Quantum Electro-Mechanical Systems (QEMS)

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ABSTRACT

We give a quantum description of a Quantum Electro-Mechanical System(QEMS) comprising a single quantum dot harmonically bound between two electrodes and facilitating a tunnelling current between them. An example of such a system is a fullerene molecule between two metal electrodes. The description is based on a quantum master equation for the density operator of the electronic and vibrational degrees of freedom and thus incorporates the dynamics of both diagonal (population) and off diagonal (coherence) terms. We derive coupled equations of motion for the electron occupation number of the dot and the vibrational degrees of freedom, including damping of the vibration and thermo-mechanical noise, and give a semiclassical description of the dynamics under a variety of bias conditions. This dynamical description is related to observable features of the system including the stationary conductance as a function of bias voltage.

Keywords: Quantum electro mechanical System, Nano electro mechanical system, NEMS, MEMS, Single electron transistor, Vibrational quanta

1. INTRODUCTION

The ever growing miniaturisation of semiconductor electronics[1] implies the need to establish means to measure and detect smaller physical quantities. Micro Electro-Mechanical Systems (MEMS) has been demonstrated to be the way to proceed, but we are approaching the limit where detection of even smaller physical quantities is necessary. This means that we need to go beyond the current micro scale range to reach the nano scale where ultimately quantum laws apply.

A Quantum-Electro Mechanical System (QEMS) consists of a mechanical oscillator with electrical driving and a motion transducer with mechanical frequency ω_o, such that the energy in the QEMS system is greater than the thermal fluctuations $\hbar\omega_o \geq k_B T$. This is known as *the quantum regime*. Indeed, QEMS opens up exciting possibilities to several application such as the means to measure ultra sensitive force, displacement detectors,[2] electrometers[3] and single spin detectors.

The small structure of QEMS suggests an increase in resonant frequency, such that it is possible to reach the order of Giga to Terra Hertz frequency. This implies that such a system would lie well within the quantum regime when the experiment is conducted at milli Kelvin temperature. Currently a high-frequency nano electro-mechanical system that operates in Giga Hz has been successfully fabricated.[4] However finding transducers of the motion that do not limit the fundamental sensitivity of the oscillator is very difficult. A very different approach to achieving a high mechanical frequency was the fullerene molecular system of Park et al.,[5] and it is this system which we take as the prototype for our theoretical description.

Another phenomenon in this regime is the *single electron charging effect* or *Coulomb Blockade effect* which manifest itself when device's capacitance is small enough so that quantized conductance and Coulomb Blockade oscillations can be observed $e^2/2C^2 \geq k_B T$.

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There are two limiting regimes of operation for tunnelling through a harmonically bound quantum dot, such as a fullerene molecule. The key parameter is the ratio of the *rms* position fluctuations of the oscillator ground state to the length scale on which the tunnelling amplitude through the dot varies. If this parameter is small, the coherent modulation of the tunnelling amplitude due to the motion of the dot can be neglected so that transport depends only on the average occupation of the vibrational levels of the dot. This is the regime that we discuss in this report. If this ratio is large, then the motion of the dot modulates the tunnelling amplitude between the leads and the dot as it moves towards and away from the leads. In this regime the device is usually refereed to as a shuttle.[6]

There are already quite a few theoretical work in the literature which try to explain various aspects of phenomena that happens in these systems either via classical and semi classical[6–9] or quantum mechanical approaches.[10–17] An early work by Gorelik et al.[6] indicates that an 'electron shuttle' mechanism will indeed give rise to the current. An electron shuttle system is produced when then movement of the central island is bigger and slower in terms of frequency compared to the C_{60} system. They investigated a system consisting of a metallic grains surrounded by soft organic molecules at room temperature numerically, treating it as an oscillator and found the existence of a dynamical instability, a limit cycle and a step-like structure of current-voltage curve similar to Coulomb staircase.

A classical analysis of the dynamics of this shuttle system then was investigated further by Isacsson[8] in which he analysed a system of a conducting grain is attached to a cantilever placed between two metallic gates. A classical treatment that yields to analytical and numerical results was presented. On this he found that there was some instability and a tendency for the system to be chaotic, depending on the voltages of the three terminal.

Another classical analysis and physical explanation of this island displacement, is also offered by Nord.[9] Using Monte Carlo simulation to find the solution to the equation of motion, Nord calculated the current as a function of bias voltage. From this, two distinct regimes of charge transport can be seen, namely the tunnelling regime and the shuttling regime. The electromechanical coupling results in a nonlinear IV curve.

Aside from these classical approaches, Boese and Schoeller[10] attempted to explain the step-like structure found in the C_{60} system using the theory of molecular vibration and local bosonic excitation. Their theoretical results compare well with the experimental results obtained by Park et al., however the dynamics of the system has not been investigated thoroughly here. Arriving from similar model, McCarthy et al.[11] studied the incoherent dynamics of the oscillator and found a strong dependence of the oscillator's potential on the electrostatics of the island. A similar setup using a micro-mechanical resonator coupled to a Cooper Pair Box is offered by Armour.[12] This provides a way to probe quantum coherence and entanglement in the system, since the electrostatic interaction causes a displacement in the cantilever which depends on which of the two charge states the Cooper box is in. Weiss and Zwerger[13] calculate the average current and fluctuations using master equation approach treated to a mechanically driven single electron shuttle.

A slightly different model consisting of a chain of three quantum dots (left dot connected to the left lead, and island dot and a righthand dot connecting to the right lead) is proposed by Armour and MacKinnon.[14] Using density matrix approach, the effect of quantized vibrational mode on electron tunnelling was investigated. Recently a new paper by Novotny et al[15] discuss this phenomenon from the quantum domain. A phase space in terms of Wigner function was plotted and shuttling driven exclusively by the quantum noise was hypothesized.

Different characteristics of QEMS system have been studied, including rate equations describing electron tunnelling via discrete quantum state,[17] elastic and inelastic transport,[18] a control to the dynamic response of the couple nano-mechanical resonator by Q-tuning[19] and the gate voltage dependence.[20] Other various aspect of QEMS such as the temperature dependance on these single molecules is investigated by Lundin and McKenzie.[21]

Although various aspects of QEMS devices has been studied, we believe that a complete quantum description which includes noise and decoherence is still lacking. In this respect, we attempt to give a full description that apply to both the classical and quantum regimes within a certain limit.

2. SYSTEM AND MODEL HAMILTONIAN

We consider a system consisting of a single electron transistor (SET) with a movable island in the middle. This island can be of a metal grain, a quantum dot or a molecule (figure 1). The interaction between the electron

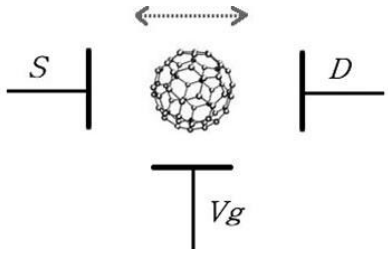

Figure 1. Illustration of the system. The island which in this case is represented by the Carbon-60 molecule can vibrate in the direction indicated between the source and drain. The flow of electrons from one electrode (the source) to the other (drain) is controlled by a third terminal (the gate) which forms a Single Electron Transistor (SET).

that jumps onto the island and the island motion produced a change in the transport properties. The single molecular transistor system reported by Park et al.[5] consists of a single C_{60} molecule weakly bound by van der Walls interactions to gold electrodes with center of mass oscillation frequency of Terra Hertz.

When the electron jumps from the source on to the C_{60}, the electron will induced an image charge on the terminal. This image will attract the electron resulting in a shift of the center of mass of the C_{60} ion. Similarly, when the electron jumps off the island into the drain, the C_{60} will again be attracted to the drain. In result, the electrostatic forces are converted into mechanical motion. This center of mass motion is what has been proposed as the main cause of the energy shift of 5 meV that is prominent in the experimental current vs. bias voltage curve (see figure 1 and 4 in Park et al.[5]).

The model we describe, figure 1, consists of a single quantum dot or single fullerene molecule coupled via tunnel junctions to two reservoirs, the source and the drain. We will assume that the coulomb blockade permits only one quasi-bound single electron state on the dot which participates in the tunnelling between the source and the drain. We will ignore spin, as the source and drain are not spin polarised. A gate voltage controls the energy of this quasi-bound state with respect to the Fermi energy in the source. The quantum dot can oscillate around an equilibrium position mid way between the source and the drain contacts due to weak restoring forces. When an electron tunnels onto the dot an electrostatic force is exerted on the dot shifting its equilibrium position. In essence this is a quantum dot single electron transistor. The dependance of the conductance on gate voltage was found to exhibit features attributed to transitions between the quantised vibrational levels of the mechanical oscillations of the molecule.

We begin analysing the system by assuming that the centre of mass of the dot is bound in a harmonic potential with resonant frequency ω_o. This vibrational degree of freedom is then described by a displacement operator $\hat{x}$ which can be written in terms of annihilation and creation operators $a, a^\dagger$ as

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega_o}}(a + a^\dagger) \tag{1}$$

The electronic state of the single quasi-bound state on the dot is described by Fermi annihilation and creation operators $c, c^\dagger$, which satisfy the anti commutation relation $cc^\dagger + c^\dagger c = 1$.

The Hamiltonian of the system can then be written as,

$$\begin{aligned} H &= \hbar\omega_I(Vg)c^\dagger c + U_c n_\uparrow n_\downarrow && (2)\\ &+ \hbar\omega_o a^\dagger a && (3)\\ &+ \hbar\omega_{kl} a_k^\dagger a_k + \hbar\omega_{kr} b_k^\dagger b_k && (4)\\ &-\chi(a^\dagger + a)\hat{n} && (5)\\ &+ \sum_k T_{sk}(a_k c^\dagger + c a_k^\dagger) + \sum_k T_{dk}(b_k c^\dagger + c b_k^\dagger) && (6)\\ &+ \sum_p \hbar\omega_p d_p^\dagger d_p + g(a^\dagger d_p + a d_p^\dagger). && (7) \end{aligned}$$

The first term of the Hamiltonian describes the free energy for the island. A particular gate voltage V_g with a corresponding $\hbar\omega_I = 15meV$ for the island is chosen for calculation. U_c is the Coulomb charge energy which is the energy that is required to put another electron in the island when there is already one electron occupying the island. We will assume this energy is large enough so that no more than one electron occupies the island at any time time. This is a Coulomb Blockade effect. The charging energy of the fullerene molecule transistor has been observed by Park to be larger than 270 meV which is two order of magnitude larger than the vibrational quantum of energy $\epsilon_o = \hbar\omega_o$. The hamiltonian for the oscillator is described in eq.(3). The Park et al. experiment gives the value $\epsilon_o = 5$ meV, corresponding to a THz oscillator. The electrostatic energy due to a source and drain reservoir can be written as eq.(4). Term (5) is the coupling between the oscillator and charge while term (6) represents the source - island tunnel coupling and the drain island tunnel coupling. The last term, (7), describes the coupling between the oscillator and the thermo-mechanical bath responsible for damping and thermal noise in the mechanical system in the rotating wave approximation.[22]

To analyse this hamiltonian, we would like to eliminate the coupling term of the oscillator and charge by doing a canonical transformation with the unitary representation, $U = e^s$, where

$$s = -\frac{\chi}{\hbar\omega_o}(a^\dagger - a)\hat{n}. \tag{8}$$

This derivation follows the approach done by Mahan.[23] The motivation behind this is as follows. The electrostatic interaction, term (5) displaces the equilibrium position of the oscillator so that the average value of the oscillator amplitude in the ground state becomes

$$\langle a \rangle = \frac{\chi}{\hbar\omega_o}. \tag{9}$$

We can shift this back to the origin by a phase-space displacement

$$\bar{a} \equiv e^s a e^{-s} = a + \frac{\chi}{\hbar\omega_o}\hat{n}. \tag{10}$$

This unitary transformation gives a conditional displacement of the oscillator, conditional on the electronic occupation the dot. One might call this a *displacement* picture. Applying U to the Fermi operator c gives

$$\bar{c} = c e^{\frac{\chi}{\hbar\omega_o}(a^\dagger - a)}. \tag{11}$$

The density matrix operator in the transformed basis is related to the original master equation by:

$$\bar{\rho} = e^s \rho e^{-s}. \tag{12}$$

To derive a master equation for the dot, we first transform to an interaction picture, within the displacement picture, to give the hamiltonian

$$\begin{aligned}
\bar{H}_I \;=\; & \sum_k T_{sk}(a_k c^\dagger e^{i(\omega_I - \epsilon - \omega_{kl})t} e^{-\lambda}(a^\dagger e^{i\omega_o t} - a e^{-i\omega_o t}) \\
& \qquad + c a_k^\dagger e^{-i(\omega_I - \epsilon - \omega_{kl})t} e^{\lambda}(a^\dagger e^{i\omega_o t} - a e^{-i\omega_o t}) \\
& + \sum_k T_{dk}(b_k c^\dagger e^{i(\omega_I - \epsilon - \omega_{kr})t} e^{-\lambda}(a^\dagger e^{i\omega_o t} - a e^{-i\omega_o t}) \\
& \qquad + c b_k^\dagger e^{-i(\omega_I - \epsilon - \omega_{kr})t} e^{\lambda}(a^\dagger e^{i\omega_o t} - a e^{-i\omega_o t}) \\
& + \sum_p g(a^\dagger d_p e^{-i(\omega_p - \omega_o)} + a d_p^\dagger e^{i(\omega_p - \omega_o)} + \lambda\hat{n}(d_p e^{-i\omega_p} + d_k^\dagger e^{i\omega_p}))
\end{aligned} \tag{13}$$

where $\epsilon = \chi^2/\hbar\omega_o$ and $\lambda = \chi/\hbar\omega_o$.

We expect an expansion to second order in λ to give an adequate description of transport. The terms of zero order in λ describe bare tunnelling through the system and do not cause excitations of the vibrational degree of freedom. The terms linear in λ describe tunnelling through the dot with the exchange of one vibrational quanta, or phonon. The terms quadratic in λ correspond to tunnelling with the exchanges of two vibrational quanta. Higher order terms could obviously be included at considerable computational expense. We will proceed to derive the master equation up to quadratic order in λ.

3. QUANTUM MASTER EQUATION

Our objective here is to find an evolution equation for the density operator for the electronic and vibrational degrees of freedom of the vibrating quantum dot. We trace out the electronic degrees of freedom for the source and drain. Unlike other approaches, we avoid tracing out the vibrational degrees of freedom for the purpose of able to look at their dynamics. We will use standard methods based on the Born and Markov approximation[22] In order to indicate where these approximations we will sketch some of the key elements of the derivation in what follows. The Born approximation assumes that the coupling between the leads and the local system is weak and thus second order perturbation theory will suffice to describe this interaction. The evolution of the density matrix operator of the system in this case can then be described as:

$$\dot{\rho} = \frac{-1}{\hbar^2}\int_0^t dt' \mathrm{Tr}[\mathrm{H_I(t)}, [\mathrm{H_I(t')}, \mathrm{R}]]. \tag{14}$$

At this point we would like to trace out the electronic degrees of freedom for the source and drain. We will assume that the states of the source and drain remain in local thermodynamic equilibrium at temperature T. This is part of the Markov approximation. Its validity requires that any correlations that develop between the electrons in the leads and the local system, as a result of the tunnelling interaction, is rapidly damped to zero on time scales relevant for the system dynamics. We need the following moments:

$$\mathrm{Tr}[a_k^\dagger a_k \rho] = f_{kl}, \qquad \mathrm{Tr}[b_k^\dagger b_k \rho] = f_{kr},$$
$$\mathrm{Tr}[a_k a_k^\dagger \rho] = 1 - f_{kl}, \qquad \mathrm{Tr}[b_k b_k^\dagger \rho] = 1 - f_{kr}.$$

where $f_{kl} = f(E_{kl})$ is the fermi function describing the average occupation number and similarly $f_{kr} = f(E_{kr})$.

The Fermi function is given by:

$$f(E) = \frac{1}{e^{E/k_B T} + 1} \tag{15}$$

where k_B is the Boltzman constant and T represents temperatures.

The next step was to convert the sum over modes to a frequency-space integral:

$$\sum_k f_{kl}|T_{sk}|^2 \rightarrow \int_0^\infty d\omega\ g(\omega) f_l(\omega)|T_s(\omega)|^2 \tag{16}$$

where here, $T_{sk}^* T_{sk} = |T_{sk}|^2$ and $g(\omega)$ is the density of states which gives the number of oscillator with frequency between $\omega + d\omega$. Evaluating the time integral:

$$\int_0^\infty d\tau e^{\pm i\epsilon\tau} = \pi\delta(\epsilon) \pm iPV(1/\epsilon) \tag{17}$$

where $\tau = t - t'$ and the imaginary term is ignored. So for example, for the term with $e^{i(\omega-\omega_0)\tau}$, ϵ in the equation above and be replaced by $\omega - \omega_0$ in which then the delta function will become $\delta(\omega_0)$.

Using the methods described above, we can combine the terms for the source and drain as γ_L and γ_R respectively

$$\int_0^\infty d\omega\ g(\omega)|T_s(\omega)|^2 \delta(\omega_0) = \gamma_L(\omega_0). \tag{18}$$

In the same way, we can define

$$\begin{aligned}
\gamma_{L1} &= \gamma_L(\hbar\omega_I - \epsilon - \mu_L) \\
f_{1L} &= f(\hbar\omega_I - \epsilon - \mu_L) \\
\gamma_{L2} &= \gamma_L(\hbar\omega_I - \epsilon - \hbar\omega_o - \mu_L) \\
f_{2L} &= f(\hbar\omega_I - \epsilon - \hbar\omega_o - \mu_L) \\
\gamma_{L3} &= \gamma_L(\hbar\omega_I - \epsilon + \hbar\omega_o - \mu_L) \\
f_{3L} &= f(\hbar\omega_I - \epsilon + \hbar\omega_o - \mu_L).
\end{aligned}$$

And similarly for $\gamma_{R1}, \gamma_{R2}\gamma_{R3}, f_{1R}, f_{2R}, f_{3R}$ replacing μ_L with μ_R and f being the fermi function described in eq. (15).

The master equation in the canonical transformed picture to the second order in λ may be written as

$$\begin{aligned}
\dot{\bar{\rho}} &= \gamma_{L1}\Big((1-\lambda^2)(f_{1L}\mathcal{D}[c^\dagger]\bar{\rho} + (1-f_{1L})\mathcal{D}[c]\bar{\rho}) \\
&\quad +\lambda^2\ (f_{1L}(-a^\dagger a c^\dagger \bar{\rho} c + a^\dagger a c c^\dagger \bar{\rho} - c^\dagger \bar{\rho} c a^\dagger a + \bar{\rho} c c^\dagger a^\dagger a) \\
&\quad +(1-f_{1L})(-a^\dagger a c \bar{\rho} c^\dagger + a^\dagger a c^\dagger c \bar{\rho} - c\bar{\rho}c^\dagger a^\dagger a + \bar{\rho} a^\dagger a c^\dagger c))\Big) \\
&+ \gamma_{L2}\lambda^2\Big(f_{2L}\mathcal{D}[ac^\dagger]\bar{\rho} + (1-f_{2L})\mathcal{D}[a^\dagger c]\bar{\rho}\Big) \\
&+ \gamma_{L3}\lambda^2\Big(f_{3L}\mathcal{D}[a^\dagger c^\dagger]\bar{\rho} + (1-f_{3L})\mathcal{D}[ac]\bar{\rho}\Big) \\
&+ \gamma_{R1}\Big((1-\lambda^2)(f_{1R}\mathcal{D}[c^\dagger]\bar{\rho} + (1-f_{1R})\mathcal{D}[c]\bar{\rho}) \\
&\quad +\lambda^2\ (f_{1R}(-a^\dagger a c^\dagger \bar{\rho} c + a^\dagger a c c^\dagger \bar{\rho} - c^\dagger \bar{\rho} c a^\dagger a + \bar{\rho} c c^\dagger a^\dagger a) \\
&\quad +(1-f_{1R})(-a^\dagger a c \bar{\rho} c^\dagger + a^\dagger a c^\dagger c \bar{\rho} - c\bar{\rho}c^\dagger a^\dagger a + \bar{\rho} a^\dagger a c^\dagger c))\Big) \\
&+ \gamma_{R2}\lambda^2\Big(f_{2R}\mathcal{D}[ac^\dagger]\bar{\rho} + (1-f_{2R})\mathcal{D}[a^\dagger c]\bar{\rho}\Big) \\
&+ \gamma_{R3}\lambda^2\Big(f_{3R}\mathcal{D}[a^\dagger c^\dagger]\bar{\rho} + (1-f_{3R})\mathcal{D}[ac]\bar{\rho}\Big) \\
&+ \kappa(\bar{n}_p+1)\mathcal{D}[a]\bar{\rho} + \kappa\bar{n}_p\mathcal{D}[a^\dagger]\bar{\rho} + \kappa\lambda^2(2\bar{n}_p+1)\mathcal{D}[c^\dagger c]\bar{\rho},
\end{aligned} \tag{19}$$

where the notation

$$\begin{aligned}
\mathcal{D}[A]B &= \mathcal{J}[A]B - \mathcal{A}[A]B \\
&= ABA^\dagger - \tfrac{1}{2}(A^\dagger AB + BA^\dagger A),
\end{aligned} \tag{20}$$

and

$$\bar{n}_p(\omega_o) = \frac{1}{e^{\hbar\omega_o/k_BT}-1}\ . \tag{21}$$

The damping of the oscillator is included using the usual thermal quantum optics master equation with mean energy damping rate of κ in order for the system to reach a steady state.[22]

4. CALCULATING CURRENT

We can now compute the current through the quantum dot. The current reflects how the reservoirs of the source and drain respond to the dynamics of the vibrational and electronics degrees of freedom. Of course in an experiment this external current is typically all we have access to. However the master equation enables us to calculate the coupled dynamics of the vibrational and electronic degrees of freedom. Understanding this dynamics is crucial to explaining the observed features in the external current. As electrons tunnel on and off the dot, the oscillator experiences a force due to the electrostatic potential. While the force is conservative, the tunnel events are stochastic (in fact a Poisson process) and thus the excitation of the oscillator is stochastic. Furthermore the vibrational and electronic degrees of freedom become entangled through the dynamics. In this section we wish to investigate these features in some detail. The average current through the left and right leads are related to the population of the dot by

$$I_L(t) - I_R(t) = \frac{d\langle c^\dagger c\rangle}{dt}. \tag{22}$$

From the master equation, the rate of change of this average occupational number of electron in the dot may be obtained:

$$\begin{aligned}\frac{d\langle c^\dagger c\rangle_{\rm CT}}{dt} &= {\rm tr}[c^\dagger c\dot{\bar\rho}] \qquad (23)\\ &= \big[\gamma_{L1}(1-\lambda^2)(f_{1L}(1-\langle c^\dagger c\rangle)-(1-f_{1L})\langle c^\dagger c\rangle)\\ &\qquad -2\gamma_{L1}\lambda^2(f_{1L}\langle a^\dagger a(1-c^\dagger c)\rangle-(1-f_{1L})\langle a^\dagger a c^\dagger c\rangle)\\ &\quad +\gamma_{L2}\lambda^2(f_{2L}\langle a^\dagger a(1-c^\dagger c)\rangle-(1-f_{2L})\langle(1+a^\dagger a)c^\dagger c\rangle)\\ &\quad +\gamma_{L3}\lambda^2(f_{3L}\langle(1+a^\dagger a)(1-c^\dagger c)\rangle-(1-f_{3L})\langle a^\dagger a c^\dagger c\rangle)\\ &\quad +\gamma_{R1}(1-\lambda^2)(f_{1R}(1-\langle c^\dagger c\rangle)-(1-f_{1R})\langle c^\dagger c\rangle)\\ &\qquad -2\gamma_{R1}\lambda^2(f_{1R}\langle a^\dagger a(1-c^\dagger c)\rangle-(1-f_{1R})\langle a^\dagger a c^\dagger c\rangle)\\ &\quad +\gamma_{R2}\lambda^2(f_{2R}\langle a^\dagger a(1-c^\dagger c)\rangle-(1-f_{2R})\langle(1+a^\dagger a)c^\dagger c\rangle)\\ &\quad +\gamma_{R3}\lambda^2(f_{3R}\langle(1+a^\dagger a)(1-c^\dagger c)\rangle-(1-f_{3R})\langle a^\dagger a c^\dagger c\rangle)\big]_{\rm CT}.\end{aligned}$$

While for the vibrational degrees of freedom, we see that

$$\begin{aligned}\frac{d\langle a^\dagger a\rangle_{\rm CT}}{dt} &= {\rm tr}[a^\dagger a\dot{\bar\rho}] \qquad (24)\\ &= \lambda^2[\gamma_{L2}(-f_{2L}\langle a^\dagger a(1-c^\dagger c)\rangle+(1-f_{2L})\langle(1+a^\dagger a)c^\dagger c\rangle)\\ &\quad +\gamma_{L3}(f_{3L}\langle(1+a^\dagger a)(1-c^\dagger c)\rangle-(1-f_{3L})\langle a^\dagger a c^\dagger c\rangle)\\ &\quad +\gamma_{R2}(-f_{2R}\langle a^\dagger a(1-c^\dagger c)\rangle+(1-f_{2R})\langle(1+a^\dagger a)c^\dagger c\rangle)\\ &\quad +\gamma_{R3}(f_{3R}\langle(1+a^\dagger a)(1-c^\dagger c)\rangle-(1-f_{3R})\langle a^\dagger a c^\dagger c\rangle)-\kappa\langle a^\dagger a\rangle+\kappa\bar n_p]_{\rm CT}.\end{aligned}$$

Here the subscript CT indicates that the quantity to which it is attached is evaluated at the canonical transformed (CT) basis. The average occupational number of electron in the dot in the original basis is the same as in the CT basis:

$$\begin{aligned}\langle c^\dagger c\rangle &= {\rm tr}[c^\dagger c\rho] \qquad (25)\\ &= {\rm tr}[c^\dagger c\ \ e^{-s}\bar\rho e^s]\\ &= {\rm tr}[c^\dagger c\bar\rho]\\ &= \langle c^\dagger c\rangle_{\rm CT}.\end{aligned}$$

While for the vibrational degrees of freedom, we have

$$\begin{aligned}\langle a^\dagger a\rangle &= {\rm tr}[a^\dagger a\rho] \qquad (26)\\ &= {\rm tr}[a^\dagger a e^{-s}e^{-i\omega_o a^\dagger at}\bar\rho e^{i\omega_o a^\dagger at}e^s]\\ &= {\rm tr}[e^{i\omega_o a^\dagger at}(a^\dagger+\lambda\hat n)(a+\lambda\hat n)e^{-i\omega_o a^\dagger at}\bar\rho]\\ &= \langle a^\dagger a\rangle_{\rm CT}+\lambda\langle(a^\dagger e^{-i\omega_o a^\dagger at}+ae^{-i\omega_o a^\dagger at})\hat n\rangle_{\rm CT}+\lambda^2\langle\hat n^2\rangle.\end{aligned}$$

We can see that the electron and vibrational degrees of freedom are entangled through the dynamics. In addition, the evolution of the of $\langle c^\dagger c\rangle$ and $\langle a^\dagger a\rangle$ depend on the higher order quantum average $\langle a^\dagger a c^\dagger c\rangle$. However, in a semi-classical approximation, if we replace $\langle a^\dagger a c^\dagger c\rangle$ by the factorized average values, i.e., $\langle a^\dagger a c^\dagger c\rangle\approx\langle a^\dagger a\rangle\langle c^\dagger c\rangle$, then the evolution equations (24) and (25) forms a closed set of equations.

We let $\gamma_{L1}=\gamma_{L2}=\gamma_{L3}=\gamma_L$ and $\gamma_{R1}=\gamma_{R2}=\gamma_{R3}=\gamma_R$ and proceed by factorising the combined average of the product of electron and phonon operator. Then the equations above can be simplified to:

$$\begin{aligned}\frac{d\langle c^\dagger c\rangle}{dt} &= A_1\langle c^\dagger c\rangle+B_1\langle a^\dagger a\rangle_{\rm CT}+C_1 \qquad (27)\\ A_1 &= -\big[\gamma_L(1-f_{2L}\lambda^2+f_{3L}\lambda^2)+\gamma_R(1-f_{2R}\lambda^2+f_{3R}\lambda^2)\big]\\ B_1 &= \lambda^2(-2f_{1L}\gamma_L+f_{2L}\gamma_L+f_{3L}\gamma_L-2f_{1R}\gamma_R+f_{2R}\gamma_R+f_{3R}\gamma_R)\\ C_1 &= (1-\lambda^2)\gamma_L f_{1L}+\gamma_L f_{3L}\lambda^2+(1-\lambda^2)\gamma_R f_{1R}+\gamma_R f_{3R}\lambda^2\ ,\end{aligned}$$

and

$$\frac{d\langle a^\dagger a\rangle_{\rm CT}}{dt} = A_2\langle c^\dagger c\rangle + B_2\langle a^\dagger a\rangle_{\rm CT} + C_2 \tag{28}$$

$$\begin{aligned} A_2 &= \lambda^2(\gamma_L(1-f_{2L}-f_{3L})+\gamma_R(1-f_{2R}-f_{3R})) \\ B_2 &= \lambda^2(-\gamma_L f_{2L}+\gamma_L f_{3L}-\gamma_R f_{2R}+\gamma_R f_{3R})-\kappa \\ C_2 &= \lambda^2(\gamma_L f_{3L}+\gamma_R f_{3R})+\kappa\bar{n}_p\ . \end{aligned}$$

These equations were then solved in MatLab and the result for various λ values are plotted in figure 2.

Here, we have been able to reproduce similar behaviours of quantized conductance that was observed experimentally. Note that in the steady state for the larger value of λ there are two steps. As one can see from figure 2(a), the current vanishes until the first Coulomb Blockade energy is overcome. The first step in the conductance is thus due to bare tunnelling though the dot. The second step represents single phonon assisted tunnelling through the dot. These results are consistent with the semiclassical theory of Boese and Schoeller[10] given that our expansion to second order in λ can only account for single phonon events. Heights of the step depends on λ which is the ratio of the value of coupling between the electron and the vibrational level χ and the oscillator energy $\hbar\omega_o$. A feature of our approach is that we can directly calculate the dynamics of the local degrees of freedom, for example the mean electron occupation of the dot as well as the mean vibrational occupation number in the oscillator.

The steady state current can be found by finding the steady state solution for each of the phonon number and electron number rate

$$\langle c^\dagger c\rangle_{\rm st} = \frac{B_1C_2-B_2C_1}{A_1B_2-A_2B_1} \tag{29}$$

$$\langle a^\dagger a\rangle_{\rm CT,st} = \frac{-A_2}{B_2}\left(\frac{B_1C_2-B_2C_1}{A_1B_2-A_2B_1}\right)-\frac{C_2}{B_2}. \tag{30}$$

The steady state current can then be found by

$$I_{\rm st} = \gamma_L[(-1+f_{2L}\lambda^2-f_{3L}\lambda^2)\langle c^\dagger c\rangle+(-2f_{1L}\lambda^2+f_{2L}\lambda^2+f_{3L}\lambda^2)\langle a^\dagger a\rangle+(1-\lambda^2)f_{1L}+f_{3L}\lambda^2]. \tag{31}$$

At the region where bias voltage is large,

$$\langle c^\dagger c\rangle_{\rm st} = \frac{\gamma_L}{\gamma_L+\gamma_R} \tag{32}$$

$$\langle a^\dagger a\rangle_{\rm st} = \left(\lambda^2+\frac{\lambda^2(-\gamma_L+\gamma_R)}{\kappa}\right)\left(\frac{\gamma_L}{\gamma_L+\gamma_R}\right)+\frac{\gamma_L\lambda^2+\kappa\bar{n}_p}{\kappa} \tag{33}$$

$$I_{\rm st} = \frac{\gamma_L\gamma_R}{\gamma_L+\gamma_R}. \tag{34}$$

Looking at figure 2, the average electron number approaching 0.5 at steady state since we have set the value of γ_L to be equal to γ_R while the average phonon number without damping grows continuously. When damping is included this phonon number will reach a value of 0.35 (figure 2(e)). As a result, the current will be steady at $e\gamma_L/2\pi$ (figure 2(f)).

At the region of the first phonon excitation level (when bias voltage is between 30 meV and 40 meV), the steady state current drops by a factor proportional to quadratic order of λ compared to the current at large bias voltage as given by

$$\Delta I_{\rm st} = \frac{\gamma_L\lambda^2(2\gamma\lambda^2+\kappa(2\bar{n}_p+1))}{4\gamma_L\lambda^2-2\kappa(\lambda^2-2)}. \tag{35}$$

The steady state current can also be obtained by solving the master equation directly from eq.(19). The steady state current for various λ values with its corresponding bias voltage can be seen in figure 3. This result compares well with the result obtained previously by solving each of the steady state solution for the electron and phonon number. This fact indicates the validity of the semi-classical approximations (eq.(27) and (28)).

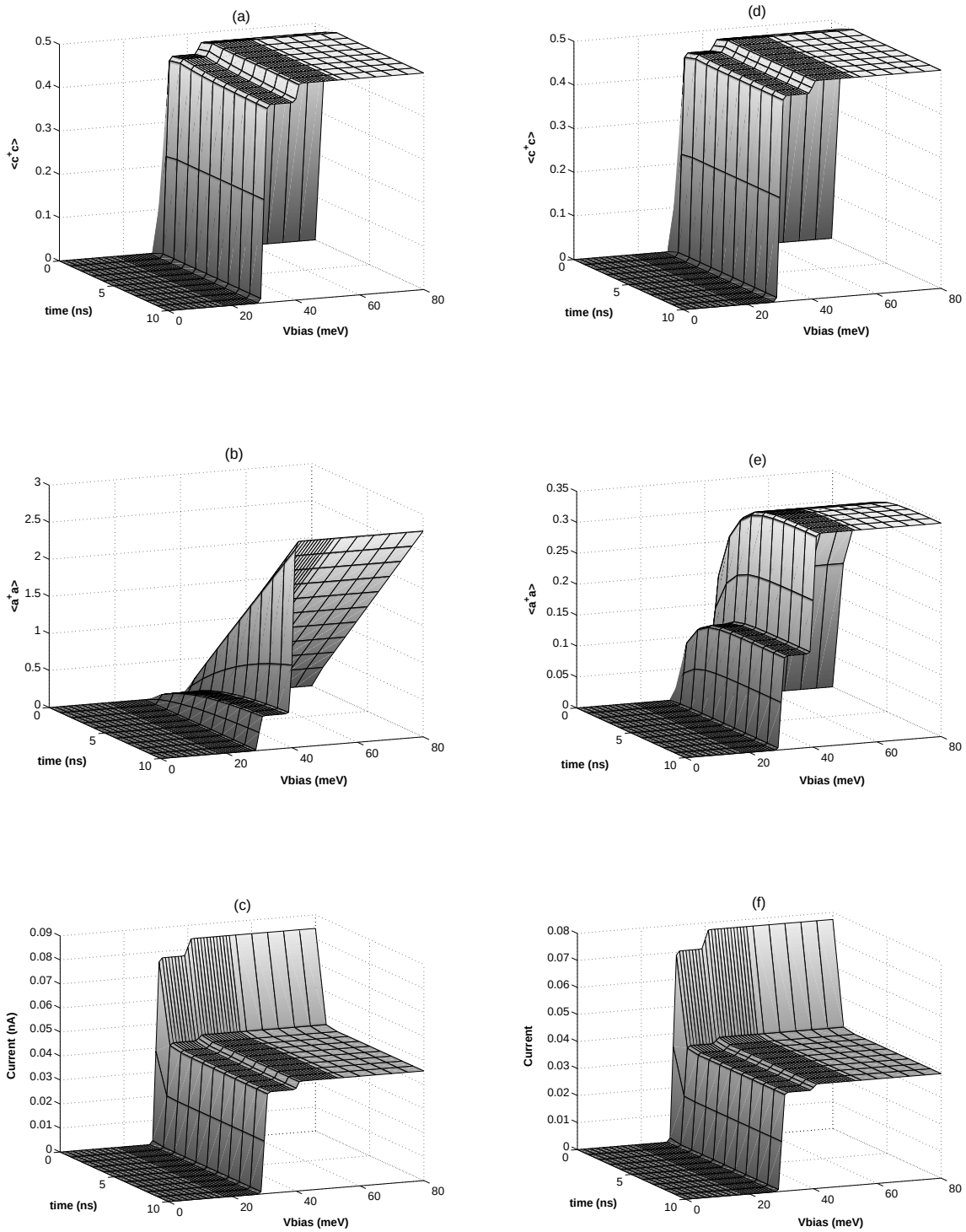

Figure 2. Average number of electron, phonon and current through the dot against bias voltage with $\hbar\omega_o = 5$ meV, $\hbar\omega_I = 15$ meV, $k_BT = 0.13$ meV, and $\hbar\gamma_L = \hbar\gamma_R = 2$ μeV for $\lambda = 0.3$. Figures (a),(b),(c) without damping and (d),(e),(f) with damping $\kappa = 0.3\gamma_L$

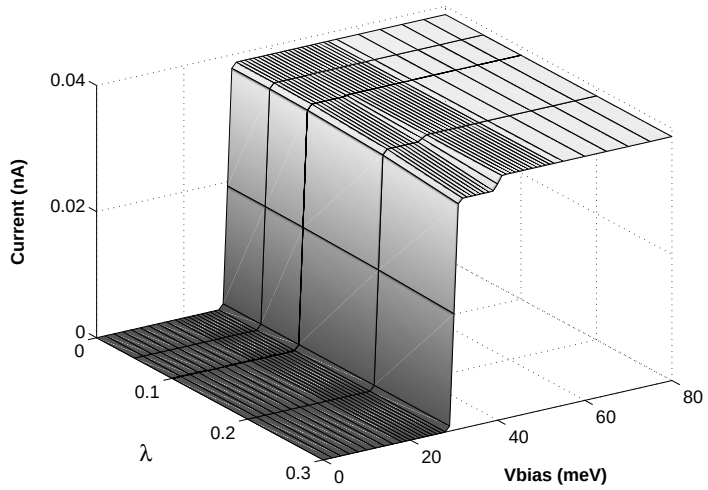

Figure 3. IV curve for different values of λ with damping $\kappa = 0.3\gamma_L$

5. CONCLUSIONS

We have been able to give a quantum description of a QEMS comprising a single quantum dot harmonically bound between two electrodes. We gave a description which is based on a quantum master equation for the density operator of the electronic and vibrational degrees of freedom and thus incorporates the dynamics of both diagonal (population) and off diagonal (coherence) terms. From this we have been able to reproduce the IV curve obtained experimentally by Park et al.[5] by our quantum master equation treatment and also of the semiclassical phenomenological theory by Boese and Schoeller.[10] However our full quantum treatment will enable us to include coherent effects which are likely to arise when a spin doped quantum dot is used in a static of RF external magnetic field.

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