On Solutions of the nonequilibrium x-ray edge problem

Bernd Braunecker
Institute of Theoretical Physics, Faculty of Basic Sciences, Swiss Federal Institute of Technology Lausanne, EPFL, CH-1015 Lausanne, Switzerland
(Received 15 November 2002; published 22 October 2003)

We rediscuss a nonequilibrium x-ray edge problem which in recent publications led to discrepancies between the results of the perturbative and of an extended Nozières-De Dominicis approach. We show that this problem results from an uncritical separation of momenta of the scattering potential, and we propose a corrected Nozières-De Dominicis solution.

DOI: 10.1103/PhysRevB.68.153104 PACS number(s): 78.70.Dm, 72.20.Ht

I. INTRODUCTION

We address a question raised recently by Combescot and Roulet[1] (CR) in the context of the nonequilibrium x-ray edge problem. The latter was studied some years ago by Ng[2] who developed an extension of the well-known Nozières and De Dominicis[3] (ND) technique. In the late 1960s, ND devised this method for the computation of the x-ray absorption spectrum. They provided with it an elegant description of the shape of the edge singularity in terms of the scattering phase shift at the Fermi surface. The approach is based on some subtle approximations, though, and thorough check of the condition of validity is required. Such a check is provided, for instance, by comparison with the perturbative parquet diagram result of Roulet, Gavoret, and Nozières,[4,5] and the validity of ND's solution for the original x-ray problem can in this sense be proven. For the nonequilibrium case, however, CR revealed an inconsistency by comparing a similar parquet diagram summation to Ng's result, yet they did not provide an explanation of its origin. In the present paper, we show that the discrepancies arise from an uncritical use of the decoupling of the momenta of the scattering potential. Further, we show how ND's method can be modified to yield a result coinciding with the perturbative one. This is illustrated on CR's academic problem for which it turns out that Ng's multichannel extensions are not required.

II. NONEQUILIBRIUM X-RAY PROBLEM

The nonequilibrium system to be discussed consists of two Fermi seas $n=1,2$, referred to as *subbands* which are characterized by the fixed chemical potentials $\mu_1<\mu_2$ and the energies $\varepsilon_1,\varepsilon_2$ at the bottom of the subbands. We assume that $\mu_1>\varepsilon_2$, so there is a nonzero overlap between the bottom of the subband 2 and the Fermi surface μ_1. A core state with energy ε_d and an infinite mass is assumed to exist below the subbands. The qualitative situation is shown in Fig. 1.

If both subbands were isolated, the x-ray absorption spectrum would be the result of a simple superposition of two independent x-ray problems, and two edge singularities corresponding to μ_1 and μ_2 could be observed. The mixture between the two subbands, however, allows for a new physical process: Particle–hole excitations with the particle in one subband and the hole in the other one become possible with energies that may be positive or negative (see Fig. 1). The form of the absorption spectrum is changed considerably. The edge singularities are broadened, the core–hole acquires a finite lifetime, and absorption below the threshold becomes possible, where the missing energy is compensated by such particle–hole excitations of negative energy.

The Hamiltonian of the system is assumed to be given by

$$H=\sum_{kn}\varepsilon_{kn}c_{kn}^{\dagger}c_{kn}+\varepsilon_d b^{\dagger}b+\sum_{kk'nn'}V_{kk'}^{nn'}c_{kn}^{\dagger}c_{k'n'}bb^{\dagger}, \tag{1}$$

where $n=1,2$ labels the subbands. Conduction electrons with momenta k in the subbands n are created and annihilated by $c_{kn}^{\dagger}$ and c_{kn}, while $b^{\dagger}$ and b operate on the core state. The interaction with the photon field is described by the operator

$$H_x=\sum_{kn}\lambda_k^n c_{kn}b^{\dagger}+\text{h.c.} \tag{2}$$

For simplicity, spin indices have been dropped.

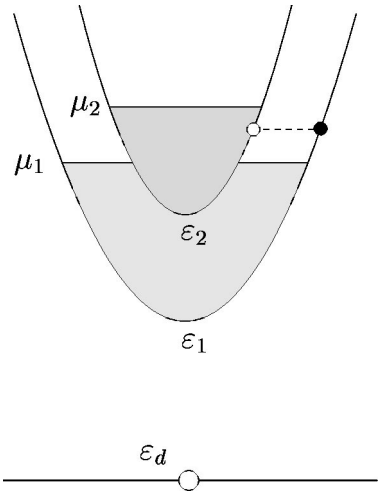

FIG. 1. Two nonequilibrium Fermi seas extending between the energies (ε_1,μ_1) and (ε_2,μ_2), respectively. A zero energy particle–hole pair between the subbands is indicated. Pairs with positive or negative energies are possible.

III. PERTURBATIVE APPROACH OF COMBESCOT AND ROULET

The problem, as it is defined by the Hamiltonians (1) and (2) above, depends on the parameters $\lambda_k^1, \lambda_k^2, V_{kk'}^{11}, V_{kk'}^{22}$, and $V_{kk'}^{12}$. With respect to the original x-ray problem the new physics must enter with the subband couplings $V_{kk'}^{12}$. To focus on the new effects we consider with CR the academic problem of $V_{kk'}^{11}=V_{kk'}^{22}=\lambda_k^2=0$. This means that a photon can excite the core electron only into the subband $n=1$, and particle–hole excitations are due only to particles tunneling between both subbands, as indicated in Fig. 1.

The perturbative approach of CR consists in assuming $V_{kk'}^{12} \equiv -V^{12}$ and in expanding the response function $\mathcal{S}(\Omega)$, which is the Fourier transform of

$$\mathcal{S}(t_2-t_1)=\langle T\{H_x(t_2)H_x(t_1)\}\rangle, \tag{3}$$

in powers of

$$\tilde{V}=V^{12}V^{21}=|V^{12}|^2. \tag{4}$$

The imaginary part of $\mathcal{S}(\Omega)$ yields the absorption rate $\mathcal{A}(\Omega)$. CR performed the sum over the most singular parquet diagrams and found an absorption rate of the x-ray problem which is, close to the threshold energy $\omega_0=\mu_1-\varepsilon_d$, of the form

$$\mathcal{A}(\Omega)\approx \mathrm{Im}\frac{\nu_{11}}{2g}\left(\frac{\xi_0}{|\Omega-\omega_0|}\right)^{2g} e^{i\pi 2g\,\theta(\Omega-\omega_0)} \tag{5}$$

for ξ_0 a cutoff of the order of the bandwidth, θ the usual step function, and g the effective coupling constant,

$$g=\nu_{11}\tilde{V}(\bar{\nu}_{21}-i\pi\nu_{21}). \tag{6}$$

Here we have used the notation $\nu_{nn'}=\nu_n(\mu_n')$ for the density of states in the subband n at the energy $\mu_{n'}$, and $\bar{\nu}_{nn'}$ for the integral

$$\bar{\nu}_{nn'}=\int_{\varepsilon_n}^{\infty} d\varepsilon\,\nu_n(\varepsilon)P\frac{1}{\mu_{n'}-\varepsilon}, \tag{7}$$

with P denoting the principal value. The approximation (5) holds for small values of the coupling constant g.

CR compared this result with Ng's extended ND approach. Their criticism refers to the appearance of the density of states $\nu_{22}=\nu_2(\mu_2)$, and not, as in the perturbative result above, of the density of states at μ_1, $\nu_{21}=\nu_2(\mu_1)$. The presence of ν_{22} implies a coupling of particles at the respective energies μ_1 and μ_2, whereas the zero energy intersubband fluctuations at μ_1 are entirely absent. This is definitely unphysical as soon as $\mu_2-\mu_1$ becomes large. The origin of this discrepancy remained unresolved in CR's paper and is discussed in the next section.

IV. ORIGIN OF THE UNPHYSICAL BEHAVIOR

The problems with ND's approach arise from an uncritical use of the momentum decoupling,

$$V_{kk'}^{nn'}\rightarrow V^{nn'}u_k^n u_{k'}^{n'}. \tag{8}$$

As CR have noticed with the perturbative results above, the important particle–hole excitations occur in the low energy sector with the particle and hole energies close to the Fermi surface μ_1. In the single-band equilibrium x-ray problem, the restriction to this energy sector can be assured by the decoupling (8). As it turns out, the explicit form of the u_k is of little importance because the form of the free propagator is controlled by the discontinuity at the Fermi surface [see Ref. 3, Eq. (33), and below] which naturally imposes the low-energy restrictions. There is consequently no risk in assuming the potential $V_{kk'}$ to be constant in the whole band as long as one introduces the adequate cutoff ξ_0 imposed by the bandwidth.

In the nonequilibrium case a similar "naive" splitting of the form (8) leads to the unphysical results mentioned above. If one assumes the potential to be constant over the whole bandwidths, the free propagators which are integrated over the u_k^n are controlled by the discontinuities at the Fermi surfaces of their respective subbands analogously to the original x-ray problem. The coupling of the subbands then leads to the mixture of the energy sectors close to the different Fermi surfaces, and therefore to large energy particle–hole excitations of the order of $\mu_2-\mu_1$, whereas the intersubband fluctuations close to μ_1 and μ_2, respectively are absent. From CR's perturbative approach, however, we know that the latter are the relevant processes and cannot be neglected.

In the sequel we propose a projection onto these low-energy sectors which is artificial in a similar way as ND's splitting (8) in the one-band case but allows us to capture the important particle–hole excitations found within the perturbative approach.

V. MODIFICATION OF THE NOZIÈRES–DE DOMINICIS APPROACH

A. Splitting of the potential: Asymptotic forms of propagators

Let us reconsider the academic problem above in which only the potentials $V_{kk'}^{12}=[V_{k'k}^{21}]^*$ are nonzero. To restrict to energies close to μ_1 we assume these potentials to be separable as

$$V_{kk'}^{12}=-V^{12}u_k^{11}u_{k'}^{21}, \tag{9}$$

where the $u_k^{nn'}$ are functions which refer to values of k in the subband n and which are maximum at the Fermi surface $\mu_{n'}$ and fall off sufficiently fast away from it. To maintain the Hermiticity of the potentials V^{12} we assume these functions to be real and equal, $u_k^{11}=u_k^{21}\equiv u_k^1$.

In ND's approach, the constant part V^{12} acts as an "external" potential on particles described by the operators $c_n^\dagger=\Sigma_k u_k^1 c_{kn}^\dagger$ during times between t_1 and t_2. The relevant physical quantities can be obtained from the so-called transient propagator, $\varphi(t,t')$, which describes the time evolution of these particles, with $t_1<t,t'<t_2$. The potential V^{12} enters as the self-energy part into the Dyson equation for the tran-

sient propagator [see Eq. (22) below]. The free part of this Dyson equation is described by the Green's functions,

$$G_n(t)=\sum_k (u_k^1)^2 G_{kn}(t)=-i\sum_k (u_k^1)^2 e^{-i\varepsilon_{kn}t} \times[\theta(t)\theta(\varepsilon_{kn}-\mu_n)-\theta(-t)\theta(\mu_n-\varepsilon_{kn})]. \tag{10}$$

Following ND we must examine the asymptotic behavior of these functions as $t\to\infty$. We first consider the case $n=1$. Here the cutoff function u_k^1 is centered at the Fermi surface μ_1 which corresponds to the situation of the original x-ray problem. Let us recall ND's arguments to obtain an approximate expression for $G_1(t)$: For large times t the behavior of $G_1(t)$ is dominated by the discontinuity at the Fermi surface. Let $\varrho_{11}(\varepsilon)=\nu^1(\varepsilon)(u^1(\varepsilon))^2$ with $\nu^1(\varepsilon)$ the density of states in the subband 1, and $u^1(\varepsilon_{k1})=u_k^1$. Then, for $t>0$,

$$G_1(t)=-i\int_{\mu_1}^{\infty} d\varepsilon\,\varrho_{11}(\varepsilon)e^{-i\varepsilon t}, \tag{11}$$

which becomes for large times $t\gg\xi_0^{-1}$ [where ξ_0 is the characteristic energy describing the decay of $u^1(\varepsilon)$],

$$G_1(t)\approx\frac{\nu^1(\mu_1)}{t}e^{-i\mu_1 t}. \tag{12}$$

The same expression holds for $t<0$. We observe that the exact shape of $u^1(\varepsilon)$ is of no importance as long as $|t|\gg\xi_0^{-1}$. To include the short-time behavior, $t\lesssim\xi_0^{-1}$, ND imposed that integrals over the product of $G_1(t)$ and some slowly varying function (the transient propagator) must yield the correct result. Hence, if a is a time cutoff such that $a\gg\xi_0^{-1}$ but still much smaller than the characteristic time scale of the transient propagator, the short-time behavior of $G_1(t)$ enters only through the integral

$$A_1=\int_{-a}^{a} dt\,G_1(t)=\int_{-\infty}^{\infty} d\varepsilon\,\varrho_{11}(\varepsilon)P\frac{1}{\varepsilon-\mu_1}\equiv-\overline{\nu}_{11}, \tag{13}$$

where we have used Eq. (11) for the second equality. This quantity can be added to the asymptotic expression (12) in the form of $A_1\delta(t)$, and we obtain the central approximation of ND's approach,

$$G_1(t)=-\nu_{11}P\frac{1}{t}e^{-i\mu_1 t}-\overline{\nu}_{11}\delta(t). \tag{14}$$

The case $n=2$ is more subtle because there is no Fermi edge discontinuity at μ_1 for electrons in the subband 2. Let us set $\varrho_{21}(\varepsilon)=\nu_2(\varepsilon)(u^1(\varepsilon))^2$ with $\nu_2(\varepsilon)$ the density of states in the subband 2. We have, from Eq. (10),

$$G_2(t)=-i\theta(t)\int_{\mu_2}^{\infty} d\varepsilon\,\varrho_{21}(\varepsilon)e^{-i\varepsilon t} +i\theta(-t)\int_{-\infty}^{\mu_2} d\varepsilon\,\varrho_{21}(\varepsilon)e^{-i\varepsilon t}. \tag{15}$$

If $\mu_2-\mu_1$ is large with respect to the cutoff ξ_0 of the function $u^1(\varepsilon)$ the first integral can be neglected. This means that the present treatment is valid for times which are much larger than $(\mu_2-\mu_1)^{-1}$ or for frequencies much smaller than $(\mu_2-\mu_1)$. Using the same argument, we can push the upper boundary of the remaining integral to infinity. Hence,

$$G_2(t)=+i\theta(-t)\int_{-\infty}^{\infty} d\varepsilon\,\nu_2(\varepsilon)(u^1(\varepsilon))^2 e^{-i\varepsilon t}. \tag{16}$$

For large times, $|t|\gg\xi_0^{-1}$, the period of oscillation of the exponential is much shorter than the time of variation of the $u^1(t)$ so that the integral averages to zero. Following the above argumentation, the short-time behavior of $G_2(t)$ can be resumed into a term $A_2\delta(t)$ with [using Eq. (16)]

$$A_2=\int_{-a}^{0} dt\,G_2(t)=i\int_{-a}^{0} dt\int_{-\infty}^{\infty} d\varepsilon\,\varrho_{21}(\varepsilon)e^{-it(\varepsilon-\mu_1)}. \tag{17}$$

The exchange of the two integrals demands some care because the integrand becomes singular. For nonzero values of ε the time integration can be performed first and yields an integrand proportional to $1/\varepsilon$. In order to handle $\varepsilon\to0$, we notice that only the advanced part of the function survives because of the constraint $t<0$. This implies that the energies entering in the exponential of Eq. (17) must be shifted by an infinitesimal imaginary amount, $\varepsilon\to\varepsilon+i\eta$, with $\eta>0$. The time integration can then be performed first, and we obtain

$$A_2=-\int_{-\infty}^{\infty} d\varepsilon\,\varrho_{21}(\varepsilon)\frac{1}{\varepsilon-\mu_1+i\eta}, \tag{18}$$

where we have suppressed the term at the lower boundary of the time integral since it is due to the sharp artificial time-cutoff a. With the formula $1/(x-i\eta)=P(1/x)+i\pi\delta(x)$ we finally find

$$A_2=-\overline{\nu}_{21}+i\pi\nu_{21} \tag{19}$$

with

$$\overline{\nu}_{21}=\int_{-\infty}^{\infty} d\varepsilon\,\varrho_{21}(\varepsilon)P\frac{1}{\varepsilon-\mu_1}, \tag{20}$$

which coincides with $\overline{\nu}_{21}$, given by Eq. (7) with a slightly modified definition because of the weight function $\varrho_{21}(\varepsilon)$.

The approximate form resulting from ND's argumentation is therefore given by

$$G_2(t)=[i\pi\nu_{21}-\overline{\nu}_{21}]\delta(t). \tag{21}$$

There is no algebraic decay in $1/t$ because the Fermi surface discontinuity for the subband $n=2$ is of no relevance for processes of energies close to $\varepsilon=\mu_1$.

B. Transient propagators and absorption rates

With the approximate forms of the initial Green's functions, Eqs. (14) and (21), we can follow ND's analysis step by step, and we focus here only on the new features in the derivation.

The computation of physical quantities is based on the transient propagators $\varphi^{nn'}$ which can be defined by the Dyson equations,

$$\varphi^{nn'}(t,t') = G_n(t-t')\delta_{nn'} - \sum_{n''} \int_{t_1}^{t_2} dt'' G_n(t-t'') V^{nn''} \varphi^{n''n'}(t'',t'). \quad (22)$$

For the academic problem under discussion, the functions φ^{11} and φ^{21} are found to form a closed set of equations,

$$\varphi^{11}(t,t') = G_1(t-t') - \int_{t_1}^{t_2} dt'' G_1(t-t'') V^{12} \varphi^{21}(t'',t'),$$

$$\varphi^{21}(t,t') = -\int_{t_1}^{t_2} dt'' G_2(t-t'') V^{21} \varphi^{11}(t'',t'). \quad (23)$$

Since $G_2(t)$ is proportional to a δ-function, we obtain a single integral equation for φ^{11},

$$\varphi^{11}(t,t') = G_1(t-t') - \int_{t_1}^{t_2} dt'' G_1(t-t'') \tilde{V}_{11} \varphi^{11}(t'',t'), \quad (24)$$

in which the effective interaction

$$-\tilde{V}_{11} = (-V^{12})[i\pi\nu_{21} - \overline{\nu}_{21}](-V^{21}) \quad (25)$$

leads to the same coupling constant g as in the perturbative approach, given by Eq. (6). The remaining problem coincides exactly with ND's original x-ray problem with the interaction potential V replaced by the effective potential $\tilde{V}_{11}$. Therefore, the absorption rate becomes, from Eq. (66) of Ref. 3,

$$\mathcal{A}(\Omega) \sim \mathrm{Im}\left[\left(\frac{\xi_0}{|\Omega - \omega_0|} \right)^{\epsilon} e^{i\pi\epsilon\theta(\Omega-\omega_0)} \right], \quad (26)$$

with

$$\epsilon = 2\frac{\delta}{\pi} - \frac{\delta^2}{\pi^2}, \quad (27)$$

and δ the complex "phase shift" at $\varepsilon = \mu_1$ induced by the effective potential $\tilde{V}_{11}$,

$$\frac{\tan\delta}{\pi} = \frac{\nu_{11}\tilde{V}_{11}}{1 + \overline{\nu}_{11}\tilde{V}_{11}}. \quad (28)$$

For small V^{12}, one has $\delta/\pi \approx \nu_{11}\tilde{V}_{11}$, and the absorption rate merges with the parquet graph result of CR. Furthermore, the imaginary part of δ leads to a broadening of the sharp Fermi edge singularities which would exist in the case of disconnected subbands.

VI. CONCLUSION

With the preceding discussion of the nonequilibrium x-ray problem we have seen that ND's technique provides an elegant calculation tool for which, however, the conditions of validity must be checked carefully at the beginning.

The key approximation is the restriction to low-energy fluctuations close to the Fermi surface(s). The separation of momenta in the interaction potentials must occur in these energy sectors. In the single-band case of the original x-ray problem, this low-energy restriction enters naturally by the discontinuity of the Green's functions at the Fermi surface which controls the large time behavior of these functions. The particular form of the weight functions $u^n(\varepsilon)$ which project onto the low-energy sector has only little importance, so that it even might be taken as constant over the whole band, as often assumed in the literature.

We have noticed with CR that the latter assumption leads to unphysical results within ND's approach in the case of nonequilibrium systems. Here the form of the weight functions becomes important, and we have shown how the approximations of the initial Green's functions must be chosen to obtain physical results. In particular, the decay in $1/t$ which is characteristic for ND's asymptotic approximation, appears only if a Fermi surface lies within the energy range in which the cutoff functions $u^n(\varepsilon)$ are nonzero.

With this taken into account, ND's method remains valid and provides us with quantitative results for the exponents of the power-law divergences at the Fermi edges. Moreover, the absence of the $1/t$-decay in the subband $n=2$ reduces the complexity of the discussed multichannel problem. Instead of systems of singular integral equations, we deal with a scalar (single-channel) problem in which the presence of the other channels is reflected by a mere renormalization of the interaction strength which, however, becomes a complex quantity.

ACKNOWLEDGMENT

I thank P.-A. Barès for many helpful discussions. The support of the Swiss National Fonds is gratefully acknowledged.

[1] M. Combescot and B. Roulet, Phys. Rev. B **61**, 7609 (2000).
[2] T.-K. Ng, Phys. Rev. B **54**, 5814 (1996).
[3] P. Nozières and C.T. De Dominicis, Phys. Rev. **178**, 1097 (1969).
[4] B. Roulet, J. Gavoret, and P. Nozières, Phys. Rev. **178**, 1072 (1969).
[5] P. Nozières, J. Gavoret, and B. Roulet, Phys. Rev. **178**, 1084 (1969).