On Nuclear Spin Measurement using Coherent Electron Spin Transport

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We propose an experimental setup to study spin-dependent magneto-transport through quantum dot. We show that due to spin-flip transitions, generated by the spin-orbit interaction, the spectral density of the tunneling current develops a distinct peak at the frequency of Zeeman splitting. We argue that under suitable conditions the peak's width can be sufficiently narrow to allow for detection of magnetization produced by few nuclear spins. The proposed g-factor engineered heterostructure can be utilized in measurements of single qubits in several schemes for quantum information processing in solid state systems.

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The problem of single spin measurement, electronic or nuclear, apart of its great fundamental importance, has recently attracted much practical interest in the light of rapid development of quantum information science and its potential applications in condensed matter systems. A number of quantum computing proposals have recently been suggested [1–3], preliminary experiments to fabricate and control a few quantum bit/qubit systems have been carried out or contemplated [4]. Among these a nuclear spin represents a perfect candidate for a role of qubit for quantum computers. Indeed, its longitudinal and transverse relaxation times in certain materials, such as in P donors in Si are seconds and can potentially be extended by at least several orders of magnitude by using special techniques [1].

There is, however, a significant disadvantage of nuclear spin qubits: because of their tiny magnetic moments the possibility of control of single nuclear spins is rather obscure. For this reason it was recently suggested to use scanning tunneling microscopy (STM) techniques for measurement of single nuclear spins, which seems to be free from the above disadvantages [3]. The proposal utilized an experimental observations of a distinct peak in the STM tunneling current spectrum in the presence of external constant magnetic field B [5]. This peak has been found at the frequency equal to that of electronic Zeeman splitting and therefore was associated with a modulation of the tunneling current by the Larmor precession of a nearby magnetic impurity. Yet, no self-consistent microscopic theory of the observed phenomenon [5] exists in the literature.

In this Letter we suggest a novel approach to the problem of local spin measurement, that may as well explain the above described STM experiments [5]. Our approach is based on resonant tunneling through microscopic/mesoscopic structures (impurities, quantum dots, etc), which energy levels are spin-split by an external magnetic field. In this case the spin-orbit coupling causes the spin-flip transitions resulting in coherent effects in the tunneling current [6]. We demonstrate below that these spin-flip transitions generate a distinct peak in the tunneling current at the Zeeman splitting frequency. If the width of this peak is rather narrow $\leq$ MHz, as observed in the experiments [5], one can hope to resolve hyperfine structure of the spin center from the peak's location in the spectrum, etc., and thus be able to measure a state of the nuclear spin of a given impurity atom [3].

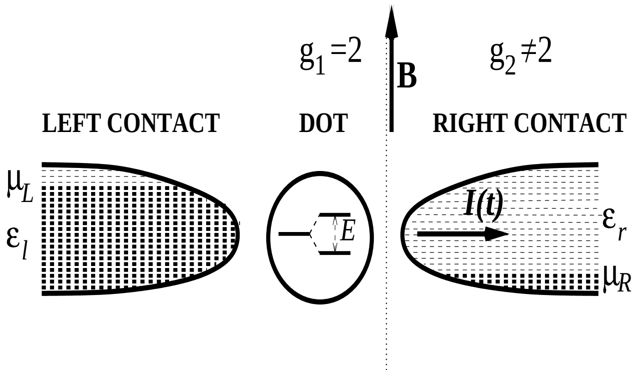

Fig. 1: Quantum dot coupled to two contacts. The right contact has a g-factor different from that of the left contact and the dot. The tunneling with spin flip generates effective coupling between the two Zeeman sublevels in the dot.

Let us consider a g-factor engineered heterostructure (for example Si/Ge) schematically shown in Fig. 1. There are two regions, to the right and to the left from the dotted line denoting the interface, that have different g-factors, $g_1 \approx 2$ for the left region and $g_2 \neq 2$. There are two contacts/Fermi reservoirs in each of the regions. The left region also contains a quantum dot so that when potential difference V is applied between the two reservoirs, electrons can tunnel from left to the right reservoirs via the dot. The states of two reservoirs are filled up to Fermi energies μ_L and μ_R respectively, where $\mu_L - \mu_R = eV$. We assume that there is a single discrete level in the dot due to spatial quantization, which is spin-split by an externally applied magnetic field. We also assume that the dot is doped with impurities, having nonzero nuclear spin. If these are spin polarized, an electron in the dot will experience a magnetic field $B = B_0 + B_{hyp}$, where B_0 is external field and B_{hyp} is an effective field produced by the hyperfine coupling of the electron and nuclear magnetic moments, which is proportional to the degree of polarization of nuclear spins. Therefore if one can detect the splitting between the two Zeeman levels of the electron in the dot, one can measure the nuclear spin polarization produced by the nuclei in the dot, provided that detection of the splitting can be carried out with sufficient precision to resolve the contribution due to B_{hyp}. In what follows we show that by measuring the power spectrum of current fluctuations in the proposed heterostructure one can resolve B_{hyp} produced by several tens of nuclear spins within the present day technology and potentially allow one to detect polarizations produced by fewer nuclei.

We model our system by the Hamiltonian $H = H_L + H_R + H_S + H_C + H_T$ where the first two terms represent the unperturbed states of two contacts, $H_L = \sum_{l,s} \epsilon_{ls} a^\dagger_{ls} a_{ls}$ and $H_R = \sum_{r,s} \epsilon_{rs} a^\dagger_{rs} a_{rs}$, where $a^\dagger_{ls}$ ($a^\dagger_{rs}$) creates a fermion/electron at the energy level ϵ_l (ϵ_r) and with spin s in the left (right) reservoir. The states in the dot are described by $H_S = \sum_s \epsilon_s \hat{n}_s$, where $\hat{n}_s = a^\dagger_s a_s$ and $a^\dagger_s$ creates an electron in the dot at the level with spin s. In the presence of magnetic field B the levels are split, so that $\epsilon_{-1/2} - \epsilon_{1/2} = g\beta B \equiv E$, Fig. 1, where g is the effective g-factor of the spin center and β is Bohr's magneton. The term $H_C = \sum_s \frac{U}{2} \hat{n}_s \hat{n}_{-s}$, where $\hat{n}_s = a^\dagger_s a_s$, and $a^\dagger_s$ corresponds to the Coulomb charging energy for the electron in the well. In what follows we will assume the case of complete Coulomb blockade, i.e., $U \to \infty$, thus allowing for only one electron to occupy the spin states in the well.

The tunneling transitions between the left reservoir, the dot and the right reservoir are represented by the Hamiltonian:

$$H_T = \sum_{l,s} \Omega_l \left(a^\dagger_{ls} a_s + a^\dagger_s a_{ls} \right) + \sum_{r,s,s'} \Omega_{rss'} \left(a^\dagger_{rs} a_{s'} + a^\dagger_{s'} a_{rs} \right) . \qquad (1)$$

Here we use gauge in which the tunneling amplitudes Ω_l and $\Omega_{rss'}$ are real. Note that our model accounts for possible spin flip in tunneling transitions from the dot to the right reservoir. The mechanism generating such transitions is similar to that of spin scattering by nonmagnetic impurities in semiconductors [9]. Due to spin-orbit interaction, relatively strong in the right contact in our case, the orbital and spin states of the electron in the right reservoir are mixed, resulting in effective g-factors for the electrons there to be different from 2. The eigenstates of H_R are represented by Kramers doublet, $|\psi_{r,s=1/2}\rangle = u_r|\uparrow\rangle + v_r|\downarrow\rangle$ and a Kramers conjugate state $|\psi_{r,s=-1/2}\rangle$, where u_r and v_r are functions of spatial coordinates only, and $|v| \sim O(|\Delta g u|)$, $\Delta g = g - 2$ [9]. We have assumed the spin orbit coupling in the left reservoir and the dot is much weaker ($g \approx 2$), so that we can neglect by the spin-orbit mixing effect there. In order to evaluate the tunneling matrix elements for transitions from the dot to the right reservoir, given by the second term in Eq. (1), one can utilize Bardeen's formula [10]: $\Omega_{rss'} = 1/2m \int d\vec{S} \cdot (\phi^*_s \vec{\nabla} \psi_{r,s'} - \psi_{r,s'} \vec{\nabla} \phi^*_s)$, where the integral is over any surface lying entirely within the tunneling barrier, separating the dot and the right reservoir, and the wave functions ϕ_s (state with spin s in the dot, $|\phi_s\rangle = |\phi\rangle|s\rangle$) and $\psi_{r,s'}$ are smoothly continued under the barrier; m is electron's mass and $\hbar = 1$. It is obvious that the states ψ_s under the barrier are still spin-orbit mixed due to the continuity condition. Therefore the tunneling matrix elements, corresponding to the transitions from the resonant level to the right reservoir without spin flip, are $\Omega_{rss} = 1/2m \int d\vec{S} \cdot (\phi^* \vec{\nabla} u_r - u_r \vec{\nabla} \phi^*)$, and the matrix elements of transitions accompanied by spin flips are $\Omega_{rs\,\bar{s}} = 1/2m \int d\vec{S} \cdot (\phi^* \vec{\nabla} v_r - v_r \vec{\nabla} \phi^*)$; $\bar{s} \equiv -s$. The two transition amplitudes are related as $|\Omega_{rs\bar{s}}| \sim O(|\Delta g \Omega_{rss}|)$.

In what follows we adopt approach developed in Refs. [7,8]. We construct the time dependent wave function of the system as

$$|\mathbf{\Psi}(t)\rangle = \Big\{ b_0(t) + \sum_{l,s} [b_{ls}(t) a^\dagger_s a_{ls} + b_{l\bar{s}}(t) a^\dagger_s a_{l\bar{s}}] + \sum_{l,r,s} [b_{lrs}(t) a^\dagger_{rs} a_{ls} + b_{lr\bar{s}}(t) a^\dagger_{rs} a_{l\bar{s}}] + \ \ldots \Big\} |\mathbf{0}\rangle , \qquad (2)$$

where the "ground" state $|\mathbf{0}\rangle$ corresponds to the situation when all states below Fermi energy in the left contact are filled, while all states above Fermi energy in the right contact are empty. The above wave function is a superposition of all possible particle-hole combinations that can be generated by the Hamiltonian H; note that H conserves the total number of particles in the system. Thus the first term in $\mathbf{\Psi}$ is the amplitude of the unperturbed state, i.e., when no excitations in the system is present, the second term describes a state in which a hole is created in the left reservoir and a particle with the same spin occupies the resonant level, etc. The above wave function satisfies the Schrodinger equation $i|\dot{\mathbf{\Psi}}\rangle = H|\mathbf{\Psi}\rangle$.

In order to describe transport in our model we introduce probabilities for the dot to be empty or occupied, provided the a certain number of electrons have been passed through the junction. The level can be either empty, with probability σ^n_{aa}, where the subscript aa indicates that there is no electrons in the dot and the superscript n describes that n electrons have arrived in the right reservoir/collector, or the level can be filled with probabilities σ_{bb}^n and σ_{cc}^n, where bb indicates that the lower Zeeman sublevel $s = 1/2$ is filled, while cc stands for the upper Zeeman sublevel $s = -1/2$ being filled. Occupation of both Zeeman levels in the dot by two electrons is prohibited in our model by the infinite charging energy U; see Refs. [7,8] for detailed discussion. We also introduce the off-diagonal elements σ_{bc}^n describing coherent superpositions of states on the upper and lower Zeeman levels of the electron in the dot. σ_{ij}^n's are related to the wave function $|\mathbf{\Psi}\rangle$ as $\sigma_{aa}^0 = |b_0|^2$, $\sigma_{bb}^0 = \sum_{l,s=1/2}|b_{ls}|^2 + \sum_{l,s=-1/2}|b_{l\bar{s}}|^2$, $\sigma_{aa}^1 = \sum_{l,r,s}[|b_{lrs}|^2 + |b_{l,r,\bar{s}}|^2]$, etc.

Following steps of Refs. [7,8] one derives the rate equations for the density matrix σ from the Schrodinger equation for the wave function $|\mathbf{\Psi}\rangle$. These rate equations for a general case are presented in [8]. One finds for our case:

$$\dot{\sigma}_{aa}^n = -2\Gamma_L\sigma_{aa}^n + \Gamma_R\left(\sigma_{bb}^{n-1} + \sigma_{cc}^{n-1}\right) + \Delta\Gamma_R\left(\sigma_{bc}^{n-1} + \sigma_{cb}^{n-1}\right)\,, \tag{3a}$$

$$\dot{\sigma}_{bb}^n = -\Gamma_R\sigma_{bb}^n + \Gamma_L\sigma_{aa}^n - \frac{\Delta\Gamma_R}{2}\left(\sigma_{bc}^n + \sigma_{cb}^n\right)\,, \tag{3b}$$

$$\dot{\sigma}_{cc}^n = -\Gamma_R\sigma_{cc}^n + \Gamma_L\sigma_{aa}^n - \frac{\Delta\Gamma_R}{2}\left(\sigma_{bc}^n + \sigma_{cb}^n\right)\,, \tag{3c}$$

$$\dot{\sigma}_{bc}^n = iE\sigma_{bc}^n - \Gamma_R\sigma_{bc}^n - \frac{\Delta\Gamma_R}{2}\left(\sigma_{bb}^n + \sigma_{cc}^n\right) \tag{3d}$$

Here $\Gamma_{L,R} = 2\pi\Omega_{L,R}^2(\epsilon_s)\rho_{L,R}(\epsilon_s)$ and $\Delta\Gamma_R = 2\pi\Omega_R(\epsilon_s)\delta\Omega_R(\epsilon_s)\rho_R(\epsilon_s)$, where we denote $\Omega_{rss} \equiv \Omega_R$, $\Omega_{rs\bar{s}} \equiv \delta\Omega_R$. In derivation of Eqs. (3) we assumed that the coupling constants Ω's and the densities of states ρ's are weakly dependent on energy, and so $\rho_{L,R}(\epsilon_s) = \rho_{L,R}(\epsilon_{\bar{s}})$, $\Omega_{L,R}(\epsilon_s) = \Omega_{L,R}(\epsilon_{\bar{s}})$ and thus rates $\Gamma_{R,L}$ for the electrons tunneling into and out of the dot are independent of energy. We also assumed that the bias voltage condition, $V \gg \Gamma_{L,R}$, which is essential for derivation of Eqs. (3). One sees from Eqs. (3) that the two Zeeman levels in the dot are coupled with each other due to spin-flip transitions through continuum with the rate $\Delta\Gamma_R$. We also assume that $\Gamma_L, \Gamma_R \geq \Delta\Gamma_R$.

By summing Eqs. (3) over the number of electrons in the right reservoir one obtains the "standard" Bloch-type equations for the reduced density matrix $\sigma_{ij} = \sum_n \sigma_{ij}^n$ with $i, j \equiv a, b, c$. These equations, which look essentially identical to Eqs. (3), describe the state of the resonant level independently of the states of the reservoirs.

From Eqs. (3) one can derive the dynamics for the expectation value of the tunneling current by assuming that the right reservoir is properly isolated from the external fields [11]. In this case the tunneling current is given by $\langle I(t)\rangle = ie\langle\mathbf{\Psi}(t)|[H, \hat{N}_R]|\mathbf{\Psi}(t)\rangle$, where H is the total Hamiltonian and $\hat{N}_R = \sum_{r,s} a_{rs}^\dagger a_{rs}$ is the operator of the electron numbers in the right reservoir. Using Eq. (2) one finds that the average current can be written as $\langle I(t)\rangle = e\langle\dot{N}_R(t)\rangle$, where $\langle N_R\rangle = \sum_n n(\sigma_{aa}^n + \sigma_{bb}^n + \sigma_{cc}^n)$. Using Eqs. (3) for $\dot{\sigma}^n$, one can sum over n thus obtaining

$$\langle I(t)\rangle = e\Gamma_R[\sigma_{bb}(t) + \sigma_{cc}(t)] + e\Delta\Gamma_R[\sigma_{bc}(t) + \sigma_{cb}(t)]\,.$$

It is easy to check that the transient behavior of the average current is an oscillatory one (due to coherence terms $\sim \sigma_{bc}$) with frequency equal to E and approaching stationary value

$$\langle I(\infty)\rangle = \frac{2e\Gamma_L\Gamma_R\left(E^2 + \Gamma_R^2 - \Delta\Gamma_R^2\right)}{\left(2\Gamma_L + \Gamma_R\right)\left(E^2 + \Gamma_R^2\right) - 2\Gamma_R\Delta\Gamma_R^2}\,. \tag{4}$$

The power spectral density of the current, $S_I(\omega) = \int_0^\infty dt\cos(\omega t)\langle I(t)I(t+\tau)\rangle$, can be evaluated from rate equations (3) utilizing MacDonald's theorem, that relates S_I to the dispersion of charge accumulated on the collector (right reservoir) [12]:

$$S_I(\omega) = e^2\omega/\pi\int_0^\infty dt\sin(\omega t)\langle\dot{N}_R^2(t)\rangle\,. \tag{5}$$

The dispersion for the number of electrons in the right reservoir can be found from the rate equations (3) as $\langle N_R^2\rangle = \sum_n n^2(\sigma_{aa}^n + \sigma_{bb}^n + \sigma_{cc}^n)$. Here we quote the final expression for spectral density $S_I(\omega)$. The general result is rather cumbersome. In the region of interest, $E \geq \Gamma_L, \Gamma_R \geq \Delta\Gamma_R$, expanding S_I in powers of $\Delta\Gamma_R$ up to $O(\Delta\Gamma_R^2)$, we obtain:

$$S_I(\omega) = \frac{e^2}{\pi}\frac{2\Gamma_L\Gamma_R}{2\Gamma_L + \Gamma_R}\frac{4\Gamma_L^2 + \Gamma_R^2 + \omega^2}{\left(2\Gamma_L + \Gamma_R\right)^2 + \omega^2} + \frac{8e^2\Gamma_L^3\Gamma_R^2}{\pi E^2\left(2\Gamma_L + \Gamma_R\right)^2}\frac{\Delta\Gamma_R^2}{\Gamma_R^2 + (\omega - E)^2}\,. \tag{6}$$

The spectrum (6) is shown in Fig. 2. The first term in (6) is the shot noise approaching the "Schottky" limit $S_I = e\langle I\rangle/\pi$ for $\omega \gg \Gamma_R, \Gamma_L$. For frequencies $\omega \leq \Gamma_L, \Gamma_R$ there is a dip in the spectrum - the result merely consistent with Refs. [13]. The second term representing a distinct peak arises due to spin-flip transitions between the Zeeman-split sublevels in the dot. It is roughly of a Lorentzian shape centered approximately at $\omega = E$ and having width Γ_R. A similar situation takes place in case of a current tunneling through a double well structure [14], where a peak in the fluctuation spectrum appears to be located at the tunneling frequency for the double well structure. The ratio of the peak's height to the noise pedestal (the signal to noise ratio) given by Eq. (6) is $S/N = 4\Gamma_L^2\Delta\Gamma_R^2/E^2\Gamma_R(2\Gamma_L + \Gamma_R)$. The S to N ratio can be significantly increased in heterostructures with greater $g_1 - g_2$ difference, and thus greater spin transition rate $\Delta\Gamma_R$, or in asymmetric heterostructures with $\Gamma_L \gg \Gamma_R$. From Eqs. (4), (6) one can evaluate the orders of magnitude for parameters needed for observation of a distinct peak in the fluctuations spectrum. The width of the peak in (6) is defined by value of current through the structure, $\Gamma_R \simeq \langle I \rangle / e$ for $\Gamma_L > \Gamma_R$. Therefore to resolve a peak due to spin flip transitions one needs to satisfy condition $E \geq \Gamma_R$, though E should not be too great as signal to noise ratio decreases with growth of E. Assuming that the Zeeman splitting E is solely due to hyperfine coupling, which is typically of order 10 - 10^2 MHz per single nuclear spin, the current through the heterostructure must be sufficiently small, < 10 pA. However measurement of magnetization produced by tens of nuclear spins requires currents of order hundreds of pA, a number within the capabilities of today's single-electronics.

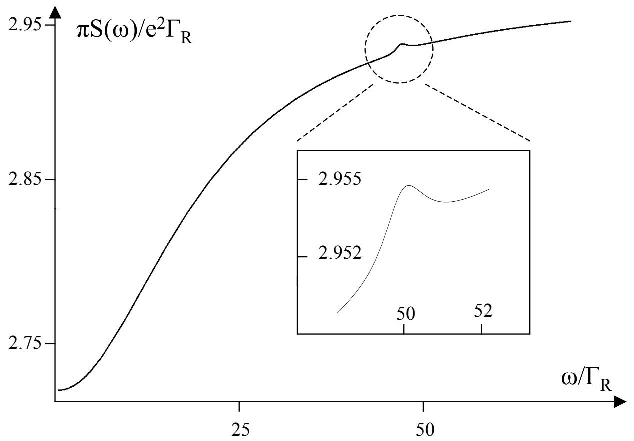

Fig. 2: Power spectrum of tunneling current fluctuations; Eq. (6). Here $E = 50\Gamma_R$, $\Delta\Gamma_R = 0.4\Gamma_R$, $\Gamma_L = 20\Gamma_R$.

The peak's broadening resulting from spin-lattice interaction can be evaluated from the results of Ref. [15]. It was shown there that the zero-dimensional character of the states in the dot leads to significant suppression of spin-flip rate as compared to that of the delocalized states, reducing the spin-flip rate to kHz for GaAs dots at low temperatures and to even smaller number for Si dots. Therefore the spin-lattice induced broadening virtually plays no role in the proposed mechanism.

In summary we have proposed a new mechanism for observation of local nuclear magnetization. We show that the spectral density of the current fluctuations for our system develops a distinct peak, whose location is determined by the Zeeman splitting of a discrete level in the dot, while the width of the peak is directly related to the value of the tunneling current. By polarizing nuclear spins in the dot one can alter the magnitude of the Zeeman splitting and therefore change the peak's location. The proposed experiment allows one to measure polarization as well as depolarization rate of a small number of nuclear spins. The later can be determined from rate of the peak's shift due to Zeeman frequency change because of the depolarization of the nuclei, provided that the nuclear relaxation rate $T_{1n}^{-1} \ll \Gamma_R$. The nuclear T_{1n}^{-1} is significantly suppressed due to large difference in Zeeman energies of electron and nuclear spins and thus one can expect that the above condition is met.

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[1] B. E. Kane, Nature (London) **393**, 133 (1998); R. Vrijen, E. Yablonovich, K. Wang, H. W. Jiang, A. Balandin, V. Roychowdhury, T. Mor and D. P. DiVincenzo, Phys. Rev. A **62**, 012306 (2000), and references therein.

[2] N. A. Gerhshefeld, I. L. Chuang, Science **275**, 350 (1997); D. Loss and D. P. DiVincenzo, Phys. Rev. A **57**, 120 (1998); V. Privman, I. D. Vagner, G. Kventsel, Phys. Lett. A **239**, 141 (1998); D. Mozyrsky, V. Privman, M. L. Glasser, Phys. Rev. Lett. **86**, 5112 (2001); A. Imamoglu, D. D. Awschalom, G. Burkard, D. P. DiVincenzo, D. Loss, M. Sherwin and A. Small, Phys. Rev. Lett. **83**, 4204 (1999).

[3] G. P. Berman, G. W. Brown, M. E. Hawley, V. I. Tsifrinovich, Phys. Rev. Lett. **87**, 097902 (2001).

[4] D. G. Cory, A. F. Fahmy, T. F. Havel, Proc. Natl. Acad. Sci. U.S.A. **94**, 1634 (1997); J. R. Tucker, T. C. Shen, Solid State Electron. **42**, 1061 (1998); R. G. Clark, unpublished results presented at a quantum computing conference held in Baltimore, MD, 2000.

[5] Y. Manassen, R. J. Hamers, J. E. Demuth, J. Castellano, Phys. Rev. Lett. **62**, 2531 (1989); D. Shachal and Y. Manassen, Phys. Rev. B **46**, 4795 (1992); Y. Manassen, I. Mukhopadhyay, N. R. Rao, Phys. Rev. B **61**, 16223 (2000).

[6] G. Usaj and H. U. Baranger, Phys. Rev. B **63**, 184418 (2001).

[7] S. A. Gurvitz and Ya. S. Prager, Phys. Rev. B **53**, 15932 (1996); S. A. Gurvitz, Phys. Rev. B **56**, 15215 (1997).

[8] S. A. Gurvitz, Phys. Rev. B **57**, 6602 (1998).

[9] V. F. Gantmakher, I. B. Levinson, *Carrier scattering in metals and semiconductors* (Elsevier Science Pub. Co., Amsterdam, New York, 1987).

[10] J. Bardeen, Phys. Rev. Lett. **6**, 57 (1961).

[11] W. Shockley, J. Appl. Phys. **9**, 635 (1938); L. Fedichkin, V. V'yurkov, Appl. Phys. Lett. **64**, 2535 (1994).

[12] D.K.C. MacDonald, Rep. Prog. Phys. **12**, 56 (1948).

[13] L. Y. Chen, C. S. Ting, Phys. Rev. B **46**, 4714 (1992); B. Elattari and S. A. Gurvitz, Phys. Lett. A, in press.

[14] A. N. Korotkov, D. V. Averin, and K. K. Likharev, Phys. Rev. B **49**, 7548 (1994).

[15] A. V. Khaetskii, Y. V. Nazarov, Phys. Rev. B **64**, 125316 (2001).