Complete quantum confinement of one-dimensional Bloch waves

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An analytical solution is given for the complete quantum confinement of one-dimensional Bloch waves in an inversion-symmetric potential. The energy spectrum of the confined Bloch states maps the energy bands exactly. For each band gap, the energy of one band-edge state does not change as the confinement length L changes. Only the energy of the other band-edge state changes and might be described by the effective-mass approximation.

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The quantum confinement is one of the most fundamental problems in low dimensional physics. A clear understanding of the physics on the quantum confinement of Bloch waves in low dimensional systems could be both theoretically very interesting and practically very important.[1] Although the quantum confinement of plane waves has been treated in almost any standard quantum mechanics textbook, theoretical investigations on the quantum confinement of Bloch waves were usually based on approximated and/or numerical approaches. The complete confinement is the simplest but also the most fundamental quantum confinement.[2] A clear understanding of the complete confinement is the basis for understanding of all other not-so-complete confinements. In this work, we give an analytical solution of the complete quantum confinement of one-dimensional Bloch waves in an inversion-symmetric potential, based on an early paper of Kohn[3] and a mathematical theorem on the Bloch functions.[4] It is found that the approximate correspondence between the bulk energy dispersion and quantum-confined energy levels noted previously by many authors[5–7] is in fact an exact correspondence for a fairly broad class of one-dimensional potentials. It also shows that the existence of confined states[5,8] whose energy is independent of the confinement length is quite general, relying on the symmetry of the periodic potential.

One-dimensional Bloch waves in an inversion symmetric potential are the solutions of Schrödinger differential equation[3]

$$H_0\phi_n(k,x)=\varepsilon_n(k)\phi_n(k,x), \tag{1}$$

where

$$H_0=-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+v(x), \quad -\infty<x<\infty \tag{2}$$

and

$$v(x+a)=v(x),$$
$$v(-x)=v(x). \tag{3}$$

We assume Eq. (1) is solved, and all energy bands $\varepsilon_n(k)$ and Bloch functions $\phi_n(k,x)$ are known. Following Kohn,[3] we assume that the energy bands do not intersect, and there are energy gaps between energy bands. The band-edge states are located at either $k=0$ or $k=\pi/a$. Due to Eq. (3), a band-edge state has a specific parity for an inversion $x\to -x$. A noteworthy point is that a band-edge state also has a specific parity for an inversion relative to $x=a/2$.[9] For the band-edge states at $k=0$, the parity does not depend on the selection of the inversion center: They are the same for either $x=0$ or $x=a/2$ to be the inversion center. However, for the band-edge states located at $k=\pi/a$, the parity does depend on the selection of the inversion center.[9] For simplicity, we assume that there is only one lowest periodic potential minimum in the interval $[0,a)$.[10] To be specific, in this work the bulk parity of a band-edge state means the parity for an inversion relative to one of these periodic potential minimum locations (PPML's).

We consider the Bloch states confined in the region $-L/2\leqslant x\leqslant L/2$ and are interested in the case where the confinement length

$$L=Na,$$

here N is a positive integer. $\pm L/2$ are located $a/2$ away from the nearest PPML.[11]

For the complete quantum confinement of Bloch waves, we look for the the eigenvalues E and eigenfunctions $\psi(x)$ of the following equation:

$$H\psi(x)=E\psi(x). \tag{4}$$

Here

$$H=H_0+V, \tag{5}$$

where H_0 is defined in Eq. (2) and

$$\begin{aligned} V&=0 \quad \text{if } -\frac{L}{2}<x<\frac{L}{2} \\ &=+\infty \quad \text{if } x\leqslant -\frac{L}{2} \text{ or } x\geqslant \frac{L}{2}. \end{aligned}$$

is the confinement potential. Thus all eigenfunctions of Eq. (4) must have

$$\psi(x)=0 \quad \text{if } x\leqslant -\frac{L}{2} \text{ or } x\geqslant \frac{L}{2}. \tag{6}$$

The confined states have a discrete energy spectrum.

We define a function $\hat{\xi}_{n,j}(x)$ as follows:

$$\hat{\xi}_{n,j}(x) = \sqrt{\frac{\pi}{L}}\left[\phi_n\left(\frac{j\pi}{L},x\right) - (-1)^j \phi_n\left(-\frac{j\pi}{L},x\right)\right],$$

$$-\infty < x < +\infty, \tag{7}$$

where $j = 1,2,3,\ldots N-1$, and $n = 0,1,2,\ldots$. The function $\hat{\xi}_{n,j}(x)$ in Eq. (7) satisfies[12]

$$\hat{\xi}_{n,j}\left(\frac{L}{2}\right) = \hat{\xi}_{n,j}\left(-\frac{L}{2}\right) = 0. \tag{8}$$

The band-edge states need special consideration. According to a mathematical theorem on the Bloch functions,[4] the two band-edge states of each band gap have the same number of zeros: Two band-edge states of the first band gap have one zero in $[0,a)$, two band-edge states of the second band gap have two zeros in $[0,a)$, ... Thus the two band-edge states of each band gap must have different bulk parity: one is odd and the other is even.[13] They have different energy, but which one is higher is dependent on the specific form of the potential $v(x)$. If the potential $v(x)$ is deep and short range around the PPML, such as used in Kittel's book[13] or Pedersen and Hemmer's work,[6] we expect that the lower band-edge state has an even bulk parity and the higher band-edge state has an odd bulk parity. In this work, we assume this is the case, while being aware that a different order of bulk parity of band-edge states is possible.[14]

We define

$$\hat{\xi}_{n,0}(x) = \sqrt{\frac{2\pi}{L}}\phi_n(0,x) \tag{9}$$

and

$$\hat{\xi}_{n,N}(x) = \sqrt{\frac{2\pi}{L}}\phi_n\left(\frac{\pi}{a},x\right). \tag{10}$$

It is easy to see that $\hat{\xi}_{n,0}(x)$ of odd bulk parity and $\hat{\xi}_{n,N}(x)$ of even bulk parity satisfies Eq. (8): They have an odd parity for an inversion relative a point $a/2$ away from a PPML. That corresponds to $\hat{\xi}_{n=\mathrm{even},0}(x)$ (Ref. 15) and $\hat{\xi}_{n=\mathrm{even},N}(x)$ for the case of deep and short-range local potential. We define another function $\xi_{n,j}(x)$ as follows:

$$\xi_{n,j}(x) = \hat{\xi}_{n,j}(x) \quad \text{if } -\frac{L}{2} \leqslant x \leqslant \frac{L}{2}$$

$$= 0, \quad \text{if } x < -\frac{L}{2} \text{ or } x > \frac{L}{2}. \tag{11}$$

Here $\hat{\xi}_{n,j}(x)$ is defined in Eqs. (7), (9), or (10). For $\hat{\xi}_{n,j}(x)$ defined in Eqs. (9) or (10), only those satisfying Eq. (8) are included in Eq. (11). Due to Eq. (8), the function $\xi_{n,j}(x)$ is a continuous function satisfying Eq. (6). Furthermore we have

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + v(x)\right)\xi_{n,j}(x) = \varepsilon_n\left(\frac{j\pi}{L}\right)\xi_{n,j}(x),$$

$$\text{if } \frac{L}{2} \leqslant x \leqslant \frac{L}{2} \tag{12}$$

and

$$\int_{-\infty}^{+\infty} \xi_{n,j}^*(x)\xi_{n',j'}(x)dx = \delta_{n,n'}\delta_{j,j'}. \tag{13}$$

The function $\psi(x)$ in Eq. (4) can be expanded in the basis of Eq. (11):

$$\psi(x) = \sum_{n,j} C_{n,j}\xi_{n,j}(x), \tag{14}$$

and thus the eigenvalues and eigenstates of Eq. (4) can be determined by

$$\det|H_{J,J'} - E\delta_{J,J'}| = 0, \tag{15}$$

where $J = (n,j)$ and

$$H_{J,J'} = \int_{-\infty}^{\infty} \xi_{n,j}^*(x) H \xi_{n',j'}(x) dx.$$

Due to Eqs. (12) and (13), we have[16]

$$H_{J,J'} = \varepsilon_n\left(\frac{j\pi}{L}\right)\delta_{n,n'}\delta_{j,j'}. \tag{16}$$

Thus the function set (11) diagonalizes the Hamiltonian (5). Hence we have the solutions of Eq. (4), the complete quantum confinement of Bloch waves, as

$$E_{n,j} = \varepsilon_n\left(\frac{j\pi}{L}\right), \tag{17}$$

and

$$\psi_{n,j}(x) = \xi_{n,j}(x), \quad -\infty \leqslant x \leqslant +\infty, \tag{18}$$

where $j = 1,2,\ldots N$ for $n = 0$, $j = 0,1,2,\ldots N$ for $n =$ even (except $n = 0$) and $j = 1,2,\ldots N-1$ for $n =$ odd, for the case of deep and short-range local potential. They can be obtained from the solutions of Eq. (1).

Figure 1 shows a comparison between the energy bands $\varepsilon_n(k)$ as the solutions of Eq. (1) and the energy spectrum $E_{n,j}$ [Eq. (17)] as the solutions of Eq. (4) for $N = 8$.

By using a Kronig-Penney potential, Pedersen and Hemmer found that the energy spectrum of the confined Bloch waves maps the energy bands.[6] The "central observation" of an investigation of Zhang and Zunger[5] is also the energy spectrum of confined electrons in Si quantum films maps the energy band structure of Si approximately. Much previous work also indicates that the eigenvalues of confined Bloch states map *closely* the dispersion relations of the unconfined Bloch waves.[7] Equation (17) shows that the map is *general* and *exact* in the one-dimensional case treated here.

The energy of most confined states changes as L changes. This is the energy quantum confinement effect in the usual

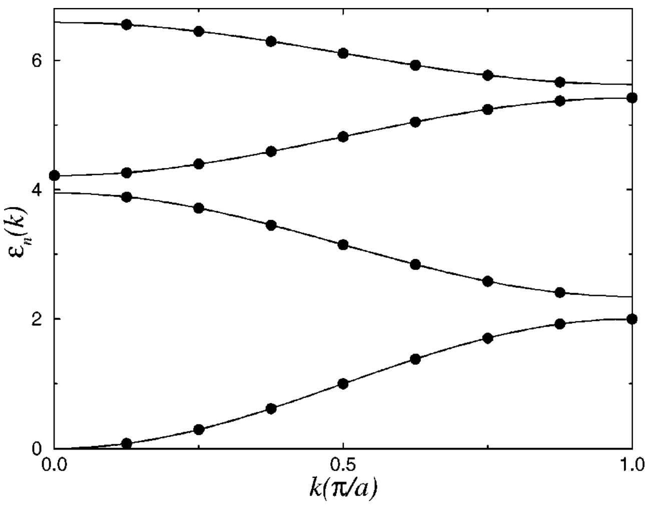

FIG. 1. A comparison between $E_{n,j}$ (solid circles) in Eq. (17) and the energy bands $\varepsilon_n(k)$ (solid lines) for the lowest four bands for the case $N=8$. Note: (i) that $E_{n,j}$ map the energy bands exactly; (ii) the existence of constant-energy confined states.

sense. However, there is always a band-edge state for each band gap whose energy does not change. For the case of deep and short-range local potential, the energy of the lower confined band-edge state near the band gap at $k=\pi/a$ is

$$E_{n,N}=\varepsilon_n\left(\frac{\pi}{a}\right) \tag{19}$$

and the state is

$$\psi_{n,N}(x)=\sqrt{\frac{2\pi}{L}}\phi_n\left(\frac{\pi}{a},x\right) \quad \text{if } -\frac{L}{2}\leqslant x\leqslant\frac{L}{2}$$
$$=0, \quad \text{if } x<-\frac{L}{2} \text{ or } x>\frac{L}{2} \tag{20}$$

for $n=0,2,4,\ldots$. The energy of the higher confined band-edge state near the band gap at $k=0$ is

$$E_{n,0}=\varepsilon_n(0) \tag{21}$$

and the state is

$$\psi_{n,0}(x)=\sqrt{\frac{2\pi}{L}}\phi_n(0,x) \quad \text{if } -\frac{L}{2}\leqslant x\leqslant\frac{L}{2}$$
$$=0, \quad \text{if } x<-\frac{L}{2} \text{ or } x>\frac{L}{2} \tag{22}$$

for $n=2,4,6.\ldots$. Thus the energy of these band-edge states does not change as the confinement length L changes. There is a such confined band-edge state for each band gap, therefore the energy of a half of confined band-edge states does not show the quantum confinement effect in the usual sense. In Fig. 2 are shown the energies of two confined band-edge states near the band gap $\Delta_{0,1}$ between the $n=0$ and $n=1$ energy bands as functions of confinement length L. In Fig. 3 are shown the energies of two confined band-edge states near the band gap $\Delta_{1,2}$ between the $n=1$ and $n=2$ energy bands as functions of confinement length L.

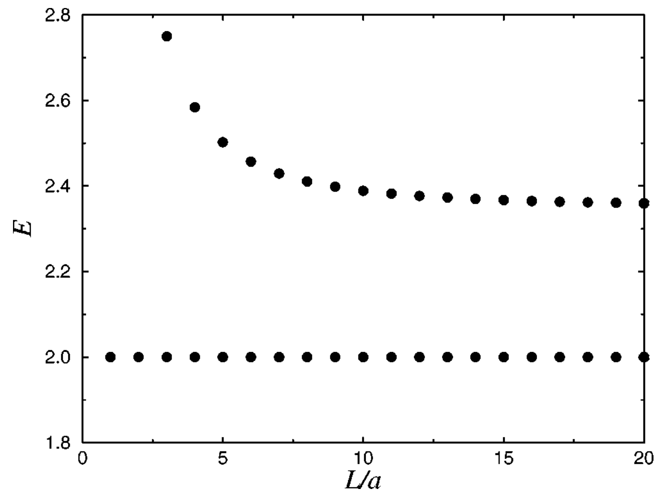

FIG. 2. The energies of two confined band-edge states near the band gap $\Delta_{0,1}$ as functions of the confinement length L. Note the energy of the lower confined band-edge state is a constant; only the energy of the higher confined band-edge state changes as L changes.

Zhang and Zunger observed a state with such behavior in their investigation on Si quantum films.[5] Franceschetti and Zunger also observed a such state in their investigations on the free standing GaAs quantum film.[8] They call it ''zero confinement state.'' In fact these states are confined: In real space they are confined in the region $-L/2\leqslant x\leqslant L/2$ [Eqs. (20) and (22)] and in the Bloch space each confined state $\langle n',k|n,j\rangle$ (Ref. 17) has a distribution, rather than being a δ function as is an unconfined Bloch wave. This distribution in the Bloch space is widened as L decreases, due to the uncertainty principle. Nevertheless, the energy of these states does not change as L changes. This is due to the fact that Eqs. (19) and (21) are eigenvalues of the confined Hamiltonian H. We

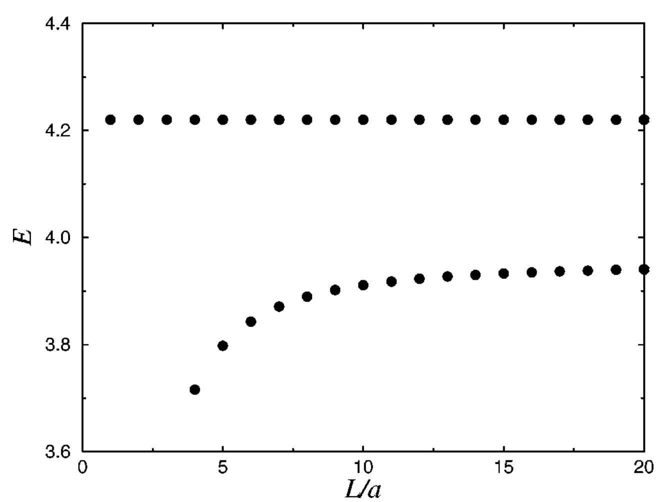

FIG. 3. The energies of two confined band-edge states near the band gap $\Delta_{1,2}$ as functions of the confinement length L. Note that the energy of higher confined band-edge state is a constant; only the energy of the lower confined band-edge state changes as L changes.

prefer to call these states constant-energy confined states. *The fundamental reason of the existence of those constant-energy confined states is due to the symmetry of the periodic potential; for each band gap there is always a band-edge state which has an odd parity for an inversion relative to a point $a/2$ away from a PPML and thus naturally satisfies* Eq. (8). Whether this is the higher band-edge state or the lower band-edge state is dependent on the location of the band gap and the specific form of $v(x)$.

Pedersen and Hemmer used a Kronig-Penney potential to investigate the quantum confinement of Bloch waves. However, they did not treat the band edge states and thus did not obtain results such as Eqs. (19)–(22).

The effective-mass approximation (EMA) has been widely used in investigating the quantum confinement of Bloch electrons. Essentially this approach is derived from the understanding on the quantum confinement of plane waves. However, originally the EMA was developed for treating the electronic states near band edges in the presence of slowly varying weak perturbations, such as an external electric and/or magnetic field, as well as the potential of shallow impurities.[18] But in quantum confinement problems, the perturbation is neither weak nor slowly varying at the confinement boundaries, and the conditions for justifying the use of EMA are thus completely violated. There has been much work on this interesting puzzle, mainly using the envelope function approach.[19]

However, we have seen that there are constant-energy confined states for which the concept of EMA is not even qualitatively correct. This point has also been noticed by Zhang and Zunger.[5] The failure of EMA for these band-edge states clearly indicates that one has to be careful in using EMA or EMA derived ideas in the quantum confinement of Bloch waves. On the other hand, for other confined band-edge states whose energy does change as L changes, as solutions of the Schrödinger Eq. (4), the *only* requirement for the EMA to be valid is that the energy band $\varepsilon_n(k)$ near the band edge can be approximated by a parabolic energy band. For example for $n=\text{odd}$, if

$$\varepsilon_n(k)\approx\varepsilon_n(0)+\frac{\hbar^2}{2m^*}k^2,$$

then the energy spectrum of the near band-edge confined states can be directly obtained from Eq. (17) as

$$E_{n,j}\approx\varepsilon_n(0)+\frac{\hbar^2}{2m^*}\frac{j^2\pi^2}{L^2}. \tag{23}$$

This is the complete confinement results of the EMA. A corresponding expression of EMA can be easily obtained for the confined states near the band gap at $k=\pi/a$.

In summary, we have given an analytical solution of the quantum confinement of one-dimensional general Bloch waves in an inversion-symmetric potential. The major result is Eqs. (17) and (18).

Any real solid always has a limited size and does not have a periodic boundary. Nevertheless, Bloch theorem based on the periodic boundary condition has been the basis of our current understanding on the electronic structures in modern solid-state physics. A similar problem on phonons was the subject of argument between Born and Raman.[20] Naturally one will be interested in the problem on what a difference there will be if a more realistic boundary condition on solids—such as the electrons being completely confined in the limited size of a real solid—is used. This work gives a complete and exact answer to this interesting problem for an inversion-symmetric potential in the one-dimensional case.

The quantum confinement of Bloch waves treated in this work—the one-dimensional case—is the simplest case. The higher dimensional cases would be more complicated. Nevertheless, since we have seen that even in the simplest one-dimensional case the quantum confinement of the Bloch waves could be fundamentally different from the quantum confinement of plane waves, it is very likely that there still could be some fundamental difference between the quantum confinements of Bloch waves and plane waves in higher dimensional cases. A clearer understanding on this interesting problem will need more work in the future.

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[1] See, for example, A.D. Yoffe, Adv. Phys. **42**, 173 (1993); M. Kelly, *Low Dimensional Semiconductors: Materials, Physics, Devices and Applications* (Oxford University Press, Oxford, 1996); Peter Y. Yu and Manuel Cardona, *Fundamentals of Semiconductors, Physics and Materials Properties* (Springer Verlag, Berlin, 1999).

[2] The electrons in a free standing thin film can be considered as completely confined in the thin film.

[3] W. Kohn, Phys. Rev. **115**, 809 (1959). In this work, Kohn investigated the analytical properties of the one-dimensional Bloch waves in an inversion-symmetric potential. The band-edge states will have either odd or even parity.

[4] M.S.P. Eastham, *The Spectral Theory of Periodic Differential Equations* (Scottish Academic Press, Edinburgh, 1973). Theorem 3.1.2. For the problem treated here, the theorem indicates: (i) $\phi_0(0,x)$ has no zeros in $[0,a]$. (ii) $\phi_{2m+1}(0,x)$ and $\phi_{2m+2}(0,x)$ have exact $2m+2$ zeros in $[0,a)$. (iii) $\phi_{2m}(\pi/a,x)$ and $\phi_{2m+1}(\pi/a,x)$ have exact $2m+1$ zeros in $[0,a)$.

[5] S.B. Zhang and A. Zunger, Appl. Phys. Lett. **63**, 1399 (1993).

[6] F.B. Pedersen and P.C. Hemmer, Phys. Rev. B **50**, 7724 (1994).

[7] For example, Z.V. Popovic, H.J. Trodahl, M. Cardona, E. Richter, D. Strauch, and K. Ploog, Phys. Rev. B **40**, 1202 (1989); Z.V. Popovic, M. Cardona, E. Richter, D. Strauchi, L. Tapfer, and K. Ploog, *ibid.* **40**, 1207 (1989); **40**, 3040 (1989); P. Malinasmata and M. Cardona, Superlattices Microstruct. **10**, 39 (1991).

[8] A. Franceschetti and A. Zunger, Appl. Phys. Lett. **68**, 3455 (1996).

[9] $a/2$ is also an inversion center because $v(-x-a/2)=v(x+a/2)=v(x-a/2)$. Due to Eq. (3), for a band-edge state we have

$$\phi_n(k,-x)=\alpha\phi_n(k,x),$$

where $\alpha=\pm 1$. Thus

$$\phi_n(k,-x-a/2)=\alpha\phi_n(k,x+a/2),$$

$$=\alpha\lambda\phi_n(k,x-a/2),$$

where $\lambda=1$ if $k=0$, $\lambda=-1$ if $k=\pi/a$.

[10] Otherwise the order of parity of the band-edge states might be different.

[11] For a monoatomic crystal, this means the Bloch waves are confined $a/2$ away from the boundary atom, because physically PPML can be considered as the locations of the atoms.

[12] By using Eqs. (4.6), (4.9), and (4.10) in Ref. 3 it can be easily proven that

$$\hat{\xi}_{n,j}(-x)=-(-1)^j\hat{\xi}_{n,j}(x).$$

From Eq. (7) we have

$$\hat{\xi}_{n,j}(x+L)=(-1)^j\hat{\xi}_{n,j}(x),$$

and Eq. (8) can be directly obtained from the two equations with $x=-L/2$.

[13] Otherwise these two states cannot be orthogonal to each other. An example can be seen in C. Kittel, *Introduction to Solid State Physics*, Seventh Edition (Wiley, New York, 1996), Chap. 7. Kittel pointed out that the two different band-edge states of a band gap in an inversion-symmetric potential have different parities is the origin of the existence of the band gap.

[14] Otherwise for some band gaps, especially the band gaps at higher energy, the order of parity of the band-edge states might be different.

[15] $\phi_0(0,x)$ has no zeros in the interval $[0,a]$, thus $\hat{\xi}_{0,0}(x)$ cannot satisfy Eq. (8) and has to be excluded.

[16] Although V is infinite outside of the confinement region, it is easy to show that $\psi(x)$ is even higher-order infinitesimal.

[17] For the widening of the confined Bloch states in the Bloch space, see, for example, S.Y. Ren, Phys. Rev. B **55**, 4665 (1997); S.Y. Ren, Solid State Commun. **102**, 479 (1997); S.Y. Ren, Jpn. J. Appl. Phys., Part 1 **36**, 3941 (1997).

[18] J.M. Luttinger and W. Kohn, Phys. Rev. **97**, 869 (1957); W. Kohn, *Solid State Physics* (Academic Press, New York, 1955), Vol. 5, p. 257.

[19] M.G. Burt, J. Phys.: Condens. Matter **4**, 6651 (1992), and references therein.

[20] See, for example M. Born and K. Huang, *Dynamical Theory of Crystal Lattices* (Oxford University Press, Oxford, 1954), Appendix IV.