

Interplay of Spin and Charge Channels in Zero-Dimensional Systems

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We study the interplay of charge and spin (zero-mode) channels in quantum dots. The latter affects the former in the form of a distinct signature on the differential conductance. We also obtain both longitudinal and transverse spin susceptibilities. All these observables, underlain by spin fluctuations, become accentuated as one approaches the Stoner instability. The nonperturbative effects of zero-mode interaction are described in terms of the propagation of gauge bosons associated with charge [$U(1)$] and spin [$SU(2)$] fluctuations in the dot, while transverse spin fluctuations are analyzed perturbatively.

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As one decreases the effective dimensionality of a conductor, the role of electron-electron interactions—notably in the charge and spin channels—is enhanced. In one dimension ($d = 1$) these two channels, responsible for a widely ranged spectrum of effects, often decouple. It is of obvious interest to study the counterpart of this physics in $d = 0$ quantum dots (QDs). An easily accessible scheme is the “Universal Hamiltonian” [1,2] where, in addition to the (impurity and geometry dependent) single-particle Hamiltonian, only zero-mode interactions (charge and spin (exchange) in our case) are included. The former leads to the phenomenon of the Coulomb blockade, while the latter leads to the Stoner instability [3] which is modified in mesoscopic systems [1]. Attention has been given to the intriguing interplay between the charge and the spin channels. This is manifest, e.g., in the suppression of certain Coulomb peaks due to “spin blockade” [4]. In a recent theoretical study [5], the effect of the spin channel on Coulomb peaks has been analyzed employing a master equation in the classical limit. Notwithstanding the success of this approach, quantum effects are expected to play an important role. A full fledged quantum mechanical analysis of the charge-spin interplay in zero dimensions is thus called for.

Here we report on the first step in this direction. In contrast to Ref. [5], we focus on the “Coulomb valley,” a regime which, in principle, is amenable to experimental study, but which so far has not been investigated thoroughly. In a future publication [6], employing essentially a similar approach, we shall address the vicinity of the Coulomb peak regime. The message to be conveyed from our present analysis is twofold: (i) quantum fluctuations play an essential role in affecting charge and spin related observables; (ii) the charge and spin channels in zero-dimensional systems are coupled, and the latter renormalizes the former.

More specifically we find that (i) as the spin modes renormalize the Coulomb blockade (CB), they modify the tunneling density of states (TDOS)—hence the differential conductance—of the dot [cf. Eq. (15)]. For an Ising-

like spin anisotropy the longitudinal mode partially suppresses the CB. Quantum fluctuations, manifest through the transverse modes, act qualitatively in the same way, but as one approaches the Stoner instability (from the disordered phase) their effect reverses its sign, giving rise to suppression of the conductance (i.e., *enhancement* of the CB). This results in a *nonmonotonic behavior of the TDOS*; (ii) the longitudinal spin susceptibility [Eq. (17)] *diverges* at the thermodynamic Stoner instability point, while the transverse susceptibility is *enhanced* by gauge fluctuations (but remains finite).

Our QD of linear size L is in the “metallic regime” (either diffusive ($l \ll L$) or ballistic-chaotic ($l \approx L$)). The Thouless energy and the mean level spacing satisfy $g \equiv E_{\text{Th}}/\Delta \gg 1$. We consider the following terms of the Universal Hamiltonian:

$$H = \sum_{\alpha,\sigma} \epsilon_{\alpha} a_{\alpha,\sigma}^{\dagger} a_{\alpha,\sigma} + H_C + H_S. \quad (1)$$

The spin (σ) degenerate levels of the single-particle Hamiltonian obey the Wigner-Dyson statistics. For simplicity we confine ourselves to the Gaussian unitary ensemble case. The charging interaction $H_C = E_c(\hat{n} - N_0)^2$ accounts for the Coulomb blockade. Here \hat{n} is the number operator; N_0 represents the positive background charge and is tuned to the Coulomb valley regime. The term

$$H_S = -J \left\{ \left(\sum_{\alpha} S_{\alpha}^z \right)^2 + \gamma \left[\left(\sum_{\alpha} S_{\alpha}^x \right)^2 + \left(\sum_{\alpha} S_{\alpha}^y \right)^2 \right] \right\}$$

represents spin, $\vec{S}_{\sigma\sigma'} = \frac{1}{2} \sum_{\alpha} a_{\alpha,\sigma}^{\dagger} \vec{\sigma}_{\sigma\sigma'} a_{\alpha,\sigma'}$, interactions within the dot. Below we allow for an easy axis anisotropy, $\gamma = J_{\perp}/J < 1$, reducing the original $SU(2)$ symmetry to $SO(2)$. There are several possible sources for such an anisotropy: geometrical, molecular anisotropy, etc. The degree of anisotropy can be controlled by introducing magnetic impurities into the system, or by applying anisotropic mechanical pressure [7].

The main steps of our analysis are as follows: (i) We first apply a Hubbard-Stratonovich transformation on our

Euclidean action (no dependence on spatial coordinates), leading to a Lagrangian quadratic in the fermionic fields, with auxiliary bosonic fields, ϕ (scalar) for the charge and $\vec{\Phi}$ (vector) for the spin degrees of freedom [cf. Eq. (3)]. (ii) We next apply a nonunitary transformation on the fields [Eq. (5)] whose effect is to gauge out both the Coulomb and the longitudinal component of the spin interaction. Next we integrate out the fermionic variables. In the absence of transverse components [$\gamma = 0$, implying a $U(1)$ symmetry], and following Ref. [8], one is then able to integrate out (exactly) the finite Matsubara frequency components of the bosonic fields, and express the dot's Green's function (GF) as a product of the bare (interaction free) GF (with a shifted chemical potential) and two gauge factors (the “charge boson” and the “longitudinal boson” [Eq. (11)]). (iii) The presence of the transverse components of $\vec{\Phi}$ gives rise to non-Abelian action [$SU(2)$ symmetry for $\gamma = 1$], which is the reason why a *simple* simultaneous gauging out of all components of $\vec{\Phi}$, similar to Ref. [8], is not possible. Instead, we expand the GF in powers of γ [Eq. (9)]. The above GF is now additionally dressed by transverse correlators. (iv) We evaluate the transverse correlator [Eq. (13)] and then calculate the first nontrivial diagram for the GF (Fig. 1). We obtain a close expression for the TDOS [Eq. (15)] which is then computed (Fig. 2). (v) In a similar manner we write and evaluate the leading diagrams to the longitudinal and transverse susceptibility.

Before proceeding we recall that beyond the thermodynamic Stoner instability point, $J_{\text{th}} = \Delta$, the spontaneous magnetization is an extensive quantity. At smaller values of the exchange coupling, $J_{\text{mesoscopic}} < J < J_{\text{th}}$, finite magnetization shows up, which, for finite systems, does not scale linearly with the size of the latter [1]. Its non-self-averaging nature gives rise [9] to strong sample-specific mesoscopic fluctuations [10]. We next provide some technical details on our analysis.

Gauge transformation.—The Euclidian action for the model (1) is given by

$$S = \int_0^\beta \mathcal{L}(\tau) d\tau = \int_0^\beta \left[\sum_\alpha \bar{\psi}_\alpha (\partial_\tau + \mu) \psi_\alpha - H \right] d\tau. \quad (2)$$

Here $\{\psi_\alpha\}$ stand for Grassmann variables representing electrons in the dot. Following a Hubbard-Stratonovich transformation the Lagrangian contains a term quadratic in Ψ , $\mathcal{L}_\Psi = \sum_\alpha \bar{\Psi}_\alpha M_\alpha \Psi_\alpha$, where we use spinor notations for $\bar{\Psi}_\alpha = (\bar{\psi}_{1\alpha} \bar{\psi}_{1\alpha})$ and the matrix M_α is given by

$$M_\alpha = \begin{pmatrix} \partial_\tau - \xi_\alpha + i\phi + \Phi^z & \sqrt{\gamma}\Phi^- \\ \sqrt{\gamma}\Phi^+ & \partial_\tau - \xi_\alpha + i\phi - \Phi^z \end{pmatrix}. \quad (3)$$

To obtain the GF we add source terms to the Lagrangian, $\mathcal{L}_{\Lambda Y} = \mathcal{L} + \bar{\Lambda}\Psi + \bar{\Psi}\Lambda + \bar{Y}\vec{\Phi}$. The fermionic (2×2) and bosonic (3×3) matrix GF's are given as derivatives of the generating (partition) function Z [8],

$$\mathcal{G}_\alpha^{\sigma\sigma'}(\tau_i, \tau_f) = \frac{\partial^2 Z}{\partial \bar{\Lambda}_{\tau_f}^\sigma \partial \Lambda_{\tau_i}^{\sigma'}}, \quad (4)$$

$$\mathcal{D}^{\mu\nu}(\tau_i, \tau_f) = \frac{\partial^2 Z}{\partial Y_{\tau_f}^\mu \partial Y_{\tau_i}^\nu},$$

with $\Lambda \rightarrow 0$, $\vec{Y} \rightarrow 0$. Here $\mathcal{G}_\alpha^{\sigma\sigma} = -\langle T_\tau \Psi_{\alpha\sigma}(\tau_f) \bar{\Psi}_{\alpha\sigma}(\tau_i) \rangle$ while $\mathcal{D}^{\mu\nu} = -\langle T_\tau \Phi^\mu(\tau_f) \Phi^\nu(\tau_i) \rangle$.

Our gauge transformation is given by $\tilde{M}_\alpha = W M_\alpha W^{-1}$, $\tilde{\Psi} = W(\tau)\Psi$ and $\tilde{\Phi} = \bar{\Psi}W^{-1}(\tau)$ with

$$W(\tau) = e^{i\theta(\tau)} \begin{pmatrix} e^{\eta(\tau)} & 0 \\ 0 & e^{-\eta(\tau)} \end{pmatrix}. \quad (5)$$

Here θ and η account for the $U(1)$ fluctuations of the charge and longitudinal fluctuations, respectively,

$$\theta = \int_0^\tau [\phi(\tau') - \phi_0] d\tau', \quad \eta = \int_0^\tau [\Phi^z(\tau') - \Phi_0^z] d\tau'. \quad (6)$$

In defining the gauge fields ϕ_0 [8] and Φ_0^z one needs to account for possible winding numbers ($k, m = 0 \pm 1, \dots$) [11]:

$$\beta\phi_0 = \int_0^\beta \phi d\tau + 2\pi k, \quad \beta\Phi_0^z = \int_0^\beta \Phi^z d\tau + 2i\pi m. \quad (7)$$

In Eq. (6) initial conditions [$W(0) = 1$] and periodic boundary conditions [$W(0) = W(\beta)$] are employed. As a result, the diagonal part of the gauged inverse electron's GF (\tilde{M}_α) does not depend on the finite-frequency components of fields. The off-diagonal part can be taken into account by a perturbative expansion in $\gamma < 1$. We represent $\tilde{M}_\alpha = (\mathcal{G}_\alpha^{[0]})^{-1} + \sqrt{\gamma}\Sigma_\Phi$ with $[\mathcal{G}_\alpha^{[0]}(\tau)]^{-1} = (\partial_\tau - \xi_\alpha + i\phi_0)\hat{1} + \Phi_0^z\sigma^z$ and the self-energy $\sqrt{\gamma}\Sigma_\Phi = \sqrt{\gamma}(\Phi^- e^{2\eta}\sigma^+ + \Phi^+ e^{-2\eta}\sigma^-)$. We next calculate the Green's function

$$\mathcal{G}_\alpha^{\sigma\sigma'}(\tau, \tilde{\mu}) = \delta_{\sigma\sigma'} \langle \mathcal{G}_\alpha^{[0]}(\tau, \tilde{\mu}) \exp(\sigma\eta_\tau + i\theta_\tau) \rangle_{\tilde{\Phi}, \phi}. \quad (8)$$

Hereafter $\langle \dots \rangle_{\tilde{\Phi}, \phi}$ denotes Gaussian averaging over fluctuations of the bosonic field ($\vec{\Phi}, \phi$) and the shifted chemical potential $\tilde{\mu} = \mu + \sigma\Phi_0^z + i\phi_0$. Integrating over all Grassmann variables and expanding \tilde{M}_α with respect to the transverse fluctuations, one obtains [12]

$$\mathcal{G}_{\alpha}^{\sigma\sigma}(\tau_i, \tau_f) = \frac{1}{Z(\mu)} \int d\vec{\Phi}_0 d\phi_0 \exp\left(-\frac{(\Phi_0^z)^2}{TJ} - \frac{(\phi_0)^2}{4TE_c} - \beta\Omega_0\right) \int \prod_{n \neq 0} d\Phi_n^z d\phi_n \exp\left\{T \sum_{n \neq 0} \left(-\frac{\Phi_n^z \Phi_{-n}^z}{J} - \frac{\phi_n \phi_{-n}}{4E_c}\right)\right\} \\ \times W(\tau_i) \left[\mathcal{G}_{\alpha}^{[0]}(\tau_i - \tau_f, \tilde{\mu}) - \sum_{k=1}^{\infty} \gamma^k \int d\tau_1 \dots \int d\tau_{2k} \langle (\mathcal{G}_{\alpha}^{[0]} \Sigma)^{2k} \rangle_{\text{tr}} \mathcal{G}_{\alpha}^{[0]}(\tau_{2k} - \tau_f, \tilde{\mu}) \right] W^{-1}(\tau_f), \quad (9)$$

where $\Omega_0(\tilde{\mu}) = -T \ln Z_0$, Z_0 is the partition function of the noninteracting electron gas. Also, computing the bosonic correlator [Eq. (4)], we find

$$\mathcal{D}^{\mu\nu}(\tau_i, \tau_f) = \frac{1}{Z(\mu)} \int D[\vec{\Phi}] \Phi^{\mu}(\tau_i) \Phi^{\nu}(\tau_f) \\ \times \exp\left(\text{Tr} \log[1 + \mathcal{G}_{\alpha}^{[0]} \Sigma_{\Phi}] - \frac{1}{J} \int_0^{\beta} \vec{\Phi}^2 d\tau\right). \quad (10)$$

In the spirit of [8], the interaction of electrons with the finite-frequency charge and longitudinal modes (ϕ_n , Φ_n^z) may be interpreted in terms of a gauge boson [13] dressing the electron propagator [cf. Fig. 1(a)]. The *exact* electronic GF which depends on the winding number [Eq. (7)] through $\tilde{\mu}$, is given by [11]

$$\mathcal{G}_{\alpha,\sigma}(\tau_i - \tau_f) = \sum_{\text{windings}} \mathcal{G}_{\alpha,\sigma}^{[0]}(\tau_i - \tau_f, \tilde{\mu}) e^{-S_{\parallel}(\tau_i - \tau_f)}, \quad (11)$$

where the Coulomb-longitudinal $U(1)$ gauge factor is

$$S_{\parallel}(\tau) = 4T \sum_{n \neq 0} \frac{E_c - J/4}{\omega_n^2} \sin^2\left(\frac{\omega_n \tau}{2}\right) \\ = \left(E_c - \frac{J}{4}\right) \left(|\tau| - \frac{\tau^2}{\beta}\right). \quad (12)$$

The exchange interaction effectively modifies the charging energy. For long-range interaction this correction is small $E_c/J \sim (k_F L)^{d-1}$ [2], while for contact interaction $E_c = J/4$ [2]. The spin effects for Ising model ($\gamma = 0$) lead therefore to a shift of the charging energy.

Transverse fluctuations.—The first nonvanishing diagram of our expansion (9) is depicted in Fig. 1(b). The bare GF, $\mathcal{G}_{\alpha,\sigma}^{[0]}(\tau) = e^{-\xi_{\alpha\sigma}\tau} [n_{\xi_{\alpha\sigma}}(1 - \theta_{\tau}) - (1 - n_{\xi_{\alpha\sigma}})\theta_{\tau}]$, depends on the transverse correlator (or \mathcal{D}^{+-}). The latter is evaluated in the Gaussian approximation

$$\langle \Phi^+(\tau_1) \Phi^-(\tau_2) \rangle_{\vec{\Phi}, \phi} = \frac{J}{2} \delta(\tau_1 - \tau_2) + \frac{\gamma J^2}{2\beta(\Delta - \gamma J)}. \quad (13)$$

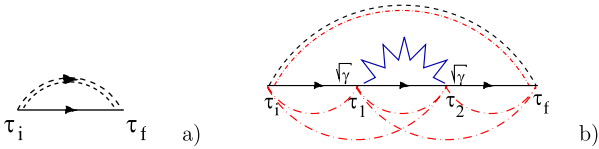


FIG. 1 (color online). Zeroth and first order Feynman diagrams contributing to electron's GF. Solid line represents $\mathcal{G}_{\alpha,\sigma}^{[0]}$; dashed lines stand for Coulomb bosons, dashed-dot lines denote longitudinal bosons, while the zigzag line represents $\langle \Phi^+(\tau_1) \Phi^-(\tau_2) \rangle$.

In Eq. (13) the first term is a manifestation of the white noise fluctuations of the fields $\vec{\Phi}$ arising from the Gaussian weight factor [cf. Eq. (10)]. The second term involves expansion of the $\text{Tr} \log$ term [(10)] and reflects the feedback of $\mathcal{G}^{[0]}$ on \mathcal{D}^{+-} . Note that the transverse components Φ^{\pm} are always accompanied by the gauge factors $e^{\mp 2\eta}$, hence the longitudinal bosons contribute to the dynamics involving the transverse fluctuations.

To proceed we now sum Eq. (9) over α . We compute perturbative corrections to the GF, $G_{\sigma}(\tau) \equiv \sum_{\alpha} \mathcal{G}_{\alpha,\sigma}(\tau)$, arising from the first term in the correlator Eq. (13) (to second order in $\frac{J}{T}$) and the second term there of (first order in $\frac{\gamma^2 J^2}{T(\Delta - \gamma J)}$). This yields

$$G_{\sigma}(\tau) = G_{\sigma}^{[0]}(\tau) e^{-S_{\parallel}(\tau)} F_{\perp}(\tau, \gamma). \quad (14)$$

Note the following technical points concerning this expansion: (i) $F_{\perp}(\gamma, \tau - \frac{\tau^2}{\beta})$ preserves the symmetry (in τ) with respect to $\beta/2$ to all orders of the expansion. (ii) Consider the term in F_{\perp} [arising from the first term in Eq. (13)], $\gamma \frac{J}{2} (\tau - \frac{\tau^2}{\beta})$. It can be exponentiated and combined with the contribution of the longitudinal boson (12), resulting in $J/4 \rightarrow J(1 + 2\gamma)/4$ in the expression for $S_{\parallel}[J(1 + 2\gamma)/4 \rightarrow JS(S + 1)$ for the isotropic model]. (iii) The second term in Eq. (13) contributes $\sim -\frac{\gamma^2 J^2}{2\beta(\Delta - \gamma J)} [\tau - \frac{\tau^2}{\beta}]^2$, which, upon exponentiation, leads to a non-Gaussian contribution to $G_{\sigma}(\tau)$. (iv) It is easy to show that below the incipient Stoner instability, $J < J_{\text{mesoscopic}}$, F_{\perp} is dominated by the “white noise” term of Eq. (13), while above this point it is the second (singular Stoner) term in (13) which dominates.

Tunneling density of states.—The conductance g_T is related to the TDOS ν through $g_T = \frac{e}{h} \int d\epsilon \nu(\epsilon) \Gamma(\epsilon) \times (-\frac{\partial f_F}{\partial \epsilon})$ where f_F is the Fermi distribution function at the

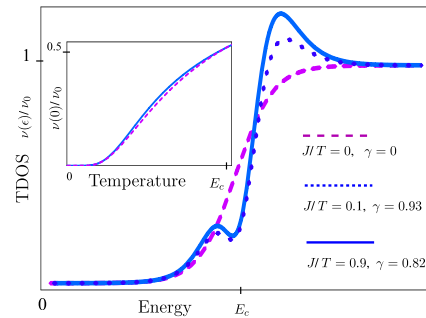


FIG. 2 (color online). The spin-normalized tunneling density of states shown as function of energy $E_c/T = 10$ and $J/\Delta = 0.92 \pm 0.02$ for all plots. Inset: TDOS as a function of temperature, $E_c/\Delta = 10$.

contact and Γ is the golden rule dot-lead broadening. To obtain the TDOS from the GF, Eq. (14), we deform the contour of integration in accordance with [8]. As a result, the TDOS is given by [14]

$$\nu(\epsilon) = -\frac{1}{\pi} \cosh\left(\frac{\epsilon}{2T}\right) \int_{-\infty}^{\infty} \sum_{\sigma} \left\langle G_{\sigma} \left(\frac{1}{2T} + it \right) \right\rangle_{k,m} e^{i\epsilon t} dt. \quad (15)$$

where $\langle \dots \rangle_{k,m}$ denotes a summation over all winding numbers for Coulomb and longitudinal zero-modes [11]. Examples for the temperature and energy dependence of the TDOS (for various γ) are depicted in Fig. 2. The energy dependent TDOS shows an intriguing nonmonotonic behavior at energies comparable to the charging energy E_c . This behavior, absent for $J = 0$ (see, e.g., [15]), is due to the contribution of the second term in Eq. (13), corresponding to the transverse spin susceptibility (see discussion below). It is amplified in the vicinity of the Stoner Instability point, and signals the effect of collective spin excitations (incipient ordered phase). One of possible experimental realizations of predicted effect is transport measurements in magnetic QD [16].

Spin susceptibilities.—These are defined through

$$\chi^{\mu\nu}(\tau_i, \tau_f) = \frac{\partial^4 Z}{\partial \bar{\Lambda}_{\tau_f}^{\mu} \partial \Lambda_{\tau_f}^{\nu} \partial \bar{\Lambda}_{\tau_i}^{\nu} \partial \Lambda_{\tau_i}^{\mu}}. \quad (16)$$

The longitudinal susceptibility (χ^{zz}) is *not* affected by the gauge bosons. By contrast, the transverse χ^{+-} acquires the gauge factor $\langle e^{2\eta(\tau)} \rangle_{m, \Phi^z}$, where the average is performed with respect to the Gaussian fluctuations of Φ^z and, in principle, the winding numbers [cf. Eq. (7)]. In practice, since $T > J$, only the $m = 0$ winding should be taken into account; $T > \Delta$ allows us to evaluate the path integral in the Gaussian approximation. One finds to leading order in γ

$$\chi^{zz}(\tau) = \frac{\chi_0}{1 - J\chi_0}, \quad \chi^{+-}(\tau) = \frac{2\gamma\chi_0 e^{J\tau}}{1 - \gamma J\chi_0}, \quad (17)$$

where $\chi_0 = 1/\Delta$. The above susceptibilities are given as function of τ . To obtain the dynamic susceptibilities one needs to Fourier transform and then continue to real frequencies. χ^{zz} (17) [17] diverges at the thermodynamic Stoner Instability point, akin to the Ising case (no γ corrections to the denominator), while χ^{+-} remains finite at the transition. Notwithstanding, the static transverse susceptibility is enhanced by the gauge fluctuations. The oscillating (in real time) factor in the dynamic χ^{+-} , Eq. (17), describes Bloch precessions in an anisotropic easy axis spin model.

Summarizing, we have studied the influence of spin and charge zero-mode interactions on the TDOS and the spin susceptibilities, χ^{zz} and χ^{+-} . Longitudinal spin fluctuations suppress the CB and the static χ^{zz} diverges at the Stoner transition. Transverse fluctuations generally tend to suppress the CB, but also contain a term which dominates

the dynamics near the Stoner instability and *enhances* the CB; χ^{+-} will be enhanced as well. The building blocks (correlators) defined here allow for various extensions of our analysis, e.g., studying the dynamic susceptibilities (including relaxation processes), γ corrections to $\chi^{\mu\nu}$, spin fluctuations modified two-particle GF, and analysis of the Coulomb peak regime. This will be discussed elsewhere [6].

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