Screening in perfect lateral surface superlattices

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Abstract. We study the electrostatic screening of a large periodic potential by a two-dimensional electron gas in zero magnetic field. For large potentials the screening is non-linear; depleted areas form which leads to the creation of either a dot or antidot lattice. The self-consistent potential is calculated numerically. The results show a significant alteration of the shape of the applied potential by the screening.

1. Introduction

In recent years there has been much study, both theoretical [1–5] and experimental [6–9], of the properties of lattices of dots and antidots. These structures are created when a two-dimensional electron gas (2DEG) is manipulated so that the electrons may only occupy certain areas. If they are restricted to small isolated regions then dots are formed; if however they are excluded from small isolated regions, antidots are created. These structures are most often periodic, the dots or antidots being arranged on a triangular [4] or square [6, 7] lattice. These structures have the generic name lateral surface superlattices (LSSL).

The realization of such structures is typically as follows. A 2DEG is formed in a semiconductor heterojunction near the surface of a crystal. Then the surface of the crystal may be etched [10]. or periodically damaged by an ion beam [8, 11] or else have a specially shaped periodic gate laid on top [6, 12, 13]. When, for example, a voltage is applied to this gate a periodic electrostatic field is set up inside the crystal. The bulk crystal will screen this potential, and the 2DEG will feel only the lowest Fourier modes. If the field is strong enough then depleted areas will form, leading either to a dot or an antidot lattice. It is experimentally possible [8] to take a dot lattice and successively raise the electron density so that the dot size increases until the system passes through a threshold into an antidot lattice.

Very little work has been done on the static response of the 2DEG to the applied field. Most textbook treatments of screening are done in the linear regime, where the modulation of the electron density is small [14, 15]. This is most certainly not the case here. Section 2 of this paper goes beyond the linear approximation to develop a screening equation for an 'incomplete' electron gas (i.e. one which has depleted areas). The solution of this equation will give the self-consistent electrostatic potential for cases where the electron density is periodic. This equation can be solved using very basic numerical iteration. The results show that the electron gas can greatly modify the shape as well as amplitude of the applied potential. This treatment is for zero magnetic field. There has been previous work on non-linear screening, for example [16, 17]. Some treatments concentrate on strong magnetic fields [18–20], or certain special geometries [21].

Many successful theoretical treatments of transport in antidot lattices involve considering the classical motion of electrons in model screened potentials [5, 7]. The shape of the actual potential may then be important as it affects the electron trajectories. Knowledge of the screening can also be important when considering the conductance of a system that is just below the threshold between a dot and an antidot lattice. This system will naturally show a dramatic rise in its conductance as threshold is approached. A theoretical treatment requires information of how the screened potential will change with Fermi level or electron number. This conductance problem will be discussed in a later paper.

Though typical conditions of the experiments are such that disorder has to be allowed for, the perfect lattice description given here can apply in extreme conditions, and it includes many of the essential ingredients for a more general treatment. In general the disorder will have a greater effect on the conductance than on the screened potential.

2. Derivation of the screening equation

Consider a 2DEG in which the charge density varies over scales large compared to the mean separation of the electrons. In such a case it is possible to write the electronic charge density $\rho(r)$ in the form

$$\rho(r) = -en(x, y)\delta(z)$$

for a 2DEG that is normal to the z direction. Following [22], inserting this into Poisson's equation, and performing a Fourier transform with respect to x and y gives

$$\left(\frac{\partial^2}{\partial z^2} - (k_x^2 + k_y^2)\right)\Phi^{\text{ind}}(k, z) = \frac{1}{\epsilon_0 \epsilon_r}en(k)\delta(z).$$

This has the solution

$$\Phi^{\text{ind}}(k, z) = -\frac{e}{2\epsilon_0\epsilon_r}\frac{1}{k}e^{-k|z|} = \phi^{\text{ind}}(k)e^{-k|z|}. \tag{1}$$

Here ϕ^{ind} is the electrostatic potential in the $z = 0$ plane created by the distribution of electronic charge. The relative permittivity ϵ_r is taken to be that of the crystal in which the 2DEG exists. For example GaAs has $\epsilon_r = 13.1$.

The electron gas will move under the influence of the *total* electrostatic potential $\phi(x, y)$, and we shall need to know the equilibrium distribution $n(x, y)$ for a given ϕ. So long as the potential varies over distances large compared to the mean electron spacing, then the number density will be given by

$$n(x, y) = \int_0^\infty g(\epsilon)\rho(\epsilon - e\phi)\,d\epsilon \tag{2}$$

where $g(\epsilon)$ is the two-dimensional density of states and $\rho(\epsilon)$ is the Fermi–Dirac distribution function. The integral can be performed exactly, and yields the result

$$n(x, y) = \frac{m}{\pi\hbar^2}\left[(\mu + e\phi(x, y)) + kT \ln\left(1 + e^{-(\mu + e\phi(x, y))/kT}\right)\right] \tag{3}$$

where μ is the chemical potential, and we have assumed a two-fold spin degeneracy. This can be written in the form

$$n(x, y) = \frac{m}{\pi\hbar^2}(\mu + e\phi(x, y))f_r(x, y, T).$$

At low temperatures where kT is small compared to μ, the function $f_{\tau}(x, y, T)$ can be replaced by the *area function* $f(x, y) = f_{\tau}(x, y, 0)$. This has the form

$$f(x, y) = 1 \qquad \mu \geqslant -e\phi(x, y)$$
$$f(x, y) = 0 \qquad \mu < -e\phi(x, y).$$

For many cases the applied potential will be periodic, such as in a dot or antidot lattice. In this situation the resulting charge density and screened potential will also be periodic. All such quantities can thus be expanded as two-dimensional Fourier series. For example

$$\phi(r) = \sum_k \phi(k) e^{ik \cdot r}.$$

At this point we have three equations which when solved together will yield the self-consistent screened field $\phi(x, y)$ created when an external field $\phi^{\text{ext}}(x, y)$ is applied to a 2DEG. When expressed in Fourier space these equations take the following form.

$$\phi(k) = \phi^{\text{ext}}(k) + \phi^{\text{ind}}(k) \tag{4}$$

$$n(k) = \frac{m}{\pi \hbar^2} \mu f(k) + \frac{me}{\pi \hbar^2} \sum_q f(k - q)\phi(q) \tag{5}$$

$$\phi^{\text{ind}}(k) = -\frac{e}{2\epsilon_0 \epsilon_r} \frac{1}{k} n(k). \tag{6}$$

Eliminating ϕ^{ind} and $n(k)$ yields the screening equation, the solution of which will give the screened potential.

$$\phi(k) \left[1 + \frac{2}{a_0 k} f(0) \right] + \frac{2}{a_0 k} \sum_{q \neq k} f(k - q)\phi(q) = \phi^{\text{ext}}(k) - \frac{2\mu}{e a_0 k} f(k). \tag{7}$$

Here a_0 is the 'reduced' Bohr radius, $me^2/4\pi\hbar^2 \epsilon_0 \epsilon_r$. This equation is difficult to solve in general because it contains an unavoidable self-consistency. This arises because the area function f which defines the boundary of the 2DEG will depend upon $n(x, y)$ which in turn depends upon the screened potential $\phi(x, y)$.

If, however, the external field is small and the chemical potential is high then there will not be any depleted regions. In this case $f(x, y) = 1$ everywhere, and the screening equation simplifies to the more familiar linear equation [15]:

$$\phi(k) \left[1 + \frac{2}{a_0 k} \right] = \phi^{\text{ext}}(k). \tag{8}$$

3. Numerical solution for a periodic two-dimensional potential

3.1. Reduction to a matrix equation

In order to proceed with the general equation (7) we shall consider the case of an external potential that is periodic and even with period a in both the x and y directions. The screened potential would be expected to have the same periodicity. If the applied potential is large enough then depleted regions will exist, and the structure will be that of a dot or antidot lattice. When the density of electrons or chemical potential μ is varied then the boundary of the electron gas will move. It is reasonable to assume that the boundaries for different values of μ do not cross. In this case specifying a point b as being on the edge of the electron gas will uniquely define both the boundary and hence the chemical potential:

$$\mu = -e\phi(b) = -e \sum_q \phi(q) \cos(q \cdot b). \tag{9}$$

This can be inserted into the screening equation (7) to obtain

$$\phi(k) + \frac{2}{a_0 k} \sum_q \left[f(k-q) - \cos(q \cdot b) f(k) \right] \phi(q) = \phi^{\text{ext}}(k). \tag{10}$$

The wavevectors k and q have the form $(2\pi m/a, 2\pi n/a)$ where n and m are positive or negative integers. Because of the square lattice symmetry of the potential all four of the Fourier components $\phi(\pm k_x, \pm k_y)$ are equal. This symmetry carries through to the Fourier components of the area function, $f(k)$. This enables the sum in (10) to be rewritten so that it runs over wavevectors q that have both q_x and q_y positive. The equation then reduces to the form

$$\sum_{q^+} A_{kq} \phi(q) = \phi^{\text{ext}}(k) \tag{11}$$

where the plus indicates that both components of q are positive. The coefficient A_{kq} has the form

$$\frac{2}{a_0 k} \left[f\left((k_x - q_x), (k_y - q_y)\right) + f\left((k_x + q_x), (k_y - q_y)\right) + f\left((k_x - q_x), (k_y + q_y)\right) \right.$$
$$\left. + f\left((k_x + q_x), (k_y + q_y)\right) + 2\cos(b_x q_x + b_y q_y) + 2\cos(b_x q_x - b_y q_y) \right] + \delta_{kq}. \tag{12}$$

If, however, either q_x or q_y are zero, then this equation gives twice the required answer (because there is then only a symmetry between two different q values rather than the usual four). In this case the first of the two terms in (12) should be divided by two.

In many circumstances the applied potential can be described well by very few Fourier components. It should then be possible to describe the screened potential well using a finite set of Fourier components. The wavevectors can be restricted to the set $(2\pi n/a, 2\pi m/a)$ where n and m are positive and $n, m \leqslant N$. The numerical results showed that $N \sim 20$ was sufficient. The screening equation, as written, does not take into account the background charge density produced by the fixed positive ions in the crystal. The effect of this background is to make $\phi(0)$ equal to zero (charge neutrality). This condition can now be included by simply removing the wavevector 0 from the set of allowed values. The total number of allowed wavevectors is then $N^2 - 1$.

Once these restrictions are applied then (11) reduces to a finite size matrix equation. This equation must still be solved self-consistently. The matrix elements of A depend upon the area function, which in turn depends upon the screened potential ϕ.

The matrix equation can be solved numerically using an iterative loop involving a standard LU decomposition routine. This method converges quickly to give the self-consistent potential.

Once the screened potential and chemical potential has been obtained, it is very easy to calculate the total number of electrons in a single dot. This is given by the following integral over a lattice square.

$$N = \frac{m_e}{\pi \hbar^2} \int \int \left(\mu + e\phi(x, y) \right) f(x, y) \, dx \, dy. \tag{13}$$

This equation is valid at $T = 0$, and assumes that the density of states is just $m_e/\pi\hbar^2$.

4. Numerical results for the screened potentials

In this section we present the results of the numerical solution of (11). For simplicity here we chose an external potential that only contains one wavelength.

$$\phi^{\text{ext}}(x, y) = V_0 \left[\cos\left(\frac{2\pi x}{a}\right) + \cos\left(\frac{2\pi y}{a}\right) \right]. \tag{14}$$

The results presented here are for the specific parameter values $a = 800$ nm (which is a typical value for a LSSL) and $V_0 = 0.5$ V (which is not typical). The numbers presented will, however, scale very simply with the parameter V_0; $\phi \propto V_0$, $N \propto V_0$.

The computational solution involved selecting a vector b which is chosen to lie on the edge of the electron gas. This in turn will have selected a unique boundary. The numerical calculations then give both the Fourier components of the screened potential and the value of the chemical potential.
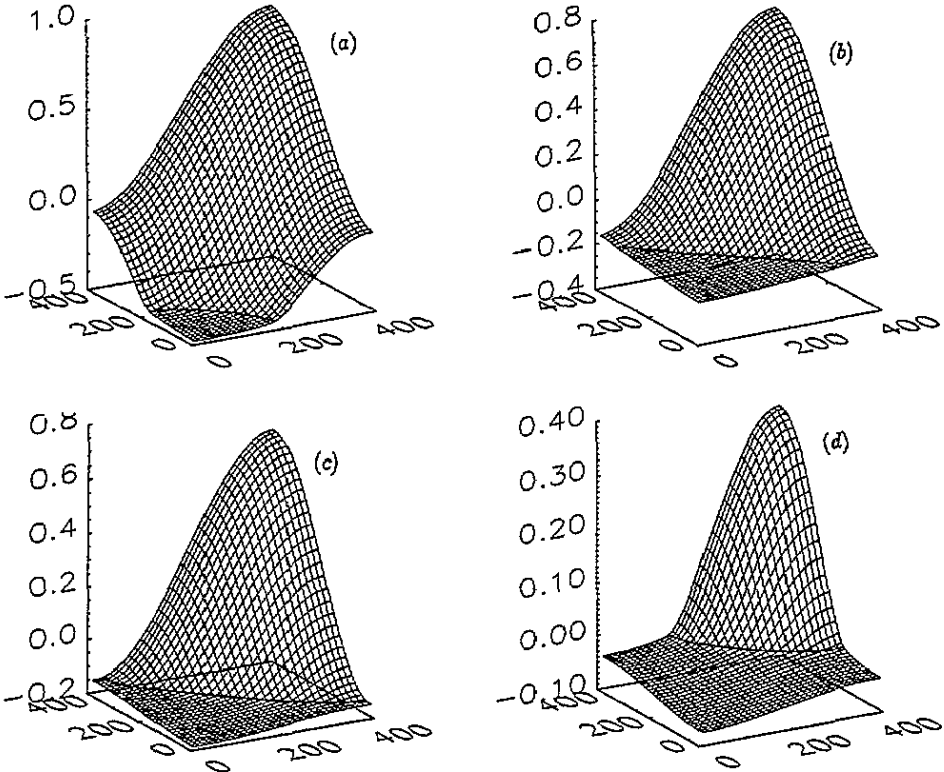

Figure 1. This shows 3D plots of the numerically calculated screened potential for four different numbers of electrons per dot. As the sequence progresses (a)–(d) the number of electrons increases. Each plot shows only one quarter of a lattice square with lattice constant $a = 800$ nm. (a) $N = 490$, $b = (188, 0)$ (b) $N = 1470$, $b = (344, 0)$ (c) $N = 1690$, $b = (400, 31)$ (d) $N = 3550$, $b = (400, 156)$. The contour line shows the edge of the electron gas.

Figure 1 shows the results of the numerical calculations for b equal to each of

$$\left(\frac{30}{128}a, 0\right) \quad \left(\frac{55}{128}a, 0\right) \quad \left(a\frac{1}{2}, \frac{5}{128}a\right) \quad \left(a\frac{1}{2}, \frac{25}{128}a\right).$$

These values cover the whole range from isolated quantum dots through threshold to an antidot lattice. For each value of b there is a 3D plot of the screened potential in the upper right-hand quadrant of a single lattice square.

All of the plots have the general feature that where the area function f is unity and there are electrons, the potential gradient is small. But, in the region beyond the edge of the electron gas where f is zero, the potential becomes far steeper. The electron gas has significantly altered the shape of the potential. This alteration of shape would effect the classical motion of an electron in the dot or antidot lattice.

The *threshold* between a dot lattice and an antidot lattice occurs when the number of electrons per dot, N_c, is 1 560. At this point each dot covers a fraction 0.41 of the area of a lattice square.
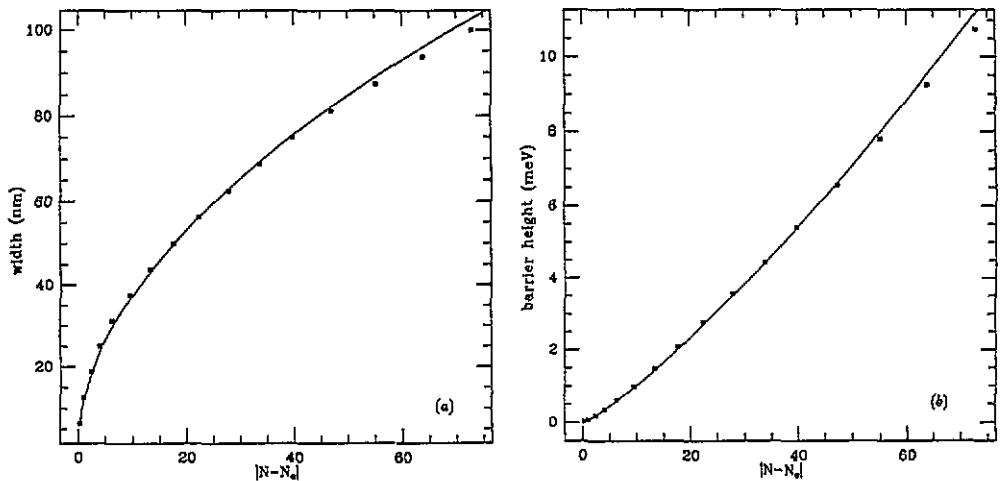

Figure 2. Plots showing the variation in (a) width and (b) minimum height of the barrier between neighbouring dots on the lattice. The points indicate the numerical values and the lines show the fitted power laws.

When the system is below threshold, the system consists of an array of isolated dots which are separated by a potential barrier. Figure 2 shows how the minimum width and minimum height of this barrier (measured from the Fermi level) varies with $|N - N_c|$, the difference between the number of electrons per dot and the number at threshold. The plots show that there is an approximate power law relationship. The barrier height varies as $|N - N_c|^{1.20\pm0.01}$ and the barrier width as $|N - N_c|^{0.52\pm0.01}$. As threshold is approached the width of the barrier very rapidly decreases. At this point there is very little change in the shape of the electron gas boundary with electron number, except at the points where the barrier is thinnest. Here the gas develops a narrow extension that eventually joins to the neighbouring dot.

When the number of electrons in a lattice square increases beyond N_c, neighbouring dots merge to form an antidot structure. Now each lattice square can be considered to contain a *reservoir* of electrons joined by a thin *constriction* to the neighbouring squares. As the number of electrons per lattice square increases further, the constriction widens and deepens. The constriction width and maximum depth (measured from the Fermi level) also show an approximate power law dependence with $(N - N_c)$. The constriction width varies as $(N - N_c)^{0.55\pm0.02}$ and the depth as $(N - N_c)^{0.65\pm0.02}$.

The lateral conductance of a dot lattice close to threshold will depend crucially on the width and height of the potential barriers separating the dots. Consequently the exponents in the power law relationships will be important in predicting the variation of the conductance with electron number.

5. Analytic considerations of the power laws

In the previous section we presented results for screening of a simple applied potential by an incomplete electron gas. This screening was highly non-linear, in the sense that as well as reducing the amplitude of the potential, the electrons also alter its shape and introduce further Fourier components. This process in turn affects the exponents of the power laws discussed in the last section. It is interesting to ask how different the numerical exponents are to those given by a linear screening theory. This will tell us how necessary it will be to use the non-linear potential in a conductance calculation.

In a linear theory the screened potential will not be changed in shape only in amplitude. The potential energy felt by the electrons would then be

$$V_s(x, y, \eta) = -e V_0(\eta) \left[\cos\left(\frac{2\pi x}{a}\right) + \cos\left(\frac{2\pi y}{a}\right) \right] \tag{15}$$

where the boundary of the electron gas is given by

$$\cos\left(\frac{2\pi x}{a}\right) + \cos\left(\frac{2\pi y}{a}\right) = \eta. \tag{16}$$

It is possible to deduce from this equation the expected exponents for the power laws neglecting the shape modification effects. If, in addition, screening was totally neglected then $V_0(\eta)$ would be constant and (15) would give the barrier/constriction width proportional to $|N - N_c|^{0.5}$ and the barrier height/constriction depth proportional to $|N - N_c|^{1.0}$. If the function V_0 is allowed to be vary then the exponents are only slightly modified

$$\text{width } (\sim \eta^{0.5}) \qquad \propto |N - N_c|^{0.5+\delta} \tag{17}$$

$$\text{height/depth } (\sim \eta V_0(\eta)) \propto |N - N_c|^{1.0+\gamma} \tag{18}$$

where δ and γ are positive and of order 10^{-2}. The linear exponents for the widths agree well with the numerical results, but there is poor agreement with them and the numerical results for the barrier height and constriction depth. These exponents are significantly modified by the non-linear aspect of the screening.

It is easy to see why the change of shape will affect these exponents if one considers trying to fit a functional form for $V_0(\eta)$ to the numerical data. One logical procedure would be to choose η to give the correct width (and hence similar boundary) and then fix the value of $V_0(\eta)$ to give the correct number of electrons. This procedure has the effect of fitting the simple $\cos(x) + \cos(y)$ potential to the true potential in the region where the electron density is non-zero. The results of this procedure are shown in figures 3 and 4. Figure 3 shows cross-sections of the true and fitted potentials taken along the line $y = 0$ for a system below threshold. Figure 4 shows cross sections of the true and fitted potentials along the line $x = a/2$ for a system above threshold.

Consider now using the fitted potential to deduce the barrier height. Figure 4 shows that this procedure would underestimate the height. As you move away from threshold and $|N - N_c|$ increases the discrepancy will get worse. This implies that the numerical barrier height will have a larger exponent than the linear prediction.
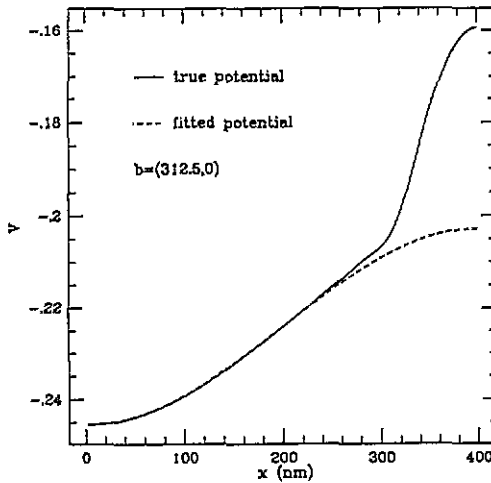
Figure 3. Cross-sections along the line $y = 0$ showing both the true screened potential and the fitted potential for a system below threshold.
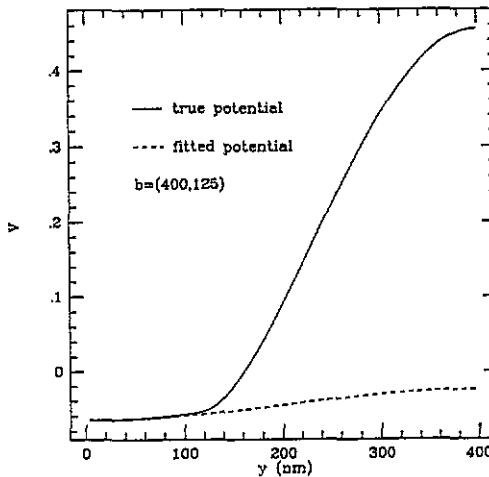

Figure 4. Cross-sections along the line $x = a/2$ showing both the true screened potential and the fitted potential for a system above threshold.

The situation is different for the constriction depth. The fitted potential will always have, at the point $(a/2, 0)$, the same curvature in the x and y directions. The true potential however has a larger curvature in the y direction. Consequently use of the fitted potential to deduce the depth will always produce an underestimate. This time, however, the discrepancy improves as $(N - N_c)$ increases. In turn this implies the numerical depth has an exponent smaller than the linear prediction.

So, for both the constriction depth and the barrier height, there is discrepancy between the linear prediction (18) and the actual numerical exponents and this due to the modification of the potential shape by screening.

6. Conclusions

In this paper we have presented a theory for the non-linear screening of a periodic external potential by a two-dimensional plane of electrons in zero magnetic field. This should be applicable to a 2DEG formed at a heterojunction to which a suitable potential is applied leading to the formation of a dot or antidot lattice. The method presented lends itself easily to numerical solution, and can be applied to any applied potential that is adequately expressed by a small set of Fourier components.

We have concentrated on the evolution of the potential as a dot lattice changes to an antidot lattice with increasing electron number. For clarity we picked the simplest applied potential that will show this behaviour, namely the sum of two cosines. The numerical calculations showed a significant change in the shape of the potential once it was screened.

Well within either the region where the electron density is non-zero ($f = 1$) or the region with ($f = 0$) the shape of the screened potential does come close to the shape of the applied potential. This is illustrated by figure 3. A simple functional form to describe the screened potential could be the following

$$V_s(x, y) = \left[V_1(N) + f(x, y)(V_2(N) - V_1(N)) \right] \left\{ \cos \left(\frac{2\pi x}{a} \right) + \cos \left(\frac{2\pi y}{a} \right) \right\}. \qquad (19)$$

In this equation the function V_1 will be much larger than V_2. Both will vary with the electron number N. The functional form given here will naturally break down when close to the edge of the electron gas.

We studied in more detail the potential barriers between dots in a lattice below threshold. The height and width of this barrier show a power law relation to $|N - N_c|$, the difference between electron number and the number at threshold. The exponents differ from those expected from linear screening.

The simple applied potential used here may not be appropriate to most experimental situations. A more realistic potential can easily be used, its form depending on the sample fabrication. In general a different potential will show different exponents. However one can consider a class of potentials which have a well defined minimum, saddle point and maximum, and which exhibit the transition from dot to antidot lattice. Numerical results show that the exponents within this class are comparable. This occurs because the exponent is dominated by the behaviour close to the saddle point, which is similar in all cases. Certain experiments may fall into this class [8]. The results of this paper will then be applicable.

In this paper we have not treated the effects of disorder. There are two main sources of disorder. Firstly the applied potential in any real system will not be perfectly periodic. The size of the deviation from periodicity will vary with fabrication technique, but can be very small for lithographic methods. Secondly many 2DEGs are created in modulation doped structures. There will be a layer of ionized donors lying above the 2DEG. These will set up a random potential that will be seen by the electrons in the 2D layer. If the length scale of the disordered potential is small compared to the lattice constant of the applied potential, then the large scale features of the screened potential will be little changed. This condition may be satisfied if the donor spacing is small enough and the lattice constant large enough. However this is not always the case. In order for the results in this paper to remain valid the amplitude of the applied potential must be large compared to the amplitude of the random potential. The typical scale of these fluctuations is 10 meV, and in certain experimental situations this is small enough to be neglected in comparison with the applied potential.

As mentioned before, the systems we discuss will show a rise in conductivity as threshold is approached. In a perfect lattice this can be viewed through the formation

of bands from the bound dot states. In systems with disorder on the scale of the lattice constant the band picture is inappropriate. In this case conduction will occur via hopping between dots. In both cases the potential shape between the dots is important. A subsequent paper will discuss in detail the mechanism for this conductance rise.

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