Golden-rule approach to the soft-x-ray-absorption problem. III. The temperature dependence

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(Received 12 June 1984)

The exact formulation of the soft-x-ray-absorption problem of previous work [Phys. Rev. B **28**, 6833 (1983)] is generalized to the case of finite temperatures. By giving a closed-form expression of the response function in terms of the overlap integrals between the initial and final electron states, we demonstrate that the exactness can be pursued quite generally. The general formula, when applied to the case of a contact core-hole potential, leads to expressions of the dispersion integral and the frequency shift, both modified from their $T=0$ forms by the temperature effect. In the near-edge region, an analytical form of the response function can be derived, which reproduces precisely the time and temperature dependences of that of Yuval and Anderson [Phys. Rev. B **1**, 1522 (1970)] and, in addition, provides an exact expression for the prefactor of the open-line contribution of the spectrum.

I. INTRODUCTION

The method of Nozières and De Dominicis[1] (cited as ND) of solving the soft-x-ray-absorption problem[2,3] is characterized by their time-space treatment of the Dyson equation. In a series of papers[4,5] [referred to as OT (Ohtaka and Tanabe) and TO (Tanabe and Ohtaka)], we developed for the same problem formulation in the frequency space, using the Fermi golden rule for the absorption cross section. Our approach is composed of calculating the matrix elements of the dipole moment operator between the initial unperturbed ground state and the final states perturbed by a core-hole potential, and then summing the transition probabilities over all possible final states. We showed how the orthogonality catastrophe of Anderson[6]—zero overlap between the initial and final ground states in the thermodynamic limit—manifests itself in the overlap integrals and how it disappears in the process of summing the cross section over the final states, to make the absorption cross section remain finite even in the limit of N (number of electrons) $\rightarrow\infty$. The expression we derived for the response function $I(t)$ is exact, whose validity is not restricted to the long-time behavior nor to some particular core-hole potential. We demonstrated that the integral equation involved, which can be solved in the near-edge region in the case of a contact core-hole potential, yields an analytical form for the prefactor of the power-law behavior of the open-line contribution, besides reproducing the exact exponent of the power-law response function obtained first by ND. It is also to be noted that the total absorption intensities of the main and secondary absorption bands in the presence of a bound state, whose exact forms are given by TO, are just the quantities determined by the value at $t=0$ of the response function. These points clarified by our approach have been rather difficult to explore in the time-space treatment of ND, because a lot of information is lost from the start in deriving the asymptotic ($t\simeq\infty$) formula of the unperturbed propagator to be used in the Dyson equation.

The purpose of the present paper is to extend the formulation of OT at absolute zero of temperature to that of finite temperatures. It is generally accepted that except for a few tens-of-percents contributions in the case of aluminum,[7] the thermal effect on the linewidth of the spectrum is rather minor, as compared to a finite lifetime of a core hole due to the phonon and Auger effects.[3] In spite of that, however, how the infrared divergence is suppressed at finite temperatures remains to be an interesting theoretical problem in its own right.

There have been a number of studies on this topic. Almbladh and Minnhagen[7] calculated the spectrum by applying the method of Schotte and Schotte[8] of approximating a particle-hole pair as an excited boson. They showed that the power-law t dependence of $I(t)$ at $T=0$ is replaced by that of $\sinh(\pi Tt)/\pi T$ in the case of a finite T. The lowest-order calculation by Ferrell[9] of the core-hole propagator involved in $I(t)$ as well as the perturbation treatment of Mahan[2] suggests strongly the exactness of this T and t dependences. The work parallel to ND at finite temperatures was given by Yuval and Anderson.[10,11] They showed that in the approximation of treating only the long-time behavior, the Dyson equation can be dealt with by generalizing the standard Hilbert problem encountered at $T=0$. They thus showed that the replacement of time t by $\sinh(\pi Tt)/\pi T$ is in fact the right way of obtaining $I(t)$ for $T\neq 0$ from the ND solution.

Our interest in the present study is the same as that of OT. We formulate the problem using the final-state wave functions and calculating the cross section of x-ray absorption. Since the multiplicity of the excited states needs to be considered even in the initial states, the calculation is naturally much more involved than before. Our results obtained finally are, however, exact.

In Sec. II we derive the matrix elements between the initial and the final many-body states. In Sec. III the summation of the cross section over the initial and final states is carried out to bring forth a closed formula for $I(t)$. In Sec. IV the response function in the case of a contact-type

core-hole potential is derived. It is shown that in order to obtain the absorption spectrum we need to solve two integral equations. One of them is solved in Sec. V. The other integral equation is solved in Sec. VI. We solve the latter in the asymptotic region of t, which appears to be the only region where an analytical treatment is possible. A summary is given in Sec. VII.

In this paper we do not consider the case where a bound state exists in the final state. However, the results of Secs. II and III may apply to this case as such, if one occupied state considered there is regarded as a bound state.

II. MATRIX ELEMENTS OF THE DIPOLE MOMENT OPERATOR

We adopt as in OT (Ref. 4) and TO (Ref. 5) the Hamiltonian of ND for the system of N (spinless) conduction electrons plus one core electron. In the initial state the core level is filled, while in the final state $N+1$ electrons in the conduction band suffer from scattering due to a created core hole. Let $\mathcal{N}$ be the total number of states of the conduction band. $\mathcal{N}-N$, the number of unoccupied states in the initial state, is denoted as M. Throughout the paper N lowest states of the initial (final) conduction band are labeled by the index $m(\mu)$, and the remaining M states are labeled by the index $b(\gamma)$. The sums $\sum_\mu$, $\sum_m$, etc., in what follows have their respective meanings in accordance with this rule. When there is no need to specify a state relative to the Fermi level, we use the index k (κ) for the initial (final) state. The ground state of N conduction electrons is expressed by the Slater determinant of the states $m=1,2,\ldots,N$ in the case of the initial state or $\mu=1,2,\ldots,N$ in the case of the final state. The energy of the state with $m=N$ defines the Fermi level (chemical potential at $T=0$).

At finite T our initial $(N+1)$-electron states are specified by the number of electron-hole pairs involved and the way they are distributed in the conduction band. Let $|n\rangle=|\bar{m}_1,\ldots,\bar{m}_n,b_1,\ldots,b_n\rangle$ be an initial state with n excited electrons at the states $b_1,b_2,\ldots,b_n$ and n holes left behind at the states $m_1,m_2,\ldots,m_n$. The bar over m_i indicates that the state m_i is empty. The existence of the core electron in $|n\rangle$ is to be understood. Likewise, the state $|\nu\rangle=|\bar{\mu}_1,\ldots,\bar{\mu}_{\nu-1},\gamma_1,\ldots,\gamma_\nu\rangle$ signifies the final state with ν excited electrons at the states $\{\gamma_i\}$ and $\nu-1$ holes at $\{\mu_i\}$. Since there is a hole in the core state, there is $\nu-1$ holes in the conduction band in the state $|\nu\rangle$. Our aim is to obtain the expression of the matrix element $\langle\nu|W|n\rangle$ for the dipole moment operator W.

As the formulation of OT, the overlap integrals between two Slater determinants for N conduction electrons are important. The inner product $\langle\kappa|k\rangle$ between the unperturbed one-particle state $|k\rangle$ and perturbed one $|\kappa\rangle$ is denoted by $a_{\kappa k}$. Let Δ be the overlap integral between the ground states of the initial and final Hamiltonian for N electrons:

$$\Delta=\det\underline{A}\ , \tag{2.1}$$

with the $N\times N$ matrix $\underline{A}$ defined by ($\mu,m=1,2,\ldots,N$)

$$(\underline{A})_{\mu m}=a_{\mu m}\ . \tag{2.2}$$

Remember that the rows and columns of $\underline{A}$ are labeled by the final and initial single-particle states, respectively. By the orthogonality catastrophe, Δ vanishes in the limit $N\to\infty$. In addition to $\underline{A}$, we need, in the following, four matrices: $\underline{A}(\bar{\mu}\gamma|\ )$, $\underline{A}(\ |\bar{m}b)$, $\underline{A}(\bar{\mu}|\bar{m})$, and $\underline{A}(\gamma|b)$. They are defined as follows: Replacement of the μth row of $\underline{A}$ [$=(a_{\mu1}\ a_{\mu2}\ \cdots\ a_{\mu N})$] by the new row γ [$=(a_{\gamma1}\ a_{\gamma2}\ \cdots\ a_{\gamma N})$] forms $\underline{A}(\bar{\mu}\gamma|\ )$; its determinant is an overlap integral between the initial ground state and an excited final state with an electron at the state γ above the Fermi level and a hole at μ. The matrix $\underline{A}(\ |\bar{m}b)$ is obtained from $\underline{A}$ by replacing its mth column by the new column b; it determines an overlap integral between a thermally excited initial state and the ground final state. The matrix $\underline{A}(\bar{\mu}|\bar{m})$ is defined to be -1 times the cofactor $\Delta_{\mu m}$ of $\underline{A}$. Finally, $\underline{A}(\gamma|b)$ is an $(N+1)\times(N+1)$ matrix obtained by adding the new row γ and the new column b to the original matrix $\underline{A}$, with $a_{\gamma b}$ being inserted as the (γ,b)th element in the augmented matrix. Let $\Delta(\bar{\mu}\gamma|\ )$, $\Delta(\ |\bar{m}b)$, $\Delta(\bar{\mu}|\bar{m})$, and $\Delta(\gamma|b)$ be their respective determinants. By definition

$$\begin{aligned}
&\Delta(\bar{\mu}\gamma|\ )/\Delta=\sum_m a_{\gamma m}(\underline{A}^{-1})_{m\mu}\ ,\\
&\Delta(\ |\bar{m}b)/\Delta=\sum_\mu(\underline{A}^{-1})_{m\mu}a_{\mu b}\ ,\\
&\Delta(\bar{\mu}|\bar{m})/\Delta=-(\underline{A}^{-1})_{m\mu}\ ,\\
&\Delta(\gamma|b)/\Delta=a_{\gamma b}-\sum_{m,\mu}a_{\gamma m}(\underline{A}^{-1})_{m\mu}a_{\mu b}\ .
\end{aligned} \tag{2.3}$$

The matrix element $\langle\nu|W|n\rangle$ will be expressed in terms of these four determinants. In OT, the expression of $\langle\nu|W|0\rangle$ is given. To avoid unnecessary complications, we derive here $\langle2|W|1\rangle$ and $\langle2|W|2\rangle$ from $\langle2|W|0\rangle$. The matrix element $\langle2|W|0\rangle$ is expressed as

$$\langle2|W|0\rangle=\Delta\det\begin{vmatrix}p(\gamma_1) & \Delta(\bar{\mu}_1\gamma_1|\ )/\Delta\\ p(\gamma_2) & \Delta(\bar{\mu}_1\gamma_2|\ )/\Delta\end{vmatrix}$$

$$=\Delta\det|\underline{a}_1\ \ \underline{a}_2|\ , \tag{2.4}$$

where

$$p(\gamma)=w_{\gamma c}-\sum_\mu[\Delta(\bar{\mu}\gamma|\ )/\Delta]w_{\mu c}\ , \tag{2.5}$$

$w_{\gamma c}$ ($w_{\mu c}$) being the optical matrix element between the state γ (μ) and the core state c. The second line of Eq. (2.4) defines two column vectors $\underline{a}_1$ and $\underline{a}_2$. In calculating $\langle2|W|1\rangle=\langle\bar{\mu}_1,\gamma_1,\gamma_2|W|\bar{m}_1,b_1\rangle$, we note that Eq. (2.4) still applies, if we replace $|0\rangle$ of the initial state by $|\bar{m}_1b_1\rangle$. Thus it holds that

$$\langle2|W|1\rangle=\Delta'\det\begin{vmatrix}p'(\gamma_1) & \Delta'(\bar{\mu}_1\gamma_1|\ )/\Delta'\\ p'(\gamma_2) & \Delta'(\bar{\mu}_1\gamma_2|\ )/\Delta'\end{vmatrix}$$

$$=\Delta'\det|\underline{a}'_1\ \ \underline{a}'_2| \tag{2.6}$$

with

$$p'(\gamma)=w_{\gamma c}-\sum_{\mu}[\Delta'(\bar{\mu}\gamma\,|\,)/\Delta']w_{\mu c}\ . \tag{2.7}$$

The quantities Δ' and $\Delta'(\bar{\mu}\gamma\,|\,)$ are the determinants of the matrices $\underline{A}'$ and $\underline{A}'(\bar{\mu}\gamma\,|\,)$, which are defined by replacing the m_1th column by the new column b_1 in $\underline{A}$ and $\underline{A}(\bar{\mu}\gamma\,|\,)$, respectively. Note that $\Delta'=\Delta(\,|\,\bar{m}_1 b_1)$, by the definition of $\Delta(\,|\,\bar{m}_1 b_1)$ given above. With regard to $\Delta'(\bar{\mu}\gamma\,|\,)$, Appendix A shows [the first relation of (A7)]

$$\frac{\Delta'(\bar{\mu}\gamma\,|\,)}{\Delta'}=\frac{\Delta(\bar{\mu}\gamma\,|\,)}{\Delta}-\frac{\Delta(\gamma\,|\,b_1)}{\Delta}\frac{\Delta(\bar{\mu}\,|\,\bar{m}_1)}{\Delta'}\ . \tag{2.8}$$

Using Eqs. (2.7) and (2.8) in Eq. (2.6), we find

$$\begin{aligned}\underline{a}_1'&=\underline{a}_1-\underline{c}\sum_{\mu}(-1)[\Delta(\bar{\mu}\,|\,\bar{m}_1)/\Delta']w_{\mu c}\ ,\\ \underline{a}_2'&=\underline{a}_2-\underline{c}[\Delta(\bar{\mu}_1\,|\,\bar{m}_1)/\Delta']\ ,\end{aligned} \tag{2.9}$$

with the column vector $\underline{c}$ defined by

$$\underline{c}=\begin{bmatrix}\Delta(\gamma_1\,|\,b_1)/\Delta\\ \Delta(\gamma_2\,|\,b_1)/\Delta\end{bmatrix}\ . \tag{2.10}$$

Putting Eq. (2.9) into Eq. (2.6), we obtain

$$\langle 2\,|\,W\,|\,1\rangle=\Delta\left[\frac{\Delta(\,|\,\bar{m}_1 b_1)}{\Delta}\det|\,\underline{a}_1\ \underline{a}_2\,|-p(\bar{m}_1)\det|\,\underline{c}\ \underline{a}_2\,|-\frac{\Delta(\bar{\mu}_1\,|\,\bar{m}_1)}{\Delta}\det|\,\underline{a}_1\ \underline{c}\,|\right]$$

$$=\Delta\det\begin{vmatrix}p(\gamma_1) & \Delta(\bar{\mu}_1\gamma_1\,|\,)/\Delta & \Delta(\gamma_1\,|\,b_1)/\Delta\\ p(\gamma_2) & \Delta(\bar{\mu}_1\gamma_2\,|\,)/\Delta & \Delta(\gamma_2\,|\,b_1)/\Delta\\ p(\bar{m}_1) & \Delta(\bar{\mu}_1\,|\,\bar{m}_1)/\Delta & \Delta(\,|\,\bar{m}_1 b_1)/\Delta\end{vmatrix}\ , \tag{2.11}$$

with

$$p(\bar{m})=-\sum_{\mu}[\Delta(\bar{\mu}\,|\,\bar{m})/\Delta]w_{\mu c}\ . \tag{2.12}$$

The expression (2.11) may now be used to derive $\langle 2\,|\,W\,|\,2\rangle=\langle\bar{\mu}_1,\gamma_1,\gamma_2\,|\,W\,|\,\bar{m}_1,\bar{m}_2,b_1,b_2\rangle$. Since the initial state $|\,2\rangle$ involves an additional excited electron at the state b_2 and a hole at m_2, we need only to replace all the quantities involved in Eq. (2.11) by the primed ones. The determinant Δ' is now defined by the replacement $m_2\rightarrow b_2$ in the column of $\underline{A}$, $\Delta'(\bar{\mu}\,|\,\bar{m})$ is obtained by the same replacement in the column of $\underline{A}(\bar{\mu}\,|\,\bar{m})$, and so on. Let us express the matrix elements in terms of three column vectors as follows:

$$\begin{aligned}\langle 2\,|\,W\,|\,1\rangle&=\Delta\det|\,\underline{b}_1\ \underline{b}_2\ \underline{b}_3\,|\ ,\\ \langle 2\,|\,W\,|\,2\rangle&=\Delta'\det|\,\underline{b}_1'\ \underline{b}_2'\ \underline{b}_3'\,|\ .\end{aligned} \tag{2.13}$$

The expressions (A7) of the primed determinants as combined with the relation $\Delta'=\Delta(\,|\,\bar{m}_2 b_2)$ then yield

$$\begin{aligned}\underline{b}_1'&=\underline{b}_1-\underline{d}\sum_{\mu}(-1)[\Delta(\bar{\mu}\,|\,\bar{m}_2)/\Delta']w_{\mu c}\\ \underline{b}_2'&=\underline{b}_2-\underline{d}[\Delta(\bar{\mu}_1\,|\,\bar{m}_2)/\Delta']\ ,\\ \underline{b}_3'&=\underline{b}_3-\underline{d}[\Delta(\,|\,\bar{m}_2 b_1)/\Delta']\ ,\end{aligned} \tag{2.14}$$

with

$$\underline{d}=\begin{bmatrix}\Delta(\gamma_1\,|\,b_2)/\Delta\\ \Delta(\gamma_2\,|\,b_2)/\Delta\\ \Delta(\,|\,\bar{m}_1 b_2)/\Delta\end{bmatrix}\ . \tag{2.15}$$

Resolving $\det|\,\underline{b}_1'\ \underline{b}_2'\ \underline{b}_3'\,|$ with respect to the column vectors as in Eq. (2.11), we obtain

$$\langle 2\,|\,W\,|\,2\rangle=\Delta\det\begin{vmatrix}p(\gamma_1) & \Delta(\bar{\mu}_1\gamma_1\,|\,)/\Delta & \Delta(\gamma_1\,|\,b_1)/\Delta & \Delta(\gamma_1\,|\,b_2)/\Delta\\ p(\gamma_2) & \Delta(\bar{\mu}_1\gamma_2\,|\,)/\Delta & \Delta(\gamma_2\,|\,b_1)/\Delta & \Delta(\gamma_2\,|\,b_2)/\Delta\\ p(\bar{m}_1) & \Delta(\bar{\mu}_1\,|\,\bar{m}_1)/\Delta & \Delta(\,|\,\bar{m}_1 b_1)/\Delta & \Delta(\,|\,\bar{m}_1 b_2)/\Delta\\ p(\bar{m}_2) & \Delta(\bar{\mu}_1\,|\,\bar{m}_2)/\Delta & \Delta(\,|\,\bar{m}_2 b_1)/\Delta & \Delta(\,|\,\bar{m}_2 b_2)/\Delta\end{vmatrix}\ . \tag{2.16}$$

Equations (2.11) and (2.16) are the results we have been looking for.

Starting from the expression of $\langle \nu | W | 0 \rangle$ given by OT, we can similarly construct $\langle \nu | W | n \rangle$. It is a determinant of a $(\nu+n)\times(\nu+n)$ matrix, whose rows are labeled by ν γ's and n m's and the columns by $(\nu-1)$ μ's and n b's. Note that the first column consists of $p(\gamma)$ and $p(\bar{m})$, as exhibited in Eq. (2.16). It is interesting to note that multiple excitations of electron-hole pairs can be described solely in terms of the five types of the overlap integrals, Δ, $\Delta(\bar{\mu}\gamma|\,)$, $\Delta(\,|\,\bar{m}b)$, $\Delta(\bar{\mu}\,|\,\bar{m})$, and $\Delta(\gamma\,|\,b)$, even in the presence of the nonorthogonality between one-particle wave functions of the initial and final states.

III. CLOSED FORM OF THE ABSORPTION CROSS SECTION

The absorption cross section is now obtained by summing $|\langle \nu | W | n \rangle|^2$ over all possible initial and final states with energy conservation taken into account. The energies of the initial state $|n\rangle = |\bar{m}_1, \ldots, \bar{m}_n; b_1, \ldots, b_n\rangle$ and the final one $|\nu\rangle = |\bar{\mu}_1, \ldots, \bar{\mu}_{\nu-1}; \gamma_1, \ldots, \gamma_\nu\rangle$ are written as

$$E_I^0 + \sum_{b=1}^{n} \epsilon_b - \sum_{m=1}^{n} \epsilon_m + \epsilon_{\text{core}} \tag{3.1}$$

and

$$E_F^0 + \sum_{\gamma=1}^{\nu} \epsilon_\gamma - \sum_{\mu=1}^{\nu-1} \epsilon_\mu \,, \tag{3.2}$$

respectively, where ϵ_{core} is the energy of the core state and E_I^0 (E_F^0) is the N-electron ground-state energy of the initial (final) conduction band. The difference of the energies (3.1) and (3.2) should be equal to the frequency ω of an x-ray quantum ($\hbar=1$). We measure all the single-particle energies from the Fermi level ($\epsilon_{\text{Fermi}}=0$). Thus

$$\omega_{\text{th}}^0 = E_F^0 - E_I^0 - \epsilon_{\text{core}} \tag{3.3}$$

defines the threshold (th) of the absorption band at $T=0$. Temperature effect is incorporated into our theory through the Boltzmann factor for the initial energy (3.1).

The absorption cross section or the response function, as obtained from the Fermi golden rule, now reads

$$I(\omega) = 2\,\text{Re}\int_0^\infty dt\, e^{i(\omega-\omega_{\text{th}}^0)t} I(t) \,, \tag{3.4}$$

where

$$I(t) = \sum_{\nu=1}^{M} \sum_{n=0}^{N} I_{\nu,n}(t) \,, \tag{3.5}$$

with

$$I_{\nu,n}(t) = \frac{1}{\mathscr{Z}} \sum_{\{\gamma\},\{m\}} \frac{\theta_\gamma(t)\theta_m(t)}{\nu!n!} \times \sum_{\{\mu\},\{b\}} \frac{\theta_\mu(t)\theta_b(t)}{(\nu-1)!n!} |\langle \nu | W | n \rangle|^2 \,, \tag{3.6}$$

the factorials being put to eliminate double countings and

$$\begin{aligned} \theta_\gamma(t) &= \prod_{\gamma=1}^{\nu} e^{-i\epsilon_\gamma t} \,, \\ \theta_m(t) &= \prod_{m=1}^{n} e^{-i\epsilon_m t^*} \,, \\ \theta_\mu(t) &= \prod_{\mu=1}^{\nu-1} e^{i\epsilon_\mu t} \,, \\ \theta_b(t) &= \prod_{b=1}^{n} e^{i\epsilon_b t^*} \,. \end{aligned} \tag{3.7}$$

The temperature T or β ($=1/T$ with $k_B=1$) is involved in $I(t)$ through the parameter t^* defined by

$$t^* = t + i\beta \tag{3.8}$$

and through the partition function $\mathscr{Z}$ of the initial state

$$e^{-\beta E_I^0}\mathscr{Z} = \sum_{\{k_i\}} \exp[-\beta(\epsilon_{k_1} + \epsilon_{k_2} + \cdots + \epsilon_{k_N})] \,, \tag{3.9}$$

the sum being over all possible different choices of N states out of $\mathscr{N}$ states of the conduction band. Note that double occupancy of the single-particle states γ, μ, etc., in $I(t)$ is automatically eliminated because the expression of $\langle \nu | W | n \rangle$ obtained in Sec. II gives zero cross section in such cases.

Our purpose is to obtain a closed form for $I(t)$ by carrying out all the summations required in the above formulas. The calculation of $I_{2,2}(t)$ is illustrative for deducing $I_{\nu,n}(t)$. The summation over $\{\mu\}$ and $\{b\}$ is first carried out. Let us denote that part of $I_{2,2}(t)$ as $I'_{2,2}(t)$:

$$I'_{2,2}(t) = \sum_{\{\mu\},\{b\}} \frac{\theta_\mu(t)\theta_b(t)}{1!2!} |\langle 2 | W | 2 \rangle|^2 \tag{3.10}$$

with $\langle 2| = \langle \bar{\mu}_1, \gamma_1, \gamma_2|$ and $|2\rangle = |\bar{m}_1, \bar{m}_2, b_1, b_2\rangle$. From Eq. (2.16) we have

$$\begin{aligned} I'_{2,2}(t) = |\Delta|^2 [\, &|p(\gamma_1)|^2 \pi_{\gamma_1} + \cdots + |p(\bar{m}_2)|^2 \pi_{m_2} \\ &- p^*(\gamma_1)p(\gamma_2)\pi_{\gamma_1\gamma_2} - \cdots \\ &- p^*(\bar{m}_2)p(\bar{m}_1)\pi_{m_2 m_1}] \,. \end{aligned} \tag{3.11}$$

Since the coefficient $\pi_{\gamma_1\gamma_2}$, for example, involves a product of two determinants [two cofactors of Eq. (2.16)], we can make use of the sum over $\{\mu\}$ and $\{b\}$ in Eq. (3.10) to combine them into a form analogous to Gram's determinant. We thus find

$$\begin{aligned} \pi_{\gamma_1} &= \sum{}^{(2)} K \begin{bmatrix} \gamma_2 & m_1 & m_2 \\ \gamma_2 & m_1 & m_2 \end{bmatrix} t \,, \\ \pi_{m_1} &= \sum{}^{(2)} K \begin{bmatrix} \gamma_1 & \gamma_2 & m_2 \\ \gamma_1 & \gamma_2 & m_2 \end{bmatrix} t \,, \\ \pi_{\gamma_1\gamma_2} &= \sum{}^{(2)} K \begin{bmatrix} \gamma_1 & m_1 & m_2 \\ \gamma_2 & m_1 & m_2 \end{bmatrix} t \,, \end{aligned} \tag{3.12}$$

etc., where we employ the notation $K(:::|\,t)$ defined by

$$K\left[\begin{matrix}a_1 & a_2 & a_3\\ b_1 & b_2 & b_3\end{matrix}\middle| t\right]=\det\begin{vmatrix}K(a_1,b_1\,|\,t) & K(a_1,b_2\,|\,t) & K(a_1,b_3\,|\,t)\\ K(a_2,b_1\,|\,t) & K(a_2,b_2\,|\,t) & K(a_2,b_3\,|\,t)\\ K(a_3,b_1\,|\,t) & K(a_3,b_2\,|\,t) & K(a_3,b_3\,|\,t)\end{vmatrix}. \tag{3.13}$$

The matrix elements therein are

$$\begin{aligned}
K(\gamma_1,\gamma_2\,|\,t)&=\sum_\mu \Delta(\bar{\mu}\gamma_1\,|\,)e^{i\epsilon_\mu t}[\Delta(\bar{\mu}\gamma_2\,|\,)]^*/|\,\Delta\,|^2,\\
K(\gamma,m\,|\,t)&=\sum_\mu \Delta(\bar{\mu}\gamma\,|\,)e^{i\epsilon_\mu t}[\Delta(\bar{\mu}\,|\,\bar{m})]^*/|\,\Delta\,|^2,\\
K(m,\gamma\,|\,t)&=\sum_\mu \Delta(\bar{\mu}\,|\,\bar{m})e^{i\epsilon_\mu t}[\Delta(\bar{\mu}\gamma\,|\,)]^*/|\,\Delta\,|^2,\\
K(m_1,m_2\,|\,t)&=\sum_\mu \Delta(\bar{\mu}\,|\,\bar{m}_1)e^{i\epsilon_\mu t}[\Delta(\bar{\mu}\,|\,\bar{m}_2)]^*/|\,\Delta\,|^2.
\end{aligned} \tag{3.14}$$

The notation $\sum^{(2)}$ in Eq. (3.12) requires explanation. Consider, for example, π_{γ_1}. There are three columns, γ_2, m_1, and m_2, in the determinant on the right-hand side. We construct a new determinant by replacing two [as indicated by the superscript (2)] of the three columns by two new columns defined by the matrix elements $K^0(\gamma_1,\gamma_2\,|\,t)$, etc., given below. For example, the column γ_2 [$=(K(\gamma_2,\gamma_2\,|\,t), K(m_1,\gamma_2\,|\,t), K(m_2,\gamma_2\,|\,t))^{\rm tr}$, with the symbol tr denoting the transpose] is replaced by the new column γ_2 [$=(K^0(\gamma_2,\gamma_2\,|\,t), K^0(m_1,\gamma_2\,|\,t), K^0(m_2,\gamma_2\,|\,t))^{\rm tr}$]. Totally, there are three different ways of choosing two columns, each giving a new determinant after the replacement. The sum $\sum^{(2)}$ represents taking the sum over the three determinants thus obtained. [In the general case of $|\langle\nu|W|n\rangle|^2$, the factors π_γ, $\pi_{\gamma m}$, etc., involve $(\nu+n-1)$-dimensional matrices, in which we should replace n columns by the new columns formed by $K^0(\gamma_1,\gamma_2\,|\,t)$, etc.] The matrix elements $K^0(\gamma_1,\gamma_2\,|\,t)$, etc., which define the new columns, are given by

$$\begin{aligned}
K^0(\gamma_1,\gamma_2\,|\,t)&=\sum_b \Delta(\gamma_1\,|\,b)e^{i\epsilon_b t^*}[\Delta(\gamma_2\,|\,b)]^*/|\,\Delta\,|^2,\\
K^0(\gamma,m\,|\,t)&=\sum_b \Delta(\gamma\,|\,b)e^{i\epsilon_b t^*}[\Delta(\,|\,\bar{m}b)]^*/|\,\Delta\,|^2,\\
K^0(m,\gamma\,|\,t)&=\sum_b \Delta(\,|\,\bar{m}b)e^{i\epsilon_b t^*}[\Delta(\gamma\,|\,b)]^*/|\,\Delta\,|^2,\\
K^0(m_1,m_2\,|\,t)&=\sum_b \Delta(\,|\,\bar{m}_1 b)e^{i\epsilon_b t^*}[\Delta(\,|\,\bar{m}_2 b)]^*/|\,\Delta\,|^2.
\end{aligned} \tag{3.15}$$

We next sum $I'_{2,2}(t)$ over $\{\gamma\}$ and $\{m\}$ and divide the result by $(2!)^2$. After the summation two terms proportional to $|p(\gamma)|^2$ in Eq. (3.11) contribute equally to $I_{2,2}(t)$. The same holds true for $|p(\bar{m})|^2\pi_m$, $p^*(\gamma_1)p(\gamma_2)\pi_{\gamma_1\gamma_2}$, and $p^*(\bar{m}_1)p(\bar{m}_2)\pi_{m_1m_2}$, while there are four identical contributions of the type $p^*(\gamma)p(\bar{m})\pi_{\gamma m}$ and $p^*(\bar{m})p(\gamma)\pi_{m\gamma}$. This fact serves to cancel a part of the factor $1/(2!)^2$. Then the sum $\sum^{(2)}$ may be carried out by using the following identity

$$\sum{}^{(2)}K\left[\begin{matrix}a_1 & a_2 & a_3\\ b_1 & b_2 & b_3\end{matrix}\middle| t\right]=\frac{1}{2\pi i}\int_C\frac{d\lambda}{\lambda^3}K_\lambda\left[\begin{matrix}a_1 & a_2 & a_3\\ b_1 & b_2 & b_3\end{matrix}\middle| t\right], \tag{3.16}$$

C being a contour enclosing the origin $\lambda=0$ in the complex λ plane. In terms of the matrix $\underline{K}$ and $\underline{K}^0$, the matrix $\underline{K}_\lambda$ is defined by

$$\underline{K}_\lambda=\underline{K}+\lambda\underline{K}^0. \tag{3.17}$$

The validity of Eq. (3.16) is checked by calculating the residue at $\lambda=0$, as combined with the definition of the summation $\sum^{(2)}$. Equation (3.16) completes the derivation of $I_{2,2}(t)$. $I_{\nu,n}(t)$ is obtained similarly.

We now proceed to sum $I_{\nu,n}(t)$ over ν and n to obtain $I(t)$. From Eqs. (3.11), (3.12), and (3.16) it follows that

$$\begin{aligned}
I(t)=\frac{|\,\Delta\,|^2}{\mathscr{L}}\frac{1}{2\pi i}\int_C d\lambda\,\lambda^{-N-1}\Bigg[&\left(\sum_\gamma|p(\gamma)|^2e^{-i\epsilon_\gamma t}+\frac{1}{\lambda}\sum_m|p(\bar{m})|^2e^{-i\epsilon_m t^*}\right)D_\lambda(t)\\
&-\sum_{\gamma,\gamma'}p^*(\gamma)e^{-i\epsilon_\gamma t}D_\lambda(\gamma,\gamma'\,|\,t)e^{-i\epsilon_{\gamma'}t}p(\gamma')\\
&-\frac{1}{\lambda}\sum_{\gamma,m}p^*(\gamma)e^{-i\epsilon_\gamma t}D_\lambda(\gamma,m\,|\,t)e^{-i\epsilon_m t^*}p(\bar{m})\\
&-\frac{1}{\lambda}\sum_{\gamma,m}p^*(\bar{m})e^{-i\epsilon_m t^*}D_\lambda(m,\gamma\,|\,t)e^{-i\epsilon_\gamma t}p(\gamma)\\
&-\frac{1}{\lambda^2}\sum_{m,m'}p^*(\bar{m})e^{-i\epsilon_m t^*}D_\lambda(m,m'\,|\,t)e^{-i\epsilon_{m'}t^*}p(\bar{m}')\Bigg].
\end{aligned} \tag{3.18}$$

Here

$$D_\lambda(t)=\sum_{n=0}^{N}\sum_{\nu=0}^{M}\sum_{\{\gamma_j\},\{m_j\}}\frac{\lambda^{N-n}}{n!\nu!}K_\lambda\begin{bmatrix}\gamma_1\cdots\gamma_\nu m_1\cdots m_n\\ \gamma_1\cdots\gamma_\nu m_1\cdots m_n\end{bmatrix}t\Big]\exp\left[-i\sum_{j=1}^{\nu}\epsilon_{\gamma_j}t-i\sum_{j=1}^{n}\epsilon_{m_j}t^*\right],$$

$$D_\lambda(a,b,|t)=\sum_{n=0}^{N}\sum_{\nu=0}^{M}\sum_{\{\gamma_j\},\{m_j\}}\frac{\lambda^{N-n}}{n!\nu!}K_\lambda\begin{bmatrix}a\,\gamma_1\gamma_2\cdots\gamma_\nu m_1\cdots m_n\\ b\,\gamma_1\gamma_2\cdots\gamma_\nu m_1\cdots m_n\end{bmatrix}t\Big]\exp\left[-i\sum_{j=1}^{\nu}\epsilon_{\gamma_j}t-i\sum_{j=1}^{n}\epsilon_{m_j}t^*\right], \tag{3.19}$$

with $a,b=\gamma,\gamma',m,m'$. The first term of $D_\lambda(t)$ with $n=\nu=0$ should be taken to be λ^N. Note that in $D_\lambda(m,m'|t)$ the term $\nu=0$ actually drops in Eq. (3.18) due to the integral over λ. This should be so, since the final states always must have at least one electron above the Fermi level.

From the theory of the Fredholm integral equation,[12] we may rewrite Eq. (3.18) as

$$I(t)=\frac{|\Delta|^2}{\mathscr{Z}}\frac{1}{2\pi i}\int_C d\lambda\,\lambda^{-N-1}\det\underline{H}_\lambda(t)\times[\underline{p}^*(\gamma)e^{-i\underline{\epsilon}_\gamma t}\underline{p}^*(\overline{m})e^{-i\underline{\epsilon}_m t^*}]\times\underline{H}_\lambda^{-1}(t)[\underline{p}(\gamma)\underline{p}(\overline{m})]^{\mathrm{tr}}, \tag{3.20}$$

where $\underline{p}^*(\gamma)e^{-i\underline{\epsilon}_\lambda t}$ is understood to be a row vector of dimension M and $\underline{p}^*(\overline{m})e^{-i\underline{\epsilon}_m t^*}$ is that of dimension N. They are row vectors within the spaces γ and m, respectively. The vector $[\underline{p}(\gamma)\underline{p}(\overline{m})]^{\mathrm{tr}}$ is a transposed row vector, i.e., a column vector of dimension $\mathscr{N}(=N+M)$. The matrix $\underline{H}_\lambda(t)$, an important matrix that determines $I(t)$, is an $\mathscr{N}\times\mathscr{N}$ matrix defined by

$$\underline{H}_\lambda(t)=\begin{bmatrix}\underline{I}_\gamma+\underline{K}_\lambda e^{-i\underline{\epsilon}_\gamma t} & \underline{K}_\lambda e^{-i\underline{\epsilon}_m t^*}\\ \underline{K}_\lambda e^{-i\underline{\epsilon}_\gamma t} & \lambda\underline{I}_m+\underline{K}_\lambda e^{-i\underline{\epsilon}_m t^*}\end{bmatrix}. \tag{3.21}$$

We have introduced four block matrices in the spaces (γ,γ), (γ,m), (m,γ), and (m,m), with $\underline{I}_\gamma$ ($\underline{I}_m$) the $M\times M$ ($N\times N$) unit matrix and two diagonal matrices $\underline{\epsilon}_\gamma$ ($M\times M$) and $\underline{\epsilon}_m$ ($N\times N$) defined by

$$(e^{-i\underline{\epsilon}_\gamma t})_{\gamma_1\gamma_2}=\delta_{\gamma_1\gamma_2}e^{-i\epsilon_{\gamma_1}t},\qquad (e^{-i\underline{\epsilon}_m t^*})_{m_1m_2}=\delta_{m_1m_2}e^{-i\epsilon_{m_1}t^*}. \tag{3.22}$$

To reduce Eq. (3.20) to the final form of $I(t)$, we first rewrite the partition function $\mathscr{Z}$. As in Eq. (3.16), the definition (3.9) of $\mathscr{Z}$ leads to[13]

$$e^{-\beta E_I^0}\mathscr{Z}=\frac{1}{2\pi i}\int_C d\lambda\,\lambda^{-N-1}\prod_{k=1}^{\mathscr{N}}(1+\lambda e^{-\beta\epsilon_k}). \tag{3.23}$$

Next, the response function (3.20) is proportional to the orthogonality factor $|\Delta|^2$, which originally comes from the Δ-proportional matrix element $\langle\nu|W|n\rangle$. This fact does not, however, imply that $I(t)$ vanishes in the limit $N\to\infty$ by the orthogonality catastrophe. It simply means that the summation over the initial and final states should be carried out before taking the limit $N\to\infty$, as we have done so far in obtaining Eq. (3.20). In fact, Appendix B shows

$$\det\underline{H}_\lambda(t)=\det\underline{H}_\lambda(0)\exp\left[\int_0^t d\tau\frac{d}{d\tau}\mathrm{Tr}\ln\underline{H}_\lambda(\tau)\right] \tag{3.24}$$

with

$$\det\underline{H}_\lambda(0)=|\Delta|^{-2}e^{\beta E_I^0}\prod_{k=1}^{\mathscr{N}}(1+\lambda e^{-\beta\epsilon_k}). \tag{3.25}$$

Thus, the factor $|\Delta|^2$ of $I(t)$ just cancels that of $\det\underline{H}_\lambda(t)$, making the response function $I(t)$ remain finite even in the limit $N\to\infty$. With Eqs. (3.24) and (3.25), we can safely take the thermodynamic limit.

Finally, we consider the λ integrals involved in $I(t)$ and $\mathscr{Z}$. In the limit $N\to\infty$, they are evaluated by looking for a saddle point in the complex λ plane. From Eqs. (3.23)—(3.25) we see that the integrand of (3.20) involves the same factor $u(\lambda)$ as the partition function $\mathscr{Z}$,

$$u(\lambda)=\lambda^{-N-1}\prod_{k=1}^{\mathscr{N}}(1+\lambda e^{-\beta\epsilon_k}), \tag{3.26}$$

whose saddle point λ_s is determined by

$$\sum_{k=1}^{\mathscr{N}}(1+\lambda_s^{-1}e^{\beta\epsilon_k})^{-1}=N\quad\text{or}\quad\lambda_s=e^{\beta\mu}, \tag{3.27}$$

μ being the chemical potential. But the integrand of Eq. (3.20) has an additional λ dependence originating from the factors $\det\underline{H}_\lambda(t)/\det\underline{H}_\lambda(0)$ and $\underline{H}_\lambda^{-1}(t)$, showing that the saddle point of Eq. (3.20) is not exactly the same as that of $\mathscr{Z}$. The point is, however, that these factors are intensive quantities which remain finite in the limit $N\to\infty$, in contrast to the factor $u(\lambda)$ whose exponent is related directly to N. This may be seen by examining the N dependence of these factors with the use of that of $\Delta(\overline{\mu}\gamma|)/\Delta$, etc., given in the next section. So that one can perform the λ integral in Eq. (3.20), only over $\lambda^{-N-1}\det\underline{H}_\lambda(0)$, and put $\lambda=\lambda_s$ in the rest. Then the λ integral of $I(t)$ cancels precisely the partition function $\mathscr{Z}$, leaving only the additional λ_s dependence due to $\det\underline{H}_{\lambda_s}(t)/\det\underline{H}_{\lambda_s}(0)$ and $\underline{H}_{\lambda_s}^{-1}(t)$. Ultimately, we arrive at

$$I(t)=\exp\left[\int_0^t d\tau\,A(\tau)\right]I_0(t) \tag{3.28}$$

with

$$A(\tau)=\mathrm{Tr}\left[\left[\frac{d}{d\tau}\underline{H}_{\lambda_s}(\tau)\right]\underline{H}_{\lambda_s}^{-1}(\tau)\right], \tag{3.29}$$

$$I_0(t)=[\underline{p}^*(\gamma)e^{-i\underline{\epsilon}_\gamma t}\underline{p}^*(\overline{m})e^{-i\underline{\epsilon}_m t^*}]\times\underline{H}^{-1}_{\lambda_s}(t)[\underline{p}(\gamma)\underline{p}(\overline{m})]^{\mathrm{tr}}\,. \tag{3.30}$$

The matrix $\underline{H}_{\lambda_s}(t)$ is, from Eq. (3.21),

$$\underline{H}_{\lambda_s}(t)=\begin{bmatrix}\underline{I}_\gamma+\underline{K}_{\lambda_s}e^{-i\underline{\epsilon}_\gamma t} & \underline{K}_{\lambda_s}e^{-i\underline{\epsilon}_m t^*}\\ \underline{K}_{\lambda_s}e^{-i\underline{\epsilon}_\gamma t} & \lambda_s\underline{I}_m+\underline{K}_{\lambda_s}e^{-i\underline{\epsilon}_m t^*}\end{bmatrix} \tag{3.31}$$

with

$$\underline{K}_{\lambda_s}=\underline{K}+\lambda_s\underline{K}^0\,. \tag{3.32}$$

Equations (3.28)–(3.32) are the final closed forms for the response function. They are exact, having, in particular, no restriction on the form of the core-hole potential.

Let us consider the limit $T\to 0$ of our result. Because of the definition (3.8) of t^*, the factors $\exp(-i\epsilon_m t^*)$ and $\exp(i\epsilon_b t^*)$ then vanish (note that $\epsilon_m<0$ and $\epsilon_b>0$). Thus in the final form of $I(t)$ all the quantities involving the block m disappear together with the matrix $\underline{K}^0$ which contains in its summand the factor $\exp(i\epsilon_b t^*)$. The present result thus reduces correctly to Eq. (2.36) of OT, as it should.

Finally, a comment is in order concerning the optical sum rule—the total intensity of the absorption band. It is determined by the magnitude of the response function in the short-time limit. In contrast to the analysis of TO, in which two absorption bands are involved because of the existence of a bound state in the final state, the sum rule concerned here is understandable intuitively. From Eq. (3.28), it is found that

$$I(t=0)=\sum_k|w_{kc}|^2(1-f_k)\,, \tag{3.33}$$

where

$$f_k=1/(1+e^{\beta(\epsilon_k-\mu)}) \tag{3.34}$$

is the occupation number of the initial state $|k\rangle$ and

$$w_{\gamma c}=\sum_k a_{\gamma k}w_{kc} \tag{3.35}$$

defines the optical matrix element w_{kc} between the state $|k\rangle$ and the core state. If the k dependence of w_{kc} is dropped by putting

$$w_{kc}=w\,, \tag{3.36}$$

the total intensity of absorption becomes $|w|^2$ times the number M of the unoccupied states. Though we omit the derivation (for details, see TO), the sum rule (3.33) illustrates the capability of our result of reproducing correctly the short-time response of electrons to the created core-hole potential.

IV. REDUCTION OF THE FORMULA IN THE CASE OF A CONTACT CORE-HOLE POTENTIAL

In order to calculate $A(t)$ and $I_0(t)$, we must know $p(\gamma)$,$p(\overline{m})$, $\underline{K}$, and $\underline{K}^0$. By Eqs. (2.5), (2.12), (3.14), and (3.15), they are related to $\Delta(\bar{\mu}\gamma\,|\,)$, etc., which are in turn obtained from the inverse of the matrix $\underline{A}$ of the overlap integrals [Eq. (2.3)]. To proceed further, therefore, we need an explicit form of the overlap integral $a_{\kappa k}$. Hereafter we restrict ourselves to a contact-type core-hole potential with the strength V:

$$V_{kk'}=-V\,. \tag{4.1}$$

The forms of $a_{\kappa k}$ and $\underline{A}^{-1}$ of this case are given in OT. The overlap integral is expressed in terms of the phase shift $\delta_\kappa=\delta(\epsilon_\kappa)$ of the final state:

$$a_{\kappa k}=\delta_{\kappa k}\cos\delta_\kappa-\frac{\sin\delta_\kappa}{\pi N_\kappa}\mathrm{P}\frac{1}{\epsilon_\kappa-\epsilon_k}\,, \tag{4.2}$$

where $\delta_{\kappa k}=\delta(\epsilon_\kappa-\epsilon_k)/N_\kappa$ with $N_\kappa=N(\epsilon_\kappa)$, the state density of the conduction band at $\epsilon=\epsilon_\kappa$. The inverse matrix $\underline{A}^{-1}$ is

$$(\underline{A}^{-1})_{m\mu}=\frac{|\bar{X}_{\mu+}|}{|\bar{X}_{m+}|}\frac{1}{N_m}\left[(\cos\delta_m)\delta(\epsilon_m-\epsilon_\mu)+\frac{\sin\delta_m}{\pi}\mathrm{P}\frac{1}{\epsilon_m-\epsilon_\mu}\right]. \tag{4.3}$$

The dispersion integral with complex variable z

$$X(z)=\exp\left[-\frac{1}{\pi}\int_0^D d\epsilon\frac{\delta(\epsilon)}{z-\epsilon}\right],\qquad \bar{X}(z)=\exp\left[-\frac{1}{\pi}\int_{\bar{D}}^0 d\epsilon\frac{\delta(\epsilon)}{z-\epsilon}\right] \tag{4.4}$$

defines $\bar{X}_{\mu+}=\bar{X}(\epsilon_\mu+i\epsilon)$ with $\epsilon=0+$, etc., where D and $\bar{D}$ are the upper and lower band edges, respectively, of the conduction band, measured from the Fermi level ($D>0$, $\bar{D}<0$).

The quantities $\Delta(\bar{\mu}\gamma\,|\,)$ and $p(\gamma)$ are also given by OT. The other quantities such as $\Delta(\bar{\mu}\,|\,\overline{m})$ are obtained similarly by using Eqs. (4.2) and (4.3) in Eq. (2.3). We have

$$\begin{aligned}
\Delta(\bar{\mu}\gamma\,|\,)/\Delta&=\frac{1}{\epsilon_\mu-\epsilon_\gamma}V|\bar{X}_{\mu+}||X_{\gamma+}|\,,\\
\Delta(\bar{\mu}\,|\,\overline{m})/\Delta&=-\frac{\cos\delta_m}{N_m}\delta(\epsilon_m-\epsilon_\mu)+\left[\mathrm{P}\frac{1}{\epsilon_\mu-\epsilon_m}\right]V|\bar{X}_{\mu+}||X_{m+}|\,,\\
\Delta(\,|\,\overline{m}b)/\Delta&=\frac{1}{\epsilon_b-\epsilon_m}V|\bar{X}_{b+}||X_{m+}|\,,\\
\Delta(\gamma\,|\,b)/\Delta&=\frac{\cos\delta_\gamma}{N_\gamma}\delta(\epsilon_\gamma-\epsilon_b)+\left[\mathrm{P}\frac{1}{\epsilon_b-\epsilon_\gamma}\right]V|\bar{X}_{b+}||X_{\gamma+}|
\end{aligned} \tag{4.5}$$

and

$$p(\gamma)=|X_{\gamma+}|w\,, \tag{4.6}$$

$$p(\overline{m})=|X_{m+}|w\,, \tag{4.7}$$

with the (k-independent) matrix element w introduced in Eq. (3.39). In case denominators vanish in Eq. (4.5), the principal part is needed as indicated therein. To obtain $\underline{K}$ and $\underline{K}^0$ from their definitions (3.14) and (3.15), we use the identity

$$-i\int_0^\infty d\tau e^{iE\tau}=\frac{1}{E+i\epsilon}=\mathrm{P}\frac{1}{E}-i\pi\delta(E)\ . \tag{4.8}$$

Then, for example,

$$\begin{aligned}K(\gamma,\gamma'\,|\,t)=&-N_0V^2\,|\,X_{\gamma+}\,|\,|\,X_{\gamma'+}\,|\\&\times\int_0^\infty d\tau\int_0^\infty d\tau' e^{-i\epsilon_\gamma\tau}e^{-i\epsilon_{\gamma'}\tau'}\\&\times\bar{\phi}(t+\tau+\tau')\ ,\\K^0(m,m'\,|\,t)=&-N_0V^2\,|\,X_{m+}\,|\,|\,X_{m'+}\,|\\&\times\int_0^\infty d\tau\int_0^\infty d\tau' e^{-i\epsilon_m\tau}e^{-i\epsilon_{m'}\tau'}\\&\times\phi_1(t+\tau+\tau')\ ,\end{aligned} \tag{4.9}$$

where N_0 is the state density at the Fermi level and

$$\begin{aligned}N_0\bar{\phi}(t)&=\sum_\mu|\,\bar{X}_{\mu+}\,|^2e^{i\epsilon_\mu t}\ ,\\N_0\phi_1(t)&=\sum_b|\,\bar{X}_{b+}\,|^2e^{-\beta\epsilon_b}e^{i\epsilon_b t}\ .\end{aligned} \tag{4.10}$$

The expression of the other matrix elements or the explicit form of the matrix $\underline{H}_{\lambda_s}(t)$ defined by Eq. (3.31) is given by (C3) of Appendix C.

With Eqs. (4.6) and (4.9), we are now ready to derive the response function $I(t)$ for a contact core-hole potential. The procedure to be taken here is made up of forming $\underline{H}_{\lambda_s}(t)$, inverting it to obtain $H_{\lambda_s}^{-1}(t)$, and arranging the terms in the expressions of $A(t)$ and $I_0(t)$ to give their final forms. The calculation is outlined in Appendix D. In writing the result, several quantities need to be introduced. First, let g_γ and $\bar{g}_m$ be

$$\begin{aligned}g_\gamma&=1/(1+e^{2i\delta_\gamma}e^{-\beta(\epsilon_\gamma-\mu)})\ ,\\\bar{g}_m&=1/(1+e^{-2i\delta_m}e^{\beta(\epsilon_m-\mu)})\ ,\end{aligned} \tag{4.11}$$

with g_b and $\bar{g}_\mu$ defined similarly. In terms of them, we define

$$\begin{aligned}N_0\Phi_{t+\tau,\tau'}&=\sum_\gamma g_\gamma\,|\,X_{\gamma+}\,|^2e^{-i\epsilon_\gamma(t+\tau+\tau')}\\&\quad+\sum_m\bar{g}_me^{\beta(\epsilon_m-\mu)}\,|\,X_{m+}\,|^2e^{-i\epsilon_m(t+\tau+\tau')}\ ,\\N_0\bar{\Phi}_{\tau,t+\tau'}&=\sum_b g_b\,|\,\bar{X}_{b+}\,|^2e^{-\beta(\epsilon_b-\mu)}e^{i\epsilon_b(t+\tau+\tau')}\\&\quad+\sum_\mu\bar{g}_\mu\,|\,\bar{X}_{\mu+}\,|^2e^{i\epsilon_\mu(t+\tau+\tau')}\ ,\\2\pi i\eta_{\tau,\tau'}&=2\pi i\eta_{t+\tau,t+\tau'}\\&=\sum_\gamma\frac{g_\gamma}{N_\gamma}e^{-\beta(\epsilon_\gamma-\mu)}(e^{2i\delta_\gamma}-1)e^{-i\epsilon_\gamma(\tau-\tau')}\\&\quad+\sum_m\frac{\bar{g}_m}{N_m}e^{\beta(\epsilon_m-\mu)}(e^{-2i\delta_m}-1)e^{-i\epsilon_m(\tau-\tau')}\ ,\\\bar{\eta}_{\tau,\tau'}&=\bar{\eta}_{t+\tau,t+\tau'}=\eta_{\tau',\tau}\ ,\end{aligned} \tag{4.12}$$

where the presence of two subscripts shows that the quantities defined here are treated in what follows as matrices with respect to these time variables. The way the variable t is involved in the labels of their rows and columns is to be noted.

Then it follows that

$$\begin{aligned}A(t)=&\int_0^\infty d\tau\int_0^\infty d\sigma\, i\bar{\eta}_{0,\sigma}(1-\Lambda)^{-1}_{\sigma,\tau}(1-i\bar{\eta})^{-1}_{\tau,0}\\&+(N_0V)^2\int_0^\infty d\tau\int_0^\infty d\sigma\,\Psi_{t,\sigma}(1-\Lambda)^{-1}_{\sigma,\tau}\bar{\Psi}_{\tau,t}\ ,\\I_0(t)=&N_0w^2\int_0^\infty d\tau\int_0^\infty d\sigma\Psi_{t,\sigma}(1-\Lambda)^{-1}_{\sigma,\tau}(1-i\bar{\eta})^{-1}_{\tau,0}\ ,\end{aligned} \tag{4.13}$$

with

$$\begin{aligned}\Lambda_{\sigma,\tau}&=(N_0V)^2\int_0^\infty d\rho\,\bar{\Psi}_{\sigma,t+\rho}\Psi_{t+\rho,\tau}\ ,\\(\Psi)_{t+\tau,\tau'}&=[(1-i\eta)^{-1}\Phi]_{t+\tau,\tau'}\ ,\\(\bar{\Psi})_{\tau,t+\tau'}&=[(1-i\bar{\eta})^{-1}\bar{\Phi}]_{\tau,t+\tau'}\ .\end{aligned} \tag{4.14}$$

The product involved in the right-hand side of Eq. (4.14) should be treated as

$$[(1-i\eta)^{-1}\Phi]_{t+\tau,\tau'}=\int_0^\infty d\rho(1-i\eta)^{-1}_{t+\tau,t+\rho}\Phi_{t+\rho,\tau'}\ , \tag{4.15}$$

for example, where we have inserted the variable $t+\rho$, in accordance with the definitions of η and Φ given by Eq. (4.12). The inverse $(1-i\eta)^{-1}$ is hence obtained by solving an integral equation.

Equations (4.13) and (4.14) show that, to push forward our program, we need to solve integral equations twice, once for obtaining $(1-i\eta)^{-1}$, $(1-i\bar{\eta})^{-1}$, and then for $(1-\Lambda)^{-1}$. The first step is taken in the next section.

V. SOLUTION OF THE FIRST INTEGRAL EQUATION

In this section we obtain $(1-i\eta)^{-1}$, $(1-i\bar{\eta})^{-1}$, Ψ, and $\bar{\Psi}$ involved in Eq. (4.13) and reduce $A(t)$ and $I_0(t)$ to their final forms by making use of them. The derivation of the four quantities are analogous. Let r be the inverse of $(1-i\eta)$:

$$r_{\tau,\tau'}=(1-i\eta)^{-1}_{\tau,\tau'}\ . \tag{5.1}$$

By definition, it satisfies

$$r_{\tau,\tau'}-i\int_0^\infty d\rho\,\eta_{\tau,\rho}r_{\rho,\tau'}=\delta(\tau-\tau')\ . \tag{5.2}$$

Note that $\eta_{\tau,\tau'}$ is a function of $(\tau-\tau')$ by Eq. (4.12), while $r_{\tau,\tau'}$ is not. Equation (5.2) has a typical form solvable by the method of Wiener and Hopf.[14] In writing the solution, the Fourier transform of the kernel $\eta_{\tau,\tau'}$ is needed. We define

$$\eta(\omega)=\int_{-\infty}^\infty\eta_{\tau,0}e^{i\omega\tau}d\tau\ . \tag{5.3}$$

From Eq. (4.12), we find

$$1-i\eta(\omega)=\begin{cases}[1+(e^{2i\delta(\omega)}-1)f(\omega)]^{-1}, & D>\omega>0\\ e^{2i\delta(\omega)}[1+(e^{2i\delta(\omega)}-1)f(\omega)]^{-1}, & 0>\omega>\bar{D}\end{cases} \tag{5.4a}$$

$$=\begin{cases}e^{-2i\delta(\omega)}[1+(e^{-2i\delta(\omega)}-1)\bar{f}(\omega)]^{-1}, & D>\omega>0\\ [1+(e^{-2i\delta(\omega)}-1)\bar{f}(\omega)]^{-1}, & 0>\omega>\bar{D}\end{cases} \tag{5.4b}$$

and

$$1-i\eta(\omega)=1, \quad \omega>D, \ \omega<\bar{D} \tag{5.5}$$

with the Fermi-distribution functions

$$f(\omega)=(1+e^{\beta(\omega-\mu)})^{-1}, \qquad \bar{f}(\omega)=1-f(\omega). \tag{5.6}$$

Note that Eqs. (5.4) and (5.5) are rewritten as

$$1-i\eta(\omega)=\begin{cases}\dfrac{\exp[-i\delta(\omega)(\omega/|\omega|)]\cosh[\beta(\omega-\mu)/2]}{\cosh\{[\beta(\omega-\mu)-2i\delta(\omega)]/2\}}, & \bar{D}<\omega<D\\ 1, \quad \omega>D, \quad \omega<\bar{D}.\end{cases} \tag{5.7}$$

Let us decompose $[1-i\eta(\omega)]$ as follows:

$$1-i\eta(\omega)=\frac{Z_-(\omega)}{Z_+(\omega)}, \tag{5.8}$$

where $Z_+(\omega)$ $[Z_-(\omega)]$ is determined so that it is regular and free of zeros in the upper (lower) half of the ω plane. Explicitly, we find[15]

$$Z_\pm(\omega)=\exp\left[-\frac{1}{2\pi i}\int_{\bar{D}}^{D}d\omega'\frac{\ln[1-i\eta(\omega')]}{\omega'-\omega\mp i\delta}\right]. \tag{5.9}$$

The required analytic properties and the validity of the relation (5.8) are easily confirmed. Now Appendix D shows

$$[(1-i\eta)]^{-1}_{0,\tau}=[(1-i\bar{\eta})]^{-1}_{\tau,0}=\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\frac{e^{i\omega\tau}}{Z_-(\omega)}. \tag{5.10}$$

With regard to the quantities other than $(1-i\eta)^{-1}$, we note that $(1-i\bar{\eta})^{-1}$ is a transpose of $(1-i\eta)^{-1}$ as shown in Eq. (5.10), $\Psi_{t+\tau,\tau'}$ defined by Eq. (4.14) is obtained if the δ function on the right-hand side of Eq. (5.2) is replaced by $\Phi_{t+\tau,\tau'}$, and, finally, $\bar{\Psi}_{\tau,t+\tau'}$ is obtained if the kernel $i\eta$ and the δ function in Eq. (5.2) are replaced by $i\bar{\eta}$ and $\bar{\Phi}_{\tau,t+\tau'}$, respectively. Their expressions are thus obtained similarly to $(1-i\eta)^{-1}$ (see Appendix D):

$$N_0\Psi_{t+\tau,\tau'}=\sum_k\bar{f}_k|X_{k+}|^2\sigma_k(\tau)e^{-i\epsilon_k(t+\tau')}, \qquad N_0\bar{\Psi}_{\tau,t+\tau'}=\sum_k f_k|\bar{X}_{k+}|^2\bar{\sigma}_k(\tau)e^{i\epsilon_k(t+\tau')}, \tag{5.11}$$

with the simplified notations of the Fermi-distribution function [Eqs. (3.34) and (5.6)],

$$f_k=f(\epsilon_k), \qquad \bar{f}_k=\bar{f}(\epsilon_k), \tag{5.12}$$

and

$$\sigma_k(\tau)=\frac{1}{2\pi i}\int_{-\infty}^{\infty}d\omega\frac{Z_+(\omega)/Z_+(\epsilon_k)}{\epsilon_k-\omega-i\delta}e^{-i\omega\tau}, \qquad \bar{\sigma}_k(\tau)=-\frac{1}{2\pi i}\int_{-\infty}^{\infty}d\omega\frac{Z_-(\epsilon_k)/Z_-(\omega)}{\epsilon_k-\omega+i\delta}e^{i\omega\tau}. \tag{5.13}$$

In $A(t)$ and $I_0(t)$ of Eq. (4.13) we only need the expression for $\tau,\tau'>0$ for $\Psi_{t+\tau,\tau'}$ and $\bar{\Psi}_{\tau,t+\tau'}$. By the analyticity of Z_+ (Z_-) in the upper (lower) half ω plane, as combined with the asymptotic property $Z_\pm(\omega)\to 1(|\omega|\to\infty)$ obtained from Eq. (5.9), we see that both $\sigma_k(\tau)$ and $\bar{\sigma}_k(\tau)$ vanish when $\tau<0$. Thus as long as the expression (5.11) is used, all the integrals in $A(t)$ and $I_0(t)$ may be changed to those from $-\infty$ to ∞.

Now we proceed to reduce $A(t)$ and $I_0(t)$. We substitute Eqs. (5.10) and (5.11) into Eq. (4.13) and evaluate all the integrals involved there. The details are given in Appendix E. The result is

$$A(t)=i\eta^0+(N_0V)^2\times\int_0^\infty d\sigma\int_0^\infty d\tau\Psi(t+\sigma)\times F(t+\sigma,t+\tau)\bar{\Psi}(t+\tau), \qquad I_0(t)=N_0w^2\int_0^\infty d\tau\Psi(t+\tau)F(t+\tau,t+), \tag{5.14}$$

where $t+=t+\epsilon$ with $\epsilon=0+$ and

$$i\eta^0=\int_{\bar{D}}^{D}\frac{d\omega}{2\pi}\left[\frac{1}{Z_-(\omega)}-\frac{1}{Z_+(\omega)}\right] \tag{5.15}$$

is the quantity independent of t. The two functions $\Psi(t)$ and $\bar{\Psi}(t)$ are given by

$$N_0\Psi(t)=\sum_k\bar{f}_k|X_{k+}|^2[Z_+(\epsilon_k)Z_-(\epsilon_k)]^{-1}e^{-i\epsilon_k t}, \qquad N_0\bar{\Psi}(t)=\sum_k f_k|\bar{X}_{k+}|^2Z_+(\epsilon_k)Z_-(\epsilon_k)e^{i\epsilon_k t}, \tag{5.16}$$

and $F(t+\sigma,t+\tau)$ is defined by the following integral equation:

$$F(t+\sigma,t+\tau)-\int_0^\infty d\rho\,\Lambda(t+\sigma,t+\rho)F(t+\rho,t+\tau) =\delta(\sigma-\tau)\,, \quad (5.17)$$

with the integral kernel

$$\Lambda(t+\sigma,t+\rho)=(N_0V)^2 \times\int_0^\infty d\xi\,\bar{\Psi}(t+\sigma+\xi)\Psi(t+\rho+\xi)\,. \quad (5.18)$$

The definitions of $[1-i\eta(\omega)]$ [Eqs. (5.4) and (5.5)] and $Z_\pm(\omega)$ [Eq. (5.9)] enable us to rewrite $i\eta^0$, $\Psi(t)$, and $\bar{\Psi}(t)$ in terms of the one-particle quantities. First, from Eq. (5.15) we have

$$i\eta^0=\int_C\frac{d\omega}{2\pi}\exp\left[-\frac{1}{\pi}\int_{\bar{D}}^0 d\epsilon\frac{\delta(\epsilon)}{\omega-\epsilon}+\frac{1}{2\pi i}\int_{\bar{D}}^D d\epsilon\frac{\ln[1+f(\epsilon)(e^{2i\delta(\epsilon)}-1)]}{\omega-\epsilon}\right],$$

where the contour C encloses the branch cut in the range $\bar{D}<\omega<D$ on the real axis of the complex ω plane. Since the integrand of the ω integral is analytic everywhere except having the cut on the real axis, we can enlarge the contour C infinitely. The residue at $\omega=\infty$ then yields

$$i\eta^0=-i\int_{\bar{D}}^0 d\epsilon\frac{\delta(\epsilon)}{\pi}+\frac{1}{2\pi}\int_{\bar{D}}^D d\epsilon\ln[1+f(\epsilon)(e^{2i\delta(\epsilon)}-1)]\,. \quad (5.19)$$

For $\Psi(t)$ and $\bar{\Psi}(t)$, Eq. (5.16) leads to

$$N_0\Psi(t)=\sum_k\bar{f}_k e^{-i\epsilon_k t}\exp\left[\frac{1}{\pi i}\int_{\bar{D}}^D d\epsilon\,\mathrm{P}\frac{\ln[1+\bar{f}(\epsilon)(e^{-2i\delta(\epsilon)}-1)]}{\epsilon_k-\epsilon}\right],$$
$$N_0\bar{\Psi}(t)=\sum_k f_k e^{i\epsilon_k t}\exp\left[-\frac{1}{\pi i}\int_{\bar{D}}^D d\epsilon\,\mathrm{P}\frac{\ln[1+f(\epsilon)(e^{2i\delta(\epsilon)}-1)]}{\epsilon_k-\epsilon}\right], \quad (5.20)$$

where use has been made of Eq. (4.4). Equation (5.14) with Eqs. (5.17)–(5.20) is the conclusion of this section.

With Eqs. (5.19) and (5.20), $A(t)$ and $I_0(t)$ are now directly comparable with those derived in OT. The limit $T\to0$ is easily taken there to show

$$(i\eta^0)_{T=0}=0\,,$$
$$[N_0\Psi(t)]_{T=0}=\int_0^D d\epsilon N(\epsilon) \times\exp\left[-\frac{2}{\pi}\int_0^D d\epsilon'\,\mathrm{P}\frac{\delta(\epsilon')}{\epsilon-\epsilon'}\right]e^{-i\epsilon t}\,, \quad (5.21)$$
$$[N_0\bar{\Psi}(t)]_{T=0}=\int_{\bar{D}}^0 d\epsilon N(\epsilon) \times\exp\left[-\frac{2}{\pi}\int_{\bar{D}}^0 d\epsilon'\,\mathrm{P}\frac{\delta(\epsilon')}{\epsilon-\epsilon'}\right]e^{i\epsilon t}\,.$$

Hence $\Psi(t)$ and $\bar{\Psi}(t)$ tend respectively to $\phi(t)$ and $\bar{\phi}(t)$ of OT [OT Eqs. (5.3) and (5.6)] and the response function reduces correctly to that of OT in the limit $T\to0$. In other words, $\Psi(t)$ and $\bar{\Psi}(t)$ of Eq. (5.20) present the exact form of the dispersion integral[16] at finite temperatures. Also, the limit $\eta(\omega)\to0$ as $T\to0$ is the reason why in the formulations in OT and TO we encountered only one integral equation.

VI. THRESHOLD BEHAVIOR AT FINITE TEMPERATURES

The spectrum of the soft-x-ray absorption now depends entirely upon the solution F of the integral equation (5.17). In this section we treat F in the region of large t and obtain the exact asymptotic t dependence of $A(t)$ and $I_0(t)$ from Eq. (5.14).

Before concentrating on F, however, we consider the constant term $i\eta^0$ [Eq. (5.19)] involved in $A(t)$. Since the response function $I(\omega)$ depends on $A(t)$ as follows [Eq. (3.28)]:

$$I(\omega)=2\,\mathrm{Re}\int_0^\infty dt\,e^{i(\omega-\omega_{\mathrm{th}}^0)t}\exp\left[\int_0^t d\tau\,A(\tau)\right]I_0(t)\,, \quad (6.1)$$

the t independence of $i\eta^0$ shows that the real part of η^0 provides us with a shift of the spectrum as a whole, while its imaginary part describing an exponential decay of $I(t)$. Although a clear-cut absorption threshold no longer exists at finite T, let us define the modified threshold frequency as follows:

$$\omega_{\mathrm{th}}=(E_F^0-E_I^0-\epsilon_{\mathrm{core}})-\mathrm{Re}\eta^0 =\omega_{\mathrm{th}}^0-\mathrm{Re}\eta^0\,, \quad (6.2)$$

ω_{th}^0 being the threshold at $T=0$ [Eq. (3.3)]. The difference $E_F^0-E_I^0$ of the ground-state energies arises from the potential scattering by the core hole. Thus, by Fumi's theorem, the exact expression of it is[17]

$$E_F^0-E_I^0=-\int_{\bar{D}}^0 d\epsilon\frac{\delta(\epsilon)}{\pi}\,. \quad (6.3)$$

The quantity η^0 is given exactly by Eq. (5.19). From Eqs. (5.19) and (6.3), therefore, we find

$$\omega_{\rm th}=-\frac{1}{2\pi}\int_{\bar D}^{D}d\epsilon\,{\rm Im}\ln[1+f(\epsilon)(e^{2i\delta(\epsilon)}-1)]-\epsilon_{\rm core}\ . \tag{6.4}$$

The first term tends in the limit $T\to 0$ just to Eq. (6.3), thus showing that the phase shift in Fumi's theorem at $T=0$ is replaced by the quantity given above, which is determined by the combined effect of the phase shift and the Fermi-distribution function. At moderate temperatures and for ordinary conduction bands, however, it holds that T/D, $T/|\bar D|\ll 1$. The deviation of $\omega_{\rm th}$ from $\omega_{\rm th}^0$ in these cases is therefore small, because $\frac{1}{2}{\rm Im}\ln[\cdots]$ in $\omega_{\rm th}$ is different from $\delta(\epsilon)$ only in the frequency region of the order of T near the chemical potential: The correction involved in $\omega_{\rm th}$ is of $O(T/D)$ relative to $\omega_{\rm th}^0$, which is in general of the order of the bandwidth of the conduction band.

The imaginary part of η^0 will be combined with another (t-dependent) term of $A(t)$ as seen later. Now we turn to solving Eq. (5.17). The analysis based on Eq. (5.17) requires an explicit form of the integral kernel $\Lambda(t+\sigma,t+\rho)$ which is determined by Ψ and $\bar\Psi$. We restrict ourselves to the asymptotic region of t. Also, in parallel to the above estimate of $\omega_{\rm th}$, we are concerned with the temperature region much lower than the band parameter D and $|\bar D|$. In the following discussion, therefore, t and T are respectively confined to

$$tD,t\,|\bar D|\gg 1 \tag{6.5}$$

and

$$T\ll D,|\bar D|\ . \tag{6.6}$$

Consistently with the second condition, we can now put μ, the chemical potential, to zero (energy of the Fermi level), neglecting the correction of $O(T/D)$ as in $\omega_{\rm th}$.

First we write ${\rm Im}\,\eta^0$, whose expression valid for $T\ll D,|\bar D|$ is obtained in Appendix F:

$${\rm Im}\eta^0=\pi T\left[\frac{\delta_0}{\pi}\right]^2, \tag{6.7}$$

where δ_0 is the phase shift at the Fermi level.

In order to obtain $I(t)$ for large t, we require only the asymptotic forms of Ψ and $\bar\Psi$, as is obvious from the way the time t is involved in Eqs. (5.14), (5.17), and (5.18). We derive $\Psi(t)$ and $\bar\Psi(t)$ using Eq. (5.16). The expressions for $Z_+(\omega)$ and $Z_-(\omega)$ needed there are obtained in Appendix G. The expressions of $|X_{k+}|^2$ and $|\bar X_{k+}|^2$ valid for $\epsilon_k\simeq 0$ are given in OT:

$$\begin{aligned}|X_{k+}|^2&=|\epsilon_k|^{-\alpha}|X(0)|^2\ ,\\ |\bar X_{k+}|^2&=|\epsilon_k|^{\alpha}|\bar X(0)|^2\ ,\end{aligned} \tag{6.8}$$

where [OT Eq. (5.10)]

$$\begin{aligned}|X(0)|^2&=D^{\alpha}\exp\left[\frac{2}{\pi}\int_0^D d\epsilon\frac{\delta(\epsilon)-\delta_0}{\epsilon}\right],\\ |\bar X(0)|^2&=|\bar D|^{-\alpha}\exp\left[\frac{2}{\pi}\int_{\bar D}^0 d\epsilon\frac{\delta(\epsilon)-\delta_0}{\epsilon}\right],\end{aligned} \tag{6.9}$$

and

$$\alpha=2\delta_0/\pi\ . \tag{6.10}$$

The combination of Eq. (6.8) with (G10) in Eq. (5.16) then leads to (G12):

$$\begin{aligned}\Psi(t)&=\left[\frac{2\pi T}{i}\right]^{1-\alpha}|X(0)|^2e^{-\pi Tt(1-\alpha)}[\Gamma(1-\tfrac{1}{2}\alpha)]^2\\ &\quad\times F(1-\tfrac{1}{2}\alpha,1-\tfrac{1}{2}\alpha,1\,|\,e^{-2\pi Tt})\ ,\\ \bar\Psi(t)&=\left[\frac{2\pi T}{i}\right]^{1+\alpha}|\bar X(0)|^2e^{-\pi Tt(1+\alpha)}[\Gamma(1+\tfrac{1}{2}\alpha)]^2\\ &\quad\times F(1+\tfrac{1}{2}\alpha,1+\tfrac{1}{2}\alpha,1\,|\,e^{-2\pi Tt})\ ,\end{aligned} \tag{6.11}$$

where $\Gamma(1\pm\frac{1}{2}\alpha)$ is the gamma function and $F(a,b,c\,|\,z)$ is the hypergeometric function.[18]

Several expressions different from Eq. (6.11) are possible, using Kummer's relation for the hypergeometric functions. One of them is given by (G13), which shows that our $\Psi(t)$ and $\bar\Psi(t)$ tends precisely to $\phi(t)$ and $\bar\phi(t)$ [OT Eq. (5.9)], respectively, in the limit $T=0$. The results derived in what follows are based upon Eq. (6.11).

It looks difficult to obtain a closed analytical form for $\Lambda(t+\sigma,t+\rho)$. Thus we express Λ as a power series with respect to the variable $e^{-2\pi Tt}$, and the integral over ξ in Eq. (5.18) then leads to

$$\Lambda(t+\sigma,t+\rho)=-\tfrac{1}{2}\pi T\alpha^2\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\exp[-\pi T(1+\alpha+2m)(t+\sigma)]\lambda_{m,n}\exp[-\pi T(1-\alpha+2n)(t+\rho)]\ , \tag{6.12}$$

where

$$\lambda_{m,n}=\left[\frac{(1+\frac{1}{2}\alpha)_m}{m!}\right]^2\frac{1}{m+n+1}\left[\frac{(1-\frac{1}{2}\alpha)_n}{n!}\right]^2, \tag{6.13}$$

with Pochhammer's symbol $(\gamma)_m\equiv\Gamma(\gamma+m)/\Gamma(\gamma)=\gamma(\gamma+1)\cdots(\gamma+m-1)$. In eliminating $|X(0)|^2$, $|\bar X(0)|^2$, and $\Gamma(1\pm\alpha/2)$ involved in Eq. (6.11), we have made use of the relation

$$|X(\epsilon_+)|\,|\bar X(\epsilon_+)|=\sin[\delta(\epsilon)]/[\pi VN(\epsilon)]$$

[OT Eqs. (3.13) and (3.14)].

With Eq. (6.12), the power-series expressions for $F(t+\sigma,t+\tau)$, $A(t)$, and $I_0(t)$ are straightforwardly obtained. They are given by (H2) and (H4). Our final task is to find analytical expressions for $A(t)$ and $I_0(t)$ by summing the infinite series for them. Since the form

(6.12) of Λ involves a double sum and $A(t)$ and $I_0(t)$ are written in terms of $(1-\Lambda)^{-1}$, the proof cannot be so simple. Though clumsy, our treatment given in Appendix H provides us with asymptotically exact solutions for $A(t)$ and $I_0(t)$,

$$A(t)=i(\mathrm{Re}\eta^0)-\pi T\left[\frac{\delta_0}{\pi}\right]^2\coth(\pi Tt)\,, \tag{6.14}$$

$$I_0(t)=N_0w^2\left[\frac{2\pi T}{i}\right]^{1-\alpha}|X(0)|^2[\Gamma(1-\tfrac{1}{2}\alpha)]^2 \times[2\sinh(\pi Tt)]^{-1+\alpha}\,, \tag{6.15}$$

where $i(\mathrm{Re}\eta^0)$ yields the first term of Eq. (6.4) whose meaning has been discussed there, and the term $\pi T(\delta_0/\pi)^2$ of Eq. (6.7) is absorbed into the second of Eq. (6.14). They are our final results, bringing forth the response function $I(t)$ as follows:

$$I(t)=N_0Dw^2A_0[\Gamma(1-\tfrac{1}{2}\alpha)]^2p_0e^{i(\mathrm{Re}\eta^0)t} \times\left[iD\frac{\sinh(\pi Tt)}{\pi T}\right]^{-1+\zeta_0}, \tag{6.16}$$

where

$$\zeta_0=2\frac{\delta_0}{\pi}-\left[\frac{\delta_0}{\pi}\right]^2,$$

$$p_0=\left[iD\frac{\sinh(\pi Tt_0)}{\pi T}\right]^{(\delta_0/\pi)^2} \times\exp[-i(\mathrm{Re}\eta^0)t_0]\exp\left[\int_0^{t_0}d\tau\,A(\tau)\right], \tag{6.17}$$

$$A_0=|X(0)|^2/D^\alpha=\exp\left[\frac{2}{\pi}\int_0^D d\epsilon\frac{\delta(\epsilon)-\delta_0}{\epsilon}\right].$$

The coefficient p_0 describes a short-time contribution of $A(t)$, as introduced in TO by assuming that the long-time form (6.14) remains to be valid down to $t\simeq t_0$.

The result (6.16) reproduces the result of Yuval and Anderson.[10,11] Also our treatment yields an exact expression for the prefactor of the power-law behavior of $I_0(t)$, the critical amplitude introduced by Penn, Girvin, and Mahan.[19] It is identical with that of $T=0$. Note the existence of an additional contribution from the short-time response summarized by the factor p_0, which shows that the exact form of the prefactor as a whole requires inherently the information on $A(t)$ in the whole region of t. Note also that within the restrictions (6.5) and (6.6) the relative magnitudes of t and T are completely free. Equation (6.16) thus shows that the power law in the case of $tT\ll 1$ is replaced by the exponential decay in the opposite limit of $tT\gg 1$.

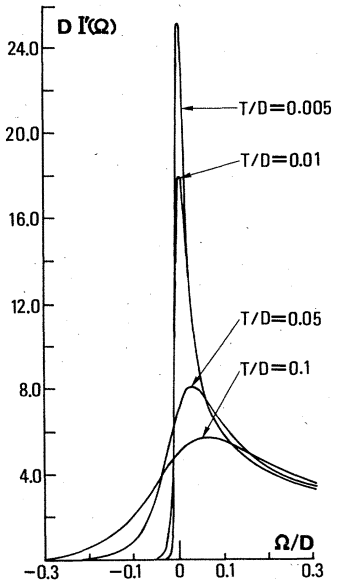

FIG. 1. Absorption spectra near the threshold at a finite temperature T. The spectrum $I'(\Omega)$ is defined by Eq. (6.18). Ω is the frequency measured from the absorption threshold at $T=0$. D is the distance between the Fermi level and the upper band edge of the conduction band, which normalizes Ω, T, and $I'(\Omega)$. The curves for four different temperatures are plotted for δ_0 (the phase shift at the Fermi level) chosen arbitrarily to be $\pi/3$.

Some typical absorption spectra are plotted in Fig. 1. We put arbitrarily $\delta_0=\pi/3$ and treat T as a parameter. Because of the ambiguity due to the factor p_0 involved in (6.16), the curves for $I'(\Omega)$ defined below are plotted instead of $I(\omega)$:

$$I'(\Omega)=\mathrm{Re}\int_0^\infty dt\,e^{i\Omega t}\left[\frac{iD\sinh(\pi Tt)}{\pi T}\right]^{-1+\zeta_0} =\frac{1}{D}\left[\frac{D}{2\pi T}\right]^{\zeta_0}\mathrm{Re}\left[e^{(\pi/2)(-1+\zeta_0)i}\frac{\Gamma\left[\frac{1}{2}-\frac{\zeta_0}{2}-\frac{i\Omega}{2\pi T}\right]\Gamma(\zeta_0)}{\Gamma\left[\frac{1}{2}+\frac{\zeta_0}{2}-\frac{i\Omega}{2\pi T}\right]}\right] \tag{6.18}$$

with

$$\Omega=\omega-\omega_{\mathrm{th}}^0\,. \tag{6.19}$$

We see that when $\Omega>1/T$ the spectra coincide nearly with that of $T=0$ (power-law spectrum of ND), while in the region $\Omega<1/T$ the divergence at $T=0$ is removed by the temperature effect to yield a rounded peak near the absorption edge. In the opposite side of the threshold

($\Omega<0$), the sharp cutoff of the spectrum at $T=0$ becomes gradually blurred with increasing T, inducing a nonzero absorption spectrum spreading roughly of the order of T below the Fermi level.

VII. SUMMARY

The present paper gives an exact treatment of the thermal effect on the soft-x-ray absorption spectrum using the Hamiltonian of Nozières and De Dominicis.[1] The formulation in the first half of the paper consists of obtaining the matrix elements of the dipole moment between two Slater determinants and summing the transition probabilities over all possible initial and final states. Because of the multiplicity of excited many-particle states, the formulation needs several careful steps before arriving at the closed formula for the response function. For example, because of the orthogonality catastrophe,[6] the summation of the cross section should precede the process of letting the system size tend to infinity.

The thermal effect is incorporated in our formulation through the Boltzmann factor. The need of treating the Slater determinants led us to consider the system with a fixed number of N electrons (canonical ensemble). This is why our final form of the response function [Eqs. (3.28)—(3.32)] involves a distinction with regard to the roles played by the states above and below the Fermi level at $T=0$. The distinction perhaps implies that the formula may be further reduced quite generally, leading to a description of the thermal effect solely in terms of the Fermi-distribution function. (The calculation for a contact core-hole potential in the rest of the paper shows that this is indeed the case.) However, to see the relationship between the exact formula for $T=0$ given in the previous work[4] to that for $T\neq 0$ obtained in this paper, the results in the present forms (3.28)—(3.32) will probably be best.

In the second half of the paper, the exact formula was applied to the case of a contact core-hole potential. The explicit use of the wave functions in the final state reduces the response function to Eqs. (5.14)—(5.20), whose validity is not restricted to the asymptotic region of t. The result shows the way the ground-state energy shift and the dispersion integral are modified by the temperature effect. We showed that the dispersion integral, when dealt with in the asymptotic region, in fact, reproduces the result of Yuval and Anderson.[10,11]

Even in the asymptotic region of t, however, the derivation of the final answer [Eq. (6.16)] has not been straightforward at all. This is because of the unwieldy form of the dispersion integral at finite temperatures [Eq. (6.11)]. But it is worth pointing out here that the complication arose mostly because we had kept with an analytical formulation for the whole problem. We have in fact confirmed that the power-law behavior exhibited by Eq. (6.16) is derived quite easily by the numerical analysis based on Eq. (6.12). In this sense, it will be interesting to test the efficiency of the formulas (5.14)—(5.20) numerically in the frequency region far from the absorption edge.

Finally our approach yields the exact form of the prefactor of the power-law formula of the open-line contribution. It is expressed by the same form as that of $T=0$, given by our previous study. The results of Yuval and Anderson are thus improved in this respect by the present analysis.

APPENDIX A: EXPRESSIONS OF $\Delta'(\bar{\mu}\gamma\,|\,)$, $\Delta'(\,|\,\bar{m}b)$, $\Delta'(\bar{\mu}\,|\,\bar{m})$, AND $\Delta'(\gamma\,|\,b)$

The determinant $\Delta'(\bar{\mu}\gamma\,|\,)$ is defined by

$$\Delta'(\bar{\mu}\gamma\,|\,)=\det|\,[\underline{A}(\bar{\mu}\gamma\,|\,)]_{m_1\to b_1}\,|\ . \tag{A1}$$

The symbol $(m_1\to b_1)$ means the replacement of the m_1th column of $\underline{A}(\bar{\mu}\gamma\,|\,)$ by the new column b_1. Expansion of $\Delta'(\bar{\mu}\gamma\,|\,)$ with respect to the row γ and column b_1 using the cofactors leads to

$$\Delta'(\bar{\mu}\gamma\,|\,)=a_{\gamma b_1}\Delta_{\mu m_1}+\sum_{\mu_1,m}{}'a_{\gamma m}a_{\mu_1 b_1}\frac{\partial^2\Delta}{\partial a_{\mu m}\,\partial a_{\mu_1 m_1}}\ , \tag{A2}$$

the primed sum meaning the exclusion of the terms with $\mu_1=\mu$ and (or) $m=m_1$. By Jacobi's theorem[20] we can transform the derivative in the second term into a determinant of the cofactors $\Delta_{\mu m}$:

$$\frac{\partial^2\Delta}{\partial a_{\mu m}\,\partial a_{\mu_1 m_1}}=\Delta\det\begin{vmatrix}\Delta_{\mu m}/\Delta & \Delta_{\mu_1 m}/\Delta\\ \Delta_{\mu m_1}/\Delta & \Delta_{\mu_1 m_1}/\Delta\end{vmatrix}\ . \tag{A3}$$

Thus

$$\Delta'(\bar{\mu}\gamma\,|\,)=a_{\gamma b_1}\Delta_{\mu m_1}+\Delta\det\begin{vmatrix}\Delta(\bar{\mu}\gamma\,|\,)/\Delta & \sum\limits_{\mu_1,m}a_{\gamma m}a_{\mu_1 b_1}\Delta_{\mu_1 m}/\Delta\\ \Delta_{\mu m_1}/\Delta & \Delta(\,|\,\bar{m}_1 b_1)/\Delta\end{vmatrix}\ . \tag{A4}$$

Combining the first term with the second and using Eq. (2.3), we find the expression of $\Delta'(\bar{\mu}\gamma\,|\,)$ given by (A7).

Likewise, the determinant $\Delta'(\bar{\mu}\,|\,\bar{m})$ is defined by

$$\Delta'(\bar{\mu}\,|\,\bar{m})=-\det|\,[\underline{A}(\bar{\mu}\,|\,\bar{m})]_{m_1\to b_1}\,|\ . \tag{A5}$$

Expansion with respect to the column b_1 yields

$$\begin{aligned}\Delta'(\bar{\mu}\,|\,\bar{m})&=\sum_{\mu_1}a_{\mu_1 b_1}\frac{\partial\Delta(\bar{\mu}\,|\,\bar{m})}{\partial a_{\mu_1 m_1}}\\&=-\sum_{\mu_1}a_{\mu_1 b_1}\frac{\partial^2\Delta}{\partial a_{\mu m}\,\partial a_{\mu_1 m_1}}\ .\end{aligned} \tag{A6}$$

Then we can make use of the identity (A3). In this way, we obtain all the primed determinants. In summary we have

$$\begin{aligned}\Delta'(\bar{\mu}\gamma\,|\,)/\Delta&=\det\begin{vmatrix}\Delta(\bar{\mu}\gamma\,|\,)/\Delta & \Delta(\gamma\,|\,b_1)/\Delta\\ \Delta(\bar{\mu}\,|\,\bar{m}_1)/\Delta & \Delta(\,|\,\bar{m}_1 b_1)/\Delta\end{vmatrix},\\ \Delta'(\,|\,\bar{m}b)/\Delta&=\det\begin{vmatrix}\Delta(\,|\,\bar{m}b)/\Delta & \Delta(\,|\,\bar{m}b_1)/\Delta\\ \Delta(\,|\,\bar{m}_1 b)/\Delta & \Delta(\,|\,\bar{m}_1 b_1)/\Delta\end{vmatrix},\\ \Delta'(\bar{\mu}\,|\,\bar{m})/\Delta&=\det\begin{vmatrix}\Delta(\bar{\mu}\,|\,\bar{m})/\Delta & \Delta(\,|\,\bar{m}b_1)/\Delta\\ \Delta(\bar{\mu}\,|\,\bar{m}_1)/\Delta & \Delta(\,|\,\bar{m}_1 b_1)/\Delta\end{vmatrix},\\ \Delta'(\gamma\,|\,b)/\Delta&=\det\begin{vmatrix}\Delta(\gamma\,|\,b)/\Delta & \Delta(\gamma\,|\,b_1)/\Delta\\ \Delta(\,|\,\bar{m}_1 b)/\Delta & \Delta(\,|\,\bar{m}_1 b_1)/\Delta\end{vmatrix}.\end{aligned} \tag{A7}$$

APPENDIX B: CALCULATION OF $\det\underline{H}_\lambda(t)$

The rows or columns of the matrix $\underline{H}_\lambda(t)$ defined by Eq. (3.21) are labeled by γ and m. We extract the factor $|\Delta|^{-2}$ from $\det\underline{H}_\lambda(t)$ by converting the representation of the matrix $\underline{H}_\lambda(t)$ to that in terms of the labels μ and b. This may be carried out by the identity $\det(\underline{I}+\underline{X}\,\underline{Y})=\det(\underline{I}+\underline{Y}\,\underline{X})$, valid for arbitrary two matrices $\underline{X}$ and $\underline{Y}$. The forms (3.14) and (3.15) show that the matrices $\underline{K}$ and $\underline{K}^0$ have in fact the form of a product of two matrices.

For our purpose, it is convenient to extend the dimension of the matrix $\underline{A}$, originally defined by Eq. (2.2). Let $\underline{\mathscr{A}}$ be an $\mathscr{N}\times\mathscr{N}$ matrix defined by

$$\underline{\mathscr{A}}=\begin{bmatrix}\underline{A}(--) & \underline{A}(-+)\\ \underline{A}(+-) & \underline{A}(++)\end{bmatrix} \tag{B1}$$

with four block matrices: the $N\times N$ matrix $\underline{A}(--)$ in the block (μ,m); the $N\times M$ matrix $\underline{A}(-+)$ in the block (μ,b), the $M\times N$ matrix $\underline{A}(+-)$ in the block (γ,m), and the $M\times M$ matrix $\underline{A}(++)$ in the block (γ,b); here the indices $+,-$, etc., are introduced in relation to the Fermi level to make explicit the labeling of the row and columns of $\underline{\mathscr{A}}$. In this notation, $\underline{A}$ used in the text is $\underline{A}(--)$. In terms of $\underline{\mathscr{A}}$, the quantities $\Delta(\bar{\mu}\gamma\,|\,)$, etc., defined by Eq. (2.3) are rewritten as

$$\begin{aligned}\Delta(\bar{\mu}\gamma\,|\,)/\Delta&=[\underline{A}(+-)\underline{A}^{-1}(--)]_{\gamma\mu}\ ,\\ \Delta(\gamma\,|\,b)/\Delta&=[\underline{A}(++)-\underline{A}(+-)\underline{A}^{-1}(--)\underline{A}(-+)]_{\gamma b}\ ,\\ \Delta(\bar{\mu}\,|\,\bar{m})/\Delta&=-[\underline{A}^{-1}(--)]_{m\mu}\ ,\end{aligned} \tag{B2}$$

etc. The identity $\det|\,\underline{I}+\underline{X}\,\underline{Y}\,|=\det|\,\underline{I}+\underline{Y}\,\underline{X}\,|$ then leads to

$$\begin{aligned}\det\underline{H}_\lambda(t)=\det&\begin{vmatrix}\underline{H}'_\lambda(--\,|\,t) & \underline{H}'_\lambda(-+\,|\,t)\\ \underline{H}'_\lambda(+-\,|\,t) & \underline{H}'_\lambda(++\,|\,t)\end{vmatrix}\\&\times\prod_{\mu=1}^{N}e^{i\epsilon_\mu t}\prod_{b=1}^{M}e^{i\epsilon_b t^*}\ ,\end{aligned} \tag{B3}$$

where the block matrices $\underline{H}'_\lambda(--\,|\,t)$, etc., labeled by μ (for minus) and b (for plus) are defined by (dagger stands for Hermitian conjugate)

$$\begin{aligned}\underline{H}'_\lambda(--\,|\,t)&=[\underline{A}^{-1}(--)]^\dagger\\&\quad\times[\,e^{-i\underline{\epsilon}_m t^*}+\lambda\underline{B}(--\,|\,t)]\underline{A}^{-1}(--)\ ,\\ \underline{H}'(-+\,|\,t)&=\lambda[\underline{A}^{-1}(--)]^\dagger\underline{B}(-+\,|\,t)\\&\quad-[\underline{A}^{-1}(--)]^\dagger[\,e^{-i\underline{\epsilon}_m t^*}+\lambda\underline{B}(--\,|\,t)]\\&\quad\times\underline{A}^{-1}(--)\underline{A}(-+)\ ,\end{aligned} \tag{B4}$$

with the $N\times N$ diagonal matrix $\underline{\epsilon}_m$ given by Eq. (3.22). $\underline{H}'_\lambda(+-\,|\,t)$ and $\underline{H}'_\lambda(++\,|\,t)$ are expressed similarly. The matrices $\underline{B}(--\,|\,t)$, etc., in (B4) are the block matrices which constitute an $\mathscr{N}\times\mathscr{N}$ matrix $\underline{\mathscr{B}}(t)$ defined by

$$\underline{\mathscr{B}}(t)=\underline{\mathscr{A}}^\dagger e^{-i\underline{\epsilon}t}\underline{\mathscr{A}}=\begin{bmatrix}\underline{B}(--\,|\,t) & \underline{B}(-+\,|\,t)\\ \underline{B}(+-\,|\,t) & \underline{B}(++\,|\,t)\end{bmatrix}. \tag{B5}$$

Its rows and columns are labeled by the unperturbed states m (for $-$) and b (for $+$) in accordance with the definition of $\underline{\mathscr{A}}$. The diagonal matrix $\underline{\epsilon}$ in (B5) is

$$\underline{\epsilon}=\begin{bmatrix}\underline{\epsilon}_\mu & \underline{0}\\ \underline{0} & \underline{\epsilon}_\gamma\end{bmatrix} \tag{B6}$$

with $\underline{\epsilon}_\mu$ and $\underline{\epsilon}_\gamma$ defined similarly to $\underline{\epsilon}_m$.

By a direct matrix multiplication, it may be shown that

$$\begin{aligned}\det\underline{H}_\lambda(t)=\det&\begin{vmatrix}[\underline{A}^{-1}(--)]^\dagger & \underline{0}\\ -\underline{A}^\dagger(-+)[\underline{A}^{-1}(--)]^\dagger & \underline{I}\end{vmatrix}\det\begin{vmatrix}e^{-i\underline{\epsilon}_m t^*}+\lambda\underline{B}(--\,|\,t) & \lambda\underline{B}(-+\,|\,t)\\ \lambda\underline{B}(+-\,|\,t) & e^{-i\underline{\epsilon}_b t^*}+\lambda\underline{B}(++\,|\,t)\end{vmatrix}\\&\times\det\begin{vmatrix}\underline{A}^{-1}(--) & -\underline{A}^{-1}(--)\underline{A}(-+)\\ \underline{0} & \underline{I}\end{vmatrix}\prod_{\mu=1}^{N}e^{i\epsilon_\mu t}\prod_{b=1}^{M}e^{i\epsilon_b t^*}\ .\end{aligned} \tag{B7}$$

From $\Delta=\det\underline{A}(---)$ and (B5), it follows that

$$\det\underline{H}_\lambda(t)=\frac{1}{|\Delta|^2}\det|\underline{I}+\lambda\underline{\mathscr{B}}(t)e^{i\underline{\epsilon}_0 t^*}| \times\prod_{\mu=1}^{N}e^{i\epsilon_\mu t}\prod_{m=1}^{N}e^{-i\epsilon_m t^*}, \tag{B8}$$

with

$$\underline{\epsilon}_0=\begin{bmatrix}\underline{\epsilon}_m & \underline{0}\\ \underline{0} & \underline{\epsilon}_b\end{bmatrix}, \tag{B9}$$

from which, as combined with

$$[\underline{\mathscr{B}}(0)]_{kk'}=(\underline{\mathscr{A}}^\dagger\underline{\mathscr{A}})_{kk'}=\delta_{kk'}$$

due to the completeness of the initial and final states, we have Eq. (3.25) for the expression of $\det\underline{H}_\lambda(0)$.

The form (3.24) is obtained by the identity

$$\det\underline{H}_\lambda(t)=\exp[\mathrm{Tr}\ \ln\underline{H}_\lambda(t)], \tag{B10}$$

and

$$f(t)=f(0)+\int_0^t d\tau\frac{df(\tau)}{d\tau}, \tag{B11}$$

with

$$f(t)=\mathrm{Tr}\ln\underline{H}_\lambda(t). \tag{B12}$$

APPENDIX C: DERIVATION OF EQ. (4.13)

First we write down the full expression of $\underline{H}_{\lambda_s}(t)$. We introduce

$$h(t)=\underline{H}_{\lambda_s}(t)\begin{bmatrix}\underline{I}_\gamma & \underline{0}\\ \underline{0} & \lambda_s^{-1}\underline{I}_m\end{bmatrix}\begin{bmatrix}\underline{g}_\lambda & \underline{0}\\ \underline{0} & \underline{\bar{g}}_m\end{bmatrix}, \tag{C1}$$

where $\underline{I}_\gamma$ ($\underline{I}_m$) is the $M\times M$ ($N\times N$) unit matrix in the space $\gamma(m)$, and

$$(\underline{g}_\gamma)_{\gamma_1\gamma_2}=g_{\gamma_1}\delta_{\gamma_1\gamma_2},\quad(\underline{\bar{g}}_m)_{m_1m_2}=\bar{g}_{m_1}\delta_{m_1m_2} \tag{C2}$$

define the diagonal block matrices $\underline{g}_\gamma$ and $\underline{\bar{g}}_m$, with g_{γ_1} and $\bar{g}_{m_1}$ given by Eq. (4.11). Substitution of $\underline{K}$ and $\underline{K}^0$ into $H_{\lambda_s}(t)$ [Eq. (3.31)] yields

$$\underline{h}(t)=\underline{I}-iV\int_0^\infty d\tau[\underline{E}_1(\tau)\underline{e}\,\underline{E}_2'(\tau)+\underline{E}_2(t+\tau)\underline{e}\,\underline{E}_1'(t+\tau)]-N_0V^2\int_0^\infty d\tau\int_0^\infty d\tau'\underline{E}_1(\tau)\underline{e}\,\bar{\Phi}_1(t+\tau+\tau')\underline{E}_1'(t+\tau'). \tag{C3}$$

All the matrices involved here are of dimension $\mathcal{N}\times\mathcal{N}$ and except for the matrix $\underline{e}$ defined by

$$(\underline{e})_{ij}=1,\quad 1\le i,j\le\mathcal{N} \tag{C4}$$

they are diagonal. In the rule of writing only the (γ,γ) and (m,m) elements in the form $((\gamma,\gamma),(m,m))$, the diagonal matrices are defined by

$$\begin{aligned}
&\underline{E}_1(\tau)=(|X_{\gamma+}|e^{-i\epsilon_\gamma\tau},|X_{m+}|e^{-i\epsilon_m\tau}),\\
&\underline{E}_1'(t+\tau)=(|X_{\gamma+}|e^{-i\epsilon_\gamma(t+\tau)}g_\gamma,|X_{m+}|e^{-i\epsilon_m(t+\tau)}e^{\beta(\epsilon_m-\mu)}\bar{g}_m),\\
&\underline{E}_2(t+\tau)=(|\bar{X}_{\gamma+}|e^{i\delta_\gamma}e^{i\epsilon_\gamma(t+\tau)}e^{-\beta(\epsilon_\gamma-\mu)},-|\bar{X}_{m+}|e^{-i\delta_m}e^{i\epsilon_m(t+\tau)}),\\
&\underline{E}_2'(\tau)=(|\bar{X}_{\gamma+}|e^{i\delta_\gamma}e^{i\epsilon_\gamma\tau}e^{-\beta(\epsilon_\gamma-\mu)}g_\gamma,-|\bar{X}_{m+}|e^{-i\delta_m}e^{i\epsilon_m\tau}e^{\beta(\epsilon_m-\mu)}\bar{g}_m).
\end{aligned} \tag{C5}$$

The quantity $\bar{\Phi}_1(t+\tau+\tau')$ in (C3) is

$$\bar{\Phi}_1(t+\tau+\tau')=\bar{\phi}(t+\tau+\tau')+\lambda_s\phi_1(t+\tau+\tau'), \tag{C6}$$

$\bar{\phi}$ and ϕ_1 being given by Eq. (4.10).

Making use of the matrix $\underline{h}(t)$ and $\underline{E}_1(t)$, etc., we can express $A(t)$ [Eq. (3.29)] and $I_0(t)$ [Eq. (3.30)] in the following form:

$$\begin{aligned}
&A(t)=iV\,\mathrm{Tr}[\underline{e}\,\underline{E}_1'(t)\underline{h}^{-1}(t)\underline{E}_2(t)]+N_0V^2\int_0^\infty d\tau\bar{\Phi}_1(t+\tau)\mathrm{Tr}[\underline{e}\,\underline{E}_1'(t)\underline{h}^{-1}(t)\underline{E}_1(\tau)],\\
&I_0(t)=w^2\mathrm{Tr}[\underline{e}\,\underline{E}_1'(t)\underline{h}^{-1}(t)\underline{E}_1(0)],
\end{aligned} \tag{C7}$$

where the derivative d/dt in $A(t)$ has been used to evaluate the integral over τ' in (C3).

The calculation of the inverse matrix $\underline{h}^{-1}(t)$ is most involved. By expanding $\underline{h}^{-1}(t)$ using (C3), the form of $\underline{h}^{-1}$ is found to be

$$\begin{aligned}
\underline{h}^{-1}(t)=\underline{I}+\int_0^\infty d\tau\int_0^\infty d\tau'[&\underline{E}_1(\tau)\underline{e}M_{11}(\tau,t+\tau')\underline{E}_1'(t+\tau')+\underline{E}_1(\tau)\underline{e}M_{12}(\tau,\tau')\underline{E}_2'(\tau')\\
&+\underline{E}_2(t+\tau)\underline{e}M_{21}(t+\tau,t+\tau')\underline{E}_1'(t+\tau')+\underline{E}_2(t+\tau)\underline{e}M_{22}(t+\tau,\tau')\underline{E}_2'(\tau')],
\end{aligned} \tag{C8}$$

with four c-number (not matrix) unknowns $M_{11}(\tau,t+\tau'),\ldots,M_{22}(t+\tau,\tau')$. They are determined so that they satisfy $\underline{h}(t)\,\underline{h}^{-1}(t)=\underline{I}$, $\underline{I}$ being an $\mathcal{N}\times\mathcal{N}$ unit matrix. A lengthy calculation using (C3) and (C8) then leads to the following matrix relation:

$$\begin{bmatrix} 1-i\bar{\eta}-\Lambda_1 & -iVN_0\bar{\Phi}_1(1-i\eta)+iN_0V\bar{\Phi} \\ -iN_0V\Phi & 1-i\eta \end{bmatrix} \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix} = \begin{bmatrix} N_0V^2\bar{\Phi}_1 & iV \\ iV & 0 \end{bmatrix}, \tag{C9}$$

where η, $\bar{\eta}$, Φ, and $\bar{\Phi}$ are defined by Eq. (4.12), $\bar{\Phi}_1$ by (C6), and Λ_1 by

$$\Lambda_1=(N_0V)^2\bar{\Phi}_1\Phi . \tag{C10}$$

The multiplication between the time-dependent quantities is understood to be the matrix multiplication, as in Eq. (4.15). The time variables defining the rows and columns of M_{ij} are shown in (C8). In accordance with the labeling made explicit in Eqs. (4.12) and (C8), the matrix elements $(\tau, t+\tau')$, $(t+\tau, t+\tau')$, (τ,τ'), and $(t+\tau,\tau')$ of the time variables are needed for the (1,1), (2,1), (1,2), and (2,2) matrix elements of (C9), respectively.

Equation (C9) is solved algebraically. The result is

$$\begin{aligned} M_{11}(\tau, t+\tau')&=N_0V^2[\bar{\Psi}(1-\bar{\Lambda})^{-1}(1-i\eta)^{-1}]_{\tau,t+\tau'} , \\ M_{12}(\tau,\tau')&=iV[(1-\Lambda)^{-1}(1-i\bar{\eta})^{-1}]_{\tau,\tau'} , \\ M_{21}(t+\tau, t+\tau')&=iV[(1-\bar{\Lambda})^{-1}(1-i\eta)^{-1}]_{t+\tau,t+\tau'} , \\ M_{22}(t+\tau,\tau')&=-N_0V^2[\Psi(1-\Lambda)^{-1}(1-i\bar{\eta})^{-1}]_{t+\tau,\tau'} . \end{aligned} \tag{C11}$$

All the quantities involved here are defined in Eqs. (4.12) and (4.14), except for $\bar{\Lambda}$, which is defined by

$$\bar{\Lambda}=(N_0V)^2\Psi\bar{\Psi} . \tag{C12}$$

The right-hand sides of (C11) and (C12) should be dealt with in a fashion similar to the example of Eq. (4.15). The inverse matrix $\underline{h}^{-1}(t)$ with M_{ij} given above is then inserted into (C7) and arranged to give the final form. To convert $\bar{\Lambda}$ to Λ, the identity

$$(1-\bar{\Lambda})^{-1}\Psi=\Psi(1-\Lambda)^{-1} , \tag{C13}$$

which is confirmed straightforwardly by the power-series expansion with respect to $\bar{\Lambda}$ or Λ, is useful. After a tedious but elementary calculation we reach the result summarized by Eq. (4.13).

APPENDIX D: DERIVATION OF EQS. (5.10) AND (5.11) BY THE METHOD OF WIENER AND HOPF

In order to solve Eq. (5.2), we introduce the following two functions,

$$r^+_{\tau,\tau'}=\begin{cases} r_{\tau,\tau'}, & \tau>0 \\ 0, & \tau<0 \end{cases}$$
$$r^-_{\tau,\tau'}=\begin{cases} 0, & \tau>0 \\ -r_{\tau,\tau'}, & \tau<0 \end{cases} \tag{D1}$$

for the extended region of $-\infty<\tau<\infty$ and $\tau'>0$. Equation (5.2) is then rewritten as

$$r^+_{\tau,\tau'}-r^-_{\tau,\tau'}-i\int_{-\infty}^{\infty}d\rho\,\eta_{\tau,\rho}r^+_{\rho,\tau'}=\Theta(\tau)\delta(\tau-\tau') , \tag{D2}$$

$\Theta(\tau)$ being the step function. In Fourier space we have

$$\frac{r^+(\omega)_{\tau'}}{Z_+(\omega)}-\frac{r^-(\omega)_{\tau'}}{Z_-(\omega)}=\frac{e^{i\omega\tau'}}{Z_-(\omega)} , \tag{D3}$$

where the decomposition (5.8) is employed, and

$$r^{\pm}(\omega)_{\tau'}=\int_{-\infty}^{\infty}d\tau\,r^{\pm}_{\tau,\tau'}e^{i\omega\tau} \tag{D4}$$

defines the Fourier transform. By (D1) and (D4), $r^+(\omega)_{\tau'}$, $[r^-(\omega)_{\tau'}]$ is regular on the upper (lower) half ω plane. Thus, solving for $r^+(\omega)_{\tau'}$ and $r^-(\omega)_{\tau'}$ of (D3) is just a standard Hilbert problem. We find[15]

$$r^+(\omega)_{\tau'}=\frac{Z_+(\omega)}{2\pi i}\int_{-\infty}^{\infty}d\omega'\frac{e^{i\omega'\tau'}}{Z_-(\omega')(\omega'-\omega-i\delta)} . \tag{D5}$$

The inverse Fourier transform leads to

$$\begin{aligned} r^+_{0,\tau'}&=\lim_{\epsilon\to 0+}r^+_{\epsilon,\tau'} \\ &=\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\frac{e^{i\omega'\tau'}}{Z_-(\omega')}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi i}\frac{Z_+(\omega)e^{-i\omega(0+)}}{\omega'-\omega-i\delta} . \end{aligned} \tag{D6}$$

Since

$$\frac{1}{2\pi i}\int_{-\infty}^{\infty}d\omega\frac{Z_+(\omega)e^{-i\omega(0+)}}{\omega'-\omega-i\delta}=\frac{1}{\pi i}\int_{-\infty}^{\infty}d\omega\frac{Z_+(\omega)}{\omega'-\omega-i\delta}$$
$$=1 , \tag{D7}$$

as obtained by making use of the contour integration, it holds that

$$r_{0,\tau'}=\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\frac{e^{i\omega'\tau'}}{Z_-(\omega')} , \tag{D8}$$

which is Eq. (5.10).

In deriving $\Psi_{t+\tau,\tau'}$ defined by Eq. (4.14), we have only to replace $e^{i\omega\tau'}$ in (D3) by

$$\int_{-\infty}^{\infty}\Theta(\tau)\Phi_{t+\tau,\tau'}e^{i\omega\tau}d\tau=\frac{i}{N_0}\left[\sum_{\gamma}g_{\gamma}\,|\,X_{\gamma+}\,|^2\frac{e^{-i\epsilon_{\gamma}(t+\tau')}}{\omega-\epsilon_{\gamma}+i\delta}+\sum_m\bar{g}_m\,|\,X_{m+}\,|^2e^{\beta(\epsilon_m-\mu)}\frac{e^{-i\epsilon_m(t+\tau')}}{\omega-\epsilon_m+i\delta}\right] . \tag{D9}$$

Using the fact that $\bar{g}_m\exp[\beta(\epsilon_m-\mu)]$ and g_{γ} defined by Eq. (4.11) are both rewritten as $\bar{f}_k(1-i\eta(\epsilon_k))$ ($k=m$ or γ) with the Fermi distribution function $\bar{f}_k=1-f_k$ [Eq. (5.12)], we obtain

$$N_0\Psi^+(\omega)_{\tau'}=i\sum_k\bar{f}_k\,|\,X_{k+}\,|^2\frac{Z_+(\omega)e^{-i\epsilon_k(t+\tau')}}{Z_+(\epsilon_k)(\omega-\epsilon_k+i\delta)} . \tag{D10}$$

For the Fourier transforms for $\bar{\Psi}$ and $i\bar{\eta}$, it is con-

venient to define them in terms of the factor $e^{-i\omega t}$ (the complex conjugate to that used in Ψ and $i\eta$), because it then holds that $\eta(\omega)=\bar{\eta}(\omega)$. In this case, $\bar{\Psi}^{+}(\omega)_{\tau}$ is regular on the lower half ω plane. We find

$$N_0\bar{\Psi}^{+}(\omega)_{\tau}=-i\sum_k f_k\,|\,\bar{X}_{k+}\,|^2\frac{Z_-(\epsilon_k)e^{i\epsilon_k(t+\tau')}}{Z_-(\omega)(\omega-\epsilon_k-i\delta)}\ . \tag{D11}$$

The inverse Fourier transform of (D10) and (D11) then gives Eq. (5.11).

APPENDIX E: DERIVATION OF EQS. (5.14)–(5.18)

In accordance with the form (4.13), we divide $A(t)$ into two parts,

$$A(t)=A_1(t)+A_2(t)\ , \tag{E1}$$

where

$$A_1(t)=[i\bar{\eta}(1-\Lambda)^{-1}(1-i\bar{\eta})^{-1}]_{0,0}$$

and

$$A_2(t)=(N_0V)^2[\Psi(1-\Lambda)^{-1}\bar{\Psi}]_{t,t} \tag{E2}$$

are the matrix forms of the first and second terms of Eq. (4.13), respectively. The prescription of the transformation is given prior to Eq. (5.14). As an example, we calculate the term of $O(\Lambda)$ of $A_2(t)$,

$$A_2^{(1)}(t)=(N_0V)^2(\Psi\Lambda\bar{\Psi})_{t,t}\ . \tag{E3}$$

Since $\Lambda=(N_0V)^2\bar{\Psi}\Psi$ [Eq. (4.14)], the explicit form of $A_2^{(1)}(t)$ is

$$A_2^{(1)}(t)=(N_0V)^4\times\int_0^\infty d\sigma\int_0^\infty d\rho\int_0^\infty d\tau\,\Psi_{t,\sigma}\bar{\Psi}_{\sigma,t+\rho}\Psi_{t+\rho,\tau}\bar{\Psi}_{\tau,t}\ . \tag{E4}$$

From Eq. (5.11), the first factor $\Psi_{t,\sigma}$ contains $\sigma_k(0+)$, which is

$$\sigma_k(0+)=\frac{1}{2\pi i}\int_{-\infty}^{\infty}d\omega\,e^{-i\omega(0+)}\frac{Z_+(\omega)/Z_+(\epsilon_k)}{\epsilon_k-\omega-i\delta}\ . \tag{E5}$$

This integral is evaluated as in (D7) by the trick of dropping the exponential factor and adding an integral along the semicircle in the upper half ω plane. The result is

$$\sigma_k(0+)=1/Z_+(\epsilon_k)\ . \tag{E6}$$

With (E6) three integrals in (E4) are easily carried out. We find

$$A_2^{(1)}(t)=iV^4\sum_{\{k\}}\bar{f}_{k_1}\,|\,X_{k_1+}\,|^2\frac{e^{-i\epsilon_{k_1}t}}{Z_+(\epsilon_{k_1})}f_{k_2}\,|\,\bar{X}_{k_2+}\,|^2\frac{Z_-(\epsilon_{k_2})/Z_-(\epsilon_{k_1})}{\epsilon_{k_2}-\epsilon_{k_1}+i\delta}$$
$$\times e^{i\epsilon_{k_2}t}\bar{f}_{k_3+}\,|\,X_{k_3+}\,|^2\frac{Z_+(\epsilon_{k_2})/Z_+(\epsilon_{k_3})}{\epsilon_{k_3}-\epsilon_{k_2}-i\delta}e^{-i\epsilon_{k_3}t}f_{k_4}\,|\,\bar{X}_{k_4+}\,|^2\frac{Z_-(\epsilon_{k_4})/Z_-(\epsilon_{k_3})}{\epsilon_{k_4}-\epsilon_{k_3}+i\delta}e^{i\epsilon_{k_4}t}\ . \tag{E7}$$

The energy denominators are then rewritten using Eq. (4.8). In addition to $\Psi(t)$ and $\bar{\Psi}(t)$ defined by Eq. (5.16), we must introduce the third quantity $\bar{\Psi}_1(t)$,

$$N_0\bar{\Psi}_1(t)=\sum_k f_k\,|\,\bar{X}_{k+}\,|^2Z_-(\epsilon_k)e^{i\epsilon_k t}\ . \tag{E8}$$

Then,

$$A_2^{(1)}(t)=(N_0V)^2\int_0^\infty d\sigma\int_0^\infty d\tau\,\Psi(t+\sigma)\left[(N_0V)^2\int_0^\infty d\rho\,\bar{\Psi}(t+\sigma+\rho)\Psi(t+\rho+\tau)\right]\bar{\Psi}_1(t+\tau)\ . \tag{E9}$$

The term in large parentheses gives $\Lambda(t+\sigma,t+\tau)$ defined by Eq. (5.18).

The higher-order terms of $A_2(t)$ and the terms $A_1(t)$ and $I_0(t)$ are similarly treated. In this way we obtain

$$\begin{aligned}A_1(t)&=\int_0^\infty d\tau\,i\eta^0(\tau)F(t+\tau,t+)\ ,\\ A_2(t)&=(N_0V)^2\int_0^\infty d\sigma\int_0^\infty d\tau\,\Psi(t+\sigma)F(t+\sigma,t+\tau)\bar{\Psi}_1(t+\tau)\ ,\\ I_0(t)&=N_0w^2\int_0^\infty d\tau\,\Psi(t+\tau)F(t+\tau,t+)\ ,\end{aligned} \tag{E10}$$

with

$$i\eta^0(\rho)=\int_{\bar{D}}^{D}\frac{d\omega}{2\pi}\left[\frac{1}{Z_-(\omega)}-\frac{1}{Z_+(\omega)}\right]e^{-i\omega\rho}\ , \tag{E11}$$

where the quantity F is the solution of the integral equation (5.17). In (E10), $I_0(t)$ has just the form given by Eq. (5.14), while in $A(t)$ some more transformations are required before reaching Eq. (5.14).

Note first that

$$N_0\bar{\Psi}_1(t)=\int_0^\infty d\rho\,N_0\bar{\Psi}(t+\rho)\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\frac{e^{-i\omega\rho}}{Z_+(\omega)}\ , \tag{E12}$$

as confirmed by integrating over ρ with the use of the definition of $\bar{\Psi}(t)$ given by Eq. (5.16). Dividing $1/Z_+(\omega)$ into two parts,

$$\frac{1}{Z_+(\omega)}=1+\left[\frac{1}{Z_+(\omega)}-1\right], \tag{E13}$$

we find

$$A_2(t)=(N_0V)^2\int_0^\infty d\sigma\int_0^\infty d\tau\,\Psi(t+\sigma)F(t+\sigma,t+\tau)\bar{\Psi}(t+\tau)$$
$$+(N_0V)^2\int_0^\infty d\sigma\int_0^\infty d\tau\int_0^\infty d\rho\,\Psi(t+\sigma)F(t+\sigma,t+\tau)\bar{\Psi}(t+\tau+\rho)\int_{-\infty}^\infty\frac{d\omega}{2\pi}\left[\frac{1}{Z_+(\omega)}-1\right]e^{-i\omega\rho}. \tag{E14}$$

Dividing F as well into two parts within $A_1(t)$, we find

$$A_1(t)=i\eta^0+\int_0^\infty d\rho\, i\eta^0(\rho)[F(t+\rho,t+)-\delta_+(\rho)], \tag{E15}$$

where $\delta_+(t)=\lim_{\epsilon\to 0+}\delta(t-\epsilon)$ and $\eta^0\,[=\eta^0(0)]$ is, from (E11), given by Eq. (5.15). The sum of the first terms of $A_1(t)$ and $A_2(t)$ is just given by Eq. (5.14). Our remaining task is thus to confirm the exact cancellation between the second term of $A_1(t)$ and that of $A_2(t)$. By means of the identities

$$\int_{-\infty}^\infty\frac{d\omega}{2\pi}=\left[\int_{-\infty}^{\bar{D}}+\int_{\bar{D}}^{D}+\int_D^\infty\right]\frac{d\omega}{2\pi}, \tag{E16}$$

$$i\eta^0(\rho)=\int_{\bar{D}}^{D}\frac{d\omega}{2\pi}\left[\frac{1}{Z_-(\omega)}-1-\left[\frac{1}{Z_+(\omega)}-1\right]\right]e^{-i\omega\rho},$$

$$Z_+(\omega)=Z_-(\omega),\quad \omega>D,\ \omega<\bar{D}$$

as combined with the series expansion of $F\,[=(1-\Lambda)^{-1}]$ with respect to the factor Λ, the cancellation may be, in fact, checked.

APPENDIX F: DERIVATION OF REAL PART OF $i\eta^0$

The real part of $i\eta^0$ is, from Eq. (5.19),

$$\mathrm{Re}(i\eta^0)=\frac{1}{4\pi}\int_{\bar{D}}^{D}d\epsilon\ln[1-4f(\epsilon)\bar{f}(\epsilon)\sin^2\delta(\epsilon)], \tag{F1}$$

with $\bar{f}(\epsilon)=1-f(\epsilon)$ [Eq. (5.6)]. The Taylor expansion of the integrand yields

$$\mathrm{Re}(i\eta^0)=-\frac{1}{4\pi}\sum_{n=1}\frac{1}{n}\int_{\bar{D}}^{D}d\epsilon[4f(\epsilon)\bar{f}(\epsilon)\sin^2\delta(\epsilon)]^n\simeq-\frac{T}{4\pi}\sum_{n=1}^{\infty}\frac{(2\sin\delta_0)^{2n}}{n}\frac{[(n-1)!]^2}{(2n-1)!}. \tag{F2}$$

In the second line we have set $\sin\delta(\omega)=\sin\delta_0$, $D=|\bar{D}|=\infty$. The procedure is obviously allowed when $T\ll D, |\bar{D}|$, because of the factor $f(\epsilon)\bar{f}(\epsilon)$. Comparing (F2) with the Taylor expansion of $(\sin^{-1}x)^2$, we find

$$\mathrm{Re}(i\eta^0)=-\frac{T}{\pi}[\sin^{-1}(\sin\delta_0)]^2=-\pi T(\delta_0/\pi)^2, \tag{F3}$$

which is Eq. (6.7).

APPENDIX G: ASYMPTOTIC FORM OF $\Psi(t)$ AND $\bar{\Psi}(t)$

We present the derivation of Eq. (6.11) based on Eq. (5.16), which is reproduced here for $\Psi(t)$,

$$N_0\Psi(t)=\sum_k\bar{f}_k|X_{k+}|^2[Z_+(\epsilon_k)Z_-(\epsilon_k)]^{-1}e^{-i\epsilon_k t} \tag{G1}$$

The quantity $Z_\pm(\omega)$ is defined by Eq. (5.9). For simplicity, let us write $Z_\pm(\omega)$ as

$$Z_\pm(\omega)=\exp[J_\pm(\omega)], \tag{G2}$$

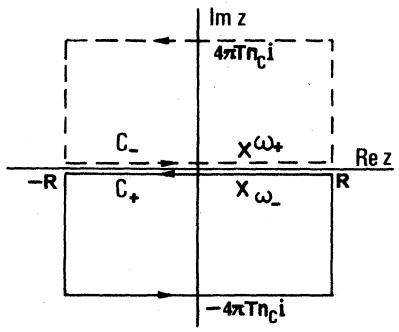

FIG. 2. Contour C_+ for $\bar{J}_+^{(3)}(\omega)$ and C_- for $\bar{J}_-^{(3)}(\omega)$ used in (G7). Since the integrands $\mathcal{J}_+(z)$ and $\mathcal{J}_-(z)$ have branch points at $z=\omega_+$ and $z=\omega_-$, respectively, the contours are chosen so that they do not include the branch point inside.

$J_{\pm}(\omega)$ being the exponent of Eq. (5.9). Substituting $1-i\eta(\omega)$ given by Eq. (5.7) into $J_{\pm}(\omega)$ and integrating it by parts, we find

$$J_{\pm}=\sum_{k=1}^{3}J_{\pm}^{(k)}(\omega)\ ,$$

with

$$J_{\pm}^{(1)}(\omega)=-\frac{1}{2\pi i}\left[\ln(\epsilon-\omega_{\pm})\ln\left[e^{i\delta(\epsilon)}\frac{\cosh(\beta\epsilon/2)}{\cosh\{[\beta\epsilon-2i\delta(\epsilon)]/2\}}\right]\Bigg|_{\bar{D}}^{0}+\ln(\epsilon-\omega_{\pm})\ln\left[e^{-i\delta(\epsilon)}\frac{\cosh(\beta\epsilon/2)}{\cosh\{[\beta\epsilon-2i\delta(\epsilon)]/2\}}\right]\Bigg|_{0}^{D}\right]$$

$$J_{\pm}^{(2)}(\omega)=-\frac{1}{2\pi}\int_{\bar{D}}^{D}d\epsilon\frac{\epsilon}{|\epsilon|}\ln(\epsilon-\omega_{\pm})\left[1-\frac{\epsilon}{|\epsilon|}\tanh\{[\beta\epsilon-2i\delta(\epsilon)]/2\}\right]\dot{\delta}(\epsilon)\ ,$$

$$J_{\pm}^{(3)}(\omega)=\frac{\beta}{4\pi}\int_{\bar{D}}^{D}d\epsilon\ln(\epsilon-\omega_{\pm})\frac{\sin\delta(\epsilon)}{\cosh(\beta\epsilon/2)\cosh\{[\beta\epsilon-2i\delta(\epsilon)]/2\}}\ .$$

From $\delta(D)=\delta(\bar{D})=0$, only the phase shift $\delta_0=\delta(0)$ at the Fermi level enters in $J_{\pm}^{(1)}(\omega)$. The integrand of $J_{\pm}^{(2)}(\omega)$ is appreciable when $\epsilon<\beta^{-1}$. The derivative $\dot{\delta}(\epsilon)=(d/d\epsilon)\delta(\epsilon)$ is generally of the order of π/D, so that $J_{\pm}^{(2)}(\omega)=O(T/D)$, which we neglect by the condition (6.6). In $J_{\pm}^{(3)}(\omega)$ the integrand is again appreciable when $\epsilon<T$, but it has a value independent of $D,\bar{D}$. In view of Eq. (6.6), we can set $D=|\bar{D}|=\infty$ and $\delta(\epsilon)=\delta_0$ therein. In this way we obtain

$$J_{\pm}(\omega)=J_{\pm}^{(1)}(\omega)+J_{\pm}^{(3)}(\omega)\ , \tag{G3}$$

where

$$J_{\pm}^{(1)}(\omega)=\begin{cases}-\dfrac{\delta_0}{\pi}(\ln|\omega|\mp\pi i), & \omega>0\\ -\dfrac{\delta_0}{\pi}\ln|\omega|, & \omega<0\end{cases} \tag{G4}$$

and

$$J_{\pm}^{(3)}(\omega)=\int_{-\infty}^{\infty}d\epsilon\,\mathcal{J}_{\pm}(\epsilon)\ , \tag{G5}$$

with

$$\mathcal{J}_{\pm}(\epsilon)=\frac{\beta}{4\pi}\sin\delta_0\frac{\ln(\epsilon-\omega_{\pm})}{\cosh(\beta\epsilon/2)\cosh[(\beta\epsilon-2i\delta_0)/2]}\ . \tag{G6}$$

$J_{\pm}^{(3)}(\omega)$ is derived by the contour integral. Let $\bar{J}_{\pm}^{(3)}(\omega)$ be

$$\bar{J}_{\pm}^{(3)}(\omega)=\int_{C_{\pm}}dz\,\mathcal{J}_{\pm}(z)\ , \tag{G7}$$

where C_+ (C_-), shown in Fig. 2, is chosen so that it may not contain the branch point $z=\omega_+$ ($z=\omega_-$) inside it. Within C_+ or C_-, therefore, there are only a series of poles due to $[\cosh\beta z/2]^{-1}$ and $[\cosh(\beta z-2i\delta_0)/2]^{-1}$. Dropping the contributions along the vertical parts which vanish in the limit $R\to\infty$, it follows that

$$\bar{J}_{\pm}^{(3)}(\omega)=\frac{\beta}{4\pi}\sin\delta_0\int_{-R}^{R}dx\frac{\ln(x-\omega_{\pm})-\ln(x\mp4\pi Tn_c i-\omega_{\pm})}{\cosh(\beta x/2)\cosh[(\beta x-2i\delta_0)/2]}\ . \tag{G8}$$

In the limit $R\to\infty$ and $n_c\to\infty$, the term with $\ln(x-\omega_{\pm})$ yields just $J_{\pm}^{(3)}(\omega)$, while the rest may be evaluated by direct integration over x by setting

$$\ln(x\mp4\pi Tn_c i-\omega_{\pm})\to\ln(\mp4\pi Tn_c i)\ .$$

On the other hand, $\bar{J}_{\pm}^{(3)}(\omega)$ is expressed as a sum of the residues at the poles inside $C_{\pm}$. Hence, we have

$$J_{\pm}^{(3)}(\omega)=\lim_{n_c\to\infty}\left[\frac{\delta_0}{\pi}\ln(\mp4\pi Tn_c i)\pm\sum_{k=0}^{2n_c-1}\ln\frac{\beta\omega_{\pm}-2i\delta_0\pm(2k+1)\pi i}{\beta\omega_{\pm}\pm(2k+1)\pi i}\right]. \tag{G9}$$

Combining (G4) and (G9) and making use of the definition of Weierstrass for the Γ function, we obtain

$$Z_{+}(\omega)=\left|\frac{\beta\omega}{2\pi}\right|^{-\delta_0/\pi}\frac{\Gamma(\frac{1}{2}-i(\beta\omega/2\pi))}{\Gamma(\frac{1}{2}-i[(\beta\omega-2i\delta_0)/2\pi])}e^{i\delta_0\omega/2|\omega|}\ ,$$

$$Z_{-}(\omega)=\left|\frac{\beta\omega}{2\pi}\right|^{-\delta_0/\pi}\frac{\Gamma(\frac{1}{2}+i[(\beta\omega-2i\delta_0)/2\pi])}{\Gamma(\frac{1}{2}+i(\beta\omega/2\pi))}e^{-i\delta_0\omega/2|\omega|}\ . \tag{G10}$$

Now substitution of (G10) into (G1), as combined with the definition of $|X_{k+}|^2$ given by Eq. (6.8), leads to

$$N_0\Psi(t)=\left[\frac{\beta}{2\pi}\right]^{2\delta_0/\pi}|X(0)|^2\sum_k \bar{f}_k\frac{\Gamma(\frac{1}{2}-i[(\beta\epsilon_k-2i\delta_0)/2\pi])\Gamma(\frac{1}{2}+i(\beta\epsilon_k/2\pi))}{\Gamma(\frac{1}{2}-i(\beta\epsilon_k/2\pi))\Gamma(\frac{1}{2}+i[(\beta\epsilon_k-2i\delta_0)/2\pi])}e^{-i\epsilon_k t},$$
$$N_0\bar{\Psi}(t)=\left[\frac{\beta}{2\pi}\right]^{-2\delta_0/\pi}|\bar{X}(0)|^2\sum_k f_k\frac{\Gamma(\frac{1}{2}+i[(\beta\epsilon_k-2i\delta_0)/2\pi])\Gamma(\frac{1}{2}-i(\beta\epsilon_k/2\pi))}{\Gamma(\frac{1}{2}+i(\beta\epsilon_k/2\pi))\Gamma(\frac{1}{2}-i[(\beta\epsilon_k-2i\delta_0)/2\pi])}e^{i\epsilon_k t}. \tag{G11}$$

The sum over k may be changed to the integral over $-\infty<\epsilon_k<\infty$, which is evaluated by adding an integral along the semicircle in the lower [for $\Psi(t)$] and upper [$\bar{\Psi}(t)$] half of the complex ϵ_k plane. We have only to calculate the residues at the poles. Noting that the poles due to $\bar{f}_k$ are removed by the zeros of $\Gamma(\frac{1}{2}-i(\beta\epsilon_k/2\pi))^{-1}$ [in the case of $\Psi(t)$], we obtain $\Psi(t)$. The calculation of $\bar{\Psi}(t)$ is similar. The result is

$$\Psi(t)=\left[\frac{2\pi T}{i}\right]^{1-\alpha}|X(0)|^2e^{-\pi Tt(1-\alpha)}\Gamma\left[1-\frac{\alpha}{2}\right]^2F\left[1-\frac{\alpha}{2},1-\frac{\alpha}{2},1\middle|e^{-2\pi Tt}\right],$$
$$\bar{\Psi}(t)=\left[\frac{2\pi T}{i}\right]^{1+\alpha}|\bar{X}(0)|^2e^{-\pi Tt(1+\alpha)}\Gamma\left[1+\frac{\alpha}{2}\right]^2F\left[1+\frac{\alpha}{2},1+\frac{\alpha}{2},1\middle|e^{-2\pi Tt}\right]. \tag{G12}$$

For the notations, see text. By means of Kummer's relation for the hypergeometric functions, we may rewrite (G12). For example, we have

$$\Psi(t)=\left[\frac{\pi T}{i\sinh\pi Tt}\right]^{1-\alpha}|X(0)|^2\Gamma\left[1-\frac{\alpha}{2}\right]^2F\left[\frac{\alpha}{2},\frac{\alpha}{2},1\middle|e^{-2\pi Tt}\right],$$
$$\bar{\Psi}(t)=\left[\frac{\pi T}{i\sinh\pi Tt}\right]^{1+\alpha}|\bar{X}(0)|^2\Gamma\left[1+\frac{\alpha}{2}\right]^2F\left[-\frac{\alpha}{2},-\frac{\alpha}{2},1\middle|e^{-2\pi Tt}\right]. \tag{G13}$$

In the limit $T=0$, the identity

$$F\left[\pm\frac{\alpha}{2},\pm\frac{\alpha}{2},1\middle|1\right]=\Gamma(1\mp\alpha)/\Gamma\left[1\mp\frac{\alpha}{2}\right]^2 \tag{G14}$$

reduces (G13) to

$$[\Psi(t)]_{T=0}=(it)^{-1+\alpha}|X(0)|^2\Gamma(1-\alpha),\quad[\bar{\Psi}(t)]_{T=0}=(it)^{-1-\alpha}|\bar{X}(0)|^2\Gamma(1+\alpha), \tag{G15}$$

which are precisely the asymptotic forms of $\phi(t)$ and $\bar{\phi}(t)$ used in Eq. (5.9) of OT for the analysis of the edge anomalies at $T=0$.

APPENDIX H: POWER-SERIES FORMS FOR $A(t)$ AND $I_0(t)$ AND THE DERIVATION OF THEIR ANALYTICAL EXPRESSIONS

Using the expression (6.12) for $\Lambda(t+\sigma,t+\rho)$, the integrals over the time variables in Eqs. (5.14) and (5.17) are now straightforward. In the following, the symbol x is used in place of $e^{-2\pi Tt}$:

$$x=e^{-2\pi Tt}. \tag{H1}$$

All the summations over the integer variables, such as $\sum_m$, are to be understood to run from zero to infinity.

From Eq. (5.17) we find

$$F(t+\sigma,t+\tau)=\delta(\sigma-\tau)-\tfrac{1}{2}\pi T\alpha^2x\sum_{m,n,l}\exp[-\pi T(1+\alpha+2m)\sigma]$$
$$\times[\underline{\lambda}(x)]_{m,l}\{[\underline{I}-\underline{L}(x)]^{-1}\}_{l,n}\exp[-\pi T(1-\alpha+2n)\tau], \tag{H2}$$

where

$$[\underline{\lambda}(x)]_{m,n}=x^m\left[\frac{(1+\alpha/2)_m}{m!}\right]^2\frac{1}{m+n+1}\left[\frac{(1-\alpha/2)_n}{n!}\right]^2x^n,\quad[\underline{L}(x)]_{m,n}=-\frac{\alpha^2}{4}x\sum_l\frac{1}{m+l+1}[\lambda(x)]_{l,n}. \tag{H3}$$

Substituting (H2) into Eqs. (5.14) and using the expressions (6.11) for $\Psi(t)$ and $\bar{\Psi}(t)$, we find

$$A(t)=i\eta^0-\tfrac{1}{2}\pi T\alpha^2xS_1(x),\quad I_0(t)=N_0w^2\left[\frac{2\pi T}{i}\right]^{1-\alpha}|X(0)|^2\Gamma\left[1-\frac{\alpha}{2}\right]^2x^{(1-\alpha)/2}S_2(x), \tag{H4}$$

where

$$S_1(x)=\sum_{m,n,l}[\underline{\lambda}(x)]_{m,l}\{[\underline{I}-\underline{L}(x)]^{-1}\}_{l,n}\ ,\quad S_2(x)=\sum_{n,l}(l+1)[\underline{\lambda}(x)]_{0,l}\{[\underline{I}-\underline{L}(x)]^{-1}\}_{l,n}\ . \tag{H5}$$

From (H3), the explicit form of $S_1(x)$ is obtained as

$$S_1(x)=\sum_{\{m\}}[\,(m_1,m_2)x^{m_1+m_2}+(-\tfrac{1}{4}\alpha^2x)(m_1,m_2,m_3,m_4)x^{m_1+\cdots+m_4}$$
$$+(-\tfrac{1}{4}\alpha^2x)^2(m_1,\ldots,m_6)x^{m_1+\cdots+m_6}+\cdots\,]\ , \tag{H6}$$

where

$$(m_1,m_2)=(+)_{m_1}\frac{1}{(1,2)_1}(-)_{m_2},\quad (m_1,\ldots,m_4)=(+)_{m_1}\frac{1}{(1,2)_1}(-)_{m_2}\frac{1}{(2,3)_1}(+)_{m_3}\frac{1}{(3,4)_1}(-)_{m_4}\ , \tag{H7}$$
$$\vdots$$

with

$$(\pm)_m=\left[\frac{(1\pm\alpha/2)_m}{m!}\right]^2,$$
$$\frac{1}{(1,2)_k}=\frac{1}{m_1+m_2+k},\quad k=0,1,2\ . \tag{H8}$$

For $S_2(x)$ we have

$$S_2(x)=\sum_{\{m\}}[\,(m_1)x^{m_1}+(-\tfrac{1}{4}\alpha^2x)(m_1,m_2,m_3)x^{m_1+m_2+m_3}$$
$$+(-\tfrac{1}{4}\alpha^2x)^2(m_1,\ldots,m_5)x^{m_1+\cdots+m_5}+\cdots\,]\ , \tag{H9}$$

with

$$(m_1)=(-)_{m_1}\ ,$$
$$(m_1,m_2,m_3)=(-)_{m_1}\frac{1}{(1,2)_1}(+)_{m_2}\frac{1}{(2,3)_1}(-)_{m_3}\ , \tag{H10}$$
$$\vdots\ .$$

A slightly different form arises in $S_2(x)$ because of the presence of the factor $[\lambda(x)]_{0,l}$ in place of $[\lambda(x)]_{m,l}$ in (H5).

Now we show that

$$S_1(x)=1/(1-x),\quad S_2(x)=(1-x)^{-1+\alpha}\ . \tag{H11}$$

If (H11) is established, substitution of (H11) into (H4) leads immediately to Eqs. (6.14) and (6.15) [note that $\mathrm{Re}(i\eta^0)=-\pi T(\delta_0/\pi)^2=-\frac{1}{4}\pi T\alpha^2$ by Eq. (6.7)]. The proof for $S_1(x)$ is given here. That for $S_2(x)$ is performed analogously if the several key relations summarized at the end are employed.

The Taylor expansion of (H6) for $S_1(x)$ is a little involved: The term of $O(x^0)$ comes from the first term of (H6), that of $O(x)$ from the first two terms, etc. Let us denote the coefficients of $1,x,x^2,\ldots,$ of S_1 as shown in Table I. S_1 is then written as

$$S_1(x)=\Sigma_0^{(0)}+\left[\Sigma_1^{(1)}+\left[-\frac{\alpha^2}{4}\right]\Sigma_0^{(1)}\right]x+\left[\Sigma_2^{(2)}+\left[-\frac{\alpha^2}{4}\right]\Sigma_1^{(2)}+\left[-\frac{\alpha^2}{4}\right]^2\Sigma_0^{(2)}\right]x^2+\cdots=\sum_{n=0}^{\infty}A_nx^n\ , \tag{H12}$$

with

$$A_n=\Sigma_n^{(n)}+\left[-\frac{\alpha^2}{4}\right]\Sigma_{n-1}^{(n)}+\left[-\frac{\alpha^2}{4}\right]^2\Sigma_{n-2}^{(n)}+\cdots+\left[-\frac{\alpha^2}{4}\right]^n\Sigma_0^{(n)}\ . \tag{H13}$$

The following key relation exists between the two neighboring columns of Table I:

TABLE I. Definition of $\sum_l^{(n)}$ used in (H12) for $S_1(x)$. The quantities (m_1,m_2), etc., are defined by (H7). If (m_1), (m_1,m_2,m_3), $(m_1,\ldots,m_5)$, etc., defined by (H10), are used in place of (m_1,m_2), $(m_1,\ldots,m_4)$, etc., respectively, with an appropriate change of the constraint for, say, $\sum^4 m_i$ to that for $\sum^3 m_i$, this table defines $\sum_l^{(n)}$ for $S_2(x)$ used in (H30).

$$\begin{bmatrix} \sum_0^{(0)} & \sum_1^{(1)} & \sum_2^{(2)} & \sum_3^{(3)} & \cdots \\ & \sum_0^{(1)} & \sum_1^{(2)} & \sum_2^{(3)} & \cdots \\ & & \sum_0^{(2)} & \sum_1^{(3)} & \cdots \\ & & & \sum_0^{(3)} & \cdots \\ & & & & \ddots \end{bmatrix} = \begin{bmatrix} \sum_{\sum_{i=1}^{2} m_i=0} (m_1,m_2) & \sum_{\sum_{i=1}^{2} m_i=1} (m_1,m_2) & \sum_{\sum_{i=1}^{2} m_i=2} (m_1,m_2) & \cdots \\ & \sum_{\sum_{i=1}^{4} m_i=0} (m_1,\ldots,m_4) & \sum_{\sum_{i=1}^{4} m_i=1} (m_1,\ldots,m_4) & \cdots \\ & & \sum_{\sum_{i=1}^{6} m_i=0} (m_1,\ldots,m_6) & \cdots \\ & & & \ddots \end{bmatrix}$$

$$\sum_l^{(n)}=\sum_{l-1}^{(n-1)}+a_l^{(n)}+\frac{\alpha^2}{4}a_{l-1}^{(n)}\,, \tag{H14}$$

with

$$\begin{aligned} &a_n^{(n)}=0\,,\\ &a_{n-1}^{(n)}=\sum_{\sum_i m_i=n-1}(m_1,m_2)\frac{1}{(m_1+1)(m_2+1)}\,,\\ &a_{n-2}^{(n)}=\sum_{\sum_i m_i=n-2}(m_1,m_2,m_3,m_4)\left[\frac{1}{(m_1+1)(m_2+1)}-\frac{1}{(m_2+1)(m_3+1)}+\frac{1}{(m_3+1)(m_4+1)}\right],\\ &\vdots\\ &a_0^{(n)}=1\,. \end{aligned} \tag{H15}$$

The first of (H15), $a_n^{(n)}=0$, is easily checked by a direct calculation of $\sum_n^{(n)}$ and $\sum_{n-1}^{(n-1)}$ using the definition of $\sum_l^{(n)}$ given in Table I. The last of (H15) holds due to the restriction $\sum m_i=0$. If the relation (H14) holds, we then have, from (H13), $A_n=A_{n-1}=\cdots=1$, i.e., the relation (H11) follows.

Our aim is thus to prove (H14) with (H15). The proof for $l=n-1$ is given below, since it is easily extended to general l. By definition, it holds that

$$\begin{aligned} (m_1,m_2,m_3,m_4)&=(m_1-1,m_2,m_3,m_4)\alpha_1\\ &=(m_1,m_2-1,m_3,m_4)\alpha_2\,,\\ &\vdots \end{aligned} \tag{H16}$$

with

$$\begin{aligned} \alpha_1&=\left[\frac{m_1+\alpha/2}{m_1}\right]^2\frac{(1,2)_0}{(1,2)_1},\\ \alpha_2&\left[\frac{m_2-\alpha/2}{m_2}\right]^2\frac{(1,2)_0(2,3)_0}{(1,2)_1(2,3)_1}\,, \end{aligned} \tag{H17}$$

$$\begin{aligned} \alpha_3&=\left[\frac{m_3+\alpha/2}{m_3}\right]^2\frac{(2,3)_0(3,4)_0}{(2,3)_1(3,4)_1}\,,\\ \alpha_4&=\left[\frac{m_4-\alpha/2}{m_4}\right]^2\frac{(3,4)_0}{(3,4)_1}\,, \end{aligned}$$

$(1,2)_1$, etc., being given by (H7). For $\sum m_i=n-1$, (H16) relates $\sum_{n-1}^{(n)}$ with $\sum_{n-2}^{(n-1)}$. When $m_1=0$, for example, the term $(m_1-1,m_2,m_3,m_4)\alpha_1$ loses its meaning. These cases are discussed later.

Let us define $p_1,\ldots,p_4$ by

$$\begin{aligned} p_1&=p_1(m_1,\ldots,m_4)=\frac{m_1}{(1,2)_0}\,,\\ p_2&=p_2(m_1,\ldots,m_4)=m_2\left[\frac{1}{(1,2)_0}-\frac{1}{(2,3)_0}\right],\\ p_3&=p_3(m_1,\ldots,m_4)=m_3\left[\frac{-1}{(2,3)_0}+\frac{1}{(3,4)_0}\right],\\ p_4&=p_4(m_1,\ldots,m_4)=m_4\frac{1}{(3,4)_0}\,, \end{aligned} \tag{H18}$$

and

$$p_1'=p_1(m_1+1,m_2,m_3,m_4)\ ,$$
$$p_2'=p_2(m_1,m_2+1,m_3,m_4)\ , \tag{H19}$$
$$\cdots\ .$$

When, e.g., $m_1=m_2=0$, the definition of (H18) for p_1 and p_2 breaks down. In these cases we define p_i by taking the limit of (H18). For example ($m_3m_4\neq 0$),

$$p_1(0,0,m_3,m_4)=\lim_{\epsilon\to 0}\frac{\epsilon}{\epsilon+\epsilon}=\frac{1}{2}\ , \tag{H20}$$
$$p_2(0,0,m_3,m_4)=\lim_{\epsilon\to 0}\epsilon\left[\frac{1}{\epsilon+\epsilon}-\frac{1}{\epsilon+m_3}\right]=\frac{1}{2}\ .$$

With these $\{p_i\}$ and $\{p_i'\}$, it holds that

$$\text{(A)}\quad p_1+p_2+p_3+p_4=1\ ,$$
$$\text{(B)}\quad p_1'\frac{(1,2)_1}{(1,2)_2}+p_2'\frac{(1,2)_1(2,3)_1}{(1,2)_2(2,3)_2}+p_3'\frac{(2,3)_1(3,4)_1}{(2,3)_2(3,4)_2}+p_4'\frac{(3,4)_1}{(3,4)_2}=1\ , \tag{H21}$$
$$\text{(C)}\quad p_1'\frac{(1,2)_1}{(m_1+1)(1,2)_2}-p_2'\frac{(1,2)_1(2,3)_1}{(m_2+1)(1,2)_2(2,3)_2}+p_3'\frac{(2,3)_1(3,4)_1}{(m_3+1)(2,3)_2(3,4)_2}-p_4'\frac{(3,4)_1}{(m_4+1)(3,4)_2}=0\ .$$

They are confirmed by direct substitution. By condition (A) as combined with (H16), it holds that

$$(m_1,\ldots,m_4)=(m_1-1,m_2,m_3,m_4)\alpha_1p_1+(m_1,m_2-1,m_3,m_4)\alpha_2p_2+\cdots\ . \tag{H22}$$

When, e.g., $m_1=0$, the first term with $(-1,m_2,m_3,m_4)$ loses its meaning. In such cases, the decomposition is revised as follows: For example ($m_3m_4\neq 0$),

$$(0,0,m_3,m_4)=(0,0,m_3,m_4)p_1+(0,0,m_3,m_4)p_2+(0,0,m_3-1,m_4)\alpha_3p_3+(0,0,m_3,m_4-1)\alpha_4p_4\ . \tag{H23}$$

Namely, when $(m_1,\ldots,m_4)$ has no zeros, we use (H22), and when there are a number of zeros, we replace the terms containing -1 in (H22) by the original $(m_1,\ldots,m_4)$ times p_i.

Suppose that we have already carried out the decomposition of all the terms in $\sum_{n-1}^{(n)}$. The result is composed of a number of terms, which are divided into two groups: group I, consisting of the terms involved in $\sum_{n-2}^{(n-1)}$ (apart from the m_i-dependent constant), and the rest, called group II. In the example of (H22), the last two terms belong to group I and the first two to group II. Group I gives $\sum_{n-2}^{(n-1)}+(\alpha^2/4)a_{n-2}^{(n)}$, and group II gives $a_{n-1}^{(n)}$, as proved in what follows.

Let us first consider the terms in group I. There are, altogether, four ways in which $(m_1',\ldots,m_4')$ (with $\sum m_i'=n-2$) arises by the decomposition mentioned above; from $(m_1'+1,m_2',m_3',m_4')$, from $(m_1',m_2'+1,m_3',m_4')$, etc. After the decomposition, therefore, $\sum_{n-1}^{(n)}$ carries the factor $(m_1',\ldots,m_4')$ in the following form:

$$\left[p_1'\left[\frac{m_1'+1+\alpha/2}{m_1'+1}\right]^2\frac{(1',2')_1}{(1',2')_2}+p_2'\left[\frac{m_2'+1-\alpha/2}{m_2'+1}\right]^2\frac{(1',2')_1(2',3')_1}{(1',2')_2(2',3')_2}+\cdots\right](m_1',m_2',m_3',m_4')\ . \tag{H24}$$

It is checked that the coefficient of $O(\alpha/2)$ thereof vanishes by condition (B) of (H21) and that of $O((\alpha/2)^0)$ is equal to unity by condition (C). Calculating the coefficient of $\alpha^2/4$ of (H24), we then find that (H24) equals

$$\left[1+\frac{\alpha^2}{4}\left[\frac{1}{(m_1'+1)(m_2'+1)}-\frac{1}{(m_2'+1)(m_3'+1)}+\frac{1}{(m_3'+1)(m_4'+1)}\right]\right](m_1',m_2',m_3',m_4')\ . \tag{H25}$$

Considering all the terms in $\sum_{n-2}^{(n-1)}$, we have

$$\sum_{n-1}^{(n)}=\sum_{n-2}^{(n-1)}+\frac{\alpha^2}{4}a_{n-2}^{(n)}+X\ , \tag{H26}$$

with $a_{n-2}^{(n)}$ just given by (H15). The first and third terms of (H14) thus arise here.

We next examine X, which represents collectively the contributions of group II in the decomposition. They come from $(m_1,\ldots,m_4)(\sum m_i=n-1)$, which has at least one zero. As an example of the term containing one zero (called the one-zero term), consider $(0,m_2,m_3,m_4)$ with $m_2m_3m_4\neq 0$. Its contribution to X is $(0,m_2,m_3,m_4)p_1$ by our rule of decomposition, which is actually zero because of $p_1(0,m_2,m_3,m_4)=0$ from (H18). The same holds true for the other one-zero terms, showing that the one-zero terms do not contribute to X. Consider next two-zero terms. There are two kinds of them, depending on the position of zeros. Two zeros of the first kind occupy separate positions such as $(0,m_2,m_3,0)$ or $(m_1,0,m_3,0)$, etc. They again contribute nothing because $p_1=p_4=0$ for $(0,m_2,m_3,0)$ and $p_2=p_4=0$ for $(m_1,0,m_3,0)$. The other terms of the first kind may be treated similarly. The terms belonging to the second kind are those which have zeros occupying two neighboring positions such as $(0,0,m_3,m_4)$. The contribution to X from this example is, by (H20) and (H23),

$$(0,0,m_3,m_4)(p_1+p_2)=(0,0,m_3,m_4)\ . \tag{H27}$$

The sum of the three two-zero terms then leads to

$$\sum_{\substack{m_i\neq 0\\ m_1+m_2=n-1}}[(0,0,m_1,m_2)-(m_1,0,0,m_2)+(m_1,m_2,0,0)]\ . \tag{H28}$$

The terms with more than two zeros are treated similarly. We find that their contributions to X amount to removing the restriction $m_i \neq 0$ in (H28). By rewriting each term of (H28) in terms of (m_1,m_2), we find

$$X=\sum_{m_1+m_2=n-1}(m_1,m_2)\frac{1}{(m_1+1)(m_2+1)}\ , \tag{H29}$$

which is $a_{n-2}^{(n)}$ defined by (H15). With (H26) and (H29), our proof for $l=n-1$ of (H14) is completed. Hence, (H11) for $S_1(x)$ follows.

The proof for $S_2(x)$ proceeds similarly. Using (H9), we define $\sum_l^{(n)}$ for $S_2(x)$ as in Table I. The key relation between $\sum_l^{(n)}$ is ($a_n^{(n)}=0$, $a_0^{(n)}=1$)

$$\sum_l^{(n)}=\sum_{l-1}^{(n-1)}\left[1-\frac{\alpha}{n}\right]+a_l^{(n)}+\frac{\alpha^2}{4}a_{l-1}^{(n)}\ , \tag{H30}$$

with new $a_l^{(n)}$ defined below. In the Taylor expansion, $S_2(x)=\sum A_n x^n$, the relation (H13), which still holds for $S_2(x)$, yields

$$A_n=\frac{n-\alpha}{n}A_{n-1}=\cdots=\frac{(1-\alpha)_n}{n!}\ . \tag{H31}$$

Thus (H30) leads to (H11). To prove (H30) for $l=n-2$, conditions (A), (B), and (C) given for $S_1(x)$ by (H21) are replaced by the following ones for five p_i's [we need five p_i, because $\sum_l^{(n)}$ with $l=n-2$ involves $(m_1,\ldots,m_5)$],

$$\text{(A)}\quad \sum_{i=1}^{5}p_i=1\ ,$$

$$\text{(B)}\quad p_1'\frac{(1,2)_1}{(1,2)_2}+p_2'\frac{(1,2)_1(2,3)_1}{(1,2)_2(2,3)_2}+\cdots+p_5'\frac{(4,5)_1}{(4,5)_2}=1\ , \tag{H32}$$

$$\text{(C)}\quad p_1'\frac{(1,2)_1}{(m_1+1)(1,2)_2}-p_2'\frac{(1,2)_1(2,3)_1}{(m_2+1)(1,2)_2(2,3)_2}+p_3'(\cdots)-p_4'(\cdots)+p_5'\frac{(4,5)_1}{(4,5)_2}=\frac{1}{n}\ .$$

If the $\{p_i\}$ are found, the proof of (H30) may be performed in exactly the same way as $S_1(x)$. Now the $\{p_i\}$ are found to be

$$p_1=\frac{m_1(1,2)_1}{n(1,2)_0},\quad p_2=\frac{m_2(1,2)_1}{n(1,2)_0},\quad p_3=\frac{m_3(3,4)_1}{n(3,4)_0}\ ,\quad p_4=\frac{m_4(3,4)_1}{n(3,4)_0},\quad p_5=\frac{m_5}{n}\ . \tag{H33}$$

In terms of (H32), the validity of (H30) is confirmed with

$$a_{n-2}^{(n)}=\sum_{\sum m_i=n-2}(m_1,m_2,m_3)\left[\frac{1}{m_1+1}+\frac{m_2+m_3+1}{(m_2+1)(m_3+1)}\right]\frac{1}{n}\ , \tag{H34}$$

$$a_{n-3}^{(n)}=\sum_{\sum m_i=n-3}(m_1,\ldots,m_5)\left[\frac{1}{m_1+1}+\frac{m_2+m_3+1}{(m_2+1)(m_3+1)}+\frac{m_4+m_5+1}{(m_4+1)(m_5+1)}\right]\frac{1}{n}\ ,$$

with (m_1,m_2,m_3), $(m_1,\ldots,m_5)$, etc., defined by (H10). The proof of (H30) for the other l can be performed similarly. Thus we obtain (H11).

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