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ESR theory for interacting 1D quantum wires

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Abstract. – We compute the electron spin resonance (ESR) intensity for one-dimensional quantum wires in semiconductor heterostructures, taking into account electron-electron interactions and spin-orbit coupling. The ESR spectrum is shown to be very sensitive to interactions. While in the absence of interactions, the spectrum is a flat band, characteristic threshold singularities appear in the interacting limit. This suggests the practical use of ESR to reveal spin dynamics in a Luttinger liquid.

The search for the Luttinger liquid (LL) behavior of one-dimensional (1D) interacting fermions [1–4] has a rather long history. Recent experimental work has reported strong evidence via the tunneling density of states in single-wall carbon nanotubes [5, 6], for the edge states in the fractional quantum Hall effect [7] (which supposedly are chiral LLs not further discussed here), and via the conductance [8] and resonant tunneling [9] in a quantum wire (QW) in semiconductor heterostructures. These studies have so far only probed the charge dynamics and are intrinsically insensitive to *spin dynamics*. However, spin dynamics can reveal some of the most interesting and spectacular aspects of the non-Fermi liquid nature of a LL, in particular the phenomena of spin-charge separation and electron fractionalization [4]. In this Letter, we suggest to probe the spin dynamics of a LL via electron spin resonance (ESR), and provide detailed theoretical predictions for the ESR spectrum in an interacting 1D QW. ESR spectra have already been obtained experimentally for the 2D electron gas in heterostructures [10], and new fabrication advances such as cleaved-edge overgrowth techniques [11] indicate that such experiments could indeed be done for QWs as well.

The ESR spectrum of a LL turns out to be extremely sensitive to the presence and precise nature of the spin-orbit coupling mechanism. This is intuitively clear as spin-orbit coupling can sometimes destroy spin-charge separation, and nearly always represents the leading term breaking $SU(2)$ invariance. Unless this symmetry is broken, the ESR spectrum (including electron-electron interactions) is simply a delta peak at the Zeeman energy. Remarkably, the spin-orbit coupling in semiconductor QWs will spoil spin-charge separation according to refs. [12, 13], while this does not happen in nanotubes [14]. Therefore ESR theory for other realizations of the LL (such as nanotubes) is quite different and will be given elsewhere [14]. Furthermore, the ESR theory of 1D spin chains [15] is also distinct due to the presence of

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Dzyaloshinskii-Moriya interactions and the absence of charge degrees of freedom. To be specific, here we focus on the practically important case of QWs. For the theoretical description of the QW including electron-electron interactions, we use the LL model.

The standard LL Hamiltonian is expressed in terms of charge and spin bosons ϕ_ν ($\nu = \rho, \sigma$) and their conjugate momenta Π_ν [4],

$$H = \sum_{\nu=\rho,\sigma} \frac{v_\nu}{2} \int dx \left[K_\nu \Pi_\nu^2 + K_\nu^{-1} (\partial_x \phi_\nu)^2 \right] \ , \tag{1}$$

with respective effective velocities v_ν and LL parameters K_ν. Under Abelian bosonization, the right- and left-moving ($r = R, L = \pm$) electron operator for spin $\alpha = \uparrow, \downarrow = \pm$ is

$$\psi_{r\alpha}(x) = \frac{1}{\sqrt{2\pi\Lambda}} \exp\left\{ i\sqrt{\pi/2} [r\phi_\rho + r\alpha\phi_\sigma + \theta_\rho + \alpha\theta_\sigma] \right\} \ , \tag{2}$$

where $\theta_\nu = -\int_{-\infty}^{x} dx' \Pi_\nu$ and Λ is a short-distance cutoff-length. To ensure $SU(2)$ invariance of eq. (1), we put $K_\sigma = 1$, while for repulsive interactions, the charge interaction parameter $K_\rho \equiv g < 1$. In addition, to respect Galilean invariance manifest in QWs, the velocities v_ν are taken as $v_\sigma = v_F$ and $v_\rho = v_F/g$ with the Fermi velocity v_F. To simplify notation, below we often put $v_F = \hbar = 1$.

The main source of spin-orbit coupling in QWs comes from the Rashba and confinement electric fields, and for sufficiently large fields leads to a deformation of each branch of the single-particle dispersion relation [12]. The net result of this deformation is the breaking of chiral symmetry, since the Fermi velocities for right- and left-moving electrons with the same spin will become different. Therefore, with $v_{R\uparrow} = v_{L\downarrow} = v_1$ and $v_{R\downarrow} = v_{L\uparrow} = v_2$, we have $\delta v = v_2 - v_1 > 0$ and $v_1 + v_2 = 2v_F$. A dimensionless measure of the spin-orbit coupling strength is then given by $\lambda \equiv \delta v / 2v_F \ll 1$. Concrete estimates for quantum wires yield values of the order $\lambda \approx 0.1$ [13]. In effect, the spin-orbit interaction produces an additional $SU(2)$ symmetry-breaking term that can be expressed as

$$H' = \lambda \int dx \left[\Pi_\rho \partial_x \phi_\sigma + \Pi_\sigma \partial_x \phi_\rho \right] \ . \tag{3}$$

Under an external static magnetic field B along the z axis, we have to add a Zeeman term,

$$H_Z = -B \int dx \, S^z(x) = -\frac{B}{\sqrt{2\pi}} \int dx \, \partial_x \phi_\sigma \ , \tag{4}$$

with $g_e \mu_B = 1$ for simplicity. Due to band curvature, the Zeeman term also gives rise to a small splitting of the spin-up and spin-down Fermi velocities [16], $\lambda_\sigma = |v_{F\uparrow} - v_{F\downarrow}|/2v_F \approx B/2E_F$. For the most interesting cleaved-edge overgrowth samples, the 1D Fermi level is $E_F > 20$ meV [11], and therefore $\lambda_\sigma \ll \lambda$ even for strong magnetic fields. Based on this observation, the Zeeman-induced splitting of the Fermi velocities is neglected here.

The ESR intensity at frequency ω is then proportional to the Fourier-transformed transverse spin correlation function,

$$I(\omega) = \int dt dx \, e^{i\omega t} \langle S^+(t,x) S^-(0,0) \rangle \ , \tag{5}$$

where $S^\pm(t,x)$ is the transverse component of the uniform part of the spin operator, $S^\pm = J_R^\pm + J_L^\pm$, with the spin currents $\vec{J}_{R,L} = \psi_{R,L}^\dagger (\vec{\sigma}/2) \psi_{R,L}$. The Zeeman term (4) can now be

transformed away by shifting the field ϕ_σ and simultaneously Π_ρ,

$$\phi_\sigma \to \phi_\sigma + \frac{Bx}{\sqrt{2\pi}}\frac{1}{1-\lambda^2} \ , \quad \Pi_\rho \to \Pi_\rho - \frac{B}{\sqrt{2\pi}}\frac{\lambda}{1-\lambda^2} \ . \tag{6}$$

This is a direct consequence of the fact that the spin-orbit term (3) spoils spin-charge separation. Albeit the magnetic field only couples to the spin, it now also affects the charge sector, and the combined shift (6) is necessary to transform away the Zeeman term. Of course, the fermion operators and the transverse components of the uniform part of spin operator are then modified,

$$\psi_{r\alpha}(x) \to \exp\left\{ ir\alpha Bx \frac{1+r\alpha\lambda}{2(1-\lambda^2)} \right\} \psi_{r\alpha}(x) \ ,$$

and therefore

$$J_R^\pm(x) \to e^{\mp ik_\sigma x} J_R^\pm(x) \ , \quad J_L^\pm(x) \to e^{\pm ik_\sigma x} J_L^\pm(x) \ , \quad v_F k_\sigma = B/(1-\lambda^2) \ . \tag{7}$$

Since the Hamiltonian remains quadratic in the boson fields, the full problem can be solved exactly. We first focus on the $T = 0$ limit where interaction effects are most pronounced. After straightforward but tedious algebra, the fermion propagator and hence the transverse spin correlation function are obtained. Using eqs. (2) and (7),

$$\langle J_R^+(t,x) J_R^-(0,0)\rangle = \frac{e^{-ik_\sigma x}}{(2\pi\Lambda)^2} \prod_{i=1,2} \left(\frac{i\Lambda}{x - u_i t + i\Lambda} \right)^{\xi_i^+} \left(\frac{-i\Lambda}{x + u_i t - i\Lambda} \right)^{\xi_i^-} \ , \tag{8}$$

with the same expression but $x \to -x$ for the left-moving part. Here the eigenmode velocities u_1 and u_2 are in units of v_F:

$$u_{1,2} = \frac{1}{\sqrt{2}} \left[g^{-2} + 1 + 2\lambda^2 \mp \sqrt{(g^{-2}-1)^2 + 8\lambda^2(g^{-2}+1)} \right]^{1/2} \ . \tag{9}$$

In the absence of spin-orbit coupling, $\lambda = 0$, these velocities reduce to the spin and charge velocities of the LL, $u_1 \to v_F$ and $u_2 \to v_F/g$, while in the non-interacting case, $g = 1$, we recover $u_1 \to v_1$ and $u_2 \to v_2$. The exponents $\xi_i^\pm$ in eq. (8) are given by

$$\xi_i^\pm = (-1)^i \frac{u_i^2 - g^{-2} + (g^{-2}+1)\lambda^2/2 \pm u_i(u_i^2 - g^{-2} - \lambda^2)}{u_i(u_2^2 - u_1^2)} \ . \tag{10}$$

The ESR intensity (5) follows from eq. (8) and the corresponding left-moving part:

$$I(\omega) = 2\,\mathrm{Re} \int dx dt \frac{e^{i\omega t - ik_\sigma x}}{(2\pi\Lambda)^2} \prod_{i=1,2} \left(\frac{i\Lambda}{x - u_i t + i\Lambda} \right)^{\xi_i^+} \left(\frac{-i\Lambda}{x + u_i t - i\Lambda} \right)^{\xi_i^-} \ . \tag{11}$$

We are unable to compute this double integral in closed analytical form for arbitrary parameters. However, it has exactly the same structure as the integrals appearing in the computation of the spectral function for the spinful LL [17,18]. As in that case, one can determine the thresholds and the singularities of the ESR spectrum.

Before that let us briefly analyze some limiting cases. In the *non-interacting* limit $g = 1$, the exponents (10) simplify to $\xi_{1,2}^+ = 1$ and $\xi_{1,2}^- = 0$. With these values for the exponents the

double integral in eq. (5) can easily be evaluated, and the ESR intensity is uniform over a finite range of frequencies with bandwidth $\Delta\omega = 2B\lambda/(1-\lambda^2)$ and zero otherwise,

$$I(\omega) = \frac{\theta(v_2 k_\sigma - \omega)\,\theta(\omega - v_1 k_\sigma)}{v_F \lambda} \ . \tag{12}$$

Clearly, in the limit of vanishing spin-orbit coupling ($\lambda \to 0$), the single delta peak at $\omega = B$ is recovered. The integrated spectrum is given by

$$\int \frac{d\omega}{2\pi}\, I(\omega) = \frac{1}{\pi}\frac{B}{v_F}\frac{1}{1-\lambda^2} \ . \tag{13}$$

Furthermore, in the absence of spin-orbit coupling but with $g < 1$, it is straightforward to recover the delta peak at $\omega = B$ directly from eq. (11).

Let us now turn to the general case with $g < 1$ and $\lambda > 0$. Following standard arguments [4], the ESR intensity vanishes identically for $\omega < u_1 k_\sigma$, with a power-law singularity approaching $\omega = u_1 k_\sigma$ from above,

$$I(\omega) \propto \theta(\omega - u_1 k_\sigma)(\omega - u_1 k_\sigma)^{\xi_1^- + \xi_2^+ + \xi_2^- - 1} \ . \tag{14}$$

To see this we change integration variables to $s = u_1 t - x$ and $s' = u_1 t + x$ in eq. (11). In the new variables, the integrand exhibits branch cuts in the upper part of the s and s' complex plane but is analytic in the lower part. This produces precisely the threshold behavior (14), where the exponent comes from a simple power-counting argument related to a rescaling of s'. In order to investigate the behavior near $\omega = k_\sigma u_2$ it is more convenient to use the change of variables $s = u_2 t - x$, $s' = u_2 t + x$. In the new variables power counting leads to the following power law near $\omega = k_\sigma u_2$:

$$I(\omega) \propto |\omega - u_2 k_\sigma|^{\xi_2^- + \xi_1^+ + \xi_1^- - 1} \ . \tag{15}$$

However, we cannot prove analytically that the intensity has a second threshold at this frequency, because the branch cuts of the integrand appear both in the upper and the lower half of the s and s' planes. More generally, one can show that because of $u_2 > u_1$ it is impossible to find a linear transformation, $s = a_{11}x + a_{12}t$ and $s' = a_{21}x + a_{22}t$, such that the position of the branch cuts of the integrand produces a $\theta(k_\sigma u_2 - \omega)$ function. However, numerical evaluation of eq. (11) indicates threshold behavior also at the upper edge. Since in general $\xi_1^+ \neq \xi_2^+$, see eq. (10), the ESR spectrum is markedly asymmetric at both thresholds. The asymmetry is quite dramatic, because near $\omega = u_1 k_\sigma$, the intensity *diverges* since the exponent is negative, whereas near $\omega = u_2 k_\sigma$ it *vanishes* since the exponent is positive.

The full ESR spectrum can be obtained numerically by direct integration of eq. (11). In the numerical integration, a finite cutoff Λ has to be employed, which leads to several artefacts that disappear for $\Lambda \to 0$, namely (i) small oscillations, (ii) finite but very small intensities outside the window discussed above, and (iii) negative intensities. Since the time discretization should resolve Λ, numerically one cannot choose arbitrarily small Λ, and typical results for two values of Λ are shown in fig. 1. Nevertheless, the data in fig. 1 are clearly consistent with the general behavior discussed above. This behavior should be compared to both the non-interacting case (where the power-law exponents are zero and a constant ESR intensity is found in the relevant window) and to the $\lambda = 0$ case (where one has a δ-peak at the lower edge). The interaction-strength-dependence of the exponents close to the lower and upper threshold is shown in fig. 2. The exponents are of different sign, but almost (yet not exactly) equal in magnitude.

Using $\xi^{\pm} = \xi_1^{\pm} + \xi_2^{\pm}$ and $\xi = \xi^+ + \xi^-$, we find for the integrated ESR spectrum

$$\int \frac{d\omega}{2\pi} I(\omega) = \frac{2^{1-\xi}}{\pi\Gamma(\xi^+)} \left[\frac{\Gamma(-1+\xi)}{\Lambda\Gamma(\xi^-)} + \frac{\Gamma(1-\xi)}{\Gamma(1-\xi^+)} (2k_\sigma)^{-1+\xi} \Lambda^{-2+\xi} \right] . \tag{16}$$

In the non-interacting limit, $\xi^- \to 0$ and $\xi^+ \to 2$, such that the first term vanishes while the second term reproduces eq. (13). Let us finally comment on the effect of thermal fluctuations ($T > 0$). Since the Hamiltonian is quadratic, these can be incorporated by substituting the $T = 0$ propagators in eq. (11) according to

$$\left(\frac{\pm i\Lambda}{x \mp u_i t \pm i\Lambda} \right) \to \left(\frac{\pm i\Lambda}{\frac{u_i}{\pi T} \sinh \frac{\pi T}{u_i} (x \mp u_i t \pm i\Lambda)} \right) .$$

In the non-interacting case, $I(\omega)$ can then be computed exactly. This solution demonstrates that thermal fluctuations wash out the thresholds, broaden the spectrum, and suppress the ESR intensity. In the interacting case, these features are also expected. In addition, scaling shows that the ESR intensity receives an overall power-law factor $T^{-2+\xi}$. The exponent is always positive, vanishes for $g = 1$, and is generally very small (for $\lambda = 0.1$, it reaches a maximum value of 0.001).

To conclude, our study of the ESR spectrum resulting from the combined presence of interactions and spin-orbit coupling in 1D quantum wires reveals dramatic changes from simple Fermi liquid modelling. The appearance of asymmetric power-law threshold behavior, with a divergence at the lower edge and a vanishing intensity at the upper edge, are manifestations of the breakdown of spin-charge separation because of spin-orbit coupling. Such features should make an experimental study of our predictions worthwhile and feasible in practice.

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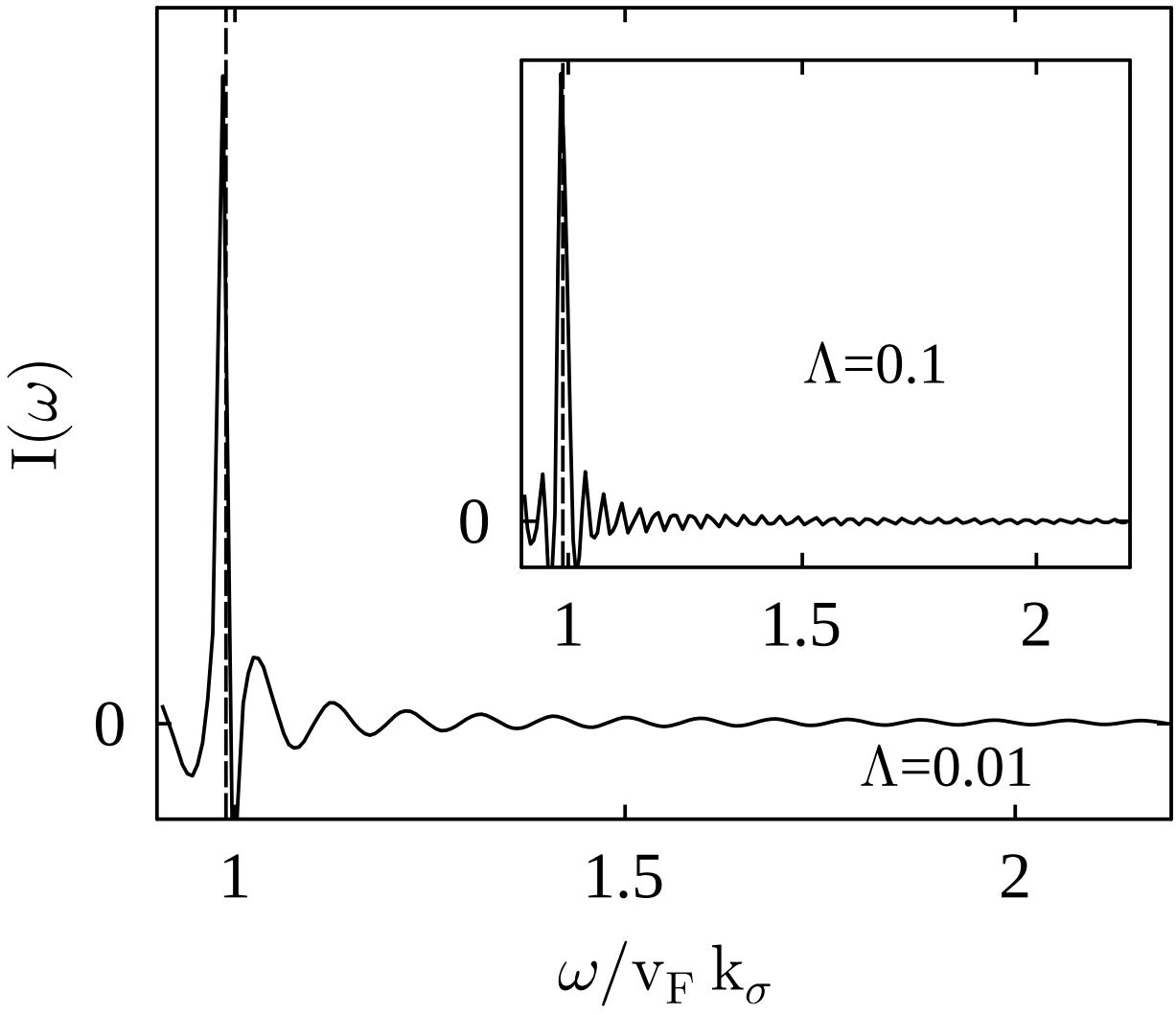

Fig. 1 – ESR intensity (in arbitrary units) for $g = 1/2$, $\lambda = 0.1$, and two values of the cutoff Λ. The threshold at $\omega = u_1 k_\sigma = 0.988$ is indicated by the dashed line, and the numerical result for $I(\omega)$ is given as the solid curve. The ESR spectrum for $\Lambda \to 0$ terminates at $\omega = u_2 k_\sigma = 2.011$.

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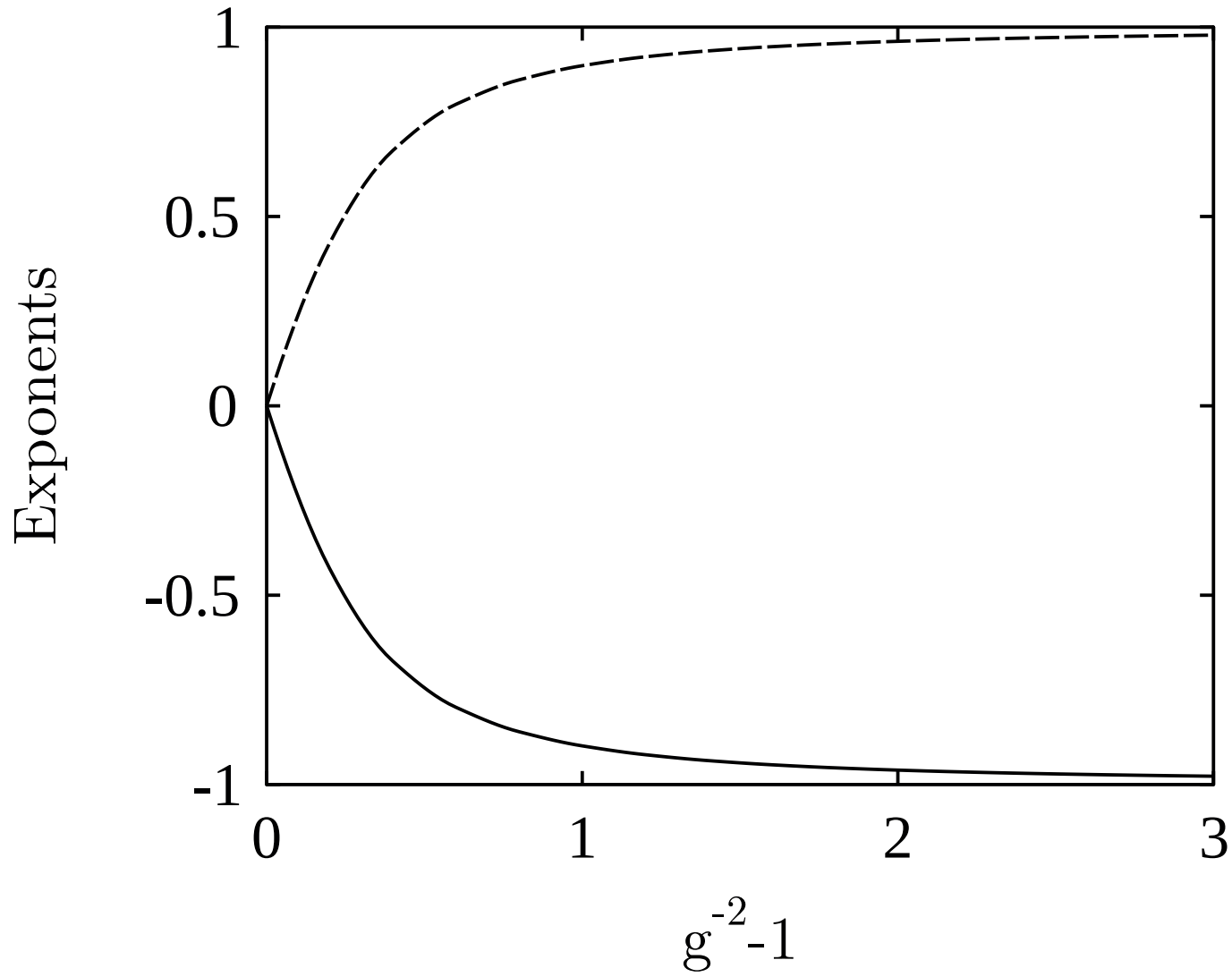

Fig. 2 – Exponents near the lower threshold $\omega = u_1 k_\sigma$ (solid curve) and near the upper threshold $\omega = u_2 k_\sigma$ (dashed curve) as function of the interaction strength for $\lambda = 0.1$.