

Electronic spectrum of a two-dimensional quantum dot array in the presence of electric and magnetic fields in the Hall configuration

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We report calculations of the electronic spectrum of a two-dimensional lattice of coupled quantum dots, subject to external electric and magnetic fields in the Hall configuration. The quantum dots array was modeled by a periodic superposition of truncated, parabolic potential wells. By adopting the Landau gauge, a single-particle Hamiltonian was formulated, and its eigenfunctions were obtained as appropriately symmetrized, magnetic field-dependent Bloch functions. The magnetic field was consistently included in the corresponding Wannier functions, which were approximated by the eigenvectors of an isolated quantum dot in the presence of the external magnetic field, and multiplied by the Peierls's phase.

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I. INTRODUCTION

The motion of electrons in two-dimensional systems, under the influence of both a periodic potential and an external perpendicular magnetic field, has been of interest to theorists and experimentalists since the early stages of solid-state quantum physics.¹ The fascinating features of these systems proceeds from the competition of two characteristic length scales: the lattice constant d , which determines the periodicity of the lattice potential, and the Landau radius l_B , which characterizes the semiclassical electronic orbits.

The first theoretical approach to the problem is due to Peierls.¹ It is based on the formulation of an effective single-band Hamiltonian, arising from a tight-binding dispersion relation $E(\mathbf{k})$, through the substitution $E[\mathbf{k} + (e/\hbar c)\mathbf{A}]$. This approximation, which assumes that the magnetic field does not alter the original Bloch-band structure of the lattice, has been discussed and extended in many classical papers.²⁻¹⁰ When combined to a semiclassical picture,¹¹⁻¹⁵ the effective Hamiltonian theory leads to the notion of quantized magnetic orbits, which can be commensurable with the lattice period. Within the framework of the effective single-band Hamiltonian theory, further investigations^{16,17} lead to butterflylike patterns for the energy spectrum. In a classical paper, Hofstadter¹⁶ achieved Harper's equation,¹⁸ whose spectrum, as a function of the magnetic field, shows a fractal structure commonly referred to as the Hofstadter butterfly. The pattern reflects, as a consequence of Harper's equation, the splitting of the single Bloch-band into magnetic subbands, according to the number of magnetic flux quanta piercing the unit cell of the lattice. This picture is generally believed to represent the weak magnetic field regime, where $d \ll l_B$,^{19,20} despite the fact that no experimental evidence has been presented yet. Indeed, its extension to higher field intensities has been severely criticized²¹ under the basis of group theoretical arguments.

In the high magnetic field regime, where $l_B \ll d$, the lattice potential is considered to be a perturbation over the free electron Landau levels. It has been shown^{22,23} that due to the presence of the periodic potential, a single Landau level is

split into subbands. A Harper's equation is then also achieved, to relate Fourier coefficients of the wave function in the reciprocal space. The effect of Landau level coupling has also been studied,²⁴ and it was shown to drastically modify the butterfly symmetries. Some experimental evidence^{25,26} supports the existence of a butterfly-type energy spectrum in the high magnetic field regime.

There seems to be a certain gap in the literature concerning to the intermediate regime, where both the lattice constant d and the Landau radius l_B are comparable in magnitude. We believe that the reason is due to the completely different criteria used to choose the appropriate basis functions in both regimes, which are strongly localized crystal-Wannier functions on one limit, versus extended Landau levels on the other. It has been already remarked by Wannier,¹³ under general group-theoretical arguments, that the Bloch-band Wannier functions do not provide an exact basis for the problem, even at weak magnetic fields. Indeed, he shows that the Bloch-band concept can be rigorously extended to this case, provided that a slightly modified manifold is defined, by incorporating the magnetic field into a new set of magnetic-consistent Wannier functions. In the present work, we applied this idea to a two-dimensional lattice of quantum dots, under the presence of a perpendicular magnetic field. By choosing the Landau gauge, after a general study of the translational symmetries involved in the Hamiltonian, we constructed appropriately symmetrized Bloch-like wave functions. The Wannier functions in this linear combination, were approximated by the eigenfunctions of a single dot under the presence of an external magnetic field. Following the original argument of Wannier,¹³ this basis is consistent with the presence of the external magnetic field, through the definition of effective energy levels. Those levels are characterized by an effective frequency Ω , which is a combination of both the quantum dot geometric frequency ω and the cyclotronic frequency ω_c . We calculated the electronic spectrum corresponding to the lowest energy level in this system, neglecting interband coupling and adopting the tight-binding approximation, and compared our results with Hofstadter's effective-Hamiltonian theory.

The effect of an external electric field on this system, what is called the Hall configuration, is also of physical interest, in particular since the discovery of the quantum Hall effect.²⁷ A characteristic electric field-dependent magnitude, known as the Stark period,^{28–31} comes into scene, interacting with the already present lattice constant and Landau radius. This subject has been previously studied, particularly in the high magnetic field^{20,22,23} regime. In the present work, we considered the inclusion of an external electric field oriented along one of the symmetry directions of the quantum dot lattice. By choosing the Landau gauge as before, we performed calculations for the electronic spectrum, under a single magnetic-band approximation. We expect these calculations to be valid in the regime of weak electric field, where interband coupling can be neglected.

II. THEORY

Semiconductor heterostructures constitute, at the atomic level, complex many-body systems. In particular, a quantum dot³² has an internal crystalline structure which, despite the relatively small size of the dot, presents electronic bands related to its semiconductor properties. Therefore, only a relatively small amount of charge carriers (1–100), either conduction-band electrons or valence-band holes, can be considered to be effectively trapped by a quantum dot. To give a reasonable description of the physical properties of such a system, at the nanoscale level, simplifications need to be made. Following the common practice, we adopt an effective-mass approximation, to take into account the effects of the crystalline atomic structure over the charge carriers. Those will be assumed to be negative charges (conduction-band electrons), as, for instance, in GaAs/InAs self-assembled quantum dot systems.³² As our interest, in this preliminary study, is to investigate the main symmetries involved in the electronic spectrum of the system, we will formulate a single-particle Hamiltonian, whose eigenfunctions can be later implemented in more realistic many-body calculations. We will neglect the Zeeman splitting and spin-orbit interactions, which are very small for GaAs systems.³²

By keeping in mind the previous statements, we modeled the two-dimensional lattice of cylindrical quantum dots, by a three-dimensional potential, periodic over the plane of the array

$$V(\rho, z) = V(\rho + \mathbf{d}_n, z), \quad (1)$$

with $\rho = (x, y)$ and $\mathbf{d}_n = (n_x d, n_y d)$. We will assume that the electrons in the dot are confined by a very narrow quantum well along the z direction. Therefore, the z -dependent degrees of freedom can be integrated, obtaining a periodic effective potential, depending only on the coordinates over the plane. This potential has been modeled by a periodic superposition of truncated parabolic wells, centered at each site of the lattice

$$V_{\text{eff}}(\rho - \mathbf{d}_n) = \sum_{\alpha=x,y} \frac{1}{2} m^* \omega^2 (\alpha - n_\alpha d)^2 \quad \text{for } |\alpha - n_\alpha d| \leq \frac{d}{2} \quad (2)$$

and equal to zero otherwise. In this expression, m^* corresponds to the effective mass over the plane, and ω is the

frequency associated with the planar geometric confinement of the quantum dots, which is characterized by the length scale $l_{\text{dot}} = \sqrt{\hbar/m^* \omega}$. When external and static electric \mathbf{F} and magnetic \mathbf{B} fields are applied, the corresponding two-dimensional, single-particle Hamiltonian for the quantum dot array is

$$H_{\parallel}(\rho) = \frac{\left[\mathbf{p}_\rho + \frac{e}{c} \mathbf{A}(\rho) \right]^2}{2m^*} + \sum_n V_{\text{eff}}(\rho - \mathbf{d}_n) + eFx. \quad (3)$$

The electric field is applied along one of the symmetry directions of the lattice, namely, $\mathbf{F} = \hat{\mathbf{x}}F$. The magnetic field, normal to the plane of the array $\mathbf{B} = \hat{\mathbf{z}}B$, will be included through the vector potential in the Landau gauge $\mathbf{A}(\rho) = \hat{\mathbf{y}}xB$. In this gauge, the Hamiltonian preserves the translational symmetry of the periodic potential, along the direction perpendicular to the electric field.

Let us assume for a moment that the electric field is turned off. In that case, it can be shown that the magnetic translation operator defined by

$$T_{\mathbf{A}}(\mathbf{d}_n) = \exp \left[-\frac{i\mathbf{d}_n}{\hbar} \left(\mathbf{p}_\rho + \frac{e}{c} \mathbf{A} \right) \right] \quad (4)$$

commutes with the Hamiltonian. This property is evident for the kinetic term, but the potential term requires some further discussion. First notice that in the gauge chosen, a direct calculation yields $[p_i, A_j] = 0$ for $i, j = 1, 2$. Therefore, the magnetic translation operator can be written as

$$T_{\mathbf{A}}(\mathbf{d}_n) = \exp \left[-\frac{ie}{\hbar c} \mathbf{A} \cdot \mathbf{d}_n \right] T_{\mathbf{d}_n}, \quad (5)$$

where $T_{\mathbf{d}_n} = \exp[-(i\mathbf{d}_n/\hbar) \cdot \mathbf{p}_\rho]$ is a normal translation operator. For an arbitrary function $f(\rho)$, the combined action of the magnetic translation operator and the periodic potential is given by

$$\begin{aligned} T_{\mathbf{A}}(\mathbf{d}_n) V(\rho) f(\rho) &= \exp \left[-\frac{ie}{\hbar c} \mathbf{A} \cdot \mathbf{d}_n \right] V(\rho - \mathbf{d}_n) f(\rho - \mathbf{d}_n) \\ &= \exp \left[-\frac{ie}{\hbar c} \mathbf{A} \cdot \mathbf{d}_n \right] V(\rho) f(\rho - \mathbf{d}_n) \\ &= V(\rho) T_{\mathbf{A}}(\mathbf{d}_n) f(\rho). \end{aligned} \quad (6)$$

As $f(\rho)$ is arbitrary, it follows that the magnetic translation operator commutes with the periodic potential, and therefore

$$[T_{\mathbf{A}}(\mathbf{d}_n), H_{\parallel}(\mathbf{F} = 0)] = 0. \quad (7)$$

This property allows the use of group theory,³³ by introducing the group of magnetic translations. This is in fact a ray group, because the product of two elements of the group yields another element, multiplied by a constant phase

$$\begin{aligned} T_{\mathbf{A}}(\mathbf{d}_1) T_{\mathbf{A}}(\mathbf{d}_2) &= e^{-(ie/\hbar c) \mathbf{d}_1 \cdot \mathbf{A}(\rho)} T_{\mathbf{d}_1} e^{-(ie/\hbar c) \mathbf{d}_2 \cdot \mathbf{A}(\rho)} T_{\mathbf{d}_2} \\ &= e^{-(ie/\hbar c) \mathbf{d}_1 \cdot \mathbf{A}(\rho)} e^{-(ie/\hbar c) \mathbf{d}_2 \cdot \mathbf{A}(\rho - \mathbf{d}_1)} T_{\mathbf{d}_1} T_{\mathbf{d}_2} \\ &= T_{\mathbf{A}}(\mathbf{d}_1 + \mathbf{d}_2) e^{-(ie/\hbar c) \mathbf{d}_2 \cdot \mathbf{A}(\mathbf{d}_1)}. \end{aligned} \quad (8)$$

As a consequence of Eq. (8), we have

$$T_{\mathbf{A}}(\mathbf{d}_1)T_{\mathbf{A}}(\mathbf{d}_2) = T_{\mathbf{A}}(\mathbf{d}_2)T_{\mathbf{A}}(\mathbf{d}_1)e^{-(ie/\hbar c)\mathbf{d}_2 \cdot \mathbf{A}(\mathbf{d}_1)}. \quad (9)$$

Notice that the magnetic phase in Eq. (8), for the gauge chosen, is given by

$$\frac{e}{\hbar c}\mathbf{d}_2 \cdot \mathbf{A}(\mathbf{d}_1) = 2\pi \frac{Bd_{1,x}d_{2,y}}{\hbar c} = 2\pi n_{x,1}n_{y,2} \frac{Bd^2}{\phi_0} \quad (10)$$

which is proportional to the ratio between the total magnetic flux Bd^2 piercing the unit cell, and the magnetic flux quanta $\phi_0 = \hbar c/e$. It is then possible, for a finite lattice of dimensions $N_x d = L_x$ and $N_y d = L_y$, to generalize the Born–von Karman boundary conditions, by restricting the eigenfunctions to be periodic under magnetic translations corresponding to the full lattice size

$$T_{\mathbf{A}}(\hat{\mathbf{x}}N_x d)\varphi(\rho) = T_{\mathbf{A}}(\hat{\mathbf{y}}N_y d)\varphi(\rho) = \varphi(\rho). \quad (11)$$

Assuming that φ is an eigenfunction, $\varphi_m = T_{\mathbf{A}}(\mathbf{d}_m)\varphi$ are also eigenfunctions. If we apply a full lattice translation over any one of those functions

$$T_{\mathbf{A}}(\hat{\mathbf{x}}N_x d)\varphi_m = T_{\mathbf{A}}(\hat{\mathbf{x}}N_x d)T_{\mathbf{A}}(\mathbf{d}_m)\varphi = e^{-(ie/\hbar c)\mathbf{d}_m \cdot \mathbf{A}(\hat{\mathbf{x}}N_x d)}\varphi_m, \quad (12)$$

where the property (9) has been applied. If we demand that all those functions satisfy the Born–von Karman periodic boundary conditions, the constant phase in Eq. (12) must be a multiple of 2π :

$$\frac{e}{\hbar c}\mathbf{d}_m \cdot \mathbf{A}(\hat{\mathbf{x}}N_x d) = 2\pi m_y N_x \frac{Bd^2}{\phi_0} = 2\pi q. \quad (13)$$

This condition can be fulfilled each time the number of magnetic flux quanta which traverses the unit cell is a rational number

$$N_\phi = \frac{Bd^2}{\phi_0} = \frac{q}{m_y N_x} \quad (14)$$

thus imposing a commensurability relation between the magnetic field intensity and the lattice size. A detailed analysis of the representations of the group of magnetic translations has been reported by Brown.³³ He showed that, when periodic Born–von Karman boundary conditions can be applied, a generalization of the Bloch's theorem leads to the definition of magnetic reciprocal lattice vectors

$$\mathbf{k} \rightarrow \mathbf{k} + \frac{e}{\hbar c}\mathbf{A}, \quad (15)$$

where \mathbf{k} is a normal reciprocal lattice vector at zero magnetic field. This formulation defines modified Bloch functions as eigenvectors of the Hamiltonian, which can be formally expanded in the corresponding magnetic Wannier functions.

After this brief preamble on the magnetic translation group, let us go back to the original case, in which the electric field is turned on, and pointing along the x direction. Despite the translation symmetry along this direction is destroyed by the presence of the electric field, the symmetry along the y direction is preserved. It follows then that $[T_{\mathbf{A}}(\hat{\mathbf{y}}d), H_I(\rho)] = 0$, where $T_{\mathbf{A}}(\hat{\mathbf{y}}d)$ denotes the operator of

discrete magnetic translations along the y direction. Therefore, a restricted form of the Bloch's theorem can be still applied to find the eigenfunctions of the Hamiltonian, provided that we restrict the full ray group of magnetic translation operators to its subgroup of magnetic translations along the y direction.

Taking into account the translational symmetry involved, and applying the Bloch's theorem, the eigenfunctions of the Hamiltonian given by Eq. (3) can be constructed by the following prescription:

$$\Psi_{k_y}(\rho) = e^{ik_y y} u_{k_y}(\rho). \quad (16)$$

The function $u_{k_y}(\rho)$ satisfies the periodicity condition along the y direction

$$u_{k_y}(\rho + d\hat{\mathbf{y}}) = u_{k_y}(\rho) \quad (17)$$

and it can be expressed in terms of Wannier functions $W(\rho - \mathbf{d}_n)$,

$$u_{k_y}(\rho) = \sum_{\mathbf{d}_n} C_{n_x} \exp\left(-i\left[k_y + \frac{e}{\hbar c}A_y(\mathbf{d}_n)\right](y - n_y d)\right) W(\rho - \mathbf{d}_n). \quad (18)$$

Therefore, the wave functions in Eq. (16) can be written as

$$\Psi_{k_y}(\rho) = \sum_{\mathbf{d}_n} C_{n_x} e^{ik_y n_y d} \exp\left[-i\frac{e}{\hbar c}\mathbf{A}(\mathbf{d}_n) \cdot (\rho - \mathbf{d}_n)\right] W(\rho - \mathbf{d}_n). \quad (19)$$

Notice that a magnetic field-dependent phase multiplies each Wannier function. This phase was first suggested by Peierls,¹ and later discussed by Wannier.¹³ The coefficients C_{n_x} in the expansion, must be obtained by solving the eigenvalue problem for the Hamiltonian (3).

Given that the Wannier functions are strongly localized on the lattice sites, the standard choice is to build them from linear combinations of "atomic orbitals." In this work, we choose $W(\rho)$ as eigenfunctions of a single-dot Hamiltonian, under the presence of the external magnetic field

$$H^{\text{dot}}(\rho) = \frac{\left(\mathbf{p}_\rho + \hat{\mathbf{y}}\frac{eB}{c}x\right)^2}{2m^*} + \frac{m^*}{2}\omega^2\rho^2. \quad (20)$$

This choice has the advantage that the magnetic field needs not to be treated as a perturbation, but it is consistently included in the basis. The eigenfunctions of this operator, in which the vector potential is in the same gauge as stated in the Hamiltonian (3), can be obtained from the well known eigenfunctions of the Fock-Darwin Hamiltonian^{34,35}

$$H^{\text{FD}}(\rho) = \frac{\left(\mathbf{p}_\rho + \frac{e}{2c}\mathbf{B} \times \rho\right)^2}{2m^*} + \frac{m^*}{2}\omega^2\rho^2 \quad (21)$$

by means of a gauge transformation. The Landau gauge is related to the symmetric gauge in the Fock-Darwin Hamiltonian, by the transformation

$$\hat{\mathbf{y}}xB = \frac{1}{2}\mathbf{B} \times \boldsymbol{\rho} + \nabla \left(\frac{B}{2}xy \right), \quad (22)$$

such that the eigenfunctions of Eq. (20) are given by the eigenfunctions of Eq. (21), modified by a magnetic field-dependent phase

$$\Phi_{n,m}^{\text{dot}}(\boldsymbol{\rho}) = \sqrt{\frac{2}{l_0^2}} \sqrt{\frac{n_r!}{(n_r + |m|)!}} \left(\frac{\boldsymbol{\rho}}{l_0} \right)^{|m|} \times \exp \left[-\frac{\rho^2}{2l_0^2} - i \frac{eB}{2\hbar c} xy \right] L_{n_r}^{|m|} \left(\frac{\rho^2}{l_0^2} \right). \quad (23)$$

In this definition, $L_{n_r}^{|m|}$ are the Laguerre polynomials. The corresponding eigenvalues are

$$\varepsilon(n,m) = \hbar\Omega(n+1) - \frac{1}{2}\hbar\omega_c m, \quad (24)$$

where $n=0,1,\dots$, is the principal quantum number, $m=-n,-n+2,\dots,n$ is the azimuthal quantum number, and $n_r=(n-|m|)/2$ is the radial quantum number.

The effective frequency Ω , as defined in Eq. (24), is given by the expression $\Omega = \sqrt{\omega^2 + \omega_c^2}/4$. The effective length scale which characterizes these functions is given by $l_0 = l_B/\sqrt[4]{1+4\omega^2/\omega_c^2}$, where $l_B = \sqrt{\hbar c/eB}$ is the Landau radius.

III. ZERO ELECTRIC FIELD

In the absence of an external electric field, the eigenvalue equation for the Bloch function (16) is

$$\left[\frac{\left[\mathbf{p}_\rho + \frac{e}{c}\mathbf{A}(\boldsymbol{\rho}) \right]^2}{2m^*} + \sum_n V_{\text{eff}}(\boldsymbol{\rho} - \mathbf{d}_n) \right] \Psi_{k_y}(\boldsymbol{\rho}) = E_{k_y} \Psi_{k_y}(\boldsymbol{\rho}). \quad (25)$$

By inserting Eq. (16) into Eq. (25), we obtain the corresponding eigenvalue equation for the periodic function $u_{k_y}(\boldsymbol{\rho})$:

$$\left[\frac{\left(\mathbf{p}_\rho + \hat{\mathbf{y}}\hbar k_y + \frac{e}{c}\mathbf{A}(\boldsymbol{\rho}) \right)^2}{2m^*} + \sum_n V_{\text{eff}}(\boldsymbol{\rho} - \mathbf{d}_n) \right] u_{k_y}(\boldsymbol{\rho}) = E_{k_y} u_{k_y}(\boldsymbol{\rho}). \quad (26)$$

Let us assume that the ratio between the magnetic flux through a unit cell, and the quantum of flux $\phi_0 = hc/e$, is a rational number, for instance,

$$N_\phi = \frac{Bd^2}{\phi_0} = \frac{p}{q} \quad (27)$$

with p an integer prime to q . Provided that this condition is satisfied, let us apply the translation operator $T_{\hat{\mathbf{x}}qd}$ over the eigenvalue equation (26). Notice that, in the Landau gauge, $\mathbf{A}(\boldsymbol{\rho} + \hat{\mathbf{x}}qd) = \mathbf{A}(\boldsymbol{\rho}) + \hat{\mathbf{y}}qdB$. Therefore, after the translation is applied, Eq. (26) becomes

$$\left[\frac{\left[\mathbf{p}_\rho + \hat{\mathbf{y}}\hbar \left(k_y + \frac{2\pi q}{d} N_\phi \right) + \frac{e}{c}\mathbf{A}(\boldsymbol{\rho}) \right]^2}{2m^*} + \sum_n V_{\text{eff}}(\boldsymbol{\rho} - \mathbf{d}_n) \right] \times u_{k_y}(\boldsymbol{\rho} + \hat{\mathbf{x}}qd) = E_{k_y} u_{k_y}(\boldsymbol{\rho} + \hat{\mathbf{x}}qd). \quad (28)$$

From the rationality condition assumed for the magnetic field, we have $k_y + (2\pi q/d)N_\phi = \bar{k}_y$, where $\bar{k}_y = k_y + 2\pi p/d$. As a consequence of the translational symmetry along the y direction, and based on the preliminary discussion about the magnetic translation group and the generalized Bloch's theorem, we conclude that both k_y and \bar{k}_y are associated to the same magnetic Bloch function, except for a constant phase. As in the standard Bloch's theorem, this associated to the periodicity in the energy spectrum $E_{\bar{k}_y} = E_{k_y}$, for $\bar{k}_y = k_y + 2\pi p/d$. Taking into account the previous statements, Eq. (28) can be expressed as

$$\left[\frac{\left[\mathbf{p}_\rho + \hat{\mathbf{y}}\hbar \bar{k}_y + \frac{e}{c}\mathbf{A}(\boldsymbol{\rho}) \right]^2}{2m^*} + \sum_n V_{\text{eff}}(\boldsymbol{\rho} - \mathbf{d}_n) \right] u_{k_y}(\boldsymbol{\rho} + \hat{\mathbf{x}}qd) = E_{k_y} u_{k_y}(\boldsymbol{\rho} + \hat{\mathbf{x}}qd). \quad (29)$$

By comparing Eq. (29) with Eq. (26), we conclude that

$$u_{k_y}(\boldsymbol{\rho} + \hat{\mathbf{x}}qd) = e^{i\alpha_q} u_{\bar{k}_y}(\boldsymbol{\rho}), \quad (30)$$

where α_q is a constant phase, as a consequence of the non-degeneracy of the energy spectrum. In other words, despite not being explicit in our construction of the magnetic Bloch functions, at zero electric field the magnetic translational symmetry exists along the x direction, in agreement with the preliminary discussion about the magnetic translations group. Its effect can be intuitively pictured as to “enlarge” the effective lattice period, along the x direction, by a factor q . As shown in Appendix A, this symmetry property imposes a necessary condition, to be satisfied by the coefficients in the expansions (18) and (19)

$$C_{n_x+q} = e^{i\alpha_q} C_{n_x}. \quad (31)$$

Therefore, under the presence of a rational magnetic field, the space of solutions to the eigenvalue equation (25) is reducible, and its reduction leads to exactly q subspaces, for $N_\phi = p/q$. As a consequence, we expect in that case for the energy spectrum to be composed of exactly q subbands.

After this preliminary discussion of the general symmetry properties involved, we will adopt the basis defined by the eigenfunctions of the single-dot Hamiltonian of Eq. (20), and we will approximate the Wannier functions by the lowest energy eigenstate Φ_0^{dot} , which is

$$\Phi_0^{\text{dot}}(\boldsymbol{\rho}) = \frac{1}{\sqrt{\pi}l_0} \exp \left(-\frac{\rho^2}{2l_0^2} - i \frac{eB}{2\hbar c} xy \right). \quad (32)$$

Therefore, according to Eq. (19), the wave functions are given by the linear combinations

$$\Psi_{k_y}(\rho) = \sum_{\mathbf{d}_n} C_{n_x} e^{ik_y n_y d} e^{-(ie/\hbar c)\mathbf{A}(\mathbf{d}_n) \cdot (\rho - \mathbf{d}_n)} \Phi_0^{\text{dot}}(\rho - \mathbf{d}_n). \quad (33)$$

Substituting Eq. (33) into Eq. (25), we obtain

$$\sum_{\mathbf{d}_n} C_{n_x} e^{ik_y n_y d} \left[\frac{\left[\mathbf{p}_\rho + \frac{e}{c} \mathbf{A}(\rho) \right]^2}{2m^*} + \sum_n V_{\text{eff}}(\rho - \mathbf{d}_n) - E_{k_y} \right] \times e^{-(ie/\hbar c)\mathbf{A}(\mathbf{d}_n) \cdot (\rho - \mathbf{d}_n)} \Phi_0^{\text{dot}}(\rho - \mathbf{d}_n) = 0. \quad (34)$$

It is straightforward to show that the magnetic phase factor can be transferred to the left of the Hamiltonian operator, by means of a translation in the argument of the vector potential, such that we have

$$\sum_{\mathbf{d}_n} C_{n_x} e^{ik_y n_y d} e^{-(ie/\hbar c)\mathbf{A}(\mathbf{d}_n) \cdot (\rho - \mathbf{d}_n)} \left[\frac{\left[\mathbf{p}_\rho + \frac{e}{c} \mathbf{A}(\rho - \mathbf{d}_n) \right]^2}{2m^*} - \sum_n V_{\text{eff}}(\rho - \mathbf{d}_n) - E_{k_y} \right] \Phi_0(\rho - \mathbf{d}_n) = 0. \quad (35)$$

We can write the expression inside the parentheses in terms of the single-dot Hamiltonian H^{dot} centered on the lattice site \mathbf{d}_n

$$\sum_{\mathbf{d}_n} C_{n_x} e^{ik_y n_y d} e^{-(ie/\hbar c)\mathbf{A}(\mathbf{d}_n) \cdot (\rho - \mathbf{d}_n)} [H^{\text{dot}}(\rho - \mathbf{d}_n) - E_{k_y} + \Delta V(\rho - \mathbf{d}_n)] \Phi_0^{\text{dot}}(\rho - \mathbf{d}_n) = 0, \quad (36)$$

where

$$\Delta V(\rho - \mathbf{d}_n) \equiv \sum_{\mathbf{d}_n} V_{\text{eff}}(\rho - \mathbf{d}_n) - \frac{m^*}{2} \omega^2 (\rho - \mathbf{d}_n)^2. \quad (37)$$

Since $\Phi_0^{\text{dot}}(\rho)$ is an eigenfunction of H^{dot} with eigenvalue $\hbar\Omega$, we have

$$\sum_{\mathbf{d}_n} C_{n_x} e^{ik_y n_y d} [\hbar\Omega - E_{k_y} + \Delta V(\rho - \mathbf{d}_n)] \langle \rho | \mathbf{d}_n \rangle = 0, \quad (38)$$

where we adopted the Dirac's notation $\langle \rho | \mathbf{d}_n \rangle = e^{-(ie/\hbar c)\mathbf{A}(\mathbf{d}_n) \cdot (\rho - \mathbf{d}_n)} \Phi_0^{\text{dot}}(\rho - \mathbf{d}_n)$.

To determine the coefficients C_{n_x} from Eq. (38), we take the internal product with the function $\langle \mathbf{d}_{n'} | \rho \rangle$

$$\sum_{\mathbf{d}_n} C_{n_x} e^{ik_y n_y d} [(\hbar\Omega - E_{k_y}) \langle \mathbf{d}_{n'} | \mathbf{d}_n \rangle + \langle \mathbf{d}_{n'} | \Delta V(\rho - \mathbf{d}_n) | \mathbf{d}_n \rangle] = 0. \quad (39)$$

The analytical expressions for the matrix elements appearing in Eq. (39) are presented in Appendix A.

In the tight-binding approximation, Eq. (39) adopts the following expression:

$$2 \cos(2\pi N_\phi n_x + k_y d) C_{n_x} + C_{n_x+1} + C_{n_x-1} = \tilde{E} C_{n_x} \quad (40)$$

with

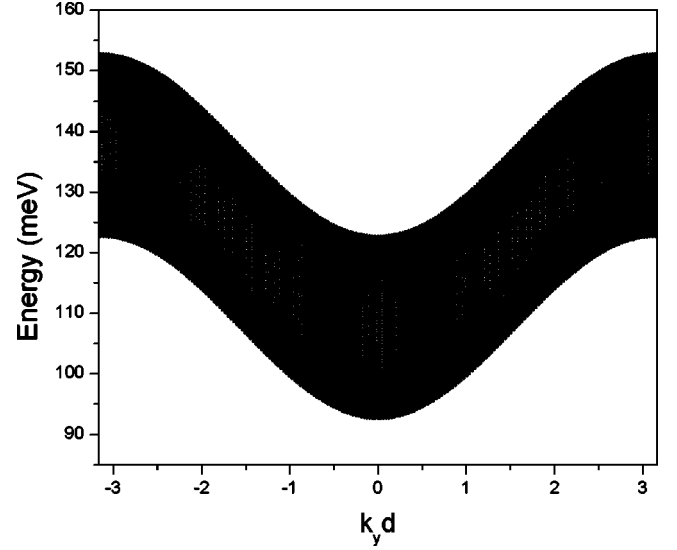


FIG. 1. Energy spectrum for the system, in the absence of external fields. $d=100 \text{ \AA}$, $l_{\text{dot}}=30 \text{ \AA}$.

$$\tilde{E} = [E_{k_y} - \hbar\Omega - E_F]/W. \quad (41)$$

The analytical expressions of the parameters W and E_F are given in Appendix B. Equation (40), which determines the nondimensional energy spectrum \tilde{E} , is Harper's equation.¹⁸

A. Results

We present results for a two-dimensional array of quantum dots with radius $l_{\text{dot}}=30 \text{ \AA}$ and lattice constant $d=100 \text{ \AA}$. For the effective mass, we assumed $m^*=0.067$, corresponding to conduction electrons in GaAs.

As a control test for the model, we calculate the energy spectrum when neither external magnetic nor electric fields are applied. For this purpose, we considered a finite size system with periodic boundary conditions, and the corresponding energy spectrum as a function of k_y is shown in Fig. 1, showing the projection of the superlattice first Brillouin zone over the y axis. The band center is located at 122.7 meV, which corresponds to the "atomic" energy $\hbar\omega$, thus recovering the expected results for a standard single-band tight-binding model. Clearly, in this last case the whole bidimensional energy surface is a function of the k_x component as well, of the form $E(k_x, k_y) = \hbar\omega + V \cos(k_x d) + V \cos(k_y d)$. However, as the model presented in this work does not involve explicitly the k_x component, its effect can be appreciated in the projected spectrum as the width of the band for a fixed value of k_y , which corresponds to $2V=30 \text{ meV}$, and the total band width which is $4V=60 \text{ meV}$.

When an external magnetic field is applied over the system, its dimensions are chosen such that commensurability with the number of magnetic flux quanta traversing the unit cell $N_\phi=p/q$ is satisfied, i.e., $L_x=L_y=mqd$. According to our previous analysis, when the number of magnetic flux quanta traversing the unit cell is a rational number $N_\phi=p/q$, a splitting of the single band spectrum into q minibands is expected. In agreement with this theoretical prediction, Fig. 2

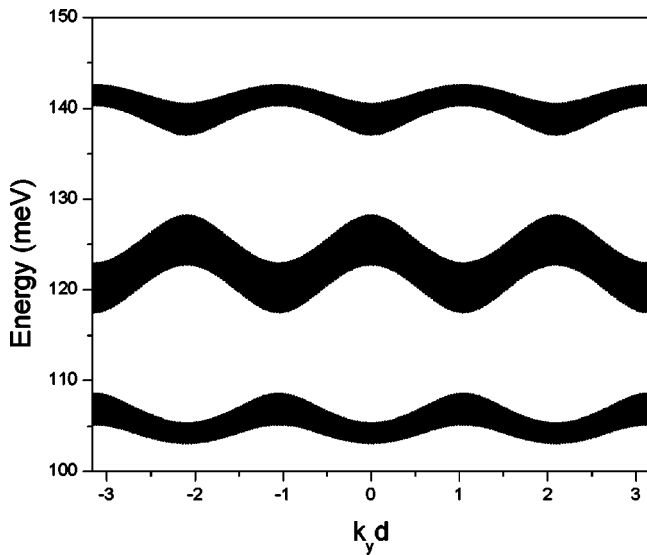


FIG. 2. Energy spectrum for the system, for a magnetic field corresponding to $N_\phi = \frac{1}{3}$. $d = 100 \text{ \AA}$, $l_{\text{dot}} = 30 \text{ \AA}$.

shows the energy spectrum as a function of k_y , when an external magnetic field equivalent to $N_\phi = \frac{1}{3}$ has been applied. By comparing with Fig. 1, one can appreciate that the single band spectrum has been split into exactly $q = 3$ subbands. It is also interesting that the effective first Brillouin zone has been reduced to $\frac{1}{3}$ of its original size, as a consequence of the already discussed magnetic translational invariance, which enlarges the effective size of the unit cell in the array by a factor of q .

The nondimensional energy spectrum, which arises as the solution of Eq. (28), is depicted in Fig. 3, as a function of the number of magnetic flux quanta which traverses the unit cell. It is the well known Hofstadter's butterfly, a fractal structure whose mathematical properties have been widely studied.¹⁶ The main assumption involved in Hofstadter's picture, is that the original band structure of the crystal is preserved, despite the presence of the external field. Therefore, he does the substitution $E(\mathbf{k}) \rightarrow E[\mathbf{k} + (e/\hbar c)\mathbf{A}]$, where $E(\mathbf{k})$ is the dis-

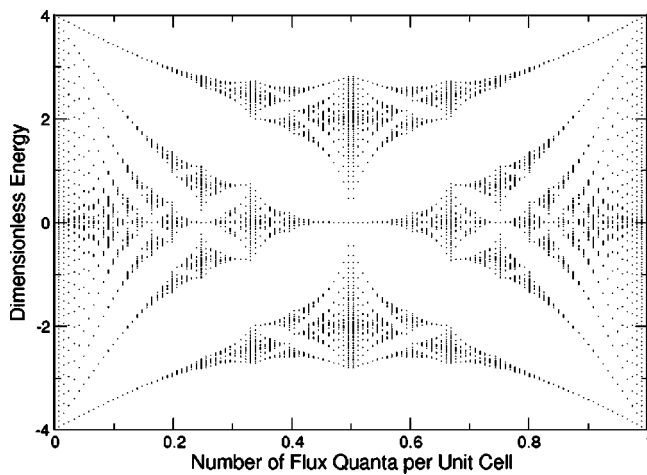


FIG. 3. Dimensionless energy spectrum, as a function of the external magnetic field intensity.

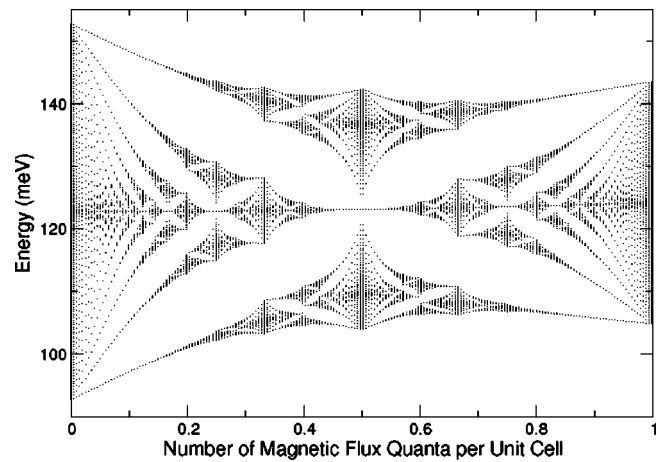


FIG. 4. Energy spectrum, as a function of the magnetic field intensity. $d = 100 \text{ \AA}$, $l_{\text{dot}} = 30 \text{ \AA}$.

persion relation for the energy band in the absence of the external field. This assumption might be justified if the magnetic field is weak, but its validity is questionable at higher intensities. In particular, as seen in Fig. 3, the butterfly is symmetric with respect to the axis $N_\phi = \frac{1}{2}$. In fact, the whole structure is periodic in the magnetic field, with period $N_\phi = 1$, as can be trivially inferred from Harper's equation. This symmetry is a characteristic of Hofstadter's approach, where the energy spectrum is scaled by a constant, that is, the energy bandwidth of the crystal at zero magnetic field.

The energy spectrum, as predicted by our model, is displayed in Fig. 4. It shows a qualitative similarity with Hofstadter's butterfly, but it does not have the magnetic field periodicity that the former possesses. This characteristic is due to the magnetic field dependence of the energy parameters W , E_F , and, in particular, of the single quantum dot energy $\hbar\Omega$. From Fig. 4, it can be observed that the effective band width diminishes as the magnetic field increases, with a slight continuous shift in the center of the band. On purely physical grounds, we argue that this behavior is qualitatively correct, due to the competence between the "geometric" confinement, characterized by the "atomic" energy $\hbar\omega$, and the magnetic confinement, characterized by the energy $\hbar\omega_c$. In this sense, as the magnetic field intensity increases, the Landau radius l_B , which characterizes the electronic semiclassical orbit length scale, decreases. Therefore, the effective confinement length scale l_0 becomes smaller than the pure geometric one, imposed by the dot radius l_{dot} . This effect decreases the overlap and hopping between nearest-neighbor wave functions, and consequently the total bandwidth is expected to diminish as the magnetic field intensity increases, according to the results shown in Fig. 4. In the limit case of an extremely high magnetic field intensity, the dot confining energy $\hbar\omega$ is expected to be a small perturbation, as compared to the magnetic energy $\hbar\omega_c$. Therefore, in this limit, the energy spectrum is expected to be well represented by Landau levels instead of dot eigenfunctions. Under this argument, one should expect for the single-band energy spectrum to continuously converge into a single Landau level, with nearly zero bandwidth, with the corresponding approximately linear dependence of the energy on the magnetic field

intensity. By means of a comparative analysis between Hofstadter's model and the one presented in this work, we conclude that the results originated by the latter show the proper physical behavior within the approximations adopted. We emphasize that the main advantage of the wave function that we propose, is that it is constructed with appropriately symmetrized combinations of "atomic" eigenfunctions of a single quantum dot, *in the presence* of the external magnetic field. Therefore, the field is not treated as a perturbation, but it is included consistently in the basis as part of the solution, such that the "atomic" energy is characterized by an effective frequency which combines both the geometric and magnetic confinement effects $\hbar\Omega = \sqrt{\omega^2 + \omega_c^2}/4$.

IV. NONZERO ELECTRIC FIELD

The effect of an external electric field, applied along the x direction, will be considered in what follows. As was previously stated, due to the Landau gauge chosen, the Hamiltonian preserves the translational symmetry along the y direction, even when the electric field is present. This property allows us to preserve the general structure of the basis functions previously introduced, showing the advantage of the gauge chosen to solve the general problem. The translational symmetry along the x direction is evidently broken by the presence of the external electric field. However, by considering discrete translations along the x direction, an interesting periodicity property of the energy density of states, related to the Stark period, can be shown as follows.

As translational invariance along the y direction is preserved, the wave-vector component k_y is still a good quantum number for the system, such that eigenfunctions and energy eigenstates are still characterized by fixed values of k_y

$$H_{||}(\rho)\Psi_{k_y}(\rho) = E_{k_y}\Psi_{k_y}(\rho). \quad (42)$$

The corresponding eigenvalue equation for the periodic function u_{k_y} is

$$\left[\frac{\left(\mathbf{p}_\rho + \hat{\mathbf{y}}\hbar k_y + \frac{e}{c}\mathbf{A}(\rho) \right)^2}{2m^*} + \sum_n V_{\text{eff}}(\rho - \mathbf{d}_n) + eFx \right] u_{k_y}(\rho) = E_{k_y} u_{k_y}(\rho). \quad (43)$$

Let us apply a discrete translation $T_{\hat{\mathbf{x}}qd}$ to the previous equation. The resulting expression, after a slight rearrangement is

$$\left[\frac{\left(\mathbf{p}_\rho + \hat{\mathbf{y}}\hbar \left(k_y + \frac{2\pi q}{d} N_\phi \right) + \frac{e}{c}\mathbf{A}(\rho) \right)^2}{2m^*} + \sum_n V_{\text{eff}}(\rho - \mathbf{d}_n) + eFx \right] u_{k_y}(\rho + \hat{\mathbf{x}}qd) = (E_{k_y} - qeFd) u_{k_y}(\rho + \hat{\mathbf{x}}qd). \quad (44)$$

As was previously pointed out, if the number of flux quanta which traverses the lattice unit cell is a rational num-

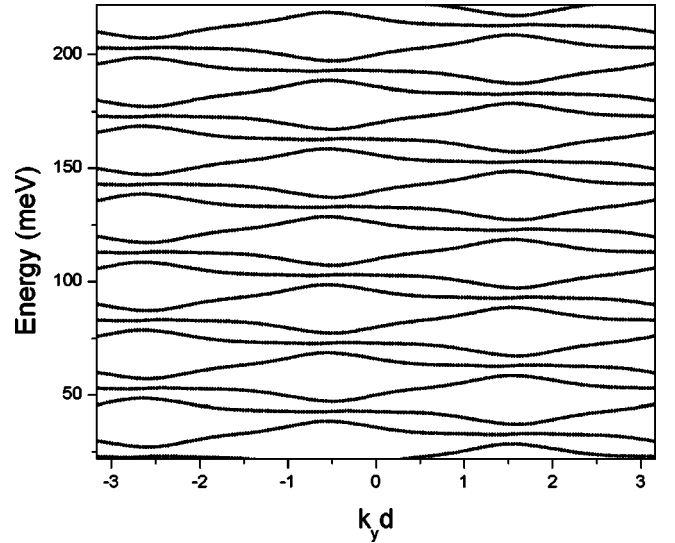


FIG. 5. Energy spectrum for the system, for a magnetic field corresponding to $N_\phi = \frac{1}{3}$, when an electric field of $F = 10$ KV/cm is also applied. $d = 100$ Å, $l_{\text{dot}} = 30$ Å.

ber, for instance, $N_\phi = p/q$, then $\bar{k}_y = k_y + (2\pi q/d)N_\phi$ is associated to the same magnetic Bloch function as k_y , as a consequence of the translational symmetry along the y direction, which is preserved even in the presence of the electric field. Therefore $E_{\bar{k}_y} = E_{k_y}$, and the eigenvalue equation (44) can be written as

$$\left[\frac{\left(\mathbf{p}_\rho + \hat{\mathbf{y}}\hbar \bar{k}_y + \frac{e}{c}\mathbf{A}(\rho) \right)^2}{2m^*} + \sum_n V_{\text{eff}}(\rho - \mathbf{d}_n) + eFx \right] \times u_{k_y}(\rho + \hat{\mathbf{x}}qd) = (E_{k_y} - qeFd) u_{k_y}(\rho + \hat{\mathbf{x}}qd). \quad (45)$$

The conclusion is that, if E_{k_y} is an eigenvalue belonging to the electronic spectrum, then $E_{k_y} - qeFd$ is another eigenvalue corresponding to the same value of k_y . Notice that this result states that the presence of the magnetic field, combined with the electric field, modifies the Stark period by a factor q , for rational magnetic fields where $N_\phi = p/q$.

Under the same assumptions which lead to Eq. (40), the presence of the external electric field modifies the finite differences equation for the coefficients in the form

$$[2 \cos(2\pi N_\phi n_x + k_y d) - n_x \tilde{F}] C_{n_x} + C_{n_x+1} + C_{n_x-1} = \tilde{E} C_{n_x}, \quad (46)$$

where $\tilde{F} = eFd/W$ and \tilde{E} is defined as before.

A. Results

The effect of an external field of $F = 10$ KV/cm, produces a rich structure in the energy spectrum of the quantum dots lattice, as shown in Fig. 5. For $N_\phi = p/q$ rational, the spectrum is periodic in a multiple q of the Stark energy eFd , for a fixed wave number k_y . In the system represented by Fig. 5, $q = 3$ and the energy period for a fixed k_y is 30 meV, which is

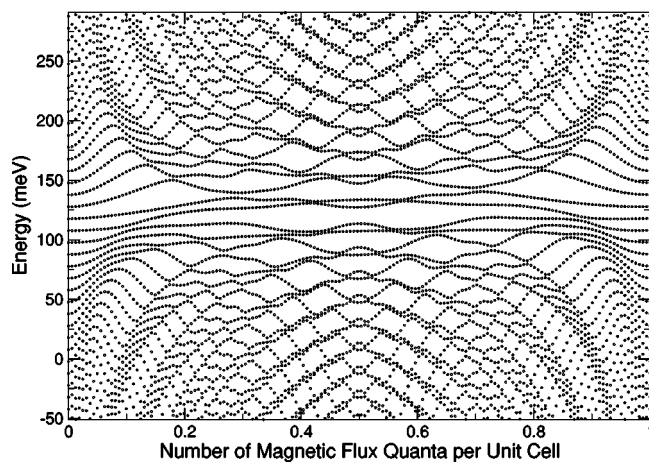


FIG. 6. Energy spectrum, as a function of the external magnetic field intensity, when an external electric field $F=10$ KV/cm is also applied. $d=100$ Å, $l_{\text{dot}}=30$ Å.

exactly three times the Stark energy $eFd=10$ meV. It is also found that for each energy value associated to one particular k_y , there exists another energy value in the spectrum, which is associated to $k'_y=k_y-G_y$, with $G_y=2\pi/qd$, which is shifted by the normal Stark period eFd .

The energy spectrum as a function of the number of magnetic flux quanta traversing the unit cell, when an electric field of $F=10$ KV/cm is applied over the system, is depicted in Fig. 6, for a fixed value of $k_y=0$. An expanded region near the center of the band is shown in detail. The modified Stark period, as before, can be appreciated in the spectrum for rational values of the number of magnetic flux quanta piercing the unit cell.

V. CONCLUSIONS

In summary, we have studied the energy spectrum of electrons in a two-dimensional lattice of quantum dots, subject to a perpendicular magnetic field and an electric field in the plane, applied along one of the symmetry directions of the array. We introduced a method to construct appropriately symmetrized, Bloch-like wave functions, which includes the magnetic field in the “atomic” orbitals. Therefore, the magnetic field is not treated as a perturbation to the band structure, but it is included in the spectrum calculations in a self-consistent way. Within a single-band approximation, we compared our results at zero electric field with the classical Hofstadter’s model, and show that our method leads to the appropriate physical behavior.

The external electric field is not included in the wave functions, so its effects are calculated by direct diagonalization of the Hamiltonian. As we adopted a single-band approximation, our results are expected to be valid for weak electric field intensities, when no interband coupling occurs.

Despite the approximations involved in this preliminary work, i.e., tight-binding and single-band “atomic” orbitals, the proposed method for constructing magnetic Bloch-like wave functions in the Landau gauge is fairly general. Therefore, it is straightforward to generalize it to perform multi-

band calculations, to be valid for a wide range of electric and magnetic field intensities. Coulomb interactions may be also included in the model, in particular to calculate the excitonic spectrum of the system.

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APPENDIX A

If the condition $N_\phi=p/q$ is satisfied, the term associated to the vector magnetic potential in the phase of Eq. (18) adopts the form

$$\frac{e}{\hbar c}A_y(\mathbf{d}_n) = \frac{2\pi N_\phi n_x}{d} = \frac{2\pi p}{d}n_x \frac{p}{q}.$$

Now, consider a translation of the periodic function (18) along the x direction, in a lattice vector $\mathbf{d}_{m_x}=\hat{x}m_xd$:

$$\begin{aligned} u_{k_y}(\rho + \mathbf{d}_{m_x}) &= \sum_{n_x} \sum_{n_y} \exp\left(-i\left[k_y + \frac{2\pi p}{d}n_x\right](y - n_yd)\right) \\ &\quad \times C_{n_x}W(\rho + \mathbf{d}_{m_x} - \mathbf{d}_n) \\ &= \sum_{\bar{n}_x} \sum_{n_y} \exp\left(-i\left[k_y + \frac{2\pi p}{d}(\bar{n}_x + m_x)\right]\right. \\ &\quad \left.\times (y - n_yd)\right) C_{\bar{n}_x+m_x}W(\rho - \mathbf{d}_{\bar{n}}). \end{aligned}$$

In the former equation, if $m_x=q$, then the y component of the quasimomentum k_y appearing in the phase can be replaced by $\bar{k}_y=k_y+(2\pi/d)p$, which is a consequence of the translational symmetry along the y direction. However, \bar{k}_y must define the same magnetic Bloch function as k_y , except for a possible constant phase

$$u_{k_y}(\rho + \mathbf{d}_q) = e^{i\alpha_q}u_{\bar{k}_y}(\rho)$$

provided that the condition $C_{\bar{n}_x+q}=e^{i\alpha_q}C_{\bar{n}_x}$ is satisfied.

APPENDIX B

The matrix elements appearing in Eq. (39) are given by

$$\langle \mathbf{d}_{n'} | \mathbf{d}_n \rangle = e^{i2\pi N_\phi(n'_x+s/2)r} A_{r,s}$$

and

$$\begin{aligned} \langle \mathbf{d}_{n'} | \Delta V(\rho - \mathbf{d}_n) | \mathbf{d}_n \rangle &= \frac{\hbar\Omega}{2} \left(\frac{l_{\text{dot}}}{l_0}\right)^4 e^{i2\pi N_\phi(n'_x+s/2)r} A_{r,s} \\ &\quad \times [B_{r,s} - 1 - D_{r,s}], \end{aligned}$$

where $r=n_y-n'_y$, $s=n_x-n'_x$ and

$$A_{r,s} = e^{-(r^2+s^2)/4[(d/l_0)^2+(\pi N_\phi l_0/d)^2]},$$

$$B_{r,s} = e^{-(s^2/4)(\pi N_\phi l_0/d)^2} \Xi^{(s)} \left(\frac{d}{l_0}, \frac{\pi N_\phi l_0 r}{d} \right) \\ + e^{-(r^2/4)(\pi N_\phi l_0/d)^2} \Xi^{(r)} \left(\frac{d}{l_0}, \frac{\pi N_\phi l_0 s}{d} \right), \\ D_{r,s} = \frac{r^2 + s^2}{4} \left[\left(\frac{d}{l_0} \right)^2 - \left(\frac{\pi N_\phi l_0}{d} \right)^2 \right].$$

The function $\Xi^{(i)}(x,y)$ is given by

$$\Xi^{(i)}(x,y) = \begin{cases} \sum_m \int_{(m-1/2)x}^{(m+1/2)x} du (u - mx)^2 e^{-u^2} \cos yu, & i \text{ even,} \\ \sum_m \int_{(m-1)x}^{mx} du [u - (m - 1/2)x]^2 e^{-u^2} \cos yu, & i \text{ odd.} \end{cases}$$

The matrix elements corresponding to the electric field contribution are given by

$$\langle \mathbf{d}_{n'} | eFx | \mathbf{d}_n \rangle = (eFd) e^{i2\pi N_\phi (n_x + s/2)r} \\ \times A_{r,s} \left[n_x + \frac{s}{2} + i \frac{\pi N_\phi r}{4} \left(\frac{l_0}{d} \right)^2 \right].$$

The parameters W and E_F are defined as

$$W = \frac{\hbar\Omega}{2} \left(\frac{l_0}{l_{\text{dot}}} \right)^4 A_{1,0} [B_{1,0} - 1 - D_{1,0}],$$

$$E_F = \frac{\hbar\Omega}{2} \left(\frac{l_0}{l_{\text{dot}}} \right)^4 [B_{0,0} - 1].$$

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