Electron Locking In Semiconductor Superlattices

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Abstract

We describe a novel state of electrons and phonons arising in semiconductor superlattices (SSL) due to strong electron-phonon interactions. These states are characterized by a localization of phonons and a self-trapping or locking of electrons in one or several quantum wells due to additional, deformational potential arising around these locking wells in SSL. The effect is enhanced in a longitudinal magnetic field.

Using the tight-binding and adiabatic approximations the whole energy spectrum of the self-trapped states is found and accurate, analytic expressions are included for strong electron-phonon coupling. Finally, we discuss possible experiments which may detect these predicted self-trapped states.

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Modern technology allows materials and structures with narrow bandwiths to be created. One example of such a structure is the semiconductor superlattice which can be manufactured in such a way that it can consist of different numbers of layers of differing thicknesses. In SSL consisting of say, for example, a sequence of layers of $GaAs$ and $Ga_xAl_{1-x}As$, an electron miniband of width t may be created, where t is the overlapping integral for an electron localized in neighboring quantum wells. The number of levels in this miniband depend on the number of layers the SSL consists of. For example, if the superlattice consists of two quantum wells, there are only two levels associated with the symmetrical and antisymmetric wave functions. For each energy level, the probability to find the electron in either well is equally distributed. The same is true when there are many levels in the miniband. However, the situation changes dramatically if electron-phonon interactions are considered. The effect of this interaction may give rise to coupled electrons and phonons where the dimensionless electron-phonon coupling constant of this system is inversely proportional to t. Since the miniband width, in SSL, is between 1 - 100 meV the electron-phonon coupling is strongly

intensified in comparison with the conventional bandwidth which is about 1 eV. Such an intensification in the electron-phonon interaction in narrow band structures may give rise to some novel, self-trapped states of the electron.

This phenomenon of the self-trapping of electrons and excitons in solids, originally predicted theoretically[1–5], has been observed and well studied in many materials (see, for example, review[4]). It arises, primarily, in low dimensional systems and in systems with a strong electron-phonon interaction.

The SSL is a new system where the effective electron-phonon coupling may become large, especially when a longitudinal magnetic field is applied. This can give rise to the locking of an electron in some wells with the creation of novel self-trapped states. The number of such states depend on how many layers the SSL consists of and how strong the electron-phonon interactions are, ie the narrowness of the miniband. The structure of these states is associated with a localization pattern. This pattern indicates where the electron is localized, ie, in which wells the electron is locked in.

The system can be described in the framework of a 1D tight-binding model. If the interaction of the electron with acoustic phonons is considered then the Schrödinger equation takes the form:

$$-\frac{\Delta\psi_n}{2m_\perp} - t\psi_{n-1} + 2t\psi_n - t\psi_{n+1} + DQ_n\psi_n = E\psi_n \tag{1}$$

where $\Delta = \partial^2/\partial x^2 + \partial^2/\partial y^2$ is a two dimensional Laplacian associated with the electron motion inside the planes of the quantum wells, $m_\perp$ is the effective, transverse mass of the electron, $\psi_n(x, y)$ is the wave function for an electron located in the n^{th} quantum well and D is a constant of the deformation potential which depends on the material the SSL is made up of. Note that deformations along all 3 coordinate axes have been included because $Q_n = \nabla.\mathbf{u} = \partial_x u_x + \partial_y u_y + \partial_z u_z$ where $\mathbf{u_n} = (u_{nx}, u_{ny}, u_{nz})$ is a vector of atomic displacements in the n^{th} quantum well. Thus, Q_n includes deformations in the x, y and z directions.

Using the adiabatic approximation, in which the lattice moves slowly in comparison with the electrons (because of the large mass of atomes M_a and small, effective mass $m_e = \hbar^2/ta^2$ of the electrons), the kinetic energy of the lattice with the parameter $m_e/M_a \to 0$ is zero. The adiabatic self-trapped states are associated with the stationary points of the adiabatic potential. In other words employing the adiabatic parameter (the ratio of electron and atomic masses $m_e/M_a << 1$) following Pekar[1] we consider different **static** deformations of the lattice and the localized electron states created by these deformations. Extreme (or critical) points of this adiabatic surface are self-trapped states.

Traditionally, adiabatic self-trapping has only been studied in continuum models[5] applicable to localized states with a large radius (in comparison to the lattice spacing), except, of course, the exciton self-trapping in rare gas solids[4]. The same is true for studies of the interaction of an electron with polar phonons (polarons), where the adiabatic Pekar type polarons have a large radius. Anti-adiabatic (or non-adiabatic) polarons with a small radius have also been intensively investigated[6]. However, the anti-adiabatic limit is completely the opposite to the adiabatic limit discussed in our paper. In the adiabatic approximation, the adiabatic potential J, consisting of the electron energy E and the elastic energy of the lattice $E_{el} = K\sum_n Q_n^2/2$, is given by

$$J = \int d^2x[\sum_n \frac{|\nabla\psi_n|^2}{2m_\perp} + t\sum_n |\psi_n - \psi_{n+1}|^2$$
$$+D\sum_n Q_n|\psi_n|^2 + K\sum_n \frac{Q_n^2}{2}] \quad (2)$$

The lowest energy self-trapped states correspond to a wave function which is homogeneous in the transverse direction $\psi_n(x,y) = \psi_n$ and is a true solution of the above equation. Then the equations describing the self-trapped states are obtained by minimization of J with respect to ψ_n and Q_n provided that $\sum_n \int d^2x|\psi_n|^2 = 1$ (see, for example,[4,5]). Doing so, ie by a minimization of J with respect to Q_n, gives $Q_n = -\frac{D}{K}|\psi_n|^2$, where K is the modulus of elasticity of the lattice. Substituting for $Q_n(\psi_n)$ in eq. (1), (2), respectively, gives the nonlinear Schrödinger equation (NSE)

$$-\psi_{n-1} + 2\psi_n - \psi_{n+1} - c|\psi_n|^2\psi_n = E\psi_n \quad (3)$$

and the corresponding expression for the adiabatic potential

$$J = \sum_n |\psi_n - \psi_{n+1}|^2 - \frac{c}{2}\sum_n \mid \psi_n \mid^4 \quad (4)$$

where $c = D^2/tK$ is the dimensionless electron-phonon coupling constant and E and J are measured in units of the miniband width t. The normalization condition is $\sum_n \mid \psi_n \mid^2 = 1/L^2$, where L^2 is the area of the transverse plane of the SSL (assuming it is a square of side L). It is convenient to make the scaling transformation $\psi_n \to \psi_n/L$. This transformation does not alter the form of the equations but it does give the conventional normalization condition for the new wave function $\sum_n \mid \psi_n^2 \mid = 1$. However, the coupling constant does change so that $c_{new} = c_{old}/L^2$. In a longitudinal magnetic field the continuum transverse spectrum of the miniband is split into Landau levels. For strong magnetic fields only the first Landau level is relevant. The electron on this level is localized in a transverse direction in an area of the order of l_B^2, where l_B is a magnetic length, such that, $l_B^2 = C\hbar/eB$ (L and l_B are measured in units of the SSL period d). Then the electron motion is only one dimensional along the direction of the magnetic field through the SSL. The coupling constant then transforms to $c_{new} \to c_{old}/l_B^2$. Thus, **with the increase of the longitudinal magnetic field, the phonon coupling constant can be strongly enhanced**.

To illustrate, consider some examples having exact solutions. The simplest is a double well structure. For a large coupling constant, $c \gg 1$, there arises the trapping of the electron in one of the two wells. The eigenvalue of this state is $E = 2 - c$ and the corresponding eigenvectors are: $\psi_1 = \frac{\sqrt{1\pm\alpha}}{\sqrt{2}}$ and $\psi_2 = \frac{\sqrt{1\mp\alpha}}{\sqrt{2}}$ where $\alpha = \sqrt{1 - \frac{A}{c^2}}$, where $A = 16$ or $A = 4$ for periodic (PBC) or open boundary conditions, respectively. These states are two-fold degenerate.

Another straight-forward example, studied analytically, consists of three superlattice layers or three quantum wells. The ground state is characterized by the localization of the electron in a single quantum well in the same manner as in the double well structure. For PBC with an increase in the value of c this state very rapidly saturates to the limit $\{\psi_1, \psi_2, \psi_3\} \Rightarrow \{0,1,0\}$ or $\{0,0,1\}$ or $\{1,0,0\}$. These three states are degenerate due to the translational symmetry associated with PBC and corresponds to the ground state energy

which in the limit $c \to \infty$ takes the simple form $E = 2 - c$, ie the same as the double well structure. There is also an excited self-trapped state, which, for $c \gg 1$, has the (degenerate) structure $\{\psi_1, \psi_2, \psi_3\} \Rightarrow \{1/\sqrt{2}, 0, 1/\sqrt{2}\}$ or $\{1/\sqrt{2}, 1/\sqrt{2}, 0\}$ or $\{0, 1/\sqrt{2}, 1/\sqrt{2}\}$. This state corresponds to the eigenvalue $E = 1 - \frac{c}{2}$ and the region of this self-trapped localization is two neighboring wells. There is also another self-trapped state in this system, which arises for very large values of c. This state has the eigenvalue $E = 3 - \frac{c}{2}$ and the associated structure has the form $\{\psi_1, \psi_2, \psi_3\} \Rightarrow \{\frac{1}{\sqrt{2}}, \frac{-1}{\sqrt{2}}, 0\}$ or analogous cyclic permutations of this pattern. An exact solution, valid for all values of c, has also been found, however, it does not appear to have a simple form. Consequently, the exact solutions are presented graphically in Fig.1. The self-trapping states emerge for values of the coupling constant, $c > 3$. From this figure it is clear that the solutions obtained in the limit $c \to \infty$ describe the spectrum of the triple quantum well structure very accurately. The first corrections to the presented eigenvectors are of order $1/c$.

Without PBC the translational invariance is broken and the degeneracy is lifted so that the number of energy levels increases. The exact spectrum for the triple quantum well structure, without PBC, is presented in Fig. 2. These new levels may also be described analytically for $c \gg 1$. A new eigenvalue, $E = 2 - \frac{c}{2}$ appears, which is associated with the localized self-trapped solution $\{\frac{1}{\sqrt{2}}, 0, \frac{\pm 1}{\sqrt{2}}\}$. Additional eigenvalues, which also satisfy the NSE, include $E = \frac{2-c}{3}, \frac{6-c}{3}, \frac{10-c}{3}$. These eigenvalues are associated with states where the electron is localized in each of the quantum wells with equal probabilities. Again, for nearly all values of coupling constant c, the amazing coincidence between the spectra obtained for $c \gg 1$ and the exact result shown in Fig.2 is seen.

From the examples discussed above, it is noticed that in the limit $c \to \infty$, the spectrum has some special features associated with the pattern of the localized states. The spectrum depends on how large the set of localizing quantum wells is and how many spots (groups of neighboring, localizing quantum wells) this set is separated into. The lowest eigenvalue always has the form $E = 2 - c$ and is associated with the localization of the electron in a single quantum well. The next eigenvalue, $E = \frac{(2-c)}{2}$, is associated with the localization of the electron in a single spot consisting of two neighboring quantum wells. However, when the localization occurs in two separate quantum wells, so that there are two spots each consisting of one well, the energy eigenvalue is $E = \frac{(4-c)}{2}$. With the localization of the electron in three quantum wells the associated eigenvalue may be written as $E = \frac{2-c}{3}$.

This observation can be used to derive exact solutions associated with an arbitrary localization pattern of an electron in SSL consisting of N quantum wells. Initially, in the zero approximation with parameter $c \gg 1$, assume that the electron is localized in a single quantum well of a $N-$well SSL, say the k^{th} well, so that $|\psi_k|^2 = 1$ and $|\psi_n|^2 = 0$ for all possible $n \neq k$. Upon making this substitution into the NSE and after some algebraic manipulation, we see that this substitution corresponds to a solution with the eigenvalue $E = 2-c$. Similarly, if it is assumed that the electron is localized in two neighboring quantum wells, say, the k^{th} and $(k+1)^{th}$, and we substitute into the NSE $\psi_k = \frac{1}{\sqrt{2}}$, $\psi_{k+1} = \frac{1}{\sqrt{2}}$ and $\psi_n = 0$ for $n \neq k, n \neq k+1$ then (after some algebra) the eigenvalue $E = \frac{2-c}{2}$ is obtained. For the localization of the electron in 3 neighboring wells, we make the substitution $\psi_k = \psi_{k+1} = \psi_{k+2} = \frac{1}{\sqrt{3}}$ and $\psi_n = 0$ for all other wells. This then yields $E = \frac{2-c}{3}$. Repeating the same procedure for the electron localized in n neighboring wells, we derive the eigenvalue $E = \frac{2-c}{n}$.

The same procedure may be applied for an electron localized in two separate spots, consisting of, say, n_1 and n_2 quantum wells. Surprisingly, we find that in this case, $E = \frac{(4-c)}{n}$, where $n = n_1 + n_2$. If this localization occurs in m distinct spots, and each spot consists of $n_1, n_2, \ldots, n_m$ neighboring quantum wells, the associated eigenvalue is $E = \frac{(2m-c)}{n}$, where $n = n_1 + n_2 + \ldots + n_m$.

However, this is still not a complete set of solutions. Note that if the electron is localized in a spot consisting of $n_1 = 2n_0$ neighboring quantum wells, then the wave function may change sign for the different quantum wells of this spot. For example, if for the first n_0 neighboring quantum wells the wave function has a positive sign and for the remaining n_0 wells the wave function is negative, then the associated eigenvalue is $E = \frac{2m+4-c}{n}$. In general, if the wave function changes sign l times in one or several localized spots the energy eigenvalue of the NSE takes the form

$$E = \frac{2m + 4l - c}{n} \tag{5}$$

where n is the total number of quantum wells in which the electron is localized. Note that, in each localizing quantum well the electron is localized with equal probability, $\psi_k^2 = 1/n$ for all numbers k associated with localizing quantum wells. This probability does not depend on the number of spots, m, the localization area is separated into. The number n may take any integer value $n = 1, 2, 3, \ldots, N$. The number m may take any integer value satisfying $m \leq n$. Similarly, the number l satisfies $l \leq n - 1$.

Eq. (5), obtained in the limit $c \to \infty$, has been compared with the exact solutions for systems consisting of up to 5 quantum wells, in the same manner as for the triple quantum well structure. Also a comparison has been made between energy spectra obtained from equation (5) and corresponding eigenvectors and energy eigenvalues from numerical calculations for SSL consisting of up to 11 quantum wells. In all these cases for nearly all values of c (except small regions of critical values where the self-trapped solutions originate) there is perfect agreement with the derived formula (5). However, in contrast with this perfect agreement between eigenvalues, a decrease in the value of c leads to a noticable deviation in the wave functions (eigenvectors) from those obtained in the limit $c \to \infty$. The first order corrections to the presented eigenvectors obtained with the use of perturbation theory is of the order of $\sqrt{n}/c$. When the coupling constant c is not very large the wave functions of some states may have interesting incommensurate and chaotic structures. The detailed analysis of such wave functions will be published elsewhere[7]. Thus, from the comparison with numerical results and with perturbation theory we conclude, that even though the spectrum of the NSE for the system with a finite, arbitrary number of wells N is well described by equation (5) the shape of appropriate wave functions for smaller values of c may have only qualitative features of the appropriate eigenvectors obtained in the limit $c \to \infty$. As c decreases the localization spots smear out and the boundaries between localizing quantum wells and quantum wells where the wave function vanishes diminish.

In general, for large ranges of the values of c the eigenvalue E_{lmn} corresponds to the state of an electron which is self-trapped or localized with near equal probability in n wells which are separated into m groups (spots). Between the spots the electron wave function is nearly vanishing while inside these spots the wave function changes sign l times, although its amplitude is nearly the same. Since the spectrum, eq.(5), is associated with a local localization pattern, it is universal and does not depend on the boundary conditions.

The eigenvalues E_{nml} are electron energies created in SSL by local deformations. Therefore, it is interesting to estimate an adiabatic potential, $J_{nml} = E_{nml} + E_{el}$, needed to create these states. With the use of the method described above the following expression for the adiabatic potential is obtained,

$$J_{nml} = \frac{4m + 8l - c}{2n} \tag{6}$$

For comparison, a state associated with the bottom of the miniband shifted by electron-phonon interaction corresponds to an adiabatic potential $J_{bs} = -c/(2N)$. For a single localization spot with no change in the sign of the wave function, $l = 0$ and $m = 1$ are substituted into (6). This corresponds to the lowest value of adiabatic potential for all values of n. From these equations one sees that for strong coupling, $c \gg 1$, there are always self-trapped states which have a lower adiabatic potential than analogous miniband states, ie $J_{110} < J_{bs}$. However, the states with very wide spots may have $J_{n10} > J_{bs}$. This will occur when the size of the spot, n, becomes larger than some critical value $n_c = N(c-4)/c$. The presence of these states (with $J_{n10} > J_{bs}$) indicates that the self-trapped states associated with the quantum numbers $n < n_c$ and the band states are separated by a self-trapped barrier, which appears only because of the lattice discreteness and finite size of the system. The self-trapping arises for a critical coupling equal to $c_{crit} = 4N/(N-1)$. In the continuum 1D case the self-trapped barrier is absent although the critical coupling for the self-trapping does exist and depends on the size of the system[8]. The self-trapped barrier exists only in the continuum 3D case, as was first discovered by Rashba[2,4].

Thus, we have described a new phenomenon of the self-organized, deformational creation of single, double, triple and in general, multiple quantum well structures in SSL with an electron locked inside. This is a local effect which depends on how many wells the SSL consists of (but exists for any number of wells) and on how perfect the SSL is. It may, therefore, be readily observed in experiments. The states with the spectrum as described by equation (5) may be detected, for example, by resonant tunneling experiments or by absorption of light. Each self-trapped state associated with different quantum numbers n, m, l will give rise to an absorption peak which lies below the miniband and is well described by equation (5). However, as the self-trapped states are associated with deformations, which maintain the localization, the main absorption of light (which follows the Franck-Condon principle) will be associated with the miniband. Since the creation of the self-trapped states takes less energy than the creation of the band states (see equation (6)), after absorbing radiation, the electrons excited at the absorption of light inside the miniband then may be self-trapped. The emission of radiation from these states will directly indicate their presence. The creation of excitons from these states is an interesting issue.

Another interesting feature of the self-trapped (or locked) states in SSL is their strong interaction with phonons or with ordinary sound waves. Each of the localizing spots of a self-trapped state is created by deformation and therefore also associated with the phonon localisation. Since inside the spot the deformation $\sim 1/n$ and vanishes outside then each spot may be viewed as a sound wave resonator. The resonant frequency and the wavelength of this resonator is related to the size of the spot. For example, for the spot consisting of n_i quantum wells the size is $n_i d$ (note that d is a period of SSL and $\sum_i n_i = n$). Then the resonance wavelength will be $\lambda = n_i d$ and the phonons with the wavevector $2\pi/(n_i d)$ will be

especially strongly scattered or trapped by the localizing spot. Based on this fact one may suggest the following scenario for experiments. When a sound wave moving through a SSL passes the self-trapped spot there will be a transfer of momentum from the sound wave to the spot. As a result of this scattering, the acoustic phonons with wave vector $q = 2\pi/(n_i d)$ will be absorbed forcing the self-trapped spot to propagate through the lattice. Such motion may give rise to the creation of current induced by sound.

Alternatively, if a bias voltage is applied to the SSL, creating a current, a constant backflow of appropriate phonons will be created. This backflow of selective phonons will be especially strong at some bias voltages equal to the interlevel spacing. Therefore, they may be observed as some minima in the current voltage characteristics of the SSL in a high magnetic field. This effect may exist only at low temperatures when there are no current carriers in the miniband. Otherwise, in doped SSL or at high temperatures the transport will be of the Bloch type. Since the number of self-trapped states increases with the total number of quantum wells in the SSL it is expected that the proposed effect will be stronger in SSL with larger numbers of quantum wells. Since the described effect of the locking of an electron in quantum wells is caused by acoustical phonons it is universal and should not depend on what material the SSL consists of. Recently we have become aware that a similar effect has been seen by L. Eaves[9] group.

In summary we have described novel, self-trapped states of an electron associated with the self-organized, deformational creation of single, double and multiple quantum wells which lock the electron in SSL. The exact energy spectrum associated with these states for a strong electron-phonon interaction, $D^2/(Kt) \gg 1$, or for a strong longitudinal magnetic field is derived. The novel states associated with local deformations have very different properties from the conventional band states and therefore may give rise to some new effects like, for example, the creation of an electric current by sound. Alternatively, such states stimulate sound absorption and prevent phonon propagation. This may give rise to unusual thermopower in SSL.

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Figure Caption

Fig. 1 The dependence of energy spectrum on the electron-phonon coupling constant c for a triple quantum well structure obtained assuming PBC. The lines of the spectrum correspond to (from bottom up on left hand side) the eigenvalues $E = 2-c$, $E = (2-c)/2$, $E = (6-c)/2$, $E = -c/3$ and $E = (8-c)/3$.

Fig. 2 The same as in Fig.1 for a triple quantum well structure obtained without assumption of PBC. The lines of the spectrum correspond to (from bottom up on LHS) the eigenvalues $E = 2-c$, $E = (2-c)/2$, $E = (4-c)/2$, $E = (6-c)/2$, $E = (2-c)/3$, $E = (6-c)/3$ and $E = (10-c)/3$.

Fig 1: Spectrum For 3 Quantum Wells