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A mean field approach to Coulomb blockade for a disordered assembly of quantum dots

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Abstract. The Coulomb blockade (CB) in quantum dots (QDs) is by now well documented. It has been used to guide the fabrication of single electron transistors. Even the most sophisticated techniques for synthesizing QDs (e.g. MOCVD/MBE) result in an assembly in which a certain amount of disorder is inevitable. On the other hand, theoretical approaches to CB limit themselves to an analysis of a single QD. In the present work we consider two types of disorders: (i) size disorder; e.g. QDs have a distribution of sizes which could be unimodal or bimodal in nature. (ii) Potential disorder with the confining potential assuming a variety of shapes depending on growth condition and external fields. We assume a Gaussian distribution in disorder in both size and potential and employ a simplified mean field theory. To do this we rely on the scaling laws for the CB (also termed as Hubbard U) obtained for an isolated QD [1]. We analyze the distribution in the Hubbard U as a consequence of disorder and observe that Coulomb blockade is partially suppressed by the disorder. Further, the distribution in U is a skewed Gaussian with enhanced broadening.

Keywords. Quantum dots; artificial atoms; Coulomb blockade; disorder in nanostructures.

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1. Introduction

Quantum dots (QDs) are structures in which charge carriers are essentially trapped in a three-dimensional potential. They are also known as 'artificial atoms' [2,3] and consist of 10^3–10^6 atoms, with system sizes in the range of 1–10 nm. They are of fundamental and technical interest for next generation electronic devices. An important goal of today's technological drive towards smaller and smaller devices is to fabricate the so-called single-electron transistor which can be operated at room temperature [4]. They may also form the basis of new generations of lasers [5].

Our aim is to understand Coulomb blockade (CB) for a distribution of QDs employing a minimal set of broad and plausible assumptions. As the name suggests, CB is the energy price paid in adding an electron to a QD. Classically, this price is $\approx e^2/C$, where e is the electron charge and C is the capacitance of the QD. In many-body quantum mechanics, this price is given a name, namely Hubbard U.

The Coulomb blockade is the model led by an effective Hubbard U which in the simplest case depends on size R of the QD in the following fashion [1]:

$$U = \frac{C}{R^\beta}, \tag{1}$$

where value of $\beta \in [0.33, 1]$ depends on the confinement potential. As demonstrated earlier, $\beta \approx 0.33$ when confinement is quasi-triangular and β approaches 1 as confinement tends towards a quasi-square well [1]. We propose to understand CB in an assembly of QDs by combining the single dot result (eq. (1)) with Kane's approach [6].

2. Size disorder

As stated in the Introduction, our aim is to understand CB for a distribution of QDs. The growth of the QDs is a stochastic process and it appears reasonable to assume dots with a Gaussian distribution of radius R centered around a mean R_0,

$$P_R = \frac{1}{\sqrt{2\pi}\sigma}\ \exp\left(-\frac{(R-R_0)^2}{2\sigma^2}\right), \tag{2}$$

$$U_0 = \frac{C}{{R_0}^\beta}, \tag{3}$$

where we pause to define a mean Hubbard U_0 related to the mean dot radius R_0.

The CB line shape is determined by transforming eq. (2) to the energy axis as is commonly done

$$P(U) = \frac{1}{\sqrt{2\pi}\sigma}\int_0^\infty \delta\left(U - \frac{C}{R^\beta}\right)\ \exp\left(-\frac{(R-R_0)^2}{2\sigma^2}\right)\mathrm{d}R. \tag{4}$$

This can be solved quite easily to obtain

$$P(U) = \frac{1}{\sigma\sqrt{2\pi}}\ \frac{C^{1/\beta}}{\beta U^{(1+\beta)/\beta}}\ \exp\left[-\frac{C^{2/\beta}}{2\sigma^2}\ \left(\frac{1}{U^{1/\beta}} - \frac{1}{U_0^{1/\beta}}\right)^2\right]. \tag{5}$$

The CB line shape is approximately Gaussian for small σ/R_0 as can be seen in figure 1. Another aspect worth noting is that the mean Hubbard U_0 and the location of the Hubbard U peak are not identical. To see this, we set derivative of $P(U)$ (eq. (5)) to zero and obtain

$$U_p = U_0\left(\frac{-R_0^2/\sigma^2 + \sqrt{R_0^4/\sigma^4 + 4(\beta+1)R_0^2/\sigma^2}}{2(\beta+1)}\right)^\beta. \tag{6}$$

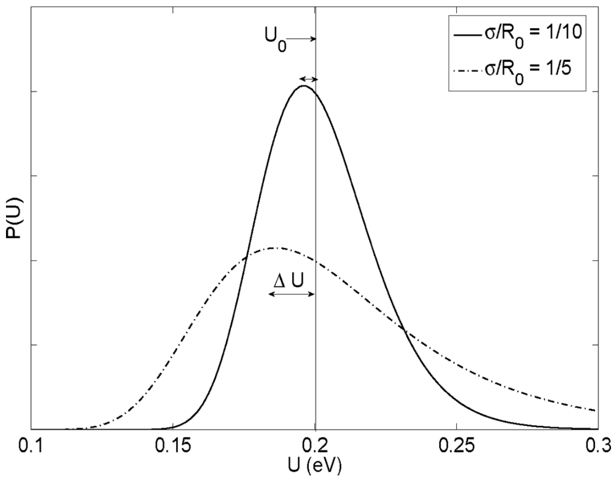

Figure 1. The distribution $P(U)$ vs. U for size disorder. Horizontal arrows indicate the downshift. The values assumed for the plot above are $U_0 = 0.2$ eV, $R_0 = 5$ nm and $\beta = 1$.

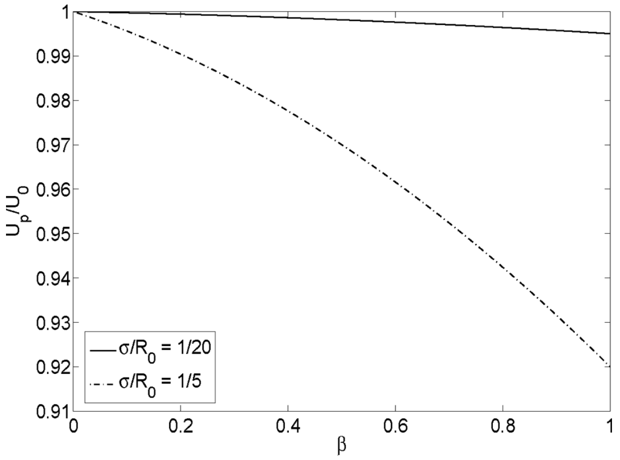

Figure 2. U_p/U_0 vs. β for size disorder. Clearly suppression of CB increases with β and also disorder. We assumed $R_0 = 5$ nm for the plot above.

For $\sigma/R_0 \to 0$, $U_p = U_0$, as expected. However, for reasonable σ the above expression can be Taylor expanded and neglecting the third- and higher-order terms, we obtain

$$U_0 - U_p = \Delta U \approx U_0(\beta + \beta^2)\frac{\sigma^2}{R_0^2}. \tag{7}$$

Thus we see a clear downshift. This is shown in figure 1 by horizontal arrows.

The peak in energy plot is at $P(U_p)$. We can obtain an approximate expression for the full-width at half-maximum (FWHM) ($U_{\rm FWHM}$) of the energy profile if the

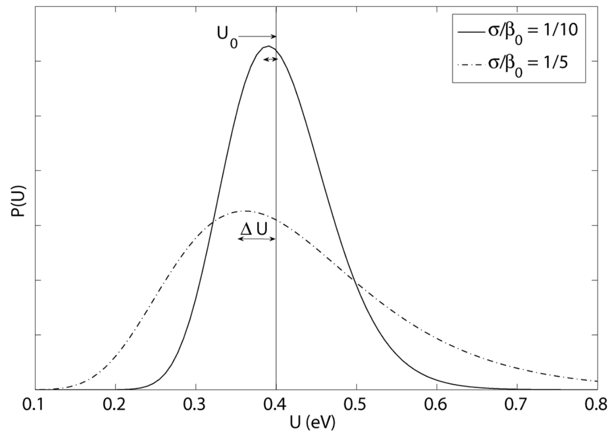

Figure 3. The distribution $P(U)$ vs. U for confinement disorder. Horizontal arrows indicate the downshift. The values assumed for the plot above are U_0 = 0.4 eV and $R = 5$ nm.

prefactor dependence $U^{(1+\beta)/\beta}$ is ignored. This is calculated for reasonably small σ/R_0 as

$$U_{\text{FWHM}} \approx \frac{C}{R_0}\,\frac{\beta}{R_0^{\beta}}\,2\sqrt{2\ln 2}\,\sigma. \tag{8}$$

Note that this is an approximate result. A larger value of U_{FWHM} is expected if the full expression is employed.

For a better insight we analyse U_p/U_0 with respect to β. This has been depicted in figure 2. It can be seen that the ratio decreases quadratically with increasing β, i.e. the suppression of CB is more pronounced for quasi-square well confinement as compared to quasi-harmonic confinement. Another feature worth noting is that ratio decreases with increasing value of σ/R_0, which implies that the suppression becomes more pronounced for greater disorder.

3. Confinement disorder

In spite of the most sophisticated experimental techniques, the growth of QDs may lead to irregular charge distribution. This, in turn, gives rise to confinement potentials with considerable disorder. We have also seen that β (eq. (1)) depends on confinement potential. For the sake of simplicity we model disorder in confinement by a Gaussian distribution in β. Here we assume radius of the QDs to be fairly constant (R) to avoid unnecessary complications. Thus we have

$$P_\beta = \frac{1}{\sigma\sqrt{2\pi}}\ \exp\left(-\frac{(\beta-\beta_0)^2}{2\sigma^2}\right) \tag{9}$$

and we pause once again to define U_0 related to mean β_0.

$$U_0 = \frac{C}{(R/R_0)^{\beta_0}}. \tag{10}$$

Here we have taken ratio of R and R_0 to ensure that the denominator is dimensionless. For the rest of the analysis, we take $R_0 = 1$ nm. Transforming eq. (9) to the energy axis as was done before, we obtain

$$P(U) = \frac{1}{U(\sigma \ln R)\sqrt{2\pi}} \exp\left[-\frac{(\ln U - \ln U_0)^2}{2(\sigma \ln R)^2}\right]. \tag{11}$$

This log normal distribution in U is depicted in figure 3. Locating the peak of the distribution obtained by the standard method of equating derivative to zero we obtain

$$U_0 - U_p = \Delta U = U_0 \left[1 - \exp\{-(\sigma \ln R)^2\}\right]. \tag{12}$$

For small $\sigma \ln R$, which is the case generally, the above expression can be appropriately approximated to

$$\Delta U \approx U_0 \ (\sigma \ln R)^2. \tag{13}$$

Once again we see a downshift in U. To obtain the dependence of downshift on disorder we need to quantify the same. We reasonably treat FWHM as the amount of disorder. For small σ, FWHM is calculated to be

$$U_{\rm FWHM} \approx C\frac{\ln R}{R^{\beta_0}}(2\sqrt{2\ln 2}\sigma). \tag{14}$$

Hence we obtain $U_{\rm FWHM} \propto \sigma$. Thus alternately we can also measure disorder in terms of σ. Equation (13) shows that suppression of CB increases with σ. Once again we are able to demonstrate the increase in suppression of CB with increasing disorder.

4. Conclusion

Some workers have argued that the size distribution in an assembly of QDs is log normal, while others have suggested bimodal distribution in the case of III–V semiconductor QDs. We are currently examining CB for such distribution.

Even in the quantum many-body calculations, the CB of the additional electron does not appear to depend on the number of electrons already added to the QD. In a series of careful calculations carried out by Pandey *et al* [1] it was found that exponent β has a very weak dependence on the number of electrons (N) in the QD.

$$\beta(N) \sim N^{\eta}, \quad \eta \approx 0.05. \tag{15}$$

Hence we are justified in ignoring this N dependence in our analysis.

Very interestingly we observe that both types of disorders (size and confinement potential) shift the CB to a lower value. Thus we may expect an attenuation in the CB. We pause to realize the physical significance of this. There is bound to be a disagreement between theoretically calculated values and experimental values as the former are obtained by usually considering a single QD while experiments are usually carried out on an assembly of QDs. This has been noticed earlier in the context of photoluminescence spectra [7,8] and band gap discrepancies [9]. We are currently examining the experimental consequences of the calculations reported herein.

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