A theorist in industry: can one fall between two stools and still land on one's feet?

VIEWPOINT

A theorist in industry: can one fall between two stools and still land on one's feet?

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Abstract
Here are reminiscences of some of my interactions with Marshall Stoneham and my career in industry, and particularly of his timely support for my work; and with some illustration of the importance of keeping a firm grasp on basic science to help see the wood from the trees in evaluating new technologies. It is interesting to see that fundamental theory established several decades ago needs to be further developed with some quite radical change of viewpoint when it is applied to new technology; and it is ironic that the impetus for such development of fundamental theory can be technological and commercial, rather than purely academic.

M Supplementary data files are available from stacks.iop.org/JPhysCM/18/S389

1. Nonradiative transitions

I first met Marshall in the 1970s. I was a post-doctoral fellow looking for a problem involving impurity or defect related deep levels in semiconductors. I was fortunate to get invited to attend a small meeting of the cognoscenti in the subject at Plessey Caswell, and Marshall was one of the prominent speakers. I am quite sure you can imagine the authority and eloquence with which he spoke on many aspects of defects and related deep levels. What most caught my attention was what he had to say on nonradiative multiphonon transitions [1]. He spoke with such aplomb, nay even insouciance, on such arcane matters as nonadiabaticity, along with promoting and accepting modes, that I was both intrigued and fascinated, if not somewhat overawed.

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[1] Visiting Professor.

Now it turned out that I got funding for work on photoexcitation of deep levels, an altogether much more sensible topic for a post-doctoral fellow to take on than anything to do with multiphonon transitions, but my enthusiasm for the latter was undiminished and I was still reading up on the subject in parallel; for instance, such classics as the paper by Huang and Rhys [2]. It was not long before I received a preprint from Marshall on an approach he had initiated [1], but continued with Ralph Bartram, on deriving a simple criterion for whether a deep centre would luminesce or not after photoexcitation [3], all part of a fruitful collaboration extending over a decade [4–6]. It was amusing to learn a little later that, unwittingly, what they had accomplished was to provide the theoretical justification for the Dexter–Klick–Russell Model.

What most struck me about this work [3] was how they had transformed what looked like an impossibly complicated problem into a possibly manageable one by adapting a recently discovered procedure from the theory of Jahn–Teller systems. They transformed to a system of effective lattice modes, which at first appeared to make the problem even more complicated, but had the saving grace of concentrating the accepting part of the electron–phonon interaction to one local effective mode. By this means, they had split the problem of how the electron-lattice system absorbs the initial optical energy and relaxes back to the ground state into three separate conceptual parts: the first was the expression of the initial total energy of the system, after optical excitation, as a sum of the electronic energy and the vibrational energy in the local effective mode, which also encapsulated the lattice distortion induced by the original optical excitation; the second was the subsequent energy dissipation by dispersal into the rest of the lattice via the coupling between the local effective mode and the remaining effective accepting lattice modes, the coupling arising from the fact that the effective modes were not orthogonal; finally, there is the discussion of the mechanism by which the electron crosses from the upper energy surface to the lower when it has cooled sufficiently to be close in energy to the crossing point. The whole paper was a real eye opener for me and was to encourage me later on, as I will explain in a moment.

It was at about this time that I made my move from academia to industry, or more precisely to industry via government. I joined the telecommunications arm of what was then called the Post Office Research Centre, part of a national corporation, which then mutated into BT Research Laboratories on privatization, which, after a few years, had a joint venture with Dupont involving the manufacture of optoelectronic devices. It was here that I became conscious of the danger of falling between two stools and the need to find a way of landing on my feet, if possible.

It is very easy when joining such a huge organization to get totally preoccupied by one's career within it. I was determined not to let that happen. So, I was very exercised as to how to keep myself interacting with academia and, indeed, other industrial research laboratories. Basically, one needs a core of work that one can publish and use to provide the justification to attend conferences. My initial wish was to concentrate on solid state theory, getting into electronic structure calculations to complement the expertise I had already begun to acquire in quantum electronic and optoelectronic processes. But near exclusive concentration on such solid state theory was difficult to justify since the organization I had joined had no experience of the benefits of this sort of work, i.e., electronic structure calculations, and I did not have the expertise to demonstrate such benefits sufficiently quickly. On the other hand, device modelling was something to which the management could relate, but, even though I might be able to smuggle some solid state theory into the device modelling, such modelling did not suit my temperament. If you are modelling a device, then someone else has already invented it; I wanted to be further upstream! So, I was in danger of falling between the two stools of solid state theory and device modelling as props to provide a presence outside my home institution.

At the time I joined the Post Office Research Centre, the development of long wavelength lasers for optical fibre telecommunications systems was a pressing problem worldwide. It turned out to be much more difficult than developing the lasers based on gallium arsenide for the earlier shorter wavelength systems. Fortunately the lack of theoretical expertise in the Post Office prior to my arrival gave me a golden opportunity to extend my quantum electronic expertise and make my mark. By learning about band to band Auger recombination in semiconductors, I was able to show that one of the laser programs, based on gallium antimonide related compounds, was doomed to failure [7], and a grateful management could then move much needed manpower on to what was to be the winning horse, a programme based on indium phosphide related compounds.

My successful application of the theory of nonradiative processes, in the form of band to band Auger recombination, to an urgent and important technological problem created a climate that made it much easier for me to rekindle my interest in multiphonon transitions, another class of nonradiative processes, especially since the related problem of phonon assisted tunnelling via deep levels was implicated in another technological problem for my colleagues, the then excessive and prohibitive leakage currents in long wavelength photodetectors.

Somewhat earlier, Brian Ridley [8] had made an important advance in the theory of multiphonon transitions. He derived an expression for the multiphonon transition rate in a deep level system, but without making the Condon approximation as had typically been used up to that time. This was and still is a real *tour de force* of a paper, and it made a big impression on me. But there was one small fly in the ointment: in order to get an algebraic expression, the Einstein model for the phonon spectrum had to be used—all phonons had the one and the same frequency. While it was still wonderful to have any algebraic expression at all, how could one justify such an approximation? Granted, the optical phonon branch of a typical semiconductor does not show great dispersion, but it would be good to have some further justification. But this is just what Marshall's work with Ralph Bartram [3] provides. If there is an effective local mode that initially accepts all the distortion energy induced by the transition, then a single effective frequency is justifiable.

Well, how could one make use of Brian Ridley's result in making comparisons with experiment? His result for the transition rate, R, had the low temperature form

$$R = [\cdots] S^p$$

in which S is the Huang–Rhys factor and p the number of phonons emitted. The prefactor, $[\cdots]$, is a complicated expression involving matrix elements of the electron–phonon interaction among other things. What is immediately apparent is the impossibility of computing R from material parameters to compare with experiment. Getting any reasonable estimate for the prefactor is daunting enough, but it fades into insignificance compared with getting anything like even an order of magnitude estimate of the term involving the Huang–Rhys factor. The point is that typically the number of phonons emitted is 20 or more. So even a 12% error in one's calculation of S will produce a factor of 10 error in R! However, if one turns the result on its head and writes

$$S = \left(\frac{R}{[\cdots]} \right)^{1/p}$$

a much more interesting opportunity presents itself: one does not need a particularly accurate value for the quantity $\frac{R}{[\cdots]}$ because even a factor of 10 error only gives a 12% error in S! So one can be quite satisfied with very modest accuracies for experimental transition rates, a blessing for one's experimental colleagues since these are by no means easy measurements even for modest accuracies, and also a rough model for the $[\cdots]$ factor will suffice. I managed to demonstrate the method by gaining what appeared to be a reasonable estimate for S for

the so-called B centre in gallium arsenide, the only case I was aware of that gave suitable data [9]. Fortunately, others took up the baton, others who were carrying out experiments on deep centres that involved different processes the magnitude of which depended on S, such as the temperature dependence of the photoionization cross section and the temperature and field dependence of emission rates. It turned out that, for a number of centres, one could get a consistent set of Huang–Rhys factors from the various measurements, which was encouraging for the effective local mode picture [10].

Another important development in multiphonon transition rate theory was a result derived by Huang [11] concerning the basis states to be used for the initial and final states. The traditional choice had been the adiabatic states of Born and Oppenheimer, for which the electron follows the nuclear/ionic motion faithfully and instantaneously; the perturbation that drives the transitions between the basis states is the nonadiabaticity operator. An alternative choice, favoured by some authors, was to use static states, for which the electron wavefunction does not depend on the nuclear/ionic motion at all and for which the appropriate perturbation is the offdiagonal part of the electron–phonon interaction. Such a basis is just that used in conventional calculations of electron–phonon scattering rates in, say, calculations of electronic conductivity or mobility. What Huang managed to show was that, to lowest order, the transition rates calculated by the two schemes, if carried out consistently, should give exactly the same transition rate. However, his proof was specific to these two choices alone and begs the question as to what happens if one chooses some other basis. After all, none of the theories to this date had tackled the vexed question as to which initial state the electron is actually in, a problem common with all internal transition rate theories.

Fortunately, I managed to come up with a general proof that any basis that differed from the static basis by terms of order of the offdiagonal part of the electron phonon interaction, which would include the adiabatic basis as a special case, would give the same transition rates to leading order in perturbation theory [12]. Hence, if working to lowest order, then one is free to choose the initial and final states as one wishes, providing only that one uses the correct interaction between the states one has chosen.

Now, as you may well appreciate, the work I have just described on Huang–Rhys factors and fundamental theory of multiphonon transition rates is not such as to give an adrenalin rush to the average member of a main stream conference programme committee. But, Marshall made sure I got invitations to speak about this work at appropriate specialist conferences so that I got the invaluable external accreditation I needed to support my work. This all helped avoid a precipitous fall between the two aforementioned stools and find a narrow bench between them as an alternative seat.

2. Envelope functions and effective mass theory

In the early 1980s an obvious topic for someone in my position to explore was the potential for quantum well technology in optoelectronics. In those days, even adapting semi-empirical methods used for bulk band structure calculations to quantum wells and superlattices was demanding in both programming effort, machine memory and run times, especially if one wanted to do more than just compute energy levels, which is necessary for any serious assessment of the influence quantum wells may have on optoelectronic processes.

The alternative to which many people turned was the particle in a box model and elaborations thereof primarily promoted by Bastard and co-workers [13–15]. Even though the justification for its application to quantum wells, with their supposedly atomically sharp boundaries, was highly dubious, it seemed to work for the most commonly grown structures.

Or did it really? It was always in the back of my mind that it was possible that errors in the method were being masked by the inevitable adjustable parameters, such as band edge discontinuities and imperfectly measured well widths and compositions, or even by the fact that the boundaries were not as abrupt as supposed.

There was relatively little discussion on the validity of the particle in a box model, the prevailing attitude being to let experiment decide. I took exception to this *a posteriori* approach. What was one doing in using experiment to decide on the validity or otherwise of a mathematical approximation? Experiment should be used only to attempt to falsify hypotheses about physical systems. If ever there were a case for using Ockham's razor, this was it.

Besides the philosophical objection to the *a posteriori* approach, there was a sound commercial objection. If one was trying to identify promising new material systems to investigate and new devices to patent, it was very burdensome if not prohibitive financially to do all this experimentally, especially as one would probably get pipped at the post by an institution that had more resources than your own.

Could one derive the correct effective mass equation/particle in a box model from phenomenological arguments alone, even supposing that such an equation existed? Maybe, for instance, the best one could ever do is use envelope functions in the well and barrier regions and then just use matching of the wavefunction at the interfaces, with all the microscopic considerations that implies, to provide connection rules. As the reader will probably recall, the main uncertainty under common discussion was whether or not the effective mass should be included in the derivative boundary condition. If the effective mass is left out, then, while the envelope function (often an ill defined concept in such discussions) and hence the wavefunction are both smooth, the hamiltonian is not hermitian. However, *a priori*, why should it be so? Without any rigorous derivation one cannot be sure that the eigenvalue equation obeyed by the envelope function should not be that for a non-hermitian operator that happens to have some real eigenvalues that approximate those of the Schrödinger equation in some range near a band edge (we now know, of course, that it is possible to derive the effective hamiltonian using unitary transformations and hermiticity maintaining approximations, but it was by no means clear that this was the case at the time); this would not have been such a ludicrous suggestion when one recalls that the electron hole energies in the solution of the Bethe–Salpeter equation for the electron hole propagator in the static screened potential approximation are the eigenvalues of a non-hermitian operator [16]. Similarly, the objection that omission of the effective mass from the derivative boundary condition leads to nonconservation of probability current is not conclusive for bound states: the current is zero everywhere anyway; and if you have not proved there must be a single universal equation for both bound and unbound states, why should there not be different equations for the two cases? Strange, perhaps, but that was no argument for exclusion in a situation which was so little understood. On the other hand, if the effective mass is included in the derivative boundary condition, then the hamiltonian is hermitian and there is always a conserved quantity, that may be the current, but there is now a kink at the boundary related to the effective mass change and this implies a kink in the wavefunction which is not acceptable *a priori*. It became clear to me that phenomenological approaches were doomed, and even if one managed to succeed, one would have no way of quantifying the errors involved in the use of any phenomenologically derived theory.

I remember my immediate aim, stimulated by a conversation with Dick Abram, was to demonstrate categorically that the equations postulated by Bastard must be incorrect in principle and the most convincing way to do that was to derive the exact equations for the envelope functions and highlight the differences [17]. The first crucial step was to appreciate that the envelope function expansion could be defined as an exact expansion of the wavefunction, not just a trial solution, as in Bastard's treatment, for some particular problem,

provided two conditions are met: (1) the same periodic functions are used throughout the well and barrier regions even though they may not be the band edge eigenstates of either material and (2) the plane wave expansion of the envelope functions are restricted to the first Brillouin zone. Defined in this way, the expansion is just as rigorous as a plane wave expansion; indeed, this point is implicit in the original paper by Luttinger and Kohn [18], but it appeared to have gone largely unappreciated. So any given wavefunction has a unique envelope function expansion without being the solution to any particular time-independent or, for that matter, any time-dependent problem. Once this point is grasped it is obvious that if the wavefunction obeys some particular Schrödinger equation, there must exist some corresponding set of exact equations that the envelope functions obey. These turned out to be coupled integral–differential equations with a nonlocality arising from the restriction on the plane wave expansion of the envelope functions. To obtain local equations, one needed to assume that the envelope functions were globally slowly varying. This does not mean that the envelope functions need to be smoothly varying everywhere. All it requires is that the significant components in their plane wave expansion correspond to small wavevector; functions which have occasional kinks and discontinuities, but are otherwise slowly varying, fall into this category [17]. Contrast this approach with that of Geller and Kohn [19, 20], in which they make the assumption of a smoothly varying effective mass, not a particularly helpful approximation in practice! The globally slowly varying envelope function is a much more appropriate and widely applicable approximation to make and in my approach leads to local equations, which can lead to a derivation of the particle in a box model and provide methods of estimating errors thereto.

Well, the upshot of all this was that the equations postulated by Bastard, were, indeed, incorrect: they ignored terms at the interface that could have an influence on the energy levels and wavefunctions. But, much to my surprise, the corrections I calculated for the quantum well structures in common use at the time turned out to be insignificant. So I had to come round to the point of view that the envelope function method/particle in a box model works well in the first instance and was certainly adequate for my purposes. However, it was not long before the cracks in the phenomenological method began to show. When more accurate and probing experiments were made, the phenomenological school, that essentially followed Bastard's approach, had to introduce arbitrary interface related terms to patch up their method. Here, if one ever doubted that it would arise, was the compelling practical justification for applying Ockham's razor. For a critique of the Bastard approach and application of the razor, I can do no better than refer the reader to the work of Brad Foreman [21].

My derivation of the effective mass equation led to the result that the effective mass should be included in the derivative boundary condition. It turns out that the kink in the envelope function at a boundary just approximates a relatively rapid variation in the exact envelope function there. As previously mentioned, the presence of such occasional kinks in the approximate envelope function does not change the globally slowly varying nature of the envelope function so the approximation is consistent.

But there turned out to be a twist in the story. If one examines the approximate multiband envelope function equations, obtained once the globally slowly varying nature of the envelope functions is exploited, then it is clear that the boundary conditions to be applied are the continuity of each envelope function and its derivative. For consistency one must include all solutions of these equations including rapidly varying out of zone solutions, those that are almost universally shunned by other authors! But, it can be shown that this is a mathematically consistent procedure and the author has demonstrated that it gives the correct wavefunction [17].

Well, as you can imagine, I had a lot of fun sorting this all out over the years, but as with multiphonon transitions, it was not the sort of thing that got the average member of a

mainstream conference programme committee jumping up and down with excitement. But fortunately I received support from Marshall and others such as Dick Abram, Volker Heine and Brian Ridley so that I got a couple of invited papers in JPCM over the years. I remember vividly getting a referee's report on one of these, in which I had been decidedly trenchant in my criticism of some other authors. The referee commented that they did not like the tone. Quite rightly, they were giving me the opportunity to reflect on what I had written. But I must admit to being a bit downcast since I felt strongly that the many and persistent errors and misrepresentations in the literature should be corrected. So, I rang Marshall up and told him about the report. He simply retorted that it was important that the paper had a tone and I felt much better!

3. Interband dipole matrix element

The first applications of quantum well technology to optoelectronics exploited interband transitions, i.e., transitions between a quantized level in the valence band and another quantized level in the conduction band. However, it was then discovered that the dipole matrix element for intraband transitions (also called intersubband transitions), for example the transition between the ground state and the first excited state within the conduction band, could be very large, typically 20% of the well width. This, taken with the rapid relaxation times and the high joint density of states, sparked off a whole subdiscipline.

The way the large size of the dipole matrix element for the intersubband transitions was portrayed was interesting. It was compared to the interband dipole matrix element, which was claimed to be of the order of atomic dimensions as it was determined by the matrix element of the dipole operator between band edge Bloch functions [22–24]. But when one calculated the size of the interband dipole matrix element needed to explain the most basic experimental facts about optical absorption in low band gap semiconductors such as indium antimonide one needs an interband dipole matrix element in the region of 30–40 Å: hardly atomic dimensions! Even for the canonical material for such investigations, gallium arsenide, the figure was about 6 Å, which should have raised suspicions, as the basic lattice translations of its face-centred cubic lattice are about 4 Å. So, there were two aspects to all this. First, where were the flaws in the argument that the interband dipole matrix element was of atomic dimensions? And, second, what were the implications for optoelectronic device development?

The question as to what the correct interband dipole matrix is for states in bulk crystals had been studied and answered many years previously by Blount [25]. Combining his results with $k \cdot p$ perturbation theory, it is clear that for all practical purposes the interband dipole matrix element is essentially given by the ratio of the interband momentum matrix element and the energy gap, the result one would obtain if one applied, erroneously as a matter of logic alone, the standard textbook result for bound states. The large interband dipole matrix elements needed to explain interband absorption data for low band gap semiconductors were and are no problem using this result. Indeed, it was this actual result everyone used in any numerical work, yet at the same time there was an almost pervasive assumption that its size was always of atomic dimensions. As far as I am aware nobody ever calculated the explicit expression given in the textbooks involving the dipole operator and the band edge Bloch functions. Yet, if one did, even for the simplest of one-dimensional models, the inconsistencies were obvious.

So where was the error in the textbook treatment of the interband dipole matrix element in quantum wells, the treatment that used the envelope function method? Since I had managed to develop a rigorous approach to envelope function theory, I must have the tools to sort this out. Indeed, I did and the results were intriguing. First, the textbook treatment assumed that only the dominant term or terms in the envelope function expansion of the wavefunction of a

quantum well state need be retained, terms that were dominant in the limit of a wide well. But, it turned out that, if such an approximation were made, the dipole matrix element between the states vanished in that limit. To get the correct answer one had to include the other terms in the envelope function expansion, terms that became vanishingly small in the wide well limit. Such terms contained all the physics, such as the transient microscopic electronic currents set up during a transition. Second, the error in the textbook treatment was in the separation in the rapidly and slowly varying terms in the integral for the interband matrix element; while the original approximate expression, in which only the dominant terms(s) in the envelope function expansion of the wavefunctions had been retained, was a well defined integral, the final expression depended on the choice of unit cell and did not have a unique value.

I sometimes wonder whether the myth that the interband dipole matrix element must be of atomic dimensions comes from a misreading of such a statement in Elliott's classic paper [26] on optical properties of bulk semiconductors (I refer to the text immediately following equation (3.5)). But Elliott's statement is perfectly correct: he was working explicitly in the tight binding approximation; and my results for wide wells and tight binding are certainly in agreement with the expression he gave both for the interband dipole matrix element and his interpretation of its size.

And what were the implications of these results for optoelectronic device development? Well, broadly speaking, if one wants a large dipole matrix element the essential feature one needs is a low energy separation between the states: while one had this for selected intersubband transitions in quantum wells, one also has it for allowed interband transitions in low band gap semiconductors! A much more important advantage for intersubband transitions near the band edge is that they offer a quasidiscrete joint density of states for optical transitions and a rapid relaxation rate. And perhaps most important for mid and far infra-red applications is the ability to use quantum well engineering to put energy levels where one wants them and at the same time use materials systems for which impressive expertise has already been demonstrated by the crystal growth community.

Not only did I find the work just described on the interband dipole matrix element useful to help me see the wood from the trees in assessing the potential of intersubband transitions in quantum well technology, but I also managed to adapt it to supporting the case for quantum dot technology, especially the use of quantum dots made by colloidal techniques for broadband amplification in optical telecommunication networks. Most of the people one was trying to influence had an electrical engineering background and talking to them at length or otherwise about subtle mathematical points was not going to help! What one needed was some imagery that would get the point across vividly.

Fortunately a way of doing this occurred to me via trying to demonstrate to physicists why the interband dipole matrix element for low direct band gap semiconductors was so surprisingly large. Consider an electron in a nonstationary quantum dot state, which is a linear superposition of the lowest quantized state in the conduction band and the uppermost state in the valence band. Such a state will have a time-varying charge density and the associated current averaged over a unit cell is essentially determined by the interband momentum matrix element. Now this quantity is roughly the same for all direct gap tetrahedral semiconductors so the currents that exist in such a state are roughly comparable, independent of the band gap, all other things being equal. But the extent of the dipole produced during an oscillatory cycle will be determined by the period of the oscillatory cycle, which will be long for superposition of stationary states with small energy difference. So the smaller the band gap the larger the oscillating dipole moment induced, which in turn implies a larger dipole matrix element between the nonstationary states.

Now a large oscillating electric dipole is powerful imagery to put in front of an electrical engineer. It signifies a strong emitter and amplifier of radiation. But large compared to

what? Fortunately that was no problem. The amplifier being developed then for use in optical fibre systems was based on erbium atoms dissolved and well separated in glass. Any charge oscillations there would be during the amplification would be confined to the individual atoms, and since it involved a transition within the f shell it would not even be a dipole. So any animation, even just for quantum confinement in one dimension, such as presented in the appendix, of the oscillating charge density for an electron in the nonstationary state described above would be fine. For band gaps corresponding to the wavelengths used in current optical fibre systems ($\sim$1500 nm) the dipole would be about 10 Å. So an animation of the nonstationary charge density showed the electric charge oscillating right across the quantum dot and the quantum dot behaving just like a giant atom. If, however, one approximated each of the stationary states by just the dominant term in the envelope function expansion, as in the textbook argument, the difference was extraordinary: the charge density virtually lost its dipole character with the oscillations restricted to just atomic dimensions. I have never seen so much physics packed into such a small part of the wavefunction. Indeed, if one takes the bulk limit, all the physics is in a vanishingly small fraction thereof!

Well, this animation certainly helped bolster the case for quantum dot work in a telecoms environment at a time when hardware research in BT was becoming very unpopular with higher management, and it helped the case in more ways than one. It kept the quantum dot work going long enough for my group to demonstrate [27] amplified spontaneous emission in a quantum dot sample that matched the gain obtained in an erbium doped fibre amplifier, which was very gratifying: our sample was about a factor of 1000 shorter than the erbium doped fibre amplifier and also demonstrated simultaneous amplification over more than 10 times the bandwidth! Quantum dots were definitely behaving as giant atoms! And it also helped my case to engage Marshall as a consultant to look further at the possibilities of quantum dots and gave us the freedom to look into other topics such as quantum computation; we had a lot of fun studying and discussing the early papers in that field. It only came to an end because BT decided to stop fundamental research in optoelectronics.

Acknowledgments

As a parting comment, Marshall, I would like to say that I could never claim to have landed on my feet in anything like the way you have managed to do throughout your career, but I can truly say that with your help and guidance I have managed to avoid landing flat on my face.

I would like to thank Tony Harker for his help in preparing the files for the animations of the charge oscillation in a nonstationary state in a quantum dot presented in the appendix.

Appendix

Simple demonstration (one dimension) of probability density (charge) oscillation in a nonstationary state in a quantum dot to demonstrate in turn that it is possible to have a dipole matrix element greater than atomic dimensions for a transition across the band gap of a low band gap semiconductor.

The microscopic potential of the model one-dimensional system used is shown in figure A.1. The potential in both the well region ($|x| \leqslant 10a$) and the barrier region ($|x| \geqslant 10a$) has the form $V_0 + V_S \cos(2\pi x/a)$ in which a, the lattice period, is 6 Å. In the well, $V_0 = 0.5$ eV and $V_S = 1.5$ eV, while in the barrier $V_0 = 0.0$ eV and $V_S = 5.0$ eV. As the reader may well anticipate, the band structures are qualitatively nearly free electron like. We consider a time-dependent state that is an equal superposition of the two stationary size quantized states either side of the first band gap at zero wavevector (see references in [17] for more detail).
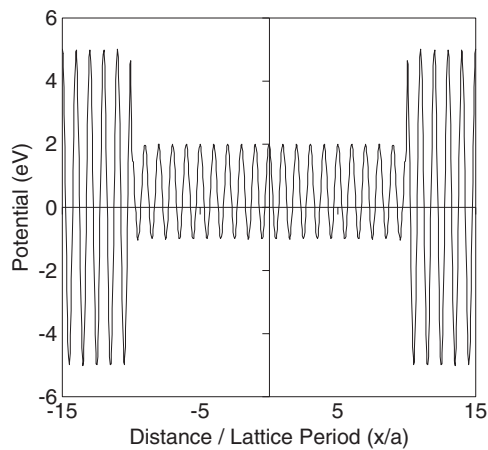
Figure A.1. Microscopic potential of the model one-dimensional system.
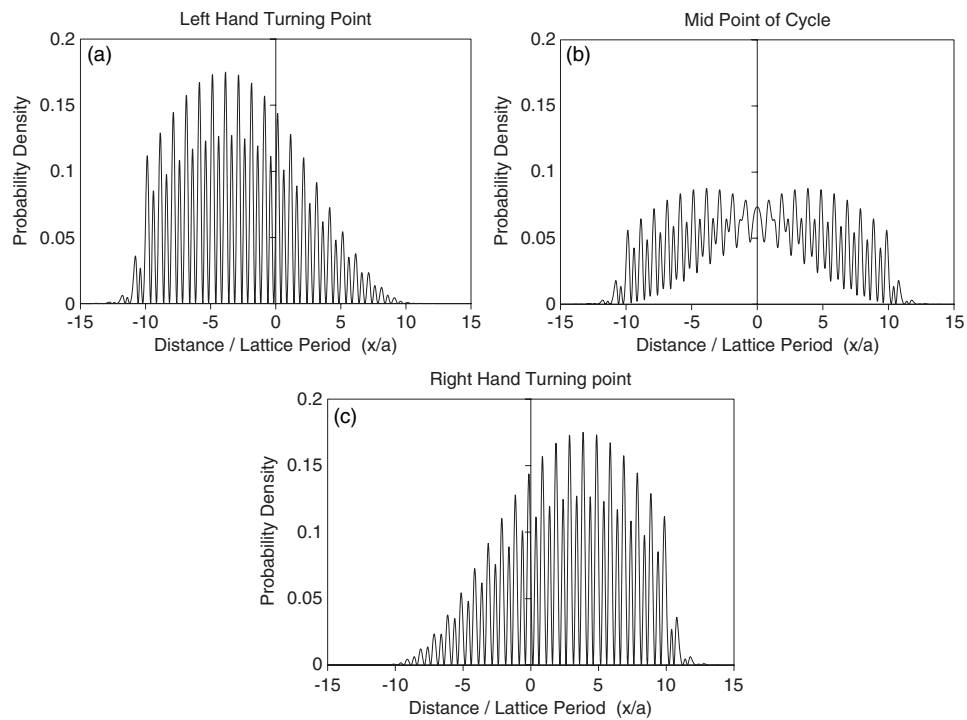
Figure A.2. Snapshots of the oscillation of the correct probability density.

In figures A.2(a), (b), (c) are shown the correct probability density for the above-mentioned time-dependent state at the left-hand tuning point, the mid-point and the right-hand turning point of the oscillatory cycle. It is clear that the displacement is considerably larger than the lattice period, a. Figures A.3(a), (b), (c) show the corresponding probability densities in which each of the wavefunctions is approximated by the dominant term in the envelope function expansion, i.e. a single product of the band edge Bloch function and the corresponding
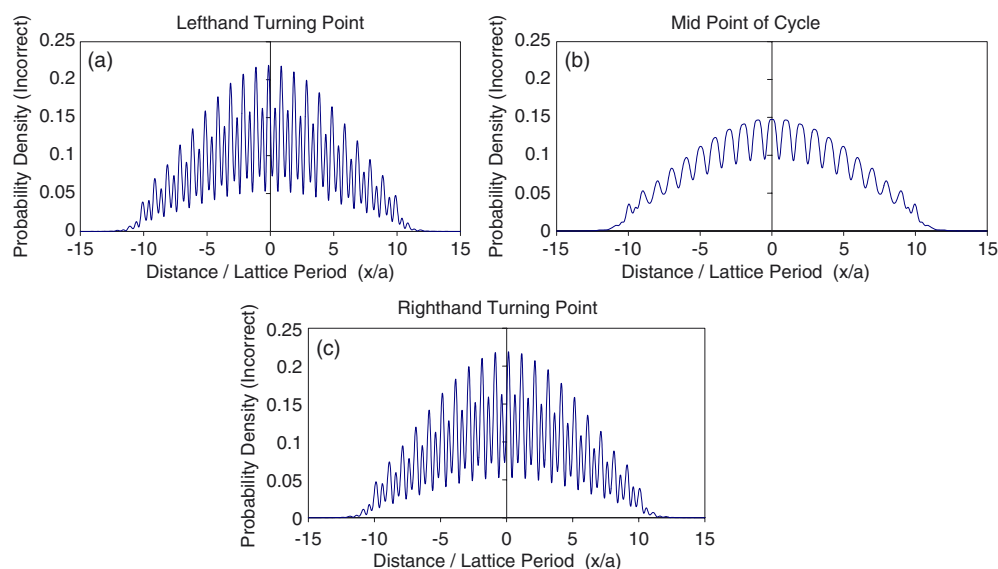
Figure A.3. Snapshots of the oscillation of the incorrectly calculated probability density.

(This figure is in colour only in the electronic version)

envelope function, Even though a relatively small part of the wavefunction has been neglected, the probability density oscillation has virtually lost its dipole character and the displacements are considerable less than the lattice period, a,

Animations of the charge oscillation of which figures A.2 and A.3 give snapshots are available in the attached files. (see stacks.iop.org/JPhysCM/18/S389)

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