The X-ray edge singularity in Quantum Dots

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(Dated: July 22, 2010)

In this work we investigate the X-ray edge singularity problem realized in noninteracting quantum dots. We analytically calculate the exponent of the singularity in the absorption spectrum near the threshold and extend known analytical results to the whole parameter regime. Additionally, we highlight the connections to work distributions and to the Loschmidt echo.

PACS numbers: 72.15.Qm,85.35.Be,73.50.Mx

Introduction. In condensed matter theory the X-ray-edge singularity constitutes one of the most important paradigms appearing in a variety of different contextes. In the X-ray edge problem one probes the response of a fermionic system, interacting or noninteracting, subject to a sudden local perturbation. Its origin lies in the study of X-ray spectra of simple metals where it was shown that the absorption or emission of a photon corresponds to the sudden switch on or off of a local potential scatterer embedded in a noninteracting Fermi sea[1–3]. Since then X-ray edge physics has been found in a variety of different systems such as Luttinger liquids with impurity[4], Anderson impurity and Kondo models[5–9], resonant tunneling current-voltage characteristics[10], gapped systems[11], decoherence in two level systems[12] or work distributions for weak local quenches[13].

In this work we focus on the realization of the X-ray edge problem in noninteracting quantum dots allowing to study it in a controlled setup. The possibility to tune the system parameters in quantum dots enables to vary the relevant quantity in the X-ray edge problem, the phase shift of the conduction band electrons. We analytically calculate the absorption lineshape near the threshold of a suitably initialized quantum dot at zero temperature extending the known analytical results[5,6] to the whole parameter regime. This is an important generalization of x-ray edge physics to an experimentally accessible setup and it constitutes one of the very few examples that allow for exact solutions. We show that the absorption spectrum can be identified with a work distribution[14] for a local quench in a resonant level model. This identification allows us to take a different point of view on the problem offering nice interpretations of the results. Moreover, we highlight the connection to the Loschmidt echo that can be related to the Fourier transform of the absorption spectrum[13,15].

The paper is organized as follows. First, we introduce the experimental setup that allows to mimic the X-ray edge problem in quantum dots. Then we calculate the absorption spectrum near the threshold by an associated Riemann-Hilbert problem[16]. In the end we show the results and point out the relation to work distributions and the Loschmidt echo.

Optical spectra of quantum dots. Below, we present a possible experimental realization of X-ray edge physics in noninteracting quantum dots following the ideas of Helmes *et al.*[8] and Türeci *et al.*[9]. In Fig. 1 a schematic picture of the setup is shown. Consider a narrow quantum dot with a large splitting of the single-particle energies coupled to an electronic reservoir. In order to decouple the two spin channels, a sufficiently large magnetic field h is applied to the dot, large enough to overcome the local Coulomb repulsion U between the spin-$\uparrow$ and spin-$\downarrow$ electrons on the dot. Thus the problem separates into two independent electronic species and we consider without restriction a single channel of spinless fermions in the following. By varying the back gate voltage V_g the quantum dot can be tuned in such a way that the topmost occupied level lies far below the Fermi surface, $(\varepsilon_F - \varepsilon_h)/\Delta \gg 1$, and the lowermost unoccupied level

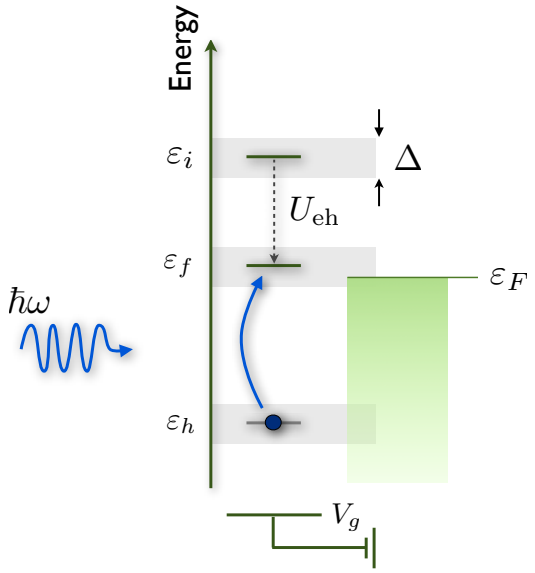

FIG. 1: (color online) Schematic picture of a quantum dot coupled to a fermionic reservoir that allows to study x-ray edge physics in absorption spectra of quantum dots. The photon absorption of a suitably initialized quantum dot implements a sudden switch on of the tunnel coupling between dot and fermionic reservoir due to a capacitative coupling between the excited electron and the residual hole. For details see text.

far above it, $(\varepsilon_i - \varepsilon_F)/\Delta \gg 1$, provided the level splitting is large enough. Here, $\Delta = \pi\rho_0 V^2$ denotes the level broadening with ρ_0 the density of states at the Fermi level and V the hopping amplitude of electrons between dot and reservoir. Thus, the lower level can be considered as occupied and the upper one as unoccupied. If an incident laser beam with angular frequency ω excites the electron from the lower level into the upper one, a positively charged hole is left behind. We assume that the quantum dot is designed such that the local capacitative coupling $U_{\rm eh}$ between the excited electron and the hole is strong shifting the upper level ε_i to lower energies ε_f to the vicinity of the Fermi level of the conduction band electrons, i.e., $|\varepsilon_f - \varepsilon_F|/\Delta \lesssim 1$. The absorption of a photon creates a local exciton. The localized hole not only interacts with the dot electron, it also establishes a local potential for the conduction band electrons. Using polarized laser light, it is possible to address just one of the two spin channels such that our description of a system of spinless fermions becomes directly relevant. Assuming that the hole is stable such that it can be considered as static, at least compared to the other time scales in the problem, we can model this system by the following initial (before absorption) and final (after absorption) Hamiltonians:

$$\begin{aligned} H_i &= \sum_k \varepsilon_k :c_k^\dagger c_k: + \varepsilon_i c_d^\dagger c_d, \\ H_f &= \sum_k \varepsilon_k :c_k^\dagger c_k: - g\sum_{kk'} :c_k^\dagger c_{k'}: + \varepsilon_f c_d^\dagger c_d + \\ &\quad + V\sum_k \left[c_k^\dagger c_d + c_d^\dagger c_k\right] + \Delta E. \end{aligned} \tag{1}$$

The hole degree of freedom already has been integrated out and is contained in a constant energy shift ΔE of the final Hamiltonian. The operator $c_k^\dagger$ creates an electron with wave vector k in the reservoir. The colons $: \ldots :$ denote normal ordering with respect to the Fermi sea. For convenience, we measure the single particle energies relative to the Fermi level, i.e., $\varepsilon_F = 0$. The operator $c_d^\dagger$ creates an electron on the upper level of the quantum dot whose energy differs depending on if a photon has been absorbed or not due to the local exciton energy.

The Hamiltonian in Eq. (1) without the potential scattering term was introduced in the context of the X-ray edge problem by Kotani and Toyozawa[5,17] to describe the X-ray spectra of metals with incomplete shells. They solved the problem analytically in the vicinity of the threshold for the case where the final local level lies far above or below the Fermi energy. A similar problem at finite temperatures has been investigated in the context of decoherence in charge qubits[18]. The combined influence of a local potential scatterer and a virtual bound state was first discussed by Kita *et al.*[6] who solved the problem analytically for the case where the final local level energy lies above the Fermi level, i.e., $\varepsilon_f > 0$.

The aim of this work is to extend the known analytical zero temperature results to the whole parameter regime with a general framework that can also be useful in other contexts. This includes, for example, decoherence in charge qubits coupled to a defect level[18,19] or absorption lineshapes of the Kondo exciton[20].

Absorption spectrum. Assuming that the coupling between the system and the light field is small, one obtains for the absorption spectrum $A(\omega)$, the rate at which photons are absorbed, in second order of the coupling (Fermi's golden rule) at zero temperature

$$A(\omega) = \kappa \sum_n \left|\left\langle e_n \left| c_d^\dagger \right| \psi_0 \right\rangle\right|^2 \delta\left[\omega - (e_n - e_{gs})\right]. \tag{2}$$

Here, $|\psi_0\rangle$ denotes the ground state of the initial Hamiltonian with energy e_{gs} and $|e_n\rangle$ is a complete orthonormal eigenbasis of the final Hamiltonian with corresponding energies e_n. The constant prefactor κ contains the experimental details such as the intensity of the incident laser beam and the system-light field coupling. Representing the δ-function by an integral over phase factors one can relate $A(\omega)$ to a dynamical correlation function $G(t)$ via Fourier transformation

$$A(\omega) = \kappa \int \frac{dt}{2\pi}\, e^{i(\omega-\varepsilon_i)t}\, G(t) \tag{3}$$

with

$$G(t) = \langle 0 | e^{iH_i t} e^{-iH_f t} | 0 \rangle. \tag{4}$$

Here, $|0\rangle = c_d^\dagger|\psi_0\rangle$ denotes a product state of the Fermi sea for the conduction band electrons with a filled local d orbital. In view of the X-ray edge problem, $G(t)$ is the equivalent to the core-hole Green's function. The dynamical correlation function $G(t)$ in Eq. (4) is an important quantity also in other physical contexts. The quantity $\mathcal{L}(t) = |G(t)|^2$ is the Loschmidt echo that allows to quantify the irreversability of a system[13,15], here H_i, under a perturbation, here $H_f - H_i$. Moreover, $G(t)$ is the characteristic funtion of a work distribution $P(\omega)$ for a quench from H_i to H_f where $P(\omega) = \kappa^{-1}A(\omega)$ is the probability of having performed the work ω on the system under this protocol[14]. The relation between absorption spectrum and work distribution has been worked out recently[21]. This relation is evident from a physical point of view. The absorbed photon provides its energy ω to the system. This is equivalent to having performed the work ω.

Analytic results for the dynamical correlation function $G(t)$ in the asymptotic long-time limit $t \to \infty$ have been obtained for the case where the final energy ε_f of the local d level lies above the Fermi level, i.e., $\varepsilon_f > 0$[6]. In the case without potential scatterer, Kotani and Toyozawa[5] calculated analytically the characteristic function $G(t)$ in the limit where the final local energy level lies far above or below the Fermi level. In both systems, the long-time behavior of the dynamical correlation function $G(t)$ is algebraic

$$G(t) \stackrel{t\to\infty}{\longrightarrow} (i\eta t)^{-\gamma}, \quad \gamma = \left(1 - \frac{\delta}{\pi}\right)^2 \tag{5}$$

with an exponent γ that only depends on the phase shift δ of the conduction band electrons at the Fermi level in presence of the local perturbation. The prefactor η of dimension energy is a high-energy scale of the order of the bandwidth. Due to the Friedel sum rule, δ/π is the screening charge that determines the exponent according to the rule of Hopfield[22].

In the following, we will extend the known results to the whole parameter regime including also the case where $\varepsilon_f \leq 0$. Although the problem is in principle quadratic, the mathematical difficulty stems from the fact that in contrast to the original X-ray edge problem an additional *dynamical* degree of freedom, the local d level, is switched on. Due to the quadratic nature of the problem, the final and initial Hamiltonians are both bilinear in fermionic operators, the characteristic function $G(t)$, that is a thermal expectation value of exponentials in H_i and H_f, can be reduced to a single-particle problem. As has been shown recently, functions such as $G(t)$ can be represented as determinants[23,24]

$$G(t) = \det M, \;\; M = 1 - f + fS, \tag{6}$$

of matrices in the single-particle space. The matrix S with matrix elements

$$S_{ll'} = \langle |c_l \hat{S} c_{l'}^\dagger| \rangle, \;\; \hat{S} = e^{iH_i t} e^{-iH_f t}, \;\; l, l' = k, d, \tag{7}$$

where $|\rangle$ is the true vacuum without any fermion, is essentially determined by the single-particle subspace of the S-matrix $\hat{S}$. Their matrix elements reduce to the retarded Green's functions of the final Hamiltonian up to a phase. The initial state is encoded in the matrix f:

$$f_{dd} = 1, \; f_{dk} = f_{kd} = 0, \;\; f_{kk'} = \delta_{kk'}\theta(-k). \tag{8}$$

It will be convenient to separate the dynamics of the additional dynamical degree of freedom, the local d level, from the dynamics of the conduction band electrons. For that purpose, we write the matrix M in a block notation

$$M = \begin{pmatrix} A & B \\ C & D \end{pmatrix} \tag{9}$$

where

$$A = M_{dd}, \; B_k = M_{dk}, \; C_k = M_{kd}, \; D_{kk'} = M_{kk'} \tag{10}$$

such that one obtains by use of an elementary property of the determinant:

$$G(t) = \det M = (A - BD^{-1}C) \det D. \tag{11}$$

The matrix D now only includes reservoir states such that $\det D$ can be calculated with techniques known from the original X-ray edge problem. But the separation of the reservoir and d level degrees of freedom comes at the cost of finding the inverse D^{-1} of an infintely large matrix. Using a technique by d'Ambrumenil and Muzykantskii[16], however, the evaluation of the determinant of D is equivalent to finding its inverse D^{-1}.

Auxiliary Riemann-Hilbert problem. The determinant of D as well as its inverse D^{-1} can be calculated by solving an auxiliary Riemann-Hilbert problem[16]. For that purpose, the determinant $\det D$ is first written as:

$$\ln \det D = \mathrm{Tr}\left[\ln(D) - f \ln S\right] + \mathrm{Tr} f \ln S \tag{12}$$

where a term $\chi^1 = \mathrm{Tr} f \ln S$ has been added and subtracted. The function $\chi^1 = i\delta E t$ contributes a term linear in t with δE the ground state energy difference between initial and final Hamiltonian. In the following, we will concentrate on the nontrivial contribution

$$\chi^2 = \mathrm{Tr}\left[\ln(1 - f + fS) - f \ln S\right]. \tag{13}$$

Introducing a new set of matrices

$$s(\lambda) = \exp(\lambda \ln S) \tag{14}$$

the logarithm appearing in the expression of χ^2 can be represented in terms of an integral over the new variable λ:

$$\chi^2 = \int_0^1 d\lambda \, \mathrm{Tr}\left[(1 - f + fs)^{-1} f - f s^{-1}\right] \frac{ds}{d\lambda}. \tag{15}$$

Thus, the problem of calculating the determinant has been transformed into the problem of inverting the matrix $1 - f + fs(\lambda)$ where for $\lambda = 1$ we have $D = 1 - f + fs(1)$. This inversion of an infinitely large matrix can be performed by solving an auxiliary Riemann-Hilbert problem. For this mapping onto the Riemann-Hilbert problem it is convient to pass over to a time representation where the Fermi-Dirac distribution, for example, takes the following form:[16]

$$f(\tau, \tau') \;=\; \frac{i}{2\pi} \frac{1}{\tau - \tau' + i0} \tag{16}$$

It remains to determine the time representation of the matrix s. As shown in Ref.[16], the Wigner transform $S(\tau, E)$ of $S_{kk'}$ can be related to the instantaneous scattering matrix provided the scattering matrix or equivalently the product $\rho(E)T(E)$ of the density of states $\rho(E)$ and the T-matrix $T(E)$ are only weakly depending on energy. Then we have that

$$\begin{aligned} S(\tau, E) \;&=\; \int d\varepsilon \, \rho(\varepsilon) S_{E+\varepsilon/2, E-\varepsilon/2} \, e^{-i\varepsilon\tau} \\ &\longrightarrow \; 1 - \theta(\tau)\theta(t-\tau) i 2\pi \rho(E) T(E) \end{aligned} \tag{17}$$

is either the identity matrix for $\tau \notin [0, t]$ or the scattering matrix for the conduction band electrons. For the long-time dynamics $t \to \infty$ we expect that only the low-energy excitations near the Fermi level are important such that we ignore the detailed dependence of the S-matrix on energy and perform the following approximation for $\tau \in [0, t]$:

$$S(\tau, E) \longrightarrow S(\tau, E = 0) = e^{2i\delta}. \tag{18}$$

Here, δ is the phase shift of the conduction band electrons at the Fermi level. Thus, the approximated $s(\lambda)$ is diagonal in its time-representation

$$s(\tau,\tau') = \sigma\delta(\tau-\tau'),\ \ \sigma = e^{2i\lambda\delta}. \tag{19}$$

The matrix $1-f+fs$ can be inverted by simply requiring

$$(1-f+fs)^{-1}(1-f+fs) = 1. \tag{20}$$

In the time representation this equation becomes a singular integral equation with a Cauchy Kernel due to the singular nature of the Fermi-Dirac distribution. Such singular integral equations exhibit an exact solution via an auxiliary Riemann-Hilbert problem[26]. Let $Y(z)$, $z\in\mathbb{C}$, be an analytic function in the complex plane except along the cut $\tau\in(0,t)$ where Y is supposed to fulfill the boundary condition

$$Y_+(\tau) = \sigma Y_-(\tau). \tag{21}$$

Here, $Y_+(\tau) = Y(\tau+i0)$ and $Y_-(\tau) = Y(\tau-i0)$. The solution to this problem is unique provided $Y(z)\to 1$ for $z\to\infty$:

$$Y(z) = \exp\left[\frac{1}{2\pi i}\int_0^t dx \frac{\ln(\sigma)}{x-z}\right]. \tag{22}$$

The knowledge of the funtion Y then allows to construct the solution of inversion problem[26]

$$\begin{aligned}&(1-f+fs)^{-1}(\tau,\tau') = \\ &= \delta(\tau-\tau') + Y_+^{-1}(\tau)f(\tau,\tau')\left[Y_-(\tau')-Y_+(\tau')\right]\end{aligned} \tag{23}$$

such that one obtains the following formula for χ^2:[16]

$$\chi^2 = \frac{i}{2\pi}\int_0^1 d\lambda \int_0^t d\tau \frac{dY_+^{-1}(\tau)}{d\tau} Y_+(\tau)\sigma^{-1}\frac{d\sigma}{d\lambda}. \tag{24}$$

For the calculation of χ^2, it is necessary to introduce a regularization scheme where the integral over τ is cut off near the boundaries of integration according to $0\to i\xi_0^{-1}$ and $t\to t+i\xi_0^{-1}$ where ξ_0 is an energy of the order of the bandwidth. Using this regularization one obtains for the asymptotic long-time behavior of $\det D$:

$$\det D \overset{t\to\infty}{\longrightarrow} e^{i\delta E t}\,(i\xi_0 t)^{-(\delta/\pi)^2} \tag{25}$$

From Eq. (23), we can deduce the inverted matrix $D^{-1} = (1-f+fs(1))^{-1}$ and thus the long-time limit of the generating function $G(t)$ according to Eq. (11)

$$G(t) \overset{t\to\infty}{\longrightarrow} (i\eta t)^{-\gamma},\ \gamma = (1-\delta/\pi)^2. \tag{26}$$

in agreement with the known result for the case $\varepsilon_f > \varepsilon_F$ in Eq. (5) and consistent with the Hopfield rule of thumb[22]. Thus, the known asymptotic behavior extends to the whole parameter regime as already shown in numerous numerical calculations[6,17,25]. This result constitutes one of the rare cases where it is possible to obtain exact analytical solutions.

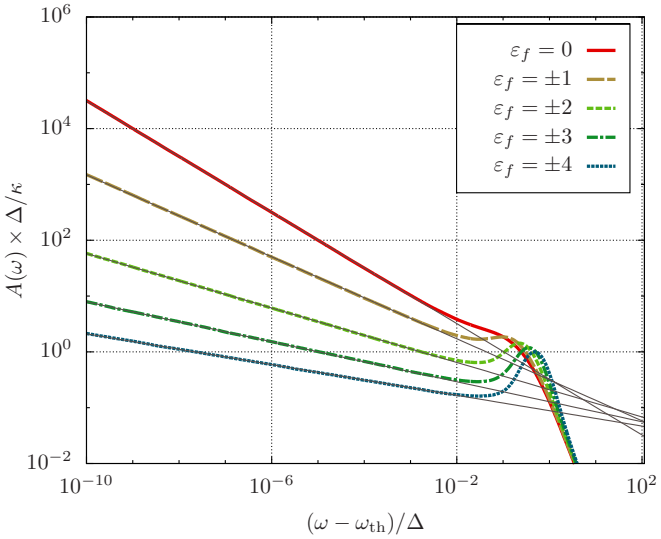

FIG. 2: Absorption spectrum $A(\omega)$ as a function of the incident light frequency ω near the threshold frequency $\omega_{\rm th}$ for different final energies ε_f of the quantum dot level. For simplicity we restrict to the case $g=0$ without potential scatterer. Here, $\Delta = \pi\rho_0 V^2$ denotes the half width of the hybridized level in the quantum dot with ρ_0 the noninteracting density of states at the Fermi level. The thick lines have been obtained by NRG calculations[27]. The thin lines show the analytic results that fit perfectly the exact NRG data in the asymptotic low frequency regime.

Loschmidt echo. As already mentioned before, the characteristic function $G(t)$ is also related to the Loschmidt echo[13,15]

$$\mathcal{L}(t) = |G(t)|^2 = \left|\langle 0\left|e^{iH_i t}e^{-iH_f t}\right|0\rangle\right|^2. \tag{27}$$

The Loschmidt echo quantifies the stability of motion in time of a system, in this case the Hamiltonian H_i, under a perturbation $H_f - H_i$. Thus, for long times t Eq. (26) states that, no matter how small the local perturbation is, the time evolution of the state $|0\rangle$ with the final Hamiltonian drives the system into a subspace of the Hilbert space that is orthogonal to the initial state. From the Anderson orthogonality catastrophe[28] it is known that the ground state of the final Hamiltonian is contained in this subspace. The system as a whole, however, does not evolve into the ground state of the final Hamiltonian as their overlap is constant in time.

Absorption lineshape. From Eq. (26), one can deduce the behavior of the absorption lineshape near the threshold analytically

$$A(\omega) \overset{\omega\to\omega_{\rm th}}{\sim} \theta(\omega-\omega_{\rm th})\,(\omega-\omega_{\rm th})^{\gamma-1} \tag{28}$$

that shows the typical power-law singularity. The singularity is a consequence of the singular behavior of the initial Fermi-Dirac distribution of the conduction band electrons at zero temperature. At finite temperatures, the singularity is cut off. In Fig. 2, NRG data for the absorption spectrum is shown. For light frequencies ω

in the vicinity of the threshold, the analytical power-law results included as thin solid lines fit perfectly to the exact NRG results. In view of the equivalence to a work distribution, the existence of the threshold in the absorption spectrum is evident. In the beginning, the system is prepared in the ground state of the initial Hamiltonian. The minimum energy, i.e., work, that has to be provided to the system by switching on the coupling to the resonant level is the ground state energy difference between initial and final Hamiltonian. Thus, it is impossible for a photon of energy less than the ground state energy difference to be absorbed. The singular behavior of the absorption spectrum shows that the dominant excitations that are created by the absorption process are low-energy excitations in the vicinity of the Fermi level.

Conclusions. In this work we have presented a general framework that allows to determine analytically the singular threshold behavior of absorption spectra in quantum dots at zero temperature. This establishes an important generalization of x-ray edge physics to experimentally accessible environments that can be used to observe x-ray edge physics in a controlled setup. Moreover, we highlighted the correspondence of the spectra to work distributions and to the Loschmidt echo. The presented framework might also be useful in other contexts such as decoherence in charge qubits or the Kondo exciton.

Acknowledgements. We acknowledge valuable discussions with J. von Delft. We thank M. Hanl and A. Weichselbaum for providing us the NRG data. This work was supported by SFB TR12 of the Deutsche Forschungsgemeinschaft (DFG), the Center for Nanoscience (CeNS) Munich, and the German Excellence Initiative via the Nanosystems Initiative Munich (NIM).

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