tending Ω (the volume of the system) to infinity.

The secular equation for the energy ϵ_κ of the state ψ_κ is obtained when the form $\psi_\kappa=\sum a_{k\kappa}\varphi_k$ is put into $h_F\psi_\kappa=\epsilon_\kappa\psi_\kappa$:

$$1+V\sum_k \frac{1}{\epsilon_\kappa-\epsilon_k}=0\ , \tag{3.2}$$

with

$$a_{k\kappa}=\frac{c_\kappa}{\epsilon_\kappa-\epsilon_k}\ , \tag{3.3}$$

c_κ being the normalization constant. Let the state ψ_κ originate from φ_{k_0} with a perturbed energy

$$\epsilon_\kappa=\epsilon_{k_0}-\frac{\delta_\kappa}{\pi}\Delta\epsilon\ , \tag{3.4}$$

where $\Delta\epsilon$ is the spacing of the unperturbed levels and

$$\delta_\kappa=\delta(\epsilon_\kappa) \tag{3.5}$$

is the phase shift. Then in the limit $\Omega\to\infty$, Eq. (3.2) turns out to be (the symbol P denotes the principal part)

$$\pi VN_\kappa\cot\delta_\kappa=1+V\int_{\bar D}^{D}N_k d\epsilon_k \mathrm{P}\frac{1}{\epsilon_\kappa-\epsilon_k}\ , \tag{3.6}$$

where

$$N_k=N(\epsilon_k) \tag{3.7}$$

is the state density of the conduction band in question, which is assumed to lie in the region $\bar D<\epsilon<D$. In deriving Eq. (3.6), we have divided the summation over k involved in Eq. (3.2) into two parts—the sum over k with $\epsilon_k\simeq\epsilon_{k_0}$ and the rest. In the first sum we have made use of the partial-fraction expansion of $\cot\delta_\kappa$ and in the rest the summation has been replaced by the principal-value integral. The summation involved in

$$\psi_\kappa=\sum_k a_{k\kappa}\varphi_k\ ,$$

with $a_{k\kappa}$ given by Eq. (3.3), may be treated similarly in the continuum limit.

When ψ_κ is normalized so that

$$\langle\psi_\kappa\,|\,\psi_{\kappa'}\rangle=\frac{1}{N_\kappa}\delta(\epsilon_\kappa-\epsilon_{\kappa'})\ , \tag{3.8}$$

it follows that

$$a_{\kappa k}=a_{k\kappa}=\delta_{\kappa k}\cos\delta_k-\frac{\sin\delta_\kappa}{\pi N_\kappa}\mathrm{P}\frac{1}{\epsilon_\kappa-\epsilon_k}\ , \tag{3.9}$$

where

$$\delta_{\kappa k}=\frac{1}{N_\kappa}\delta(\epsilon_\kappa-\epsilon_k)\ . \tag{3.10}$$

Note that we have neglected the difference between the state densities of the initial and final states. The procedure is obviously valid as long as the band states k and κ are concerned [however, see Appendix B for the derivation of Eq. (3.12b)]. Note also that the first term of Eq. (3.9) is apparently different from the expression of $a_{\kappa k}$ with k treated as discrete (see, e.g., Ref. 13). However, we shall use $a_{\kappa k}$ always within the summand of Eq. (2.8), for example. It is straightforward to check that the form of $a_{\kappa k}$ with discrete k, when combined with the partial-fraction expansion to be used in the summation over k, amounts in the continuum limit to using Eq. (3.9) with Eq. (3.10).

Let us denote the inverse of the left-hand side of Eq. (3.2) as $X_0(z)$, with the complex variable z in place of ϵ_κ:

$$X_0(z)=\left[1+\sum_k\frac{V}{z-\epsilon_k}\right]^{-1}\ . \tag{3.11a}$$

Noting the location of poles and zeros in the complex z plane, we have an alternate form

$$X_0(z)=\frac{\prod_k(\epsilon_k-z)}{\prod_\kappa(\epsilon_\kappa-z)}\ . \tag{3.11b}$$

In the continuum limit, we have

$$X_0(z)=\left[1+V\int_{\bar D}^{D}N(\epsilon)d\epsilon\frac{1}{z-\epsilon}\right]^{-1}\ , \tag{3.12a}$$

$$X_0(z)=\exp\left[-\frac{1}{\pi}\int_{\bar D}^{D}\frac{\delta(\epsilon)}{z-\epsilon}\right]\ . \tag{3.12b}$$

For the derivation of Eq. (3.12b), see Appendix B. The phase shift $\delta(\epsilon)$ determined by Eq. (3.6) has a simple relationship with $X_0(\epsilon_+)$ defined by Eq. (3.12) with $z=\epsilon+i\delta$:

$$\frac{\sin\delta(\epsilon)}{|X_0(\epsilon_+)|}=\pi V N(\epsilon)\ ,$$
$$\frac{\cos\delta(\epsilon)}{|X_0(\epsilon_+)|}=1+V\int_{\bar{D}}^{D}N(\epsilon')d\epsilon'\mathrm{P}\frac{1}{\epsilon-\epsilon'}\ . \tag{3.13}$$

Now we divide $X_0(z)$ into two parts,

$$X_0(z)=X(z)\bar{X}(z)\ , \tag{3.14}$$

with

$$X(z)=\exp\left[-\frac{1}{\pi}\int_0^D d\epsilon\frac{\delta(\epsilon)}{z-\epsilon}\right]\ ,$$
$$\bar{X}(z)=\exp\left[-\frac{1}{\pi}\int_{\bar{D}}^0 d\epsilon\frac{\delta(\epsilon)}{z-\epsilon}\right]\ . \tag{3.15}$$

They are nothing but the dispersion integral used by Mahan and co-workers.[8-11] They are important factors determining $\Delta(\bar{\mu};\gamma)$, $p(\gamma)$, and finally $I(\omega)$.

With these preparations, let us now determine $\Delta(\bar{\mu};\gamma)$ for a contact core-hole potential. From Eq. (2.8), we must first determine the inverse matrix $\underline{A}^{-1}$. One can obtain it by solving $\underline{A}\,\underline{A}^{-1}=\underline{1}$, i.e.,

$$\sum_{m(<)}a_{\mu m}(\underline{A}^{-1})_{m\nu}=\delta_{\mu\nu}\ . \tag{3.16}$$

When transformed into an integral equation, the left-hand side has a typical form of a singular integral equation, with the kernel $a_{\mu m}$ having a factor $\mathrm{P}(\epsilon_\mu-\epsilon_m)^{-1}$ as defined in Eq. (3.9). Since the mathematics to solve it is familiar from the ND formulation, we only write the result, which is the unique solution of Eq. (3.16):

$$(\underline{A}^{-1})_{m\nu}=\frac{|\bar{X}_{\nu+}|}{|\bar{X}_{m+}|}\frac{1}{N_m}\left[(\cos\delta_m)\delta(\epsilon_m-\epsilon_\nu)+\frac{\sin\delta_m}{\pi}\mathrm{P}\frac{1}{\epsilon_m-\epsilon_\nu}\right]\ , \tag{3.17}$$

where

$$\bar{X}_{\nu+}=\bar{X}(\epsilon_{\nu+})\ ,$$
$$\bar{X}_{m+}=\bar{X}(\epsilon_{m+})\ . \tag{3.18}$$

Owing to the presence of the factor $\bar{X}_{m+}$, $(\underline{A}^{-1})_{m\nu}$ is singular when $\epsilon_m\to 0$ [for a constant phase shift $\delta(\epsilon)=\delta$, $|\bar{X}_{m+}|=|\epsilon_m/(\epsilon_m-\bar{D})|^{\delta/\pi}$; note that Eq. (3.17) is valid for an arbitrary $N(\epsilon)$ or $\delta(\epsilon)$]. It is interesting to note that in the context of the golden rule we must solve the singular integral equation in a very early stage of the formalism, while in the ND formalism we need solve it only once in a final stage.

From $\underline{A}^{-1}$, Eq. (2.8) yields $\Delta(\bar{\mu};\gamma)$. Treating the sum over $m\,(<)$ as an integral, we find

$$\frac{\Delta(\bar{\mu};\gamma)}{\Delta}=\frac{1}{\epsilon_\mu-\epsilon_\gamma}\frac{\sin\delta_\gamma}{\pi N_\gamma}\frac{|\bar{X}_{\mu+}|}{|\bar{X}_\gamma|}\ . \tag{3.19}$$

Note that $\epsilon_\mu<0$ and $\epsilon_\gamma>0$. Although the detailed derivation is omitted, the key relation involved in the derivation is the identity

$$\frac{\sin\delta_m}{|X_{m+}|}=\frac{1}{2i}\left[\frac{1}{X_{m-}}-\frac{1}{X_{m+}}\right]\ , \tag{3.20}$$

which converts the integral in the range $\bar{D}<\epsilon_m<0$ into a contour integral encircling the branch cut on the real axis, thereby enabling the integral over ϵ_m to be carried out exactly. Making use of Eqs. (3.13) and (3.14), we can rewrite Eq. (3.19) into the form which reveals the particle-hole symmetry:

$$\frac{\Delta(\bar{\mu};\gamma)}{\Delta}=\frac{V}{\epsilon_\mu-\epsilon_\gamma}|\bar{X}_{\mu+}|\,|X_{\gamma+}|\ . \tag{3.21}$$

From Eq. (3.19) or Eq. (3.21) we see that $\Delta(\bar{\mu};\gamma)$ is proportional to Δ, so that it vanishes by AOC in the limit $N\to\infty$.

In order to obtain $p(\gamma)$ from Eq. (2.16), we need the quantity $\sum[\Delta(\bar{\mu};\gamma)/\Delta]a_{\mu b}$. The sum over μ can be treated in the same way as the sum over m in the above. We have

$$\sum_{\mu(<)}\frac{\Delta(\bar{\mu};\gamma)}{\Delta}a_{\mu b}=-\mathrm{P}\left[\frac{1}{\epsilon_\gamma-\epsilon_b}\right]\left[\frac{\sin\delta_\gamma}{\pi N_\gamma}-\frac{|X_{\gamma+}|}{|X_{b+}|}\frac{\sin\delta_b}{\pi N_b}\right]\ . \tag{3.22}$$

The second term contains the phase shift $\delta_b=\delta(\epsilon_b)$. Now substituting Eq. (3.22) into Eq. (2.16), we find

$$p(\gamma)=|X_{\gamma+}|\,w\ . \tag{3.23}$$

The result, still exact for a contact potential, is remarkably simple.

Equation (3.19) or Eq. (3.21) with Eq. (3.15) yields the kernel $K(\gamma,\gamma'\,|\,t)$ introduced in Sec. II. The combination of $K(\gamma,\gamma'\,|\,t)$ given by Eq. (3.23) then determines $D(t)$ and $I_0(t)$ and hence the absorption spectrum $I(\omega)$.

IV. COMPARISON WITH THE RESULTS OF MAHAN AND CO-WORKERS

Before we proceed to obtain the spectrum for a contact potential, let us see the relationship between our results and those given by Mahan and co-workers, because the latter results apply to a contact or separable core-hole potential and are directly comparable with our results. As stated in Sec. I, Mahan and co-workers treated the core-hole propagator (Ref. 11) and the open-line propagator (Ref. 10). They decomposed them into the contributions of multipair excitations, trying to resum the series thereby obtained.

As regards the core-hole propagator, Mahan gives the expression of $P_n(t)$, the contribution from the n-pair excitation. By comparing Eq. (2.37) with Eq. (9) of Ref. 11, the following relation is established:

$$\frac{D(t)}{D(0)}=\sum_{n=0}^{\infty}P_n(t)\ . \tag{4.1}$$

His expression for $P_n(t)$ [Eq. (14) of Ref. 11] is just the nth-order term of the Fredholm series of $D(t)$ given by Eq. (2.27):

$$\frac{|\Delta|^2}{n!}\sum_{\{\gamma(>)\}}\det\begin{vmatrix}K_{11} & K_{12} & \cdots & K_{1n}\\ \vdots & \vdots & & \vdots\\ K_{n1} & K_{n2} & \cdots & K_{nn}\end{vmatrix}\times\exp\left[-\sum_{i=1}^{n}\epsilon_{\gamma_i}t\right]=P_n(t)\ , \tag{4.2}$$

with $K_{ij}=K(\gamma_i,\gamma_j\,|\,t)$. To verify the above relation, it suffices to change Mahan's notations $[(R/\pi)dk_\alpha \rightarrow N_\alpha d\epsilon_\alpha,\ e^{p(\epsilon)}\rightarrow X(\epsilon),\ e^{\Delta(\epsilon)}\rightarrow\bar{X}(\epsilon)]$ and use the identity (2.23) (trivially extended to a general $n\times n$ case) and the form (3.19) suitable for a contact potential. The equivalence as combined with the relation (4.1) shows that the series $P_n(t)$ can be indeed resummed, and our (2.27) represents the summed result, valid not only for a contact but also for an arbitrary core-hole potential.

Mahan attempted the linked-cluster expansion of $G(t)$ by writing

$$\sum_{n=0}P_n(t)=\exp\left[-\int_0^\infty du\,\rho(u)(1-e^{-iut})/u\right]\ ,$$
$$\rho(u)=\sum_{n=1}^{\infty}\rho^{(n)}(u)\ , \tag{4.3}$$

$\rho^{(n)}(u)$ being the contribution from the n electron-hole—pair excitation. Since $\rho^{(n)}(u)$ involves complicated correlations of $P_k(t)$ $(k\le n)$, Mahan did not succeed in obtaining $\rho^{(n)}(u)$ for general n nor in resumming $\rho^{(n)}(u)$ over n. Instead, he gives only $\rho^{(1)}(u)$ and $\rho^{(2)}(u)$ for a separable potential. The calculation of $\rho^{(2)}(u)$ was already rather cumbersome. The fact that we successfully resummed the series of $P_n(t)$ in a closed form implies that the resummation of $\rho^{(n)}(u)$ is possible. Indeed, comparing Eqs. (2.32) and (2.34) with Eqs. (4.1) and (4.3), we obtain

$$\rho(u)=-\frac{1}{2\pi i}\int_{-\infty}^{\infty}d\tau A(\tau)e^{iu\tau}$$
$$=\frac{u}{2\pi}\int_{-\infty}^{\infty}d\tau e^{iu\tau}\mathrm{Tr}\ln[\underline{\mathbb{1}}+\underline{K}(\tau)e^{-i\underline{\epsilon}\tau}]\ . \tag{4.4}$$

The result is again valid for any core-hole potential. Furthermore, the expression for $\rho^{(n)}(u)$ is obtained from Eq. (4.4) in a straightforward manner, with the correlation of $P_k(t)$ stated above being exactly taken into account. We see that Mahan's expression for $\rho^{(2)}(u)$ may be extended to $\rho^{(n)}(u)$ if we make the following replacement in Eq. (16) of his paper,

$$-\frac{1}{2\pi^4}\rightarrow(-1)^{n+1}\frac{1}{n\pi^{2n}}\ ,$$

and increase the number of the denominators and the times of integrations appropriately.

As regards the open-line propagator, the following relation is established between $R(\omega)$ given by Eq. (3.14) of Ref. 10 and our result;

$$R(\omega)=\sum_{n=0}R_n(\omega)$$
$$=\int_{-\infty}^{\infty}dt\,e^{i\omega t}I_0(t)/w^2\ . \tag{4.5}$$

To see it we need only expand $I_0(t)$ into the series expansion with respect to $K(\gamma,\gamma'\,|\,t)$ using Eq. (2.35). We have therefore succeeded in summing the series $R_n(\omega)$ over n into a closed form:

$$R(\omega)=\int_{-\infty}^{\infty}dt\,e^{i\omega t}\times\sum_{\gamma,\gamma'(>)}p(\gamma)e^{-i\epsilon_\gamma t}\{[\underline{\mathbb{1}}+\underline{K}(t)e^{-i\underline{\epsilon}t}]^{-1}\}_{\gamma\gamma'}\times p(\gamma')/w^2\ . \tag{4.6}$$

This relation, when applied near the threshold, gives us the critical amplitude defined by Mahan, which is one of the topics to be discussed in the next section. In summary, our formulation is complete in that it may be applied without any restriction to the form of the core-hole potential, reproduces in the case of a contact potential what has already been obtained, and gives a number of expressions that have not been derived so far.

V. THRESHOLD BEHAVIOR

We are now in a position to derive $A(t)$ and $I_0(t)$ for a contact core-hole potential. We are interested in the threshold region, i.e., $\omega\simeq\omega_{\mathrm{th}}$. Our purpose is twofold: to see that the result of ND is reproduced and the prefactor of the spectrum is obtained.

Substitution of Eq. (3.21) into Eq. (2.21) yields the kernel $K(\gamma,\gamma'\,|\,t)$ for a contact potential:

$$K(\gamma,\gamma'\,|\,t)=V^2\,|\,X_{\gamma+}\,|\,\,|\,X_{\gamma'+}\,|\sum_{\mu(<)}\frac{|\,\bar{X}_{\mu+}\,|^2e^{i\epsilon_\mu t}}{(\epsilon_\mu-\epsilon_\gamma)(\epsilon_\mu-\epsilon_{\gamma'})}\ .$$

The kernel thus contains two energy denominators. Because of this it appears that solving the integral equation (2.29) would be difficult. Here we describe our method of obtaining $A(t)$ and $I_0(t)$, where the energy denominators of $K(\gamma,\gamma'\,|\,t)$ are removed by the identity

$$-i\int_0^\infty d\tau e^{iE_+\tau}=\frac{1}{E_+}\ . \tag{5.1}$$

Since $\epsilon_\mu<0$ and $\epsilon_\gamma>0$ in K, the denominator $\epsilon_\mu-\epsilon_\gamma+i\delta$, for example, is the same as $\epsilon_\mu-\epsilon_\gamma$. In what follows, the energy variables in exponents should be understood to have a small imaginary part as in Eq. (5.1).

We start from

$$K(\gamma,\gamma'\,|\,t)=-N_0V^2\,|\,X_{\gamma+}\,|\,\,|\,X_{\gamma'+}\,|\times\int_0^\infty d\tau\int_0^\infty d\tau'\,e^{-i\epsilon_\gamma\tau-i\epsilon_{\gamma'}\tau'}\bar{\phi}(t+\tau+\tau')\ , \tag{5.2}$$

the double integral being due to the two energy denominators. Here

$$N_0\bar{\phi}(t)=\int_{\bar{D}}^{0}N_\mu d\epsilon_\mu\,|\,\bar{X}_{\mu+}\,|^2e^{i\epsilon_\mu t}\ , \tag{5.3}$$

N_0 being the state density at the Fermi level. Corresponding to Eq. (5.2) the integrals with respect to one-particle energies in $A(t)$ and $I_0(t)$ are transformed into those of the time variables. An elementary but somewhat lengthy calculation by iteration shows that Eqs. (2.34) and (2.35) become

$$A(t)=N_0^2V^2\int_0^\infty d\sigma\int_0^\infty d\tau\,\phi(t+\sigma)F(t+\sigma,t+\tau)\bar{\phi}(t+\tau)$$
$$=-\int_0^\infty d\sigma\int_0^\infty d\tau\left[\frac{d}{dt}\Lambda(t+\tau,t+\sigma)\right]\times F(t+\sigma,t+\tau) \tag{5.4}$$

and

$$I_0(t)=N_0w^2\int_0^\infty d\tau\,\phi(t+\tau)F(t+\tau,t+)\ . \tag{5.5}$$

Here $\phi(t)$ and Λ are defined by

$$N_0\phi(t)=\int_0^D N_\gamma d\epsilon_\gamma\,|X_{\gamma+}|^2e^{-i\epsilon_\gamma t}\ , \tag{5.6}$$

$$\Lambda(t+\tau,t+\sigma)=N_0^2V^2\int_0^\infty d\xi\,\bar{\phi}(t+\tau+\xi)\times\phi(t+\sigma+\xi)\ , \tag{5.7}$$

and F is the solution of the integral equation

$$F(t+\tau,t+\sigma)-\int_0^\infty d\rho\,\Lambda(t+\tau,t+\rho)\times F(t+\rho,t+\sigma)=\delta(\tau-\sigma) \tag{5.8a}$$

or

$$F(t+\tau,t+\sigma)-\int_0^\infty d\rho\,F(t+\tau,t+\rho)\times\Lambda(t+\rho,t+\sigma)=\delta(\tau-\sigma)\ . \tag{5.8b}$$

Once we know F by solving Eq. (5.8), Eqs. (5.4) and (5.5) as combined with Eq. (2.36) give the spectrum. Equations (5.4)—(5.8) are exact for a contact core-hole potential. It is important to realize the role of the argument $t+$ ($=t+\delta$ with a small but positive δ) involved in Eq. (5.5). The first iteration of Eq. (5.8a)

$$F^{(0)}(t+\tau,t+)=\delta(\tau-\delta)$$

leads precisely to

$$I_0^{(0)}(t)=N_0w^2\phi(t)\ .$$

If we incorrectly use t instead of $t+$, the first iteration yields $I_0^{(0)}(t)=\frac{1}{2}N_0w^2\phi(t)$, i.e., one half of the correct value, because

$$\int_0^t d\tau\,\delta(\tau)=\tfrac{1}{2}\ .$$

It is easily checked that the difference of the factor $\frac{1}{2}$ between the correct $I_0(t)$ defined by Eq. (5.5) and the incorrect $I_0(t)$ defined by Eq. (5.5) in which $t+$ is replaced incorrectly by t persists to all orders of the iteration of Eq. (5.8a).

Now in order to obtain the threshold behavior, the long-time behavior of $\phi(t)$ and $\bar{\phi}(t)$ is necessary. In this situation some simplifications that allow an analytical treatment may be employed. For example (see Appendix C),

$$\phi(t)=(it)^{-1+\alpha}\Gamma(1-\alpha)\,|X(0)|^2\ ,$$
$$\bar{\phi}(t)=(it)^{-1-\alpha}\Gamma(1+\alpha)\,|\bar{X}(0)|^2\ , \tag{5.9}$$

with

$$|X(0)|^2=D^\alpha\exp\left[\frac{2}{\pi}\int_0^D d\epsilon\frac{\delta(\epsilon)-\delta_0}{\epsilon}\right]\ ,$$
$$|\bar{X}(0)|^2=|\bar{D}|^{-\alpha}\exp\left[\frac{2}{\pi}\int_{\bar{D}}^0 d\epsilon\frac{\delta(\epsilon)-\delta_0}{\epsilon}\right]\ , \tag{5.10}$$

where

$$\delta_0=\delta(0) \tag{5.11a}$$

is the phase shift at the Fermi energy and

$$\alpha=2\delta_0/\pi\ . \tag{5.11b}$$

With the change of variables

$$t+\tau=t/x\ ,$$

etc., and the definition of the new function

$$\bar{F}(x,y)=t\frac{y^{\alpha-1}}{x^{\alpha+1}}F\left[\frac{t}{x},\frac{t}{y}\right]\ , \tag{5.12}$$

it follows that (Appendix C)

$$tA(t)=-\frac{\delta_0\tan\delta_0}{\pi^2}\int_0^1\int_0^1\bar{F}(x,y)dx\,dy\ , \tag{5.13}$$

$$I_0(t)=N_0w^2\phi(t)\int_0^1 dx\,\bar{F}(x,1-)\ , \tag{5.14}$$

where

$$\bar{F}(x,y)+\frac{\tan\delta_0}{2\pi}\int_0^1 dz\frac{1-(z/x)^\alpha}{x-z}\bar{F}(z,y)=\delta(x-y)\ . \tag{5.15}$$

Note the argument $1-$ ($=1-\delta$) in Eq. (5.14) in accordance with Eq. (5.5).

Before solving Eq. (5.15), we consider briefly its iterative solution. We are concerned with it because, as discussed by Mahan,[11] the first-order term of $tA(t)$ in the iteration is $-\delta_0\tan\delta_0/\pi^2$, while the exact result of ND is $-(\delta_0/\pi)^2$. We would like to know the type of series for $A(t)$ the iterative solution of Eq. (5.15) will give rise to.

The first iteration is now trivial, since $\bar{F}^{(0)}(x,y)=\delta(x-y)$. From Eq. (5.13), we have

$$tA^{(0)}(t)=-\delta_0\tan\delta_0/\pi^2\ . \tag{5.16a}$$

This is the result of Mahan. In the second iteration, calculation shows

$$tA^{(1)}(t)=\frac{1}{4}\left[\frac{\tan\delta_0}{\pi}\right]^2[1-2\delta_0\cot(2\delta_0)]\ . \tag{5.16b}$$

It is impossible to hypothesize about the general form of $A^{(n)}(t)$, based on Eqs. (5.16a) and (5.16b). When, however, the trigonometric functions involved are expanded with respect to δ_0, one sees that

$$tA^{(0)}(t)=-\left[\frac{\delta_0}{\pi}\right]^2(1+\tfrac{1}{3}\delta_0^2+\cdots)\ ,$$
$$t[A^{(0)}(t)+A^{(1)}(t)]=-\left[\frac{\delta_0}{\pi}\right]^2(1-\tfrac{8}{45}\delta_0^4+\cdots)\ .$$

Now the structure of the iteration is evident: The next

iteration will bring forth $A^{(2)}(t)$, whose leading term, when Taylor-series expanded with respect to δ_0, is

$$tA^{(2)}(t)=-\left[\frac{\delta_0}{\pi}\right]^2\frac{8}{45}\delta_0^4+\cdots\ , \tag{5.16c}$$

so that

$$t\sum_{n=0}^{2}A^{(n)}(t)=-\left[\frac{\delta_0}{\pi}\right]^2[1+O(\delta_0^6)]\ .$$

Actually, the exact result for $A^{(2)}(t)$ is obtained as

$$tA^{(2)}=-\left[\frac{\delta_0\tan\delta_0}{\pi^2}\right]^3\left[\frac{\pi^2}{2\delta_0}\right]^2\left[\frac{2}{3}-\frac{\cot 2\delta_0}{\delta_0}+2\cot^2(2\delta_0)\right]\ . \tag{5.16d}$$

It is straightforward to check Eq. (5.16c). From this result, we may convince ourselves that the ND solution is correct, in spite of the fact that a few lower-order terms in the golden-rule series obscure the validity of the ND solution.

So far we have considered $A(t)$, the exponent of the core-hole propagator. As for the open-line propagator, Eq. (5.14) exhibits already the exact power-law behavior through the factor $\phi(t)$, i.e., $I_0(t)\propto t^{-1+2\delta_0/\pi}$ from Eq. (5.9). The solution of the integral equation thus determines the prefactor of the power-law behavior involved in $I_0(t)$.

Our remaining task is to solve Eq. (5.15) in order to see that the iteration, in fact, converges to the ND result for $A(t)$ and to derive an explicit formula of the prefactor of $I_0(t)$. Now let us return to Eqs. (5.13)—(5.15). By means of the change of variables, the integral equation (5.15) may be transformed into a form solvable by the method of Wiener and Hopf.[19] The details are given in Appendix D. The result is

$$A(t)=-(\delta_0/\pi)^2/t\ , \tag{5.17}$$

$$I_0(t)=N_0A_0w^2\Gamma(1-\delta_0/\pi)^2(iDt)^{2\delta_0/\pi}/(it)\ , \tag{5.18}$$

with

$$A_0=\exp\left[\frac{2}{\pi}\int_0^D d\epsilon\frac{\delta(\epsilon)-\delta_0}{\epsilon}\right]\ . \tag{5.19}$$

Combining Eqs. (5.17) and (5.18) with Eq. (2.36), the spectrum near the threshold is obtained as

$$I(\omega)\propto 1/(\omega-\omega_{\rm th})^{2\delta_0/\pi-(\delta_0/\pi)^2}\ . \tag{5.20}$$

Thus the exponent of the ND solution is reproduced precisely in the golden-rule approach without recourse to the coupling-constant integration.[3,4]

In terms of the spectrum of $I_0(\omega)$, Mahan and coworkers defined the critical amplitude Ξ [$A(0)$ in their notation[10]]

$$I_0(\omega)=2\pi N_0w^2\Xi\left[\frac{D}{\omega-\omega_{\rm th}}\right]^{2\delta_0/\pi}\ . \tag{5.21}$$

From Eq. (5.18) we have

$$I_0(\omega)=2\pi N_0w^2A_0\frac{\Gamma(1-\delta_0/\pi)^2}{\Gamma(1-2\delta_0/\pi)}\left[\frac{D}{\omega-\omega_{\rm th}}\right]^{2\delta_0/\pi}\ . \tag{5.22}$$

Thus

$$\Xi=A_0\frac{\Gamma(1-\delta_0/\pi)^2}{\Gamma(1-2\delta_0/\pi)}\ , \tag{5.23}$$

i.e., we have an analytic expression for the critical amplitude.

Let us compare our Ξ with the exact numerical result obtained by Mahan. For a step-function density of states with $D=|\bar{D}|=-\frac{1}{2}$ and $\delta_0=\pi/5$, Mahan and coworkers obtained[10]

$$\Xi=0.910A_0\ . \tag{5.24}$$

When the values $\Gamma(1-\delta_0/\pi)=\Gamma(0.8)$ and $\Gamma(1-2\delta_0/\pi)=\Gamma(0.6)$ are inserted into Eq. (5.23), our formula yields

$$\Xi=0.9102A_0\ . \tag{5.25}$$

The agreement is thus quite satisfactory, meaning convincingly the exactness of our expression (5.23) of the prefactor. Note that because of the factor A_0, which is determined by the phase shifts over the whole conduction band above the Fermi energy, the prefactor is not determined solely by the phase shift at the Fermi level.

Also interesting is the comparison of our prefactor with the result obtained by Oliveira and Wilkins through the numerical renormalization-group scheme.[20] Since their calculation corresponds to the prefactor of $I(\omega)$, not of $I_0(\omega)$, we must take into account the effect of $A(t)$. To obtain the core-hole propagator, Eq. (2.32) shows that we must integrate $A(\tau)$ in the range $0<\tau<t$. If the long-time behavior of $A(\tau)$ shown in (5.17) is assumed to be correct down to $t=0$, we find

$$\Xi=A_0\frac{\Gamma(1-\delta_0/\pi)^2}{\Gamma(1-2\delta_0/\pi+(\delta_0/\pi)^2)}\ . \tag{5.26}$$

Using $A_0=0.866$ obtained by Mahan, we find $\Xi=0.836$, to be compared with the result 0.82 by Oliveira and Wilkins. The agreement is again satisfactory. Note, however, that the prefactor given by Eq. (5.26) is based on the long-time behavior (5.17) of $A(t)$. We cannot say definitely whether or not the short-time behavior of $A(t)$ can be neglected in the prefactor. Unfortunately, therefore, we may not attribute the cause of the discrepancy between 0.836 and 0.82 to the numerical analysis, which is reported to have an error of a few percent.

VI. SUMMARY

The most elementary way of calculating the optical absorption cross section is perhaps to use the Fermi golden rule. In this paper we have followed this approach in deriving the soft-x-ray absorption cross section. Our method is thus composed of specifying final states of the optical transition, calculating the transition probability for electrons in the ground state to jump to them, and finally

summing the probabilities over all possible final states.

In our formalism we have focused our attention on showing how the factor associated with the orthogonality theorem of Anderson[13] arises in the expression of each transition probability and how it gets canceled in the course of summation over the various final states. It is this cancellation that leads to an absorption cross section that remains finite even in the limit of N (number of electrons) $\rightarrow \infty$.

The expression of the cross section we have arrived at is compactly written in terms of an integral kernel K. We have given the expression of K [Eq. (2.21), valid for an arbitrary core-hole potential]. Consequently, the final form of the closed-loop and the open-line contributions we have obtained are applicable irrespective of the form of the core-hole potential. We would like to emphasize the exactness and generality of our formulas.

For the special model of a contact core-hole potential, a detailed comparison is made between the present results and those of Mahan and co-workers,[10,11] which are the most extensive contributions related to ours in the literature. It is found that our formulas have a number of improvements over the formulas of Mahan and co-workers. The extension achieved in the expression of the core-hole propagator was especially emphasized.

As for the integral equation with the kernel K, we have shown that the exact power-law behavior in the near-edge region was correctly reproduced and the prefactor of the power law could be obtained analytically. Our formula for the prefactor shows good agreement with the numerical values known already.[10,20]

Finally, one brief remark is in order on the work of other authors. Except for the work of Mahan and co-workers discussed in this paper, there recently have been a number of developments in the analytical aspect of the x-ray absorption problem, and those by Hänsch and Ekardt[21] and Hänsch and Minnhagen[22] should be mentioned in particular. The iterative step developed by these authors is not directly connected with our iteration scheme in terms of K. Nevertheless, the rapid convergence of their scheme is remarkable in the near-edge region of the closed-loop contribution.[22] From a practical point of view, therefore, their formulas have perhaps some advantages over those obtained in the present paper or achieved by Mahan and co-workers by the golden-rule approach.

APPENDIX A: TRANSFORMATION OF $D(t)$

We prove Eqs. (2.32)—(2.34) and (2.37) by rewriting $D(t)$ defined by Eq. (2.27) into a different form. For an $N\times M$ matrix $\underline{X}$ and an $M\times N$ matrix $\underline{Y}$, there is an identity

$$\det|\underline{1}+\underline{X}\,\underline{Y}|=\det|\underline{1}+\underline{Y}\,\underline{X}| \ . \tag{A1}$$

The left-hand side involves an $N\times N$ matrix, while the right-hand side involves an $M\times M$ matrix. The equality will be shown by expanding both sides into the Fredholm series. When the definition (2.21) of $K(\gamma_1,\gamma_2\,|\,t)$ is substituted, Eq. (2.27) becomes

$$D(t)=\det\left|\delta_{\gamma_1\gamma_2}+\sum_{\mu(<)}\frac{\Delta(\bar{\mu};\gamma_1)}{\Delta}e^{i\epsilon_\mu t}\frac{\Delta(\bar{\mu};\gamma_2)^*}{\Delta^*}e^{-i\epsilon_{\gamma_2}t}\right| . \tag{A2}$$

By (A1)

$$D(t)=\det\left|\delta_{\mu_1\mu_2}+\sum_{\gamma(>)}\frac{\Delta(\bar{\mu}_1;\gamma)^*}{\Delta^*}e^{-i\epsilon_\gamma t}\frac{\Delta(\bar{\mu}_2;\gamma)}{\Delta}e^{i\epsilon_{\mu_2}t}\right| . \tag{A3}$$

The matrix with respect to the unoccupied states γ_1,γ_2 is converted into the matrix with respect to the states μ_1,μ_2 below the Fermi level. The sum over $\gamma(>)$ in (A3) is transformed into the sum over all the states above and below the Fermi level:

$$\sum_{\gamma(>)}\frac{\Delta(\mu_1;\gamma)^*}{\Delta^*}e^{-i\epsilon_\gamma t}\frac{\Delta(\bar{\mu}_2;\gamma)}{\Delta}e^{i\epsilon_{\mu_2}t}$$
$$=\sum_{\gamma(\text{all})}\frac{\Delta(\bar{\mu}_1;\gamma)^*}{\Delta^*}e^{-i\epsilon_\gamma t}\frac{\Delta(\bar{\mu}_2;\gamma)}{\Delta}e^{i\epsilon_{\mu_2}t}-\delta_{\mu_1\mu_2} . \tag{A4}$$

This relation results from

$$\Delta(\bar{\mu};\gamma)=\delta_{\gamma\mu} \tag{A5}$$

for the state γ *below* the Fermi level.

Substituting (A4) into (A3), we find

$$D(t)=\det\left|\sum_{\gamma(\text{all})}\frac{\Delta(\bar{\mu}_1;\gamma)^*}{\Delta^*}e^{-i\epsilon_\gamma t}\frac{\Delta(\bar{\mu}_2;\gamma)}{\Delta}e^{i\epsilon_{\mu_2}t}\right| . \tag{A6}$$

Now substituting Eq. (2.8) into (A6) and arranging the result using matrix notation, we find

$$D(t)=[\det(\underline{A}^{-1})]^*\det\underline{B}(t)\det(\underline{A}^{-1})\prod_{\mu(<)}e^{i\epsilon_\mu t} , \tag{A7}$$

with an $N\times N$ matrix $\underline{B}(t)$ defined by

$$[\underline{B}(t)]_{k_1k_2}=\sum_{\gamma(\text{all})}a^*_{\gamma k_1}e^{-i\epsilon_\gamma t}a_{\gamma k_2} . \tag{A8}$$

Note that the unperturbed states k_1 and k_2 below the Fermi level label the row and column of $\underline{B}(t)$, and by the completeness of $\{\psi_\gamma\}$, it holds that $[\underline{B}(0)]_{k_1k_2}=\delta_{k_1k_2}$. By definition [Eqs. (2.4) and (2.5)]

$$\det(\underline{A}^{-1})=1/\Delta , \tag{A9}$$

$$\prod_{\mu(<)}e^{i\epsilon_\mu t}=e^{i\Delta E^0 t}\prod_{m(<)}e^{i\epsilon_m t} , \tag{A10}$$

where ΔE^0 is the ground-state energy shift and ϵ_m the unperturbed one-particle energy.

From (A7) and (A9) we obtain Eq. (2.33):

$$D(0)=|\det(\underline{A}^{-1})|^2=1/|\Delta|^2 . \tag{A11}$$

When N factors $e^{i\epsilon_m t}$ ($m=1,2,\ldots,N$) are put inside the matrix $\underline{B}(t)$, it follows that

$$D(t)=D(0)\det|\underline{B}(t)e^{i\underline{\epsilon}t}|\,e^{i\Delta E^0 t} . \tag{A12}$$

The determinant involved in the right-hand side is exactly the determinant used by CN. Thus Eq. (2.37) is proved.

The remaining equation (2.32) with Eq. (2.34) is obtained by transforming Eq. (2.27) into

$$D(t)=\exp[\ln\det|\underline{1}+\underline{K}(t)e^{-i\underline{\epsilon}t}|] =\exp\{\mathrm{Tr}\ \ln[\underline{1}+\underline{K}(t)e^{-i\underline{\epsilon}t}]\}\ . \tag{A13}$$

The identity

$$f(t)=f(0)+\int_0^t d\tau\frac{df(\tau)}{d\tau}$$

then leads to the exponent given by Eq. (2.34).

APPENDIX B: DERIVATION OF EQ. (3.12b)

We derive Eq. (3.12b) from Eq. (3.11b). Let $N_I(\epsilon)$ and $N_F(\epsilon)$ be the state densities of the initial and the final states, respectively. From Eq. (3.11b), it holds that

$$\frac{d}{dz}\ln X_0(z)=\sum_\kappa\frac{1}{\epsilon_\kappa-z}-\sum_k\frac{1}{\epsilon_k-z}\ . \tag{B1}$$

In the continuum limit

$$\frac{d}{dz}\ln X_0(z)=\int_{\bar D}^{D}d\epsilon\frac{N_F(\epsilon)-N_I(\epsilon)}{\epsilon-z}\ . \tag{B2}$$

By means of the well-known relation

$$N_F(\epsilon)=N_I(\epsilon)+\delta'(\epsilon)/\pi \tag{B3}$$

and the integration by parts, we obtain

$$\frac{d}{dz}\ln X_0(z)=-\frac{d}{dz}\left[\frac{1}{\pi}\int_{\bar D}^{D}d\epsilon\frac{\delta(\epsilon)}{z-\epsilon}\right], \tag{B4}$$

from which Eq. (3.12b) follows.

APPENDIX C: SOME FORMULAS IN THE LIMIT $t\to\infty$

In this appendix we describe the approximations that lead to Eqs. (5.13)–(5.15), used for the spectrum near the threshold. From the definitions (5.3) and (5.6), the long-time behavior ($t\to\infty$) of $\phi(t)$ and $\bar\phi(t)$ can be determined by $X_{\gamma+}$ and $X_{\mu+}$ with $\epsilon_\gamma,\epsilon_\mu\simeq 0$. In this limit the dispersion integral involved in $X_{\gamma+}$ [Eq. (3.15)] is transformed as follows:

$$\mathrm{P}\int_0^D\frac{\delta(\epsilon)}{\epsilon_\gamma-\epsilon}d\epsilon=\delta_0\mathrm{P}\int_0^D\frac{d\epsilon}{\epsilon_\gamma-\epsilon}+\mathrm{P}\int_0^D\frac{\delta(\epsilon)-\delta_0}{\epsilon_\gamma-\epsilon}d\epsilon \simeq\delta_0\ln\epsilon_\gamma-\left[\delta_0\ln D+\int_0^D\frac{\delta(\epsilon)-\delta_0}{\epsilon}d\epsilon\right]. \tag{C1}$$

In the same way,

$$\mathrm{P}\int_{\bar D}^0\frac{\delta(\epsilon)}{\epsilon_\mu-\epsilon}d\epsilon\simeq-\delta_0\ln|\epsilon_\mu| -\left[-\delta_0\ln|\bar D|+\int_{\bar D}^0\frac{\delta(\epsilon)-\delta_0}{\epsilon}d\epsilon\right]. \tag{C2}$$

Thus

$$|X_{\gamma+}|^2=\epsilon_\gamma^{-\alpha}|X(0)|^2\ , \qquad |\bar X_{\mu+}|^2=|\epsilon_\mu|^\alpha|\bar X(0)|^2\ , \tag{C3}$$

with $\alpha=2\delta_0/\pi$ and $|X(0)|^2$ and $|\bar X(0)|^2$ defined by Eq. (5.10).

In the integrals over ϵ_μ [in Eq. (5.3)] and ϵ_γ [Eq. (5.6)] in deriving $\bar\phi(t)$ and $\phi(t)$, we observe that the limits of integration $\bar D$ and D can be replaced by $-\infty$ and $+\infty$, respectively, when Dt, $|\bar D|t\gg 1$ and that the integrals are well-behaved for $|\alpha|<1$. The first condition for t is satisfied in the long-time behavior, and the second condition for the phase shift is usually satisfied in the absence of bound states. Equation (C3) leads to Eq. (5.9).

The definition (5.7) of Λ as combined with Eq. (5.9) gives

$$\Lambda(t+\tau,t+\sigma) =[N_0V|X(0)|\ |\bar X(0)|]^2\Gamma(1-\alpha)\Gamma(1+\alpha) \times\int_0^\infty d\xi[i(t+\tau+\xi)]^{-1-\alpha} \times[i(t+\sigma+\xi)]^{-1+\alpha}\ . \tag{C4}$$

The integral over ξ is evaluated by transforming the integral variable from ξ to

$$\zeta=\frac{t+\tau+\xi}{t+\sigma+\xi}\ .$$

The result is further simplified using

$$|X(0)|^2|\bar X(0)|^2=|X_0(\epsilon=0)|^2\ , \tag{C5}$$

$$\Gamma(1-\alpha)\Gamma(1+\alpha)=\pi\alpha/\sin(\pi\alpha)\ , \tag{C6}$$

and the identity (3.13). Finally

$$\Lambda(t+\tau,t+\sigma)=\frac{\tan\delta_0}{2\pi}\frac{1}{\tau-\sigma}\left[\left[\frac{t+\sigma}{t+\tau}\right]^\alpha-1\right]. \tag{C7}$$

With this expression of Λ and the new function $\bar F$ defined by Eq. (5.12), transforming Eqs. (5.4), (5.5), and (5.8a) into Eqs. (5.13)–(5.15) is straightforward.

APPENDIX D: SOLUTIONS OF $A(t)$ AND $I_0(t)$ BY THE METHOD OF WIENER AND HOPF

In terms of the new variables u,v,w defined by

$$x=e^{-u},\quad y=e^{-v},\quad z=e^{-w}\ , \tag{D1}$$

Eq. (5.15) becomes ($\alpha=2\delta_0/\pi$)

$$\bar F(u,v)+\frac{\tan\delta_0}{2\pi}\int_0^\infty dw\frac{1-e^{\alpha(u-w)}}{e^{-(u-w)}-1}\bar F(w,v)=\delta(u-v)e^v\ . \tag{D2}$$

Here we have used the simplified notations $\bar F(u,v)$ in place of $\bar F(e^{-u},e^{-v})$. Although we need consider only the region $u,v>0$ Eq. (D2) automatically defines $\bar F(u,v)$ for $u<0$. In terms of the two auxiliary functions defined by

$$F_+(u,v)=\begin{cases}0, & u>0\\ \bar{F}(u,v), & u<0\end{cases}$$
$$F_-(u,v)=\begin{cases}-\bar{F}(u,v), & u>0\\ 0, & u<0\end{cases} \tag{D3}$$

Eq. (D2) is reexpressed as

$$F_+(u,v)-F_-(u,v)-\frac{\tan\delta_0}{2\pi}\int_{-\infty}^{\infty}dw\frac{1-e^{\alpha(u-w)}}{e^{-(u-w)}-1}F_-(w,v)=\delta(u-v)e^{v}\ . \tag{D4}$$

We solve (D4) using the Laplace transform. Let

$$\int_{-\infty}^{\infty}du\,e^{-su}F_{\pm}(u,v)=\Phi^{\pm}(s)_v\ . \tag{D5}$$

The Laplace transform of the kernel is found to be

$$\int_{-\infty}^{\infty}du\,e^{-su}\frac{1-e^{\alpha u}}{e^{-u}-1}=\pi\{\cot[(s-\alpha)\pi]-\cot(s\pi)\}\ . \tag{D6}$$

Draw a straight line l in the complex s plane parallel to the imaginary axis in the region $0<\alpha<\mathrm{Re}s<1$ ($0<\mathrm{Re}s<1+\alpha$ for $-1<\alpha<0$). By considering the analyticity, one sees that $\Phi^+(s)_v$ [$\Phi^-(s)_v$] is regular on the left-hand (right-hand) half plane of the line l. From (D5) and (D6), Eq. (D4) reduces to

$$\Phi^+(s)_v-U^{-1}(s)V^{-1}(s)\Phi^-(s)_v=e^{-(s-1)v}\ , \tag{D7}$$

with

$$U(s)=\frac{\Gamma(s-\alpha/2)^2}{\Gamma(s)\Gamma(s-\alpha)}\ ,$$
$$V(s)=\frac{\Gamma(1-s+\alpha/2)^2}{\Gamma(1-s)\Gamma(1-s+\alpha)}\ . \tag{D8}$$

We have made use of (C6). Note that $U(S)$ [$V(S)$] is regular and free from zeros on the right- (left-) hand side of l. Equation (D7) determines a gap along l between $\Phi^+(s)_v$ and $\Phi^-(s)_v$ when s approaches l from the left- and right-hand sides, respectively. One can solve Eq. (D7) in terms of the Hilbert transform, as in the ND formulation.

In the homogeneous equation of (D7)

$$\varphi^+(s)=[V(s)]^{-1}\ ,$$
$$\varphi^-(s)=U(s) \tag{D9}$$

are the solutions that are in accord with the regularity requirement. In terms of φ^+ and φ^-, Eq. (D7) becomes

$$\frac{\Phi^+(s)_v}{\varphi^+(s)}-\frac{\Phi^-(s)_v}{\varphi^-(s)}=\frac{e^{-(s-1)v}}{\varphi^+(s)}\ . \tag{D10}$$

The solution of (D10) that vanishes at $s=\infty$ is

$$\Phi^{\pm}(s)_v=\frac{\varphi^{\pm}(s)}{2\pi i}\int_l d\tau\frac{e^{-(\tau-1)v}}{\varphi^+(\tau)(\tau-s)}\ . \tag{D11}$$

Now the right-hand sides of Eqs. (5.13) and (5.14) turn out to be

$$\int_0^1\int_0^1 dx\,dy\,\bar{F}(x,y)=-\int_0^{\infty}dv[\Phi^-(s=1)]_v e^{-v}\ , \tag{D12}$$

$$\int_0^1 dx\,\bar{F}(x,1-)=-[\Phi^-(s=1)]_{v=0+}\ . \tag{D13}$$

To evaluate (D12), first integrate over v and next carry out the τ integral of (D11) by closing the contour on the left-hand half of the complex τ plane. Calculation of (D13) is rather delicate. The subscript $v=0+$, which originates from the variable $t+$ in Eq. (5.5), means that in evaluating (D13) the contour used in (D11) should be closed on the right-hand half of the τ plane where $\varphi^+(\tau)^{-1}$ has an infinite number of poles. Instead, put $v=0$ in place of $v=0+$. Then we can close the contour as we wish. Close it in the left-hand half and calculate the contribution of the integral along the added arc of the closed contour. In this way we get $[\Phi^-(s=1)]_{v=0}$. Now the difference between $[\Phi^-(s=1)]_{v=0+}$ and $[\Phi^-(s=1)]_{v=0}$ is a factor of $\frac{1}{2}$ [see the comment given below Eq. (5.8)]. In this way we find

$$\int_0^1\int_0^1\bar{F}(xy,)dx\,dy=\frac{\varphi^-(1)}{\varphi^+(0)}=\delta_0\cot\delta_0\ , \tag{D14}$$

$$\int_0^1\bar{F}(x,1+)dx=\varphi^-(1)=\frac{\Gamma(1-\delta_0/\pi)^2}{\Gamma(1-2\delta_0/\pi)}\ . \tag{D15}$$

Combining these results with Eqs. (5.13) and (5.14), we arrive at Eqs. (5.17) and (5.18).

Although (D14) and (D15) are derived under the assumption that $-1<\alpha<1$ ($-\pi/2<\delta_0<\pi/2$ in terms of the phase shift), the range of α where (D14) and (D15) still apply may be shown to be extended to $-2<\alpha<2$. In the presence of a bound state in the final state (planned to be treated in a separate paper), this property of the solution of the integral equation (5.8) plays an important role in deducing the correct power-law behavior.[4]

[1] G. D. Mahan, Phys. Rev. 163, 612 (1967).
[2] B. Roulet, J. Gavoret, and P. Nozières, Phys. Rev. 178, 1072 (1969); P. Nozières, J. Gavoret, and B. Roulet, *ibid.* 178, 1084 (1969).
[3] P. Nozières and C. T. De Dominicis, Phys. Rev. 178, 1097 (1969).
[4] M. Combescot and P. Nozières, J. Phys. (Paris) 32, 913 (1971).
[5] C. A. Swarts, J. D. Dow, and C. P. Flynn, Phys. Rev. Lett. 43, 158 (1979).
[6] J. D. Dow and C. P. Flynn, J. Phys. C 13, 1341 (1980).
[7] L. C. Davis and L. A. Feldkamp. Phys. Rev. B 23, 4269 (1981).
[8] W. J. Pardee and G. D. Mahan, Phys. Lett. 45A, 117 (1973).
[9] G. D. Mahan, Phys. Rev. B 21, 1421 (1980).
[10] D. R. Penn, S. M. Girvin, and G. D. Mahan, Phys. Rev. B 24, 6971 (1981).
[11] G. D. Mahan, Phys. Rev. B 25, 5021 (1982).
[12] J. Friedel, Comments Solid State Phys. 2, 21 (1969).
[13] P. W. Anderson, Phys. Rev. Lett. 18, 1049 (1967).

[14]F. G. Fumi, Philos. Mag. 46, 1007 (1955).
[15]A. C. Aitken, *Determinants and Matrices* (Interscience, New York, 1964), p. 97.
[16]S. Doniach and M. Šunjić, J. Phys. C 3, 285 (1970).
[17]G. D. Mahan, *Many-Particle Physics* (Plenum, New York, 1981), p. 771.
[18]R. Courant and D. Hilbert, *Methods of Mathematical Physics* (Interscience, New York, 1966), Vol. 1, p. 112.
[19]V. I. Smirnov, *A Course of Higher Mathematics* (Addison-Wesley, Reading, Mass., 1965), Vol. IV, p. 1.
[20]L. N. Oliveira and J. W. Wilkins, Phys. Rev. B 24, 4863 (1981).
[21]W. Hänsch and W. Ekardt, Phys. Rev. B 24, 5497 (1981).
[22]W. Hänsch and P. Minnhagen, Phys. Rev. B 26, 2772 (1982).