Charge density mapping of strongly-correlated few-electron two-dimensional quantum dots by the scanning probe technique

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Abstract
We perform a numerical simulation of the mapping of charge confined in quantum dots by the scanning probe technique. We solve the few-electron Schrödinger equation with the exact diagonalization approach and evaluate the energy maps as a function of the probe position. Next, from the energy maps we try to reproduce the charge density distribution using an integral equation given by the perturbation theory. The reproduced density maps are compared with the original ones. This study covers two-dimensional quantum dots of various geometries and profiles with the one-dimensional (1D) quantum dot as a limiting case. We concentrate on large quantum dots for which strong electron–electron correlations appear. For circular dots the correlations lead to the formation of Wigner molecules that in the presence of a tip appear in the laboratory frame. The unperturbed rotationally-symmetric charge density is surprisingly well reproduced by the mapping. We find in general that the size of the confined droplet as well as the spatial extent of the charge density maxima is underestimated for a repulsive tip potential and overestimated for an attractive tip. In lower symmetry quantum dots Wigner molecules with single-electron islands nucleate for some electron numbers even in the absence of a tip. These charge densities are well resolved by the mapping. These single-electron islands appear in the laboratory frame provided that the classical point charge density distribution is unique, in the 1D limit of confinement in particular. We demonstrate that for electron systems which possess a few equivalent classical configurations the repulsive probe switches between the configurations. In consequence the charge density evades mapping by the repulsive probe.

(Some figures may appear in colour only in the online journal)

1. Introduction

Local properties of semiconductor nanostructures can be probed by scanning gate microscopy (SGM) [1], in which the charge of an atomic force microscope tip perturbs the potential landscape below the surface of the semiconductor within the space occupied by confined charge carriers. SGM covers both open systems (quantum point contacts [2], resonant cavities [3], quantum rings [4]) in which the probe is used to read out the wavefunction at the Fermi level from the conductance perturbations and systems that are weakly coupled to reservoirs, i.e. closed quantum dots [5–8, 10–14]. For the latter, the current flows through the quantum dot only outside Coulomb blockade conditions [15], i.e., when the chemical potential \( \mu_N = E_N - E_{N-1} \) of \( N \) confined electrons lies within the transport window defined by the Fermi levels of the source and drain. In experiments, the tip-induced variation of \( E_N \) is determined from the shift of voltages that is necessary for restoration of the current flow [5, 7, 8, 12]. Since the variation depends on the electron density beneath the tip this technique allows for visualization of the charge density. The details of this technique is called Coulomb blockade microscopy by some groups [13, 14].
the variation of the charge density can be detected only for large quantum dots exceeding the range of the tip potential. In large dots and at low electron densities the SGM technique can—at least potentially—resolve single-electron islands within the few-electron quantum dots which are formed as an effect of strong electron–electron correlations with the charge density nucleating to Wigner molecules [17, 18].

Work on extraction of the confined charge density by scanning gate microscopy has mostly concerned quasi-one-dimensional (1D) quantum dots defined within a quantum wire [6, 8–11, 13, 14]. Wigner molecules in 1D quantum dots [16] are relatively stable against external perturbations due to the fact that in one dimension the electrons cannot exchange their positions. In circular 2D quantum dots at low carrier densities the electron localization acquires a molecular form [17, 18] only in the inner coordinates of the system and not in the charge density which remains rotationally invariant. The Wigner form of the electron density with separate single-electron islands can be observed in the laboratory frame for quantum dots of lower symmetry only for some $N$, for which the classical [19] charge distribution reproduces the symmetry of the confinement potential [20].

To date, scanning gate microscopy experiments on closed two-dimensional (2D) quantum dots defined within the two-dimensional electron gas (2DEG) have concerned imaging of the single-electron quantum dot [5], mapping of the position of the floating double dot defined electrostatically [7], and determination of the effective tip potential as seen by the confined electrons [12]. In this paper we consider the extent to which the energy variation induced by the tip can be used for visualization of the few-electron charge density in 2D quantum dots. We investigate the relation between Wigner molecule formation in the laboratory frame and the reaction of the confined density to the potential of the tip. We perform configuration interaction calculations taking into account both the electron–electron correlation and the reaction of the quantum dot to the tip potential. The study covers up to four electrons and quantum dots of various symmetries and profiles. We discuss the adequacy of the perturbative approach for extraction of the electron density [5, 10, 11] confined in quantum dots and the fidelity of charge images outside the perturbative regime. We find that images obtained with a repulsive (attractive) tip potential tend to overestimate (underestimate) the electron localization. We demonstrate that the confined charge density is best resolved when the classical electron configuration agrees with the symmetry of the confinement potential. We also identify cases where the confined electron density evades visualization even for a weak perturbation introduced by the tip.

The experimental technique which is referred to in this paper—Coulomb blockade microscopy—with the tip of the atomic force microscope operating in the non-contact mode is suitable for investigation of electron systems that are buried several nanometers below the semiconductor surface, in particular the ones defined in 2DEG. Interaction effects in one-dimensional electron systems are also discussed [21–26] in the context of scanning tunneling microscopy in which the flow of the current between the tip and the leads through the electron system is observed. This kind of experiment can be performed on unburied systems such as free standing quantum wires [21, 23] or carbon nanotubes [22, 23, 26]. In particular, the signature of Wigner molecule formation in the conductance of the tip–quantum dot contact has been discussed [23, 25, 26] using the Luttinger liquid formalism [25, 26] or an exact diagonalization technique [23] similar to the one applied here. It was demonstrated that the Wigner localization can be deduced from the spatial dependence of the spectral function [23] for temperatures exceeding the threshold value set by the exchange interaction. Scanning tunneling microscopy opens the possibility of resolution of the local spatially resolved density of states also on the energy scale [23] by changing the voltage applied to the tip. The present simulation concerns the chemical potential change induced by the tip charge which in experiments is determined by switching the current off and on. The influence of the tip position on the conductance, i.e. the height of the peaks of the current [15], in conditions of lifted Coulomb blockade is outside the scope of this work.

2. Theory

In this work we assume a strictly two-dimensional model of confinement which is usually justified by the strong confinement of 2DEG in the growth direction $z$. The Hamiltonian of the $N$-electron system is taken in the form

$$H = \sum_{i}^{N} h(r_{i}) + \frac{\hbar^{2}}{4\pi\varepsilon\varepsilon_{0}} \sum_{i=1}^{N} \sum_{j=i+1}^{N} \frac{1}{r_{ij}},$$

(1)

where $r_{i}$ is the position of the $i$th electron and $h$ is the single-electron Hamiltonian,

$$h = -\frac{\hbar^{2}}{2m} \nabla^2 + V(r) + V(t; r_{i}).$$

(2)
Results for a circular harmonic oscillator potential with \( \hbar \omega = 0.5 \text{ meV} \) and the potential of the tip of the Lorentz form (equation (8) with \( d_{\text{tip}} = 20 \text{ nm} \)). The columns correspond to various electron numbers from \( N = 1 \) to 4. The first (last) row of the plots shows the energies and chemical potentials for \( V_T = -0.5 \text{ meV} \) (\( V_T = 2 \text{ meV} \)). The rows from the second ((e)–(h)) to the fifth ((q)–(t)) show the electron densities: the unperturbed one (\( n_\text{brown} \) solid lines), the one reproduced with the perturbative formula (5) (\( n_\text{r} \), blue dots) and the one obtained under the assumption of a delta-like perturbation (\( n_\delta \), green triangles). Subsequent rows correspond to various values of \( V_T \).

In equation (2), \( m^* \) is the effective mass, \( \epsilon \) is the dielectric constant (we use GaAs material parameters \( m^* = 0.067 \text{ m}_0, \epsilon = 12.5 \)), \( V \) stands for the external potential, \( V_t \) denotes the tip potential as seen by the electrons within the plane of confinement and \( r_t \) is the position of the tip.

The single-electron eigenequation is diagonalized (\( h\phi_n = \epsilon_n \phi_n \)) using a basis of Gaussian functions

\[
\phi_n(x, y) = \sum_{i=1}^{M=K} \sum_{k} c_k^{(n)} \sqrt{\frac{2a}{\pi}} \exp\left(-a \left[(x-X_k)^2 + (y-Y_k)^2\right]\right),
\]

where the centers of the Gaussians \((X_k, Y_k)\) are distributed on a rectangular lattice of \( M \times K \) points (typically several hundred centers are taken—see for instance the crosses in figure 1) and \( a \) is optimized variationally [27]. The applied multicenter Gaussian basis allows for the description of any smooth potential with arbitrary or no symmetry [27]. The few-electron eigenproblem is solved with the configuration interaction approach using the eigenstates of operator (2) for construction of the basis. The single-electron eigenfunctions \((\phi_n)\) are used for construction of Slater determinants that are used as the basis for the \( N \)-electron Schrödinger equation for Hamiltonian (1),

\[
\Psi ([x_i, y_i, \sigma_i; i = 1, \ldots, N]) = \sum_k d_k A [\phi_{k1}(x_1, y_1)\chi_{k1}(\sigma_1)\ldots\phi_{kN}(x_N, y_N)\chi_{kN}(\sigma_N)],
\]

where \( A \) is the antisymmetrization operator, and \( \chi_k \) is one of the eigenstates of the spin Pauli \( \sigma_z \) matrix. For construction of the basis of determinants we use up to 38 single-electron spin-orbitals.

In an experiment the maps of the chemical potential \( \mu_N(x_t, y_t) = E_N - E_{N-1} \) can be gathered by re-tuning the conditions for the current flow (i.e. lifting the Coulomb blockade) with varied back-gate potential or bias. Since \( \mu_1 = E_1 \), the energy maps as functions of the tip position can be deduced for any \( N \). Simulation of the confined charge density mapping by the SGM technique is performed in the following sequence. We first calculate the energy of an \( N \)-electron system as a function of the tip position. The charge density extracted from the energy map \( n_r \) is obtained under the
assumption that the action of the tip is perturbative [5, 10, 11]

\[ E_N(r_t) = E_N(\infty) + \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dx \, dy \, V_1(r; r_t) n_t(r). \]  

Equation (5) is a convolution of the tip potential and the confined charge density. The charge density can be extracted from the energy dependence of the tip position using the Fourier transform technique [5, 10]. Alternatively equation (5) can be treated as the Fredholm-type integral equation for \( n_t \). We apply the Nyström approach replacing the integral by a quadrature (rectangle rule). Upon replacement we obtain a linear system of equations for the charge density in the mesh points used for the quadrature. In the following we compare the charge density deduced in this way (\( n_t \)) with the exact one (\( n \)) that is calculated from the few-electron wavefunction

\[ n(r) = \langle \Psi \rangle \sum_{i=1}^{N} \delta(r - r_i)|\Psi\rangle. \]  

For comparison we calculate also the charge density \( n_3 \) assuming that the tip potential is point-like, \( V_p = V_T \delta(x - x_t, y - y_t) \). Then, equation (5) reduces to

\[ E_N(r_t) = E_N(\infty) + V_T n_3(r_t). \]  

The normalized charge density \( n_3 \) derived from this formula is simply proportional to the energy variation.

As the tip approaches the 2DEG its charge density reacts by deformation which results in screening of the tip potential. Previous Schrödinger–Poisson calculations [28] for the reaction of the 2DEG to the tip have indicated that the effective (i.e. screened) tip potential is close to the Lorentz form

\[ V_t(r; r_t) = \frac{V_T}{(x-x_t)^2 + (y-y_t)^2 + 1}, \]  

where the width of the tip \( d_{tip} \) turns out to be of the order of the tip–2DEG distance [28] independent of the charge at the tip and the density of the 2DEG, which only influence the strength of the perturbation \( V_T \) and not its range. The Lorentz form of the effective tip potential for SGM measurements on 2DEG was also found in experimental studies of 2D quantum dots [12]. Therefore, in the bulk of this work we mainly use the Lorentz model potential of the tip and assume \( d_{tip} = 20 \text{ nm} \), which seems to be the smallest reasonable value for the potential width. For comparison we also consider the reaction of the confined system to the long-range Coulomb potential

\[ V_c(r; r_t) = \frac{Qe}{4\pi \epsilon_0} \left( \frac{1}{(x-x_t)^2 + (y-y_t)^2 + z_{tip}^2} \right)^{1/2}, \]  

where \( Q \) is the tip potential, and \( z_{tip} \) is the position of the tip above the 2DEG plane.

An ample discussion of the potentials of electrostatic quantum dots defined within 2DEG was given in [29]. The calculations [29] indicated that depending on the geometry of the device one can obtain both parabolic and quantum well profiles. The latter can only be realized for large dots [29] with a linear extent of the order of a few hundred nm, i.e. the ones which are studied in the present work. Since our purpose is to determine the relation between the \( N \)-dependent classical electron distribution and the quantum dot geometry we consider a number of potentials: parabolic

\[ V(x, y) = \frac{m}{2} \left( \omega_x^2 x^2 + \omega_y^2 y^2 \right), \]  

of circular \( \omega_x = \omega_y = \omega \) and elliptic \( \omega_x \neq \omega_y \) symmetry, as well as non-parabolic dots modeled by the formula

\[ V(x, y) = V_0 \left( 1 - \frac{1}{1 + \left( \frac{x}{X} \right)^{10} + \left( \frac{y}{Y} \right)^{10}} \right), \]  

which produces a well-like potential with a flat bottom of nearly rectangular shape with dimensions \( 2X \times 2Y \). For equation (11) we discuss the dots from a nearly 1D (\( X \gg Y \)) to square (\( X = Y \)) geometry.

3. Results and discussion

3.1. Circular potential

Let us first consider a circular parabolic quantum dot with \( \hbar \omega = 0.5 \text{ meV} \). The solid lines in figures 2(e)–(h) show the
Figure 4. Results for an elliptic parabolic potential with $\hbar \omega_x = 0.8 \text{ meV}$, $\omega_y = 1.2 \omega_x$, and the potential of the tip of the Lorentz form (equation (8) with $d_{\text{tip}} = 20 \text{ nm}$). The columns correspond to various electron numbers. The first row of plots ((a)–(d)) shows the charge density in the absence of the tip. The second ((e)–(h)) and third ((i)–(l)) rows show the energies as a function of the tip position for $V_T = -2 \text{ meV}$ and $V_T = 2 \text{ meV}$, respectively. The next three rows show the charge density reproduced by the perturbative formula, and the last one shows the density calculated for the assumption of a point-like tip potential.

unperturbed radial charge density for 1, 2, 3 and 4 electrons, respectively. When a tip modeled by the attractive Lorentzian with $V_T = -0.5 \text{ meV}$ moves above the system, the changes in the energy are of the order of 0.2 meV only (figures 2(a)–(d)). The reproduced charge density $n_r$ (circles) agrees very well with the unperturbed density, which is also the case for a weak repulsive tip potential (figures 2(m)–(p)). A stronger amplitude of the energy variation should be useful for the signal to noise ratio of the experimental maps. For a stronger attractive perturbation ($V_T = -2 \text{ meV}$, figures 2(i)–(l)) we notice that the size of the charge droplet is overestimated with an extra oscillation of a small amplitude. On the other hand, a stronger repulsive potential ($V_T = 2 \text{ meV}$, figures 2(q)–(t)) gives a smaller size of the droplet.

Figure 3 shows the two- and three-electron densities: unperturbed (figures 3(a) and (b)), and in the presence of the tip (figures 3(c)–(f)). The attractive tip $V_T = -2 \text{ meV}$ captures a part of the density underneath (figures 3(c) and (d)), the positions of the other electron islands become well resolved. The repulsive tip also pins the orientation of the Wigner molecule in the laboratory frame (figures 3(e) and (f)), but with a void under the tip position. The impact of the tip on the electron density is therefore a drastic one for both negative and positive tip potentials, so the success of the perturbative
formula given by equation (5) for reproduction of the radial density as calculated in the absence of the tip found in figure 2 is quite remarkable, even if the original density lacks finer details.

3.2. Elliptic potential

The finer details of the unperturbed electron density appear for dots of lowered symmetry: see the results for an elliptic ($\hbar \omega_2 = 0.8$ meV, $\omega_2 = 1.2 \omega_0$) quantum dot in figure 4. For two electrons, single-electron islands are formed (figure 4(b)) along the $x$ axis, as in the classical solution (figure 5(a)). For three electrons, two equivalent classical charge distributions exist (see figure 5(b)) each with symmetry lower than the elliptical one, and in consequence single-electron islands do not appear in the laboratory frame of the quantum system (figure 4(c)). For each $N$, similarly to the circular potential, for a weak perturbation with both a negative tip ($V_T = -0.5$ meV—figures 4(m)–(p)) and a positive tip (not shown), the $n_0$ density very well reproduces the unperturbed one.

The second and third rows of figure 4 show the energy of the system as a function of the tip position for stronger attractive and repulsive tip potentials, $V_T = \pm 2$ meV. For the negative tip we obtain a flat minimum, within more or less the entire region occupied by the unperturbed charge density (figures 4(e)–(h)). The minimum appears since the tip creates its own potential minimum and the electron system follows the minimum as the tip is translated. The reproduced density (figures 4(q)–(t)) occupies a larger space than the original one (as in the circular case for $V_T = -2$ meV—see figures 2(i)–(l)), and a variation of smaller amplitude appears within the maximal density area.

For the positive tip the energy maximum is more strongly localized (figures 4(i)–(l)) around the center of the dot, and the amplitude of $n_t$ variation (figures 4(u)–(x)) is drastically increased with respect to $n$. Also, the reproduced density occupies a visibly smaller area than the original one. Nevertheless, the configuration of the maxima of $n_t$ agrees with the ones present for $n$.

For $V_T = 2$ meV, the density $n_0$ reproduced with the assumption that the energy map—obtained in fact for the Lorentz function—is due to the delta-like tip potential gives a closer (figures 4(y)–(ab)) idea about the size of the charge droplet. Nevertheless, the details of the density maxima are not reproduced by $n_0$.

3.3. Square quantum dot

Let us now consider a square quantum dot (confinement potential given by equation (11) for $X = Y = 200$ nm). For $N > 1$ the unperturbed electron density distinctly sticks to the corners of the square dot (figures 6(b)–(d)) as should be expected for interacting charge density within a box. For $N = 2$ and 3 an increase of the density along the dot edges is also observed. The classical system of four electrons possesses a single lowest energy configuration (figure 7(d)) which coincides with the charge density of figure 6(d). Systems of two and three electrons possess two and four equivalent configurations, respectively (figures 7(a)–(c)). The few-electron wavefunction contains contributions from all these configurations. Since one or two corners of the square are unoccupied in the classical configurations, the amplitude of the maxima is lower at the corners than in the case of $N = 4$. As the negative tip scans the dot (figures 6(e)–(h)) we observe a rather flat dependence of the energy on the tip position with minima at the corners—where the unperturbed electron density is the largest. Remarkably, for the positive tip and $N = 2$ and 3 the energy extrema lie on the axes of the dot (figures 6(j) and (k)), and not at the corners. The reason for this behavior is given in figure 8, which displays the charge distribution when the tip is present. When the tip is above the corner of the dot (figures 8(g) and (h)) we can see that the electron density becomes nearly identical with the classical systems of electrons (cf figures 7(a)–(c)). The other equivalent lowest energy configurations of the charge density were excluded by the presence of the tip above one of the corners. On the other hand, for two electrons when the tip is above the center of a side of the dot (figure 8(e)) the electrons, instead of occupying the opposite corners of the dot, go to its other side and approach each other, hence the corresponding maximum of the energy (figure 6(j)). For three electrons, the formation of four instead of three charge maxima is found (figure 8(f)), which also increases the electrostatic energy of the system above the minimal one.

The charge density $n_t$ as reproduced for the negative tip (figures 6(m)–(l)) exhibits maxima near the maxima of
Figure 6. Results for a square quantum dot, $X = Y = 200$ nm (equation (11)), and the tip potential of the Lorentz form (equation (8) with $d_{tp} = 20$ nm). The columns correspond to various electron numbers. The first row of plots ((a)–(d)) shows the charge density in the absence of the tip. The second ((e)–(h)) and third ((i)–(l)) rows show the energies as a function of the tip position for $V_T = -2$ meV and $V_T = 2$ meV, respectively. The next three rows show the charge density reproduced by the perturbative formula, and the last one shows the density calculated for the assumption of a point-like tip potential.

For a stronger tip potential (figures 6(q)–(t)) the charge density localization near the potential edges is overestimated. When a weak positive tip potential ($V_T = 0.5$ meV) is applied (figures 6(u) and (v)) we notice that the maxima are pushed to the interior of the dot from the edges. We also notice for two electrons (figure 6(v)) that the positions of the $n_r$ maxima are shifted to the axes of the dot, which is the result of the energy increase for the tip above the sides of the dot discussed above. For $V_T = 2$ meV we notice a similar phenomenon also for three electrons (figure 6(aa)). For one and four electrons (figures 6(y), (ab)) the maxima are localized in the correct positions, and they distinctly shrink in size as compared to the maxima of $n$.

We also considered the mapping of the charge density confined in a square quantum dot by the long-range Coulomb potential (equation (9)), i.e. for neglected screening of the
Figure 7. Classical lowest energy configurations of point charges for the potential of figure 6. For $N = 2$ (panel (a)) two equivalent configurations exist which are marked by different symbols. For $N = 3$ four equivalent configurations appear (b), (c)).

Figure 8. Charge densities for $N = 2$ and 3 electrons for the parameters of figure 6. The cross marks the tip position.

tip potential—see figure 9. We considered the tip localized $z_{tip} = 30$ nm above the dot for charges at the tip of $Q = \pm 1$ and $\pm 0.1$ (e), for which the maximal value of the perturbation below the tip is equal to 3.8 meV and 0.38 meV, respectively. The weak ($Q = -0.1$) attractive perturbation (figures 9(u)–(x)) gives an $n_r$ which agrees well with $n$. On the other hand, already for the weak repulsive perturbation ($Q = 0.1$) the maxima of $n_r$ for $N = 2$ and 3 go to the axes of the dot—the phenomenon observed above for the Lorentz perturbation. For $Q = \pm 1$ the calculated $n_r$ differs drastically from the unperturbed density $n$. For $Q = -1$, $n_r$ (figures 9(y)–(ab)) drifts to the edges of the dot. This density localization convolved (equation (5)) with the Coulomb potential gives the flat energy curve of figures 9(i)–(l). On the other hand, for the positive potential $Q = 1$ the derived $n_r$ density (figures 9(ag)–(aj)) is localized in tiny islands inside the dot and only for a single and four electrons—for which a single classical configuration of the charge exists—are their positions close to the original ones. For $N = 2$ and 3 the switching between similar configurations of the type presented in figure 8 becomes so strong that the reproduced charge density (figures 9(ah) and (ai)) has little in common with the original one.

3.4. Rectangular quantum dot near the 1D limit

Finally, let us consider a rectangular quantum dot near the 1D limit ($X = 250$ nm, $Y = 50$ nm). The results for Lorentz and Coulomb tip potentials are displayed in figures 10 and 11, respectively. For this dot the classical few-electron systems for $N = 2–4$ possess two equivalent zig-zag configurations (figure 12). The electron positions in the two configurations differ only slightly and these differences are not resolved in the quantum charge density, which presents well resolved single-electron islands that are clearly visible in the original electron density for all $N$ (figures 10(a)–(d)). The single-electron islands are also well resolved in the maps obtained for all the Lorentz tip potentials considered in figures 10(m)–(x), as well as in the crudest assumption of a point-like potential (figures 10(y)–(ab)). The charge density islands obtained for $V_T = -2$ meV (figures 10(q)–(t)) are distinctly more extended along the axis of the dot, which results from the fact that the islands follow the attractive tip as it moves. On the other hand, for $V_T = 2$ meV (figures 10(u)–(x)) an extension of the $n_r$ densities in the direction perpendicular to the axis is found. When the repulsive tip localized near the edges of the dot
Figure 9. Results for a square quantum dot $X = Y = 200$ nm (equation (11)) and the tip potential of the Coulomb form (equation (9) with $z_{\text{tip}} = 30$ nm, $Q = \pm 0.1$ e and $Q = \pm 1$ e). The columns correspond to various electron numbers. The first row of plots ((a)–(d)) shows the charge density in the absence of the tip. Plots ((e)–(t)) show the energies as a function of the tip position. The next four rows show the charge density reproduced by the perturbative formula, and the last one shows the density calculated for the assumption of a point-like tip potential.
its width in the $y$ direction is effectively reduced. In this way the tip increases not only the local potential energy but also the kinetic energy due to the localization. For this reason, the perturbative formula produces a charge density which penetrates the region outside the dot, where the original density vanishes.

The repulsive Coulomb potential reproduces the charge localization correctly (figures 11(q)–(t)) with an enhanced effect of elongation of the charge density island perpendicular to the dot. On the other hand, the attractive Coulomb potential (figures 11(m)–(p)) misses the details of the charge density which is seen as equally spread along the dot. For $Q = \pm 0.1$ (not shown) the 1D Wigner molecule is well reproduced by $n_r$.

4. Summary and conclusions

We have performed simulations of the charge density mapping for electron systems confined in two-dimensional quantum dots using model tip potentials of the Lorentz and Coulomb forms, several confinement potentials and the exact solution of the few-electron Schrödinger equation. We investigated large quantum dots, where the electron–electron correlation is strong, which can give rise to the formation of single-electron islands in the laboratory frame, i.e. Wigner molecules.

For circular dots we found that the molecular electron distributions appear in the laboratory frame pinned by the tip potential. The Wigner molecule follows the tip as it moves...
Figure 11. The same as figure 10 but for the tip potential of the Coulomb form (equation (9)) with $z_{tip} = 30$ nm, $Q = \pm 0.1$ (e) and $Q = \pm 1$ (e). The last row of plots ((y)–(ab)) shows the energy map as obtained for the frozen charge density ((a)–(d)) and the Coulomb potential with $Q = 1$ (e).

Figure 12. Classical lowest energy configurations of point charges for the potential of figure 10. For each $N$ considered two equivalent configurations appear.
above the dot. In consequence, the energy map as a function of the tip position is rotationally invariant, and the density map reproduced by the perturbative formula is very close to the original one. We noticed that a stronger repulsive (attractive) tip leads to underestimate (overestimate) of the charge density size. This conclusion for the size of the droplet holds for all dot profiles studied. Moreover, for elliptical and square quantum dots single-electron islands appear in the charge density for some $N$, and they are resolved in the charge density that is reproduced from the integral perturbative formula. We have found that in 1D dots the Wigner molecule is clearly visible in the charge density mapped from the energy dependence for all $N$ and for most of the tip potential studied, with the exception of the negative Coulomb potential for the single-electron islands are lost. We demonstrated that the charge densities of electron systems which possess a few equivalent classical configurations are generally difficult to resolve by the scanning probe technique for the repulsive tip potential, since the tip switches between equivalent configurations. In consequence, the mapped charge density maxima do not overlap with the original ones.

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