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Electron Dynamics near a Metallic Island Array

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The motion of a point charge near a two-dimensional periodic array of metallic islands has been studied. The appearance of 'image charges' in the neighborhood of the test charge not only affects its local electrostatic energy, but also its dynamical properties. We are interested in the effective dynamical behavior of the quasi-particle created this way, as it can dominate magneto-transport properties. The point charge is assumed to move on a plane parallel and very close to the two dimensional plane of the metallic islands. Through classical electromagnetic theory the response of the metallic islands due to the external charge is calculated for two different limits: First, square and spatially extended metallic islands with finite conductance are used. Second, and more appropriate to the 'far-field' description of the problem, islands are assumed to be well represented as classical dipoles which respond infinitely fast to the electrical field from the test point charge. We study the dynamically-averaged characteristics of the particle trajectories, such as energy and associated fields and potentials, in order to provide a classical evaluation of the effective mass of the test charge.

Introduction Small metallic regions play an essential role in electronic devices. As these get down to the nanometer scale, single electron interactions with these metallic regions become important. Quantum mechanically this can be viewed as the interaction of charged quasi-particles with a large number of discrete point charges in the metal, which collectively result in an effective interaction potential which changes the dynamic properties (mass) of the sample charge and causes its dephasing.

Classically, the effective interaction can be viewed as coming from the high concentration of electrons in the metallic surfaces which shield the external electrical field. For simple geometries, the resulting field can be well-described via image charges. Even when in the dynamic case the response will be slightly delayed, the response of the metallic charges can be taken as immediate for small velocities of a sample point charge. This is also related to the assumption of the metal being ideal, while in real systems some dissipation occurs. Small velocities also imply that magnetic contributions can be neglected.

In this paper, the classical view is explored. Periodic 2D arrangements of metallic islands are proposed. A sample charge is placed in a plane slightly above the array, producing an effective polarization in them. Sample charge, together with the induced charge 'cloud' in the islands, can be viewed as a quasi-particle which is moving in a two dimensional plane. This is the experimental situation of a 2D electron near a structured gate, as those used in semiconductor SET [1, 2].

The polarization of each square island configuration with a sample charge at different positions is calculated numerically for the static case as explained below. The result-

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ing effective potential for the sample charge is then used to obtain several long classical trajectories. These are analyzed statistically to obtain a classical analog for the effective mass[2]) of the overall 'classical' quasi-particle.

Setup The typical square island setup is given in Fig. 1. The grid spacing a and the metallic island size s in Fig. 1b fix the *coverage* of metal on the plane. The sample charge indicated in this figure is placed on each grid point, and the structure is energetically relaxed to find the (static) interaction potential for the sample charge. For the actual calculation of the periodic potential, a finite 3×3 matrix of islands was considered. Due to the periodicity, the potential only needs to be evaluated in one unit cell as indicated. The square symmetry further reduces the evaluation to only $1/8$ of that cell.

The square island geometries are scaled from $a = 1$ μm to 1 nm. The distance of the sample charge to the plane of the islands d is taken to be $d = 1$ nm throughout the paper. However, for large d/a, one can rely on a description where the islands are replaced by idealized dipoles. This limit is also investigated.

Figure 1a shows the approximate sampling that is applied for the square islands. Since most of the induced charge gathers preferably at the corners, these are sampled in the determination of charge transfer between them. In addition, a fifth point is introduced for each island, to account for the symmetry and the image charge of the problem. The position of this fifth point depends on the position of the sample charge.

Relaxation towards the static case is done in an iterative scheme: charge transfer among the five sampling points is allowed until the potentials within each island reach a constant value within the desired accuracy. This procedure can be interpreted as the minimization of the total electrostatic energy. In the case of the square islands, the

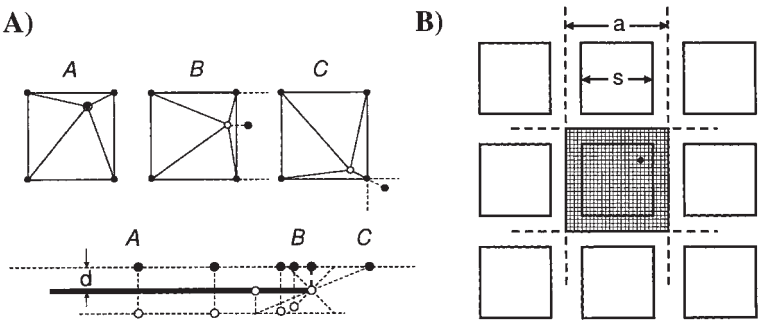

Fig. 1. a) Sampling of square islands at corners (point charges with varying spatial *extension* to account for self-energy), and at one additional point, the *image point*. Charge transfer is allowed along the solid lines. The image point changes position with respect to the sample point charge in the plane slightly above, as indicated by the white circles (spacing d); the corners appear as black dots. Bottom: The position of the image charge is given for several different positions labeled A, B, C in a side view. As the sample charge goes over the edge of the island, the model is setup so that the image directly approaches the edge and stays in the plane of the island. b) Periodic metallic island array: a is the lattice spacing, and s the island size. The grid setup for consequent positions of the sample charge is indicated in the center region

[2]) The term effective mass is normally applied in a quantum mechanical description of a quasiparticle which will also be undertaken and reported elsewhere.

expression used is

$$E_{\text{total}} = \frac{1}{2} \sum_{i,j}^{\text{all pts}} \frac{q_i q_j}{\tilde{d}_{ij}} + \sum_{i}^{\text{island pts}} \frac{q_i^2}{\tilde{d}_i} , \tag{1}$$

where q_i is the charge at point i, $\tilde{d}_{ij}$ the distance of sample point i to sample point j, and modified if both points belong to the same island, and one of them is the image point, to allow smooth merging of sample points so that they behave like a single sample point with the charge added up. The summation in the first term in Eq. (1) goes over all sample points and sample charge. Similar considerations hold true for the second sum which represents the self-energy, crucial to prevent infinite accumulation of charge at certain locations. $\tilde{d}_i$ approximately accounts for the *spatial extension* of the charge at point i, taken to be $1/3$ of the average distance to its connected neighbor points. It is smoothly changed to the distance of that point to the sample charge when the two approach.

In the case of interaction with point dipoles Eq. (1) is rewritten as

$$E_{\text{total}} = \frac{1}{2} \sum_{i}^{\text{dipoles}} \mathbf{p}_i \cdot (\mathbf{E}_i + \mathbf{E}_{si}^{(c)}) , \quad \text{where} \quad \mathbf{E}_i = \mathbf{E}_{si}^{(\text{c})} + \sum_{j \neq i}^{\text{dipoles}} \mathbf{E}_{ji}^{(\text{d})} . \tag{2}$$

Here, $\mathbf{E}_{si}^{(\text{c})}$ is the Coulomb field contribution of the sample charge s to the field at point i, $\mathbf{E}_{ji}^{(\text{d})}$ is the dipole field contribution of dipole j to the field at point i [3], and $\mathbf{E}_i$ is the local field at point i. The dipole moment is assumed to be proportional to the electric field at its location $\mathbf{E}_i$ ($\mathbf{p}_i = \alpha \mathbf{E}_i$ with $\alpha = 10^{-28}$ m^3). The $1/2$ accounts for double counting of the dipole–dipole interactions. However, the dipole–sample charge interaction is not double counted, so the $1/2$ needs to be corrected by considering this term ($\mathbf{E}_{si}^{(\text{c})}$) explicitly a second time.

Ordinary Runge Kutta fourth order with self-adaptive time step control is used to calculate classical trajectories of the sample charge on the fully-relaxed potential landscape. Total energy is monitored and conserved.

For a description of the system as a *classical* quasi-particle, a classical analog of an effective mass is considered. Looking at one cell, the trajectory provides information about the entrance point, the amount of time the particle spent in the given cell Δt and the exit point. Repeating this many times, statistical information about the velocity can be gathered, such as average or standard deviation. In this sense, the following scheme is used to extract a *classical* value for the effective mass m^*

$$E_{\text{total}} \equiv \frac{1}{2} m^* \left(\frac{\Delta x}{\Delta t} \right)^2 , \tag{3}$$

where Δx is the direct distance between entrance and exit points. Note, that $\Delta x / \Delta t$ is nothing else but the average velocity $\langle v \rangle$ in the period t to $t + \Delta t$. Running several trajectories at different total energies and using Eq. (3) provides information about the *classical* effective mass m^*.[3])

[3]) In order to have a comparison with a full electrostatic calculation, we considered a 1D island and calculated the potential on a grid matrix [3]: an open outer boundary, an island at constant potential of pin-like shape in the middle with a sample charge close by. The resulting potential profile had similar features as the ones obtained numerically in the approach described here. The details are somewhat different, but the overall behavior and the result for an effective mass are well described qualitatively by our approximate (but numerically feasible) scheme.

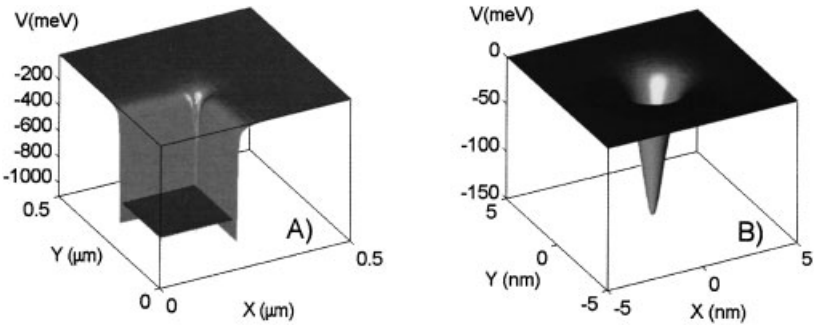

Fig. 2. a) Potential landscapes for a square metallic island ($a = 1$ μm, $s = 0.4$ μm) – only one fourth of the basis cell is shown (the rest is easily added using the square symmetry). b) Potential landscapes for a dipole array (note the different scales in x and y direction)

Results Typical potential landscapes are shown in Fig. 2. For the square metallic island (Fig. 2a) there are essentially two regions: away from the island ($|x|, |y| > s/2$), it goes rapidly to zero; above the island ($|x|, |y| < s/2$), the potential is nicely flat (just the interaction with the image charge). In the transition region ($|x|, |y| \approx s/2$), and especially at the corners of the island, the potential has sharp features, indicating a more attractive region to the sample charge as expected intuitively. On the other hand for dipoles, the typical potential is given in Fig. 2b. This potential falls off rapidly if the horizontal distance is a few times larger than the distance of the sample charge to the plane of the dipole (it has a $1/r^4$ dependence consistent with the dipole scheme, Eq. (2)). Note also the much shallower potential well in this case (~ -140 meV compared to ~ -750 meV in the center plateau of the square island).

Typical trajectories are shown in Fig. 3. Panels A and B show trajectories for the square island with high and low initial kinetic energy, respectively. It can be seen that due to the square geometry of the 2D well, the particle can get trapped by subsequent reflections. This would not be possible in a 1D well since classically the particle has enough energy to make it out of the well. In 2D however, if the particle comes in at a flat angle to the edge of the boundary, it can be reflected. It is this fact which makes predictions on how long the particle will stay in the well much harder. Panel C and D show trajectories near the dipole array for high and low initial kinetic energy, respectively. Due to the nearly circular symmetry of the potential (as neighbor interaction is almost negligible due to the short range of the dipole interaction) trapping does not occur in this case.

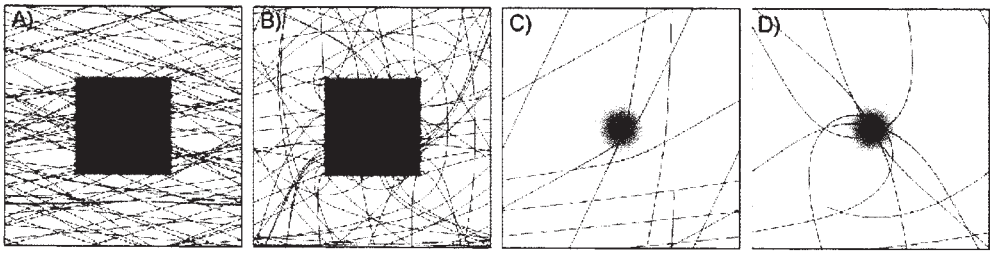

Fig. 3. Short sequences of typical trajectories for square island (A and B) and dipole (C and D) arrays

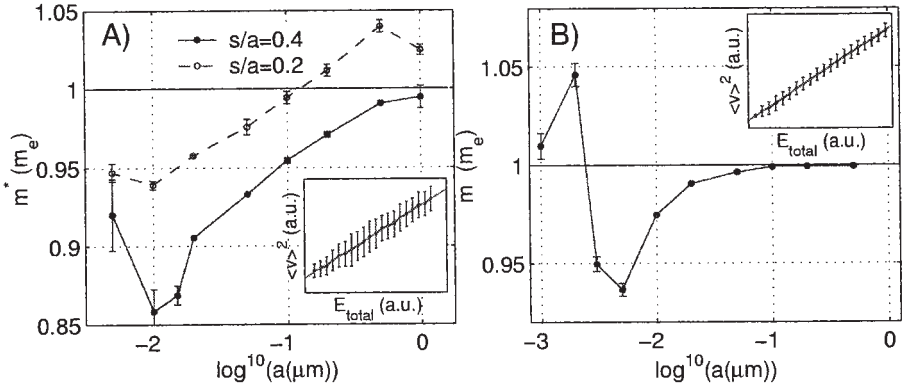

Fig. 4. a) Effective mass m^* extracted for two different a and s values ($s/a = 0.4$ and 0.2). Inset: Sample of statistical velocity data (derived from average and standard deviation) for square island setup ($a = 0.02$ μm). A line fit directly relates to an effective mass. Part b) and inset are similar to a) but for dipole configuration

The effective mass is evaluated according to Eq. (3). Panel A in Fig. 4 shows that a small island, compared to the basic cell size ($s/a = 0.2$), directly relates to an effective mass m^* that is closer to 1, e.g. closer to a free particle. Whether the effective mass is greater or smaller than 1, is not clear ab initio, since complex processes can occur while the sample charge is within a cell. For dipoles (panel B), the interaction is generally weaker, which translates into an effective mass that is closer to 1. As the arrays are downscaled, e.g. same planar geometry but smaller lattice constant a, at some point the islands get closer than the sample charge is away from the plane. Mutual interaction and cancellation smooths the potential landscape for the sample charge in such a way that the effective mass gets closer to 1 again. This process actually starts earlier, as can be seen in panel A, as the minimum for m^* is found for a lattice constant $a \approx 5$–10 nm, 5 to 10 times larger than the distance d of the sample charge to the plane of islands.

Using Eq. 3 to evaluate the *classical* analog of the effective mass m^*, one can see in Fig. 4 that it is not straightforward to decide whether m^* is greater or smaller than 1 given an overall attractive potential. In fact, we find that both results occur, depending on the geometry and the scales, as panels B and D show. Classical trapping near an island is reminiscent of quantum resonances with long lifetimes and effectively large phase shifts. Quantization of the classical motion considered here should provide for interesting resonant behavior [4].

Summary An effective mass for a particle interacting with a periodic array of metallic islands was calculated via classical means. Our calculation allows the inclusion of realistic many-body effects on the dynamics of the test charge. A quantum mechanical calculation, to be reported elsewhere, gives different values of m^* at different energies. Comparisons between the two approaches will be of interest.

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