Nonlinear voltage dependence of shot noise

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I. INTRODUCTION

Due to the particle nature of electron, electric current in a conductor fluctuates with time giving rise to shot noise. The spectra of shot noise contain information which can be used to characterize electron transport in the conductor. For instance it may be used to probe the kinetics of electrons and investigate correlations of electronic wave function. For this reason shot noise of mesoscopic systems has been studied extensively. A classical conductor is characterized by Poissonian noise, where the current fluctuation $\langle (\Delta I)^2 \rangle$ in a frequency range $\Delta \nu$ is proportional to the electrical current $I$: $\langle (\Delta I)^2 \rangle = 2qI\Delta \nu$ where $q$ is the electron charge. In a mesoscopic conductor, on the other hand, shot noise is also influenced by two other factors: the Pauli exclusion principle and the Coulomb interaction. Pauli exclusion reduces the classical shot noise by a factor proportional to $(1 - T)$ for each transmission subband, assuming the transmission coefficient $T$ to be insensitive to electron energy. Coulomb interaction, on the other hand, can contribute to reduce or enhance shot noise depending on system details.

The quantum suppression of shot noise has been convincingly demonstrated by several experiments. The universal suppression by Coulomb interaction in nondegenerate diffusive conductors has been observed in computer simulations and confirmed theoretically using Boltzmann-Langevin equation. The quantum enhancement of shot noise from the classical value due to Coulomb interaction has recently been explored experimentally. For a tunneling structure with or without a magnetic field, shot noise versus voltage increases drastically in the region of negative differential resistance (NDR). If one assumes sequential tunneling of the electron transport, numerical results were in good agreement with those of the experiment and it indicated that the enhancement of shot noise was caused by Coulomb interaction. From the scattering matrix theory point of view, Ref. examined the effect of Coulomb interaction and the enhancement of shot noise was found to be related to the multistability when a tunneling system is out of equilibrium. So far, comparison between experimental and theoretical results suggests a need for a microscopic theory.

From a theoretical point of view, focused attention has been devoted to cases where the external bias voltage strength which drives the current flow is very small. In this case the current due to each subband is a linear function of the bias voltage: $I_i = (2e^2/h)V_{\text{bias}}T_i$, where $T_i$ is the zero bias transmission coefficient of the $i$-th subband. Indeed, experiment of Ref. on quantum point contact (QPC) has shown that the peak value of shot noise due to first subband is a linear function of $V_{\text{bias}}$. Similar linear behavior was also found in QPC experiment of Ref. On the other hand, in many nonlinear devices the electric current is a nonlinear function of bias: $I = I(V_{\text{bias}})$. A notable example is the resonance tunneling structure where current $I$ varies with bias in a nonlinear fashion, giving rise to NDR regions. Previous investigations indicated that the nonlinear I-V characteristics has a profound influence on the shot noise spectra, including the enhancement of it.

The purpose of the present work is to report a microscopic theory for calculating shot noise at the nonlinear regime in mesoscopic conductors. Our theory is based on nonequilibrium Green’s functions where the electron-electron interaction is treated in a self-consistent density functional form at the Hartree level. A direct consequence of self-consistency is that shot noise becomes only a function of voltage difference, which is the required physical condition (gauge invariance) for a nonlinear theory. We derive the nonlinear shot noise formula at zero temperature, which, in the wideband limit, can be exactly evaluated. For more general situations we derive shot noise spectra order by order in the bias voltage.

In the next section we present the derivation of the nonlinear shot noise spectra. Sections III and IV present the wideband limit result with numerical evaluations, as well the weakly nonlinear analysis of the shot noise. The last section summarizes the main findings of this work.
II. NONLINEAR SHOT NOISE FORMULA

The theoretical approaches to shot noise include scattering matrices, semiclassical kinetic theory, nonequilibrium Green’s function (NEGF), etc. For a full nonlinear analysis of quantum transport in the mesoscopic regime, we have found that it is most convenient to use NEGF, but with the necessary extension of including the internal potential build up due to electron-electron interactions.

We start from the combined DC thermal and shot noise spectra derived in Ref. [7] which is appropriate for a conductor with non-interacting electrons ($\hbar = 1$),

$$<\Delta I_\alpha \Delta I_\beta> = \Delta \nu \sum_{\gamma \delta} \int dE Tr[A_{\gamma \delta}(\alpha)A_{\delta \gamma}(\beta)] \times f_\gamma (1 - f_\delta)$$

(1)

where

$$A_{\gamma \delta}(\alpha) = \delta_{\alpha \beta} s_{\alpha \gamma} - s_{\alpha \beta} s_{\delta \gamma}$$

(2)

where $f_\alpha = f(E - qV_\alpha)$ is the Fermi distribution function and $s_{\alpha \beta}$ is the scattering matrix. The subscripts denote probes which connect our conductor to the reservoirs.

In order to correctly explore nonlinear voltage dependence in a quantum transport theory, it is essential to include the long range Coulomb potential as pointed out by Büttiker. It is well known that interacting systems are most conveniently dealt within the NEGF formalism. For this purpose, we will rewrite Eq. (1) using Green’s functions where the internal Coulomb potential can be explicitly included. This way, our nonlinear theory satisfies the gauge invariant condition, where the noise spectra remains unchanged when the voltages of all probes are shifted by the same constant amount. Recently, Gransesperger and Büttiker have discussed the relationship between scattering matrix theory and the Hamiltonian approach in which the transmission coefficient is expressed in terms of Green’s function. We will use this approach to rewrite Eq. (1) in terms of the Green’s functions. We will then supplement it with the necessary steps of determining the internal electro-static potential build-up due to Coulomb interactions.

In the following, we consider a quantum coherent multi-probe conductor specified by the following Hamiltonian

$$H = \sum_{k \alpha} \epsilon_{k \alpha} c_{k \alpha}^\dagger c_{k \alpha} + H_{cen}\{d_n, d_n^\dagger\} + \sum_{k \alpha n} [T_{k \alpha n} c_{k \alpha}^\dagger d_n + c.c.]$$

(3)

where $\epsilon_{k \alpha} = \epsilon_k^0 + qV_\alpha$. The first term of Eq. (3) describes the probes where DC signal is applied far from the conductor; the second term is the general Hamiltonian for the scattering region; the last term gives the coupling between probes and the scattering region with the coupling matrix $T_{k \alpha n}$. Here $c_{k \alpha}^\dagger$ ($c_{k \alpha}$) is the creation (annihilation) operator of electrons inside the $\alpha$-probe. Similarly $d_n^\dagger$ ($d_n$) is the operator for the scattering region. It is important to note that we will include the internal Coulomb potential $U$ inside the scattering region so that the actual Hamiltonian of the scattering region is $H_{cen} + qU$.

The retarded scattering Green’s function $G^r = G^r(E, U)$, where $U = U(r)$ is the electro-static potential build-up inside the scattering region due to interacting electrons, is given by

$$G^r(E, U) = \frac{1}{E - H - qU - \Sigma^r}$$

(4)

where the self-energy $\Sigma^r = \sum_\alpha \Sigma^r_\alpha (E - qV_\alpha)$ is defined as,

$$\Sigma^r_\alpha(E) = \frac{1}{2\pi} \int \frac{\Gamma_\alpha(E') dE'}{E - E' + i\eta}$$

(5)

and $\eta$ is a positive infinitesimal and $\Gamma_\alpha(E)$ is the linewidth function

$$(\Gamma_\alpha(E))_{mn} = 2\pi \sum_k T^r_{k \alpha m} T_{k \alpha n} \delta(E - \epsilon_{k \alpha})$$

(6)

The scattering matrix can be expressed in terms of Green’s functions by the Fisher-Lee relation

$$s_{\alpha \beta} = \delta_{\alpha \beta} - 2\pi i W_{\alpha}^\dagger G^r W_{\beta}$$

(7)

where $W_\alpha$ satisfies $2\pi W_\alpha W_{\alpha}^\dagger = \Gamma_\alpha$. Using this relation, it is straightforward to show that Eq. (1) becomes

$$<\Delta I_\alpha \Delta I_\beta> = \frac{q^2}{\pi} \sum_{\gamma \delta} \int dE Tr[(i\delta_{\alpha \delta} \Gamma_\alpha G^r - i\delta_{\alpha \gamma} \Gamma_\gamma G^r)(\delta_{\beta \gamma} \Gamma_\gamma G^r - i\delta_{\beta \delta} \Gamma_\delta G^r)] f_\gamma (1 - f_\delta)$$

(8)

where $G^r = G^r(E, U)$ is the advanced Green’s function and we have used the notation $\Gamma_\alpha = \Gamma_\alpha(E - qV_\alpha)$ for the linewidth function.

Notice that we have explicitly included the internal potential landscape $U(r)$ into the Green’s functions, but this landscape can only be obtained self-consistently. This is a crucial step in the development of a gauge invariant nonlinear DC theory. We determine the internal potential $U(r)$ by the self-consistent Poisson equation

$$\nabla^2 U = 4\pi i q \int (dE/2\pi) G^<(E, U)$$

(9)

where the lesser Green’s function $G^<$ is related to the retarded and advanced Green’s functions $G^r$ and $G^a$,

$$G^<(E, U) = G^r \sum_\beta i \Gamma_\beta (E - qV_\beta) f(E - qV_\beta) G^a$$

(10)

Eq. (1) is, in general, a nonlinear equation because $G^r,a$ depends on $U(r)$ (see Eq. (9)). By self-consistently solving Eqs. (3), (4), (10), we obtain the Green’s functions as well.
as the internal potential $U$. Then we can calculate shot noise from Eq. (6) which is a general nonlinear function of the external bias $\{V_{\alpha}\}$. This theoretical procedure can be carried out at least numerically, but in this work we are interested in cases where analytical derivations are possible.

For a two-probe system, Eq.(6) reduces to

$$< (\Delta I)^2 > = \frac{q^2}{\pi} \Delta \nu \int dE \{ f_{1}(1 - f_{1}) + f_{2}(1 - f_{2}) \}
\times T r [\hat{T}] + (f_{1} - f_{2})^{2} T r [(\hat{T} - \hat{T})^2] \quad (11)$$

where $\hat{T}(E, U) = \Gamma G(E) G^\ast(U)$ is the transmission operator such that $T r [\hat{T}(E, U)]$ is the transmission coefficient, here the trace is over the matrices written in real space.

To end this section, we discuss the gauge invariance condition. It is easy to prove that the noise spectra Eqs. (6) and (11) are gauge invariant: shifting the potential everywhere by a constant $V_{\alpha}$, $U \rightarrow U + V_{\alpha}$ and $V_{\alpha} \rightarrow V_{\alpha} + V_{\alpha}$, $< (\Delta I)^2 >$ calculated from these expressions remains the same. It is useful to note that in Eqs. (6,11) the quantity $\Gamma$ depends on bias voltage: without such a voltage dependence the gauge invariance can not be satisfied.

### III. THE WIDEBAND LIMIT

In this section we evaluate the shot noise spectra at the wideband limit. In this commonly used limit$^{[3]}$, the coupling matrix $\Gamma$ is assumed to be independent of energy which drastically simplifies the algebra. The wideband limit corresponds to cases where the probes have no feature, thus the internal potential $U(r)$ becomes a space-independent constant $U_{0}$ (the value of $U_{0}$ depends on the voltages $\{V_{\alpha}\}$ and it still needs to be determined). For a single level system, as far as the nonlinear current-voltage curve is concerned, the wideband limit corresponds to a resonance tunneling system where the scattering matrix has the Breit-Wigner form.

In wideband limit the steady state Green’s function takes a very simple form, $G_{0}^{\ast} = 1/(E - E_{0} + i\Gamma/2)$, thus the integral in Eq. (11) can be done exactly at zero temperature. We obtain,

$$< (\Delta I)^2 > = \frac{q^2}{\pi} \Delta \nu \frac{4 \Gamma^2 \Gamma_{2}^{\ast}}{\Gamma_{3}^2} \left\{ \frac{\Gamma_{1}^2 + \Gamma_{2}^{\ast}}{2 \Gamma_{1} \Gamma_{2}^{\ast}} \left( \frac{\Delta E_{1}}{\Gamma/2} \right) \right. 
\left. - \arctan \left( \frac{\Delta E_{2}}{\Gamma/2} \right) - \frac{\Gamma}{2} \left[ \frac{\Delta E_{1}}{\Gamma/2} \right]^{2} \right\}
\frac{\Delta E_{2}}{(\Gamma/2)^2 + (\Delta E_{2})^2} \right\} \quad (12)$$

where $\Delta E_{\beta} = E_{F} - E_{0} - qU_{\beta} + qV_{\beta}$.

While the internal potential $U_{0}$ can be determined by the Poisson equation $\hat{E}$, which requires numerical analysis, we instead determine it by introducing the geometrical capacitances $C_{1}$ and $C_{2}$ of the left and the right coupling regions (regions where our conductor connects to the two probes) respectively. The charge in the well due to the Coulomb interaction is given by

$$\Delta Q = -i \int (dE/2\pi) [G^{\ast}(E, U_{0}) - G^{\ast}_{0}]
= C_{1}(U_{0} - V_{1}) + C_{2}(U_{0} - V_{2}) \quad (13)$$

where $\Delta Q$ is the total charge in the well and $G^{\ast}_{0}$ is the equilibrium lesser Green’s function. In the wideband limit, this equation reduces to

$$\sum_{\beta} \Gamma_{\beta} \arctan \left[ \frac{\Delta E_{0}}{\Gamma/2} \right] - \Gamma \arctan \left[ \frac{E_{F} - E_{0}}{\Gamma/2} \right]
= \frac{\pi \Gamma}{q} [C_{1}(U_{0} - V_{1}) + C_{2}(U_{0} - V_{2})]. \quad (14)$$

When $C_{1} = C_{2} = 0$, Eq. (14) corresponds to the quasi-neutrality approximation which neglects the charge polarization in the system. Thus using two phenomenological constants $C_{1}$ and $C_{2}$ we can determine $U_{0}$ from the last equation. Hence the noise spectra of Eq. (12) is now completely specified. Finally, we can check the gauge invariance of Eq. (12): the wideband approximation and the charging model for $U_{0}$ do not disrupt the satisfaction of it. Indeed, raising both $V_{0}$ and $U_{0}$ by the same amount does not alter the shot noise given by Eq. (12).

In Fig.1, we have plotted the differential shot noise $d < (\Delta I)^2 > /dV'$ as a function of the voltage for four different set of system parameters: symmetric structures with $\Gamma_{1} = \Gamma_{2} = 0.5$, $C_{1} = C_{2} = 0.5$ (solid line); $\Gamma_{1} = \Gamma_{2} = 0.5$, $C_{1} = C_{2} = 0.1$ (dotted line); $\Gamma_{1} = \Gamma_{2} = 0.1$, $C_{1} = C_{2} = 0.4$ (dot-dashed line); and an asymmetric structure with $\Gamma_{1} = 0.1$, $\Gamma_{2} = 0.8$, $C_{1} = 0.1$, and $C_{2} = 0.8$ (dashed line). For symmetric structures, we always observe two peaks for the differential shot noise whereas for the asymmetric structure there is only one. This can be understood qualitatively as follows. Since the shot noise at small voltage is proportional to $\frac{\pi \Gamma}{q} T^{-2}$, the suppression reaches maximum near the resonant point for the symmetric structure because $T \approx T^{2} \approx 1$ at resonance. As a result, a peak appears on each side of the resonant point giving rise to the two peaks in Fig. 1.

For an asymmetric structure, however, the shot noise suppression is not as strong as that of the symmetric case (see Fig. 2). For the very asymmetric structure used here, the quantum resonance is very weak, resulting to only one peak in the differential shot noise spectra. For the symmetric cases, the separation between two peaks is proportional to $\Gamma$. The different resonant positions for solid line and dotted line in Fig.1 (the dips near voltage equals 4 and 6 respectively) is due to the Coulomb interaction in the well. Smaller capacitance coefficients (dotted line) correspond to large internal potential, which shifts the level position from $E_{0}$ to higher values $E_{0} + qV_{0}$. This is why that the resonant position for the dotted curve (with smaller capacitance coefficients) is shifted further relative to the solid curve (with larger capacitances).
As discussed in the Introduction, the classical shot noise is given by $2qI\Delta\nu$. The deviation from this classical value is usually characterized by the Fano factor which is defined as

$$\gamma \equiv \frac{(\langle \Delta I \rangle^2) - \langle I \rangle^2}{2qI\Delta\nu}.$$ (15)

In the wideband limit, it is easy to derive the current $I$ to be,

$$I = \frac{q\Gamma_1\Gamma_2}{\pi\Gamma}[\arctan(\frac{2\Delta E_1}{\Gamma}) - \arctan(\frac{2\Delta E_2}{\Gamma})].$$

Before presenting the plot of $\gamma$ for our nonlinear analysis, two observations are in order. First of all, it is easy to show that in the limit $(V_1 - V_2) \to 0$ and $\Gamma \to 0$, the Fano factor $\gamma \to 1$. Secondly, in the opposite limit when voltage difference is very large, the Fano factor is given by the well known expression $\gamma = (\Gamma_1^2 + \Gamma_2^2)/\Gamma^2$. For symmetrical systems ($\Gamma_1 = \Gamma_2$) this large voltage limit of $\gamma$ is 0.5. The same behavior has been observed in experiment except near the NDR region. Physically, the currents from both leads contribute to the Fano factor. At large voltage, the current from the low biased lead can be neglected and the shot noise is suppressed.

In Fig. 2, we have depicted the Fano factor versus voltage. The system parameters are the same as that of Fig. 1. As expected, the Fano factors approach to 0.5 for symmetrical systems ($\Gamma = 1$) this large voltage limit of $\gamma$ is 0.5. The same behavior has been observed in experiment except near the NDR region. Physically, the currents from both leads contribute to the Fano factor. At large voltage, the current from the low biased lead can be neglected and the shot noise is suppressed.

In Fig. 2, we have depicted the Fano factor versus voltage. The system parameters are the same as that of Fig. 1. As expected, the Fano factors approach to 0.5 for symmetrical structures at large voltage. We also see that the Fano factors are minimum near the resonance. In the wideband limit, the Fano factor can be smaller than 0.5 for the symmetric case. For smaller $\Gamma$, the transition from $\gamma \approx 1$ to $\gamma \approx 0.5$ is much sharper (dot-dashed line). Hence this result suggests a more pronounced noise reduction for conductors which are more weakly coupled to the leads (smaller $\Gamma$). On the other hand, for the asymmetric case the suppression of the Fano factor is not as strong (dashed line). This is due to the fact that quantum resonance is not as well established in an asymmetric system as that in a symmetric one.

The reason that our full nonlinear results of Fig. 2 only shows shot noise reduction in a resonance system is due to the fact that we have applied the wideband limit for the Green’s function. Since wideband limit does not allow negative differential resistance, we can not observe NDR and hence the enhancement of shot noise. To obtain NDR within the wideband approximation, we assume the leads to have a finite occupied bandwidth by introducing an energy cutoff in the integration of Eq. (12), as suggested by Jauho et al. A result of this simple procedure indeed produced a Fano factor which can be greater than unity, as shown in Fig. 3. Our analysis thus reconfirms that shot noise can be enhanced by the existence of a NDR region. However, the experimental results showed a much sharper increase of the Fano factor when bias is varied than that showed by Fig. 3. It thus seems that one needs to go beyond the wideband limit to obtain a detailed quantitative agreement.

IV. WEAKLY NONLINEAR LIMIT

The wideband limit discussed above reduces the system to essentially a single level and zero-dimensional quantum dot, but this allows us to obtain closed form results for the full nonlinear shot noise spectra including large bias voltages. In this section we examine the another limit, namely the weakly nonlinear limit where the bias is finite but not large. In this case we can expand the shot noise formula order by order in bias, and derive the weakly nonlinear shot noise spectral coefficients.

For small bias voltages, we expand the noise spectra of two-probe systems Eq. (11) in terms of it,

$$< (\Delta I)^2 > = P_0 + P_1(V_1 - V_2) + P_2(V_1 - V_2)^2 + ...$$ (16)

where the equilibrium noise $P_0$ and the linear noise spectra $P_1$ have been considered in detail before. Here we derive an expression for the second order non-linear noise spectra $P_2$ at zero temperature. To proceed, we first need to determine the internal potential $U$. In the last section we applied a phenomenological nonlinear capacitance charging model to find $U$, here we will solve $U$ self-consistently order by order in the bias. We expand the internal potential $U$ in powers of voltages,

$$U = U_{eq} + \sum_{\alpha} u_{\alpha}V_{\alpha} + \frac{1}{2}\sum_{\alpha\beta} u_{\alpha\beta}V_{\alpha}V_{\beta} + ...$$ (17)

where $U_{eq}$ is the equilibrium potential and $u_{\alpha}(r)$, $u_{\alpha\beta}(r)$ are the characteristic potentials. They are determined by the Poisson like equations which are obtained by expanding Eq. (1) in powers of voltage,

$$-\nabla^2 u_{\alpha}(x) + 4\pi q^2 \int \Pi(x, x')u_{\alpha}(x')dx' = 4\pi q^2 \frac{dn_{eq}(x)}{dE}$$ (18)

and

$$-\nabla^2 u_{\beta\gamma}(x) + 4\pi q^2 \int \Pi(x, x')u_{\beta\gamma}(x')dx' = 4\pi q^2 \left[ \frac{d^2n_{\beta}(x)}{dE^2} \delta_{\beta\gamma} - \int \frac{d\Pi_\beta(x, x')}{dE} u_{\beta}(x')dx' \right]$$

$$- \int \frac{d\Pi_\gamma(x, x')}{dE} u_{\gamma}(x')dx'$$

$$+ \int \Pi(x, x', x'')u_{\beta}(x')u_{\gamma}(x'')dx'dx''$$ (19)

$\Pi(x, x')$ is the Lindhard function defined as

$$\Pi(x, x') = -i \int \left( \frac{dE}{2\pi} \right) f(G_0^a(x, x')G_0^b(x', x)$$

$$- G_0^a(x, x')G_0^b(x', x))$$

$$= \delta\Pi_0(x)$$

$$= \frac{q\delta U(x')}{q\delta U(x')}$$ (20)
where \( f = f(E), \) \( G_0^r \) is the equilibrium Green’s function, and the generating function \( \Pi_0(x) \) is given by
\[
\Pi_0(x) = -i \int (dE/2\pi) f [G_0^r(x,x) - G_0^a(x,x)]
\] (21)
and \( \delta/\delta U(x') \) is the functional derivative defined in Ref. 28. In Eq. (19), \( \Pi(x,x',x'') \) is the second order nonlinear response function defined as
\[
\Pi(x,x',x'') = -\frac{\delta^2 \Pi_0(x)}{q^2 \delta U(x') \delta U(x'')}
\] (22)
and \( \Pi_\alpha \) the Lindhard function for lead \( \alpha \)
\[
\Pi_\alpha(x,x') = \int (dE/2\pi) f [(G_0^r \Gamma_\alpha G_0^a)_{xx'} (G_0^a x'x + c.c.)]
\] (23)
so that \( \Pi_\alpha(x,x') = \sum_\alpha \Pi_\alpha(x,x') \). The partial local density of state at contact \( \alpha \), \( d\rho_\alpha/dE \), called the injectivity is given by,
\[
d\rho_\alpha(x)/dE = \int \Pi_\alpha(x,x') dx'
\] (24)
and \( d^2\rho_\alpha/dE^2 \) is the energy derivative of the injectivity. Finally, \( dn/dE = \sum_\alpha d\rho_\alpha/dE \) is the local DOS. It can be shown that the characteristic potential satisfy the following sum rules,
\[
\sum_\alpha u_\alpha = 1
\] (25)
and
\[
\sum_{\gamma \beta} u_{\alpha(\beta)l} = 0.
\] (26)

Here the subscript \( \{\beta\} \) is a short notation of \( l \) indices \( \gamma, \delta, \eta, \ldots \).

With these prepartations we can now derive the second order nonlinear shot noise coefficient \( P_2 \). At zero temperature, the shot noise formula Eq. (11) reduces to
\[
< (\Delta I)^2 > = \Delta \nu \frac{q^2}{\pi} \int_{E_F+qV_1}^{E_F+qV_2} dE Tr[(1 - \hat{T})\hat{T}].
\] (27)
Denoting \( g(E,U) \equiv (1 - \hat{T})\hat{T} \), we expand \( g(E,U) \) with respect to \( E \) and \( V \):
\[
g(E,U) \approx g(E,0) + \frac{dg(E,0)}{dU} U \\
\approx g_0 + \frac{dg_0}{dE} (E - E_F) + \frac{dg_0}{dU} U
\] (28)
where \( U \) is the diagonal matrix for the internal potential, \( g_0 = g(E_F,0) \) and \( (dg_0/dU)U \equiv \sum_{\alpha} (dg_0/\delta U(x))U(x) \). Substitute the above equation into Eq. (27) and complete the integral over energy \( E \), the noise spectra up to the second order in voltage is
\[
P_2(V_1 - V_2)^2 = \Delta \nu \frac{q^2}{\pi} Tr \left[ \frac{q^2}{2} \frac{dg_0}{dU} (V_1 - V_2)^2 + \frac{dg_0}{dU} [g(u_1 V_1 + u_2 V_2)(V_1 - V_2)] \right]
\] (29)
Using the relation \( q dg_0/dE = -dg_0/dU \) for gauge invariance and Eq. (25), we arrive at
\[
P_2 = \Delta \nu \frac{q^3}{2\pi} Tr \left[ \frac{dg_0}{dU} (2u_1 - 1) \right].
\] (30)
Following the same line of development, we can derive higher order nonlinear shot noise coefficients. For instance, the third order nonlinear noise spectra is found to be,
\[
P_3 = \Delta \nu \frac{q^3}{6\pi} Tr \left[ \frac{dg_0}{dU} u_{11} \right]
\] (31)

As an explicit example, let’s derive \( P_2 \) and \( P_3 \) for a resonance tunneling system using scattering approach and comparing with the result of NEGF. Using the Breit-Wigner form factor for the scattering matrix near a resonance energy \( E_0, \) \( s_{a\beta}(E) \sim \delta_{a\beta} - i \sqrt{\Gamma_a} / \Delta \), where \( \Gamma_a \) is the decay width of barrier \( \alpha, \) \( \Delta = E - E_0 + i\Gamma/2 \) with \( \Gamma = \Gamma_1 + \Gamma_2, \) we obtain,
\[
P_2 = \delta \nu \frac{q^4}{2\pi} \frac{\Gamma_2 - \Gamma_1}{\Gamma} (1 - 2T) \frac{dT}{dE}
\] (32)
and
\[
P_3 = -\delta \nu \frac{q^5}{6\pi} \left\{ \frac{6}{\Gamma^2} (E - E_0) T(2T - 1) \frac{dT}{dE}
\right.

\right. + \frac{\Gamma_1^2 + \Gamma_2^2 - \Gamma_1 \Gamma_2}{\Gamma^2} \left[ (2T - 1) \frac{dT}{dE} \right] \left( \frac{dT}{dE} \right)^2 \}
\] (33)
where \( T = \Gamma_1 \Gamma_2 / \Delta \). In the derivation of Eqs. (25) and (26), we have used the quasi-neutrality condition to determine the characteristic potential so that \( u_1 = \Gamma_1 / \Gamma \) and \( u_{11} = -2(E - E_0) T / \Gamma^2 \). Since resonance tunneling with Breit-Wigner scattering matrix is equivalent to the wideband limit of the last section, expressions (25, 26) can be directly obtained by expanding the wideband limit results (12, 13) to the appropriate order in voltage. It is straightforward to prove that the same results are obtained from this direct expansion. This gives a confirmation on the validity of the weakly nonlinear analysis presented here.

**V. SUMMARY**

In this work, we have developed a general nonlinear DC theory for calculating the shot noise spectra in the mesoscopic regime. The framework is based on nonequilibrium Green’s functions with the important extension of
solving the internal potential build up self-consistently. A direct advantage of our method is that the final expression for shot noise becomes gauge invariant which is an essential requirement for any nonlinear transport theory. Eqs. \ref{eq:negeq} completely determine the nonlinear shot noise spectra of an arbitrary multi-probe conductor, they form the basic results of our theory. Practically, one must solve the quantum scattering problem which gives the Green’s functions, in conjunction with the Poisson equation. Technically these expressions form a convenient basis for numerical predictions of shot noise spectra at finite bias voltages. For instance one can easily compute various Green’s functions and the coupling matrix $\Gamma$ for multi-probe conductors using tight-binding models, and the Poisson equation can be solved in real space using very powerful numerical techniques.

In the wideband limit and the weakly nonlinear limit, the basic equations \ref{eq:negeq} can be analyzed in closed form. Our nonlinear theory reveals that the shot noise of a mesoscopic conductor can be quite sensitive to the external bias strength, and in general the suppression of noise is most efficient near a quantum resonance point, and is stronger for symmetric systems than asymmetric ones. The suppression is also more efficient for conductors weakly coupled to the leads. In the presence of negative differential resistance region of the nonlinear current-voltage characteristics, our result confirms the existence of shot noise enhancement which has been observed experimentally. For weakly nonlinear transport regime, we have derived the shot noise nonlinear coefficients order by order in bias, and these coefficients should be adequate when the external bias is finite but not large.

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\section*{FIGURE CAPTIONS}

Fig. (1) The differential shot noise versus the voltage. Solid line: $\Gamma_1 = \Gamma_2 = 0.5$ and $C_1 = C_2 = 0.5$; dotted line: $\Gamma_1 = \Gamma_2 = 0.5$ and $C_1 = C_2 = 0.1$; dot-dashed line: $\Gamma_1 = \Gamma_2 = 0.1$ and $C_1 = C_2 = 0.4$; and dashed line: 
\[ \Gamma_1 = 0.1, \Gamma_2 = 0.8, C_1 = 0.1, \text{ and } C_2 = 0.8. \text{ Here } E_F - E_0 = -2.0. \]

Figure (2) The corresponding Fano factor of Fig.(1).

Figure (3) The Fano factor versus the voltage when the energy cut off is introduced for \( \Gamma_1 = \Gamma_2 = 0.5, C_1 = C_2 = 0.5 \) and \( E_F - E_0 = -2.0. \)
