Band structure for small lattice constant: dependence on lattice granularity

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Abstract. This paper addresses the question: how does the band structure for a regular lattice change as the lattice itself is allowed to go smoothly to its continuum limit (alternatively: how does lattice granularity affect band structure)? The energy of the lowest allowed band in a general one-dimensional lattice is obtained explicitly as a power series in the lattice constant and in wave vector. The band structure is shown to be robustly free-electron-like for small but finite lattice constant. The study was suggested by questions arising in delta-doping in semiconductors.

1. Introduction

The existence of electron energy bands in solids, and their general properties, have been the subject of intense study since the early days of the subject. Many results have become standard knowledge. Recent developments in semiconductors, and the advent of new fabrication techniques for quantum electronic systems, have brought some of the basic questions concerning band theory into new focus. Questions which did not seem interesting at one time have tended to become matters of practical interest in these new situations. This is the context of the present paper.

The question considered here is the following (we consider one dimension, for simplicity). We think of an electron as living in the space defined by the underlying lattice on which the electron lives. In the absence of its lattice, the electron is the usual free electron. In the presence of its lattice (a 'standard' lattice, say, with standard potential strength and standard lattice constant), the electron reacts to the lattice via its energy band structure, in a way studied in depth, for example, by Kohn [1].

Now consider changing the *granularity* of the underlying lattice. By this is meant that the lattice spacing is allowed to shrink to zero, but in such a way that the average potential strength per unit length remains constant (a more precise definition is given in section 3). An analogy would be a set of identical equally spaced point charges on a line. The spacing between charges is then shrunk, while the magnitude of the charges is decreased in such a way that the average charge per unit length of line remains constant.

In the limit of vanishing lattice constant one has a constant potential; the electron reacts to this by behaving like a free electron. But how, precisely, does the electron react when the granularity of its lattice is increased? In other words, how soon, and in what fashion, do lattice-dependent corrections arise to free-electron motion as the lattice becomes more granular?

This question has been suggested by delta-doping experiments in semiconductors [2–4]. In layer-by-layer semiconductor growth, a random collection of donors can be placed on

a single crystal plane. The donated electrons feel the Coulomb attraction of the plane of ionized donors and become trapped in the vicinity of that plane, forming a two-dimensional electron gas. This process is very well described by approximating the plane of ionized donors by a uniform plane sheet of positive charge [5–8].

The fact that the approximation is so good is puzzling in itself, since it seems to work well even when the individual charges are very far apart, of the order of an effective Rydberg. Screening of the donor potential will surely play some role. On the other hand, the approximation still seems to be a good one even in physical situations [9,10] such that very few electrons are trapped in the well. Is there any good reason why this should be the case?

To answer this question in full generality, for a disordered collection of donors, is a challenging and unsolved problem. In the first instance we therefore consider a similar but much simpler problem of the reaction of an electron to a regular collection of potentials, to see whether an apparent insensitivity of an electron to the underlying granularity of the space in which it lives might for some reason be a general property of the band structure. As will be seen, one can indeed obtain a *general* answer to this question, at least for a one-dimensional lattice.

2. Dispersion relation from the transfer matrix

The formalism used here differs slightly from that found in many textbooks [11], and we therefore set it out briefly for clarity and convenience.

The Schrödinger equation

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right)\psi = E\psi$$

for an electron of mass m and charge $-e$ can be written in the form

$$\frac{d}{dx}\Psi(x) = \mathbf{C}(x)\,\Psi(x) \tag{1}$$

where Ψ is defined to be the two-component vector

$$\Psi \equiv \begin{pmatrix} d\psi/dx \\ \psi \end{pmatrix} \tag{2}$$

and $\mathbf{C}$ is the 2×2 matrix

$$\mathbf{C}(x) \equiv \begin{pmatrix} 0 & -(2m/\hbar^2)[E - V(x)] \\ 1 & 0 \end{pmatrix}. \tag{3}$$

Standard notation is used. $V(x)$ is a one-dimensional periodic potential with period a and E is the energy of an electron in this potential.

A transfer matrix $\mathbf{T}$ can be defined by the relation

$$\Psi(a) = \mathbf{T}\,\Psi(0) \tag{4}$$

where a matrix product is understood. $\mathbf{T}$ can be calculated iteratively by integrating (1) between 0 and a:

$$\Psi(a) = \Psi(0) + \int_0^a dx_1\,\mathbf{C}(x_1)\Psi(x_1)$$

and using this result repeatedly to replace the rightmost term in the same equation

$$\Psi(a) = \Psi(0) + \int_0^a dx_1\,\mathbf{C}(x_1)\left(\Psi(0) + \int_0^{x_1} dx_2\,\mathbf{C}(x_2)\Psi(x_2)\right)$$

and so on. The transfer matrix defined by (4) can thus be expressed in terms of the 'component matrices' **C** by the relation

$$\mathbf{T} = \mathbf{I} + \int_0^a \mathrm{d}x_1\, \mathbf{C}(x_1) + \int_0^a \mathrm{d}x_1 \int_0^{x_1} \mathrm{d}x_2\, \mathbf{C}(x_1)\mathbf{C}(x_2) + \cdots. \tag{5}$$

We note in passing that this infinite sum may be expressed more succinctly by use of a space-ordering operator $\mathcal{R}$ defined in analogy to the time-ordering operator familiar from quantum field theory [12]: $\mathcal{R}$ acting on any product $f(x_1)\ldots f(x_n)$ re-orders the terms of the product in such a way that any position argument x_i is $\geq$ than the arguments of terms to the right of it, and $\leq$ the arguments of terms to its left. In terms of this space-ordering operator $\mathcal{R}$, the transfer matrix **T** can be written symbolically as

$$\mathbf{T} = \mathcal{R}\left[\exp\left(\int_0^a \mathrm{d}x\, \mathbf{C}(x)\right)\right].$$

The band structure (dispersion relation) for the lattice is given, as in the standard approach [11], by the equation

$$\cos(ka) = \tfrac{1}{2}\mathrm{Trace}\,\mathbf{T} \tag{6}$$

where k is the lattice wave vector and a the lattice constant. Note that, although **C**, and thus **T**, are of mixed dimensions, the diagonal elements of **T** are dimensionless, as they must be for (6) to be meaningful.

3. Isolation of small parameter (non-dimensional transfer matrix; how to define a potential for a shrinking lattice)

To discuss an infinite lattice with a lattice constant which shrinks to zero, one must have a ruler (that is, a reference length) which does not shrink. We label this arbitrary reference length a_0. We want to determine how the band structure behaves as we shrink the lattice, letting $(a/a_0) \to 0$. To ensure that this limit is taken in a consistent fashion, we change the formalism somewhat, to make dependence on the small parameter a/a_0 completely explicit. We therefore go back to the Schrödinger equation itself and write it in non-dimensional terms:

$$\left[\left(\frac{E}{\mathcal{E}_0}\right) - \left(\frac{V(\tilde{x})}{\mathcal{E}_0}\right) + \frac{\mathrm{d}^2}{\mathrm{d}\tilde{x}^2}\right]\psi = 0. \tag{7}$$

Here

$$\tilde{x} \equiv (x/a_0) \tag{8}$$

and

$$\mathcal{E}_0 \equiv \hbar^2/2ma_0^2 \tag{9}$$

is the reference energy automatically associated with the reference length a_0, This leads to a dimensionless transfer matrix **T** which is defined in terms of $\psi(\tilde{x})$ by

$$\begin{pmatrix} \psi' \\ \psi \end{pmatrix}_{\tilde{x}=1} = \mathbf{T}\begin{pmatrix} \psi' \\ \psi \end{pmatrix}_{\tilde{x}=0}$$

where the derivative ψ' is by definition

$$\psi'(\tilde{x}) \equiv (\mathrm{d}\psi/\mathrm{d}\tilde{x}).$$

The new transfer matrix **T** can be written in analogy to (5) as

$$\mathbf{T} = \mathbf{I} + \int_0^{a/a_0} \mathrm{d}\tilde{x}_1\, \mathbf{D}(\tilde{x}_1) + \int_0^{a/a_0} \mathrm{d}\tilde{x}_1 \int_0^{\tilde{x}_1} \mathrm{d}\tilde{x}_2 \mathbf{D}(\tilde{x}_1)\mathbf{D}(\tilde{x}_2) + \cdots \tag{10}$$

with component matrices

$$\mathbf{D}(\tilde{x}) = \begin{pmatrix} 0 & -[E - V(\tilde{x})]/\mathcal{E}_0 \\ 1 & 0 \end{pmatrix} \tag{11}$$

which are now dimensionless.

It is convenient to change variables in (10), defining

$$y \equiv (x/a) \tag{12}$$

or equivalently

$$\tilde{x} = (a/a_0)\, y.$$

Let us also assume that by 'shrinking the lattice' we mean that

$$V = V(x, a) = V(y). \tag{13}$$

This is in fact what has been assumed implicitly all along, and implies that the potential retains its original *shape* (over a unit cell) as the lattice shrinks. It also gives, as a bonus, the required property that the potential strength is constant per unit (invariant) length of lattice, since

$$\frac{1}{a} \int_0^a dx\, V(x) = \bar{V} = \int_0^1 dy\, V(y). \tag{14}$$

Since $V = V(y)$, then also $\mathbf{D}(\tilde{x}, a) = \mathbf{D}(y)$, and (8) can now be written

$$\mathbf{T} = \mathbf{1} + \left(\frac{a}{a_0}\right) \int_0^1 dy\, \mathbf{D}(y) + \left(\frac{a}{a_0}\right)^2 \int_0^1 dy_1 \int_0^{y_1} dy_2\, \mathbf{D}(y_1)\mathbf{D}(y_2) + \cdots. \tag{15}$$

Equation (15) is a crucial result: an explicit expansion of the transfer matrix in powers of the lattice constant.

The final point to note is that, although the transfer matrix of (15) is not the same as its dimensional counterpart $\mathbf{T}$ in (5), both matrices have the same diagonal elements. The band structure is thus given by

$$\cos(ka) = \tfrac{1}{2}\text{Trace}\,\mathbf{T} = 1 + \frac{1}{2}\left(\frac{a}{a_0}\right)^2 \int_0^1 dy_1 \int_0^{y_1} dy_2\, \text{Trace}\left[\mathbf{D}(y_1)\mathbf{D}(y_2)\right]$$

$$+ \frac{1}{2}\left(\frac{a}{a_0}\right)^4 \int_0^1 \int_0^{y_1} \dots \int_0^{y_3} dy_1 \dots dy_4\, \text{Trace}\left[\mathbf{D}(y_1)\mathbf{D}(y_2)\mathbf{D}(y_3)\mathbf{D}(y_4)\right] + \dots. \tag{16}$$

We note that terms in odd powers of (a/a_0) drop out of (16) because they have zero trace (since $\mathbf{D}$ itself is off-diagonal, from (11)).

4. Evaluation of transfer matrix

It is convenient to write the component matrices $\mathbf{D}_i \equiv \mathbf{D}(y_i)$ in (11) as

$$\mathbf{D}_i = \begin{pmatrix} 0 & -[\varepsilon - v(y_i)] \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & -\varepsilon \\ 1 & 0 \end{pmatrix} + \begin{pmatrix} 0 & v_i \\ 0 & 0 \end{pmatrix} \equiv \mathbf{d} + \mathbf{v}_i \tag{17}$$

where the terms $\mathbf{d}$ and $\mathbf{v}_i$ in the second line are respectively the first and second of the 2×2 matrices defined in the previous step of (17). Of these, only $\mathbf{v}_i$ depends on y_i, the relative position within the unit cell. Here

$$\varepsilon \equiv (E - \bar{V})/\mathcal{E}_0 \tag{18}$$

and

$$v_i \equiv (V(y_i) - \bar{V})/\mathcal{E}_0 \tag{19}$$

with $\bar{V}$ being the average potential defined in (14).

The products in the dispersion relation (16) can be built up from pairwise products of $\mathbf{D}$:

$$\mathbf{D}_i\mathbf{D}_j = (\mathbf{d} + \mathbf{v}_i)(\mathbf{d} + \mathbf{v}_j) = \mathbf{d}^2 + \mathbf{v}_i\mathbf{d} + \mathbf{d}\mathbf{v}_j + \mathbf{v}_i\mathbf{v}_j = \begin{pmatrix} -\varepsilon & 0 \\ 0 & -\varepsilon \end{pmatrix} + \begin{pmatrix} v_i & 0 \\ 0 & v_j \end{pmatrix} + 0. \tag{20}$$

Thus, for example, fourth-order products are given by

$$\mathbf{D}_i\mathbf{D}_j\mathbf{D}_k\mathbf{D}_l = \left[-\varepsilon\mathbf{1} + \begin{pmatrix} v_i & 0 \\ 0 & v_j \end{pmatrix} \right]\left[-\varepsilon\mathbf{1} + \begin{pmatrix} v_k & 0 \\ 0 & v_l \end{pmatrix} \right] \tag{21}$$

and so on.

To evaluate the dispersion relation (16), we need the traces of these even products of $\mathbf{D}$. The Trace of $\mathbf{1}$ is 2.

The Trace of $\mathbf{D}_i\mathbf{D}_j$ (the term in $(a/a_0)^2$) is

$$2(-\varepsilon) + \sum_{n=1}^{2}(v_n) \tag{22}$$

where the summation stands for $(V_i + V_j)$.

The Trace of $\mathbf{D}_i\mathbf{D}_j\mathbf{D}_k\mathbf{D}_l$ (the term in $(a/a_0)^4$) is

$$2(-\varepsilon)^2 + (-\varepsilon)\sum_{n=1}^{4}(v_n) + (v_iv_k + v_jv_l). \tag{23}$$

The Trace of $\mathbf{D}_i\mathbf{D}_j\mathbf{D}_k\mathbf{D}_l\mathbf{D}_m\mathbf{D}_n$ (the term in $(a/a_0)^6$) is

$$2(-\varepsilon)^3 + (-\varepsilon)^2\sum_{n=1}^{6}(v_n) + (-\varepsilon)\left\{ \begin{matrix} v_iv_k + v_kv_m + v_mv_i \\ + \quad v_jv_l + v_lv_n + v_nv_j \end{matrix} \right\} + \left\{ \begin{matrix} v_iv_kv_m \\ + \quad v_jv_lv_n \end{matrix} \right\} \tag{24}$$

and so on. These and succeeding traces form the integrands for the multiple integrals appearing in the dispersion relation expansion of (16).

5. Expansion of the dispersion relation

The dispersion relation expansion we have obtained may now be evaluated in terms of ordered integrals of terms such as those given in (22)–(24). These integrals are conveniently defined and labelled as in appendix A: terms I_j indicate j-fold integration of sums of pairwise products of v; J refer to integrals of sums of products of three v; K refer to integrals of products of four v; and so on. These sets can be thought of as 'standard integrals', whose values depend upon the particular potential of interest, but which are all 'of order unity', since they have no hidden dependence on the small parameter (a/a_0).

Expanding both sides of the dispersion relation (16), one obtains

$$\begin{aligned} \cos(ka) &= 1 - \left(\frac{a}{a_0}\right)^2\frac{(ka_0)^2}{2!} + \left(\frac{a}{a_0}\right)^4\frac{(ka_0)^4}{4!} + \dots \\ &= 1 + \left(\frac{a}{a_0}\right)^2\frac{(-\varepsilon)}{2!} + \left(\frac{a}{a_0}\right)^4\left(\frac{(-\varepsilon)^2}{4!} + \tfrac{1}{2}I_4\right) + \left(\frac{a}{a_0}\right)^6\left(\frac{(-\varepsilon)^3}{6!} + \tfrac{1}{2}(-\varepsilon)I_6 + \tfrac{1}{2}J_6\right) \\ &\quad + \left(\frac{a}{a_0}\right)^8\left(\frac{(-\varepsilon)^4}{8!} + \tfrac{1}{2}(-\varepsilon)^2 I_8 + \tfrac{1}{2}(-\varepsilon)J_8 + \tfrac{1}{2}K_8\right) + \dots \end{aligned} \tag{25}$$

where I, J, K and so one are defined in appendix A.

It is a general property of the expansion (25) that there is no term of the form ε^{n-1} in the bracket which multiplies $(a/a_0)^{2n}$; this follows from (A5). This fact has important implications for the band structure. In particular, it will follow that the band structure near the continuum limit (small lattice parameter) will be very insensitive to expansion of the lattice. Another way of saying this is that, as will become evident, the band structure is much more robustly free-electron-like than one might expect *a priori*, as the underlying lattice becomes progressively more granular.

The dispersion relation $E = E(k)$, or alternatively $\varepsilon \equiv [E(k) - \bar{V}]/\mathcal{E}_0 = \varepsilon(ka_0)$, can be obtained easily from (25), either by a perturbation expansion, or else iteratively as illustrated in appendix B Using such a procedure, we obtain

$$
\varepsilon = \left[\left(\frac{a}{a_0} \right)^2 I_4 + \left(\frac{a}{a_0} \right)^4 J_6 + \left(\frac{a}{a_0} \right)^6 \left(K_8 - I_4 I_6 + \frac{2}{4!} I_4^2 \right) \cdots \right]
$$
$$
+ (ka_0)^2 \left[1 + \left(\frac{a}{a_0} \right)^4 \left(\frac{I_4}{3!} - I_6 \right) + \left(\frac{a}{a_0} \right)^6 \left(\frac{J_6}{3!} - J_8 \right) \cdots \right]
$$
$$
+ (ka_0)^4 \left[\left(\frac{a}{a_0} \right)^6 \left(\frac{I_3}{3!3!} - \frac{I_4}{5!} - \frac{I_6}{3!} \right) \cdots \right].
\tag{26}
$$

Equation (26) gives an explicit construction for the band structure of the lowest allowed band, for a general one-dimensional potential $V(x)$. This expansion is expected to be valid for small lattice parameter $(a/a_0) < 1$ and for k-vectors up to order $(ka_0) \sim 1$.

6. Results: why is the band structure so parabolic?

The band structure for the continuum lattice $(a/a_0 \to 0)$ is simply

$$
\varepsilon = (ka_0)^2.
\tag{27}
$$

The band-edge energy is given by $\varepsilon = 0$, that is by $E(0) = \bar{V}$, while the k-dependence of the energy is that of a free electron. The precise effects of lattice expansion reside in the a-dependence of the electron energy, and these effects are different depending on which property is of interest.

The effect of lattice granularity will show up most strongly in the position of the band edge. The top line of (26) indicates that band-edge corrections will be evident to order $(a/a_0)^2$, the lowest order to which lattice corrections enter. The effective mass is inversely proportional to the square bracket in the second line of (26). In contrast to the band edge, (26) implies that the effective mass is only modified by lattice corrections to order $(a/a_0)^4$. Moreover, non-parabolicity of the band structure is even more insensitive to the granularity of the lattice, since it only enters (26) at order $(a/a_0)^6$. It is therefore true quite generally that the band structure $[E(k) - E(0)]$ will be extremely insensitive to the fact that the electron lives in the underlying space of a granular lattice. In fact, inspection of particular examples (such as that of appendix B) indicates very little change indeed in band structure even for lattice constants as big as $a \sim a_0$.

7. Results: lattice roughness

The band structure we obtained is expressed in standard integrals 'of order unity' This statement should be qualified, however. In particular, it may become false if the potential strength should become very large compared to the reference energy $\mathcal{E}_0$ (in some way yet

to be defined). Actually, what is at issue is not the average strength, but rather the relative strength of the deviation $v = (V - \bar{V})/\mathcal{E}_0$ from that average, a sort of measure of the 'roughness' of the potential.

Instead of looking for some general definition of lattice roughness, one can instead obtain some idea of its effects by seeing how the predictions of (26) are modified when v is multiplied by the number λ ($\lambda = 1$ in (26)). This corresponds to a change $V \rightarrow \lambda V$ in the potential itself. It does not represent a simple change in the roughness of the potential, since a change in λ also changes the band-edge energy when the lattice goes to its continuum limit; but we take the point of view that the position of the band edge is of little interest in the present context, especially since it depends in any case upon the arbitrary position of the zero of energy (we note, however, that for an arbitrary energy band the position of the band edge is often of experimental interest [9]).

The effects of increased lattice roughness on the band structure of a general one-dimensional potential $V(x)$ can be obtained from (26) almost by inspection. If the potential roughness is varied by letting $v \rightarrow \lambda v$, then (from appendix A) the standard integrals I, J, $K \ldots$ change as

$$I_n \rightarrow \lambda^2 I_n \qquad J_n \rightarrow \lambda^3 J_n \qquad K_n \rightarrow \lambda^4 K_n \ldots. \tag{28}$$

Equation (26) shows that this change has various effects on the band structure, depending upon the aspect of interest. Explicitly

$$\varepsilon = \left[\lambda^2 \left(\frac{a}{a_0} \right)^2 I_4 + \lambda^3 \left(\frac{a}{a_0} \right)^4 J_6 + \lambda^4 \left(\frac{a}{a_0} \right)^6 \left(K_8 - I_4 I_6 + \frac{2}{4!} I_4^2 \right) \cdots \right]$$

$$+ (ka_0)^2 \left[1 + \lambda^2 \left(\frac{a}{a_0} \right)^4 \left(\frac{I_4}{3!} - I_6 \right) + \lambda^3 \left(\frac{a}{a_0} \right)^6 \left(\frac{J_6}{3!} - J_8 \right) \cdots \right]$$

$$+ (ka_0)^4 \left[\lambda^2 \left(\frac{a}{a_0} \right)^6 \left(\frac{I_3}{3!3!} - \frac{I_4}{5!} - \frac{I_6}{3!} \right) \cdots \right]. \tag{29}$$

Various conclusions follow from (29). For instance, the band edge itself depends linearly on λ even in the limit $(a/a_0) \rightarrow 0$, with granularity corrections of order $\lambda^2 (a/a_0)^2$.

It might seem that our expansion of $E(k)$ in powers of $(a/a_0)^2$ would cease to be meaningful for a potential so strong that, say, $\lambda = (a_0/a) >> 1$. Equation (29) suggests, however, that this is not the case. Ignoring changes in the band edge itself, if the potential is made so strong that $V \rightarrow (a_0/a)^2 V$, (29) predicts a band structure which depends more strongly on lattice granularity than that for the unmodified potential, in that effective mass corrections enter to order $(a/a_0)^2$ rather than to order $(a/a_0)^4$. But corrections to band parabolicity are still suppressed, entering only to order $(a/a_0)^4$. Even for such strong potentials, then, the band structure is strongly parabolic, although less robustly so than for more moderate lattice potentials, when we are considering shrunken lattices $a < a_0$.

8. Points for further study

It is of interest to determine whether results similar to those presented here will hold for band structures in the vicinity of higher band minima. It is also of importance to determine whether results similar to those obtained here apply to lattices of higher dimensions.

The present study was suggested by questions arising in the context of delta doping, where it is commonly assumed for practical purposes that the attractive donor potential arising from a disordered planar collection of ionized donors can be adequately approximated by a uniform plane sheet of charge with the same average charge density, both with respect

to subband energies and wavefunctions resulting from quantum confinement, and to the electron band structure in the plane of the well. The present work would seem to touch most directly on the second of these approximations. These and other implications of present results will be discussed elsewhere.

We also note that the 'general' results presented here do not apply within the tight-binding model. This might have been guessed from the fact that, for instance, the effective mass emerging from the nearest-neighbour tight-binding Hamiltonian with constant off-diagonal elements is not the free-electron mass, but instead is inversely proportional to the strength of the off-diagonal potential [13]. Study of specific tight-binding examples also seems to indicate (a) that the continuum limit $a \rightarrow a_0$ need not give a parabolic band structure over the whole range $(ka_0) \lesssim 1$, and (b) that the limiting band structure may or may not be robust against changes in the lattice constant. These questions will be discussed in more detail elsewhere.

9. Summary

Given a one-dimensional periodic potential, the band structure $E(k)$ of the associated lattice has been written in a way that demonstrates explicitly its transition to the continuum (free electron) limit. The continuum limit itself is specified as the limit $a/a_0 \rightarrow 0$ with the lattice potential $V(x)$ required to be of the form $V(x/a)$, where a is the lattice constant and a_0 some fixed reference length. It has also been possible to see explicitly the interplay between lattice granularity effects and effects due to increasing the overall strength of the lattice potential.

The results, (26) and (29), show that for $(a/a_0) < 1$ the band structure is very robustly parabolic and free-electron like, even for lattices so granular that a approaches a_0 for all the k-vectors that can legitimately be considered, that is for k up to $ka_0 \sim 1$. These conclusions also hold, though less strongly, if the potential itself is allowed to become very strong. Specific illustrations of these results will be presented elsewhere.

Acknowledgments

Appendix A. Standard integrals

It is helpful to give convenient labels to the different terms which arise in the calculation of the dispersion relation expansion (14). The following 'standard integrals' form the calculational ingredients in this expansion.

(i) Integrals I_{2n}:

$$I_4 = \int_0^1 \ldots \int_0^{y_3} \mathrm{d}y_1 \ldots \mathrm{d}y_4 \, [v_1 v_3 + v_2 v_4]$$

$$I_6 = \int_0^1 \ldots \int_0^{y_5} \mathrm{d}y_1 \ldots \mathrm{d}y_6 \, [v_1 v_3 + v_3 v_5 + v_1 v_5 + v_2 v_4 + v_4 v_6 + v_2 v_6] \qquad (A1)$$

and so on. Here v_i denotes $v(y_i)$, and successive integrals of type I integrate the sum of all possible pairwise 'even' products $v_i v_j$ (that is, products $v_i v_j$ with different even subscripts) plus all possible pairwise 'odd' products.

(ii) Integrals J_{2n}:

$$J_6 = \int_0^1 \ldots \int_0^{y_5} dy_1 \ldots dy_6 \, [v_1 v_3 v_5 + v_2 v_4 v_6]$$

$$J_8 = \int_0^1 \ldots \int_0^{y_7} dy_1 \ldots dy_8 \, [v_1 v_3 v_5 + v_3 v_5 v_7 + v_5 v_7 v_1 + v_7 v_1 v_3 + v_2 v_4 v_6$$
$$+ v_4 v_6 v_8 + v_6 v_8 v_2 + v_8 v_2 v_4]$$
(A2)

and so on. Here successive integrals of type J integrate the sum of all possible three-member 'odd' products $v_i v_j v_k$ plus all possible 'even' ones.

(iii) Integrals K_{2n}:

$$K_8 = \int_0^1 \ldots \int_0^{y_7} dy_1 \ldots dy_8 \, [v_1 v_3 v_5 v_7 + v_2 v_4 v_6 v_8]$$

$$K_{10} = \int_0^1 \ldots \int_0^{y_9} dy_1 \ldots dy_{10} \, [v_1 v_3 v_5 v_7 + v_3 v_5 v_7 v_9 + \ldots + v_2 v_4 v_6 v_8 + v_4 v_6 v_8 v_{10} + \ldots]$$
(A3)

and so on. Integrals of type K involve the sum of all possible products of four v_i with different odd indices plus all those with different even indices.

(iv) Integrals L_{2n}:

$$L_{10} = \int_0^1 \ldots \int_0^{y_9} dy_1 \ldots dy_{10} \, [v_1 v_3 v_5 v_7 v_9 + v_2 v_4 v_6 v_8 v_{10}]$$
(A4)

and so on. Integrals L have integrands having all possible different 'odd' plus all possible 'even' products of five v_i.

The values of the integrals I, J, K, ... will depend upon the particular potential under consideration, but are all 'of order unity', since the dependence on the small parameter (a/a_0) has been made explicit by taking it outside the integrations.

Finally, we note that the integrals of the form

$$\int_0^1 \ldots \int_0^{2n-1} dy_1 \ldots dy_{2n} \sum_{i=1}^{2n} v_i = 0$$
(A5)

vanish identically. This follows because

$$\int_0^1 dy \, v(y) = 0$$
(A6)

in consequence of its definition (19), and because it can be shown (for example by induction) that

$$\int_0^b dy_1 \ldots \int_0^{y_{n-1}} dy_n \, [v(y_1) + \ldots + v(y_n)] = \frac{b^{n-1}}{(n-1)!} \int_0^b dy \, v(y).$$
(A7)

Appendix B. Iterative solution of dispersion relations (an example)

Here we illustrate the iterative method used to solve (25) by applying it to the equation

$$\cos(ka) = \cosh(qa) - \frac{1}{2}\left(\frac{a}{a_0}\right)^2 \frac{\sinh(qa)}{(qa)}.$$
(B1)

Equation (B1) is the dispersion relation for the simple Kronig–Penney potential

$$V(y) \equiv V(x/a) = -\mathcal{E}_0 \sum_{n=-\infty}^{\infty} \delta(x/a - n).$$
(B2)

Here k is the lattice momentum, while q is the wave vector of the electron

$$q^2 = -2mE/\hbar^2.$$

Equation (B1) may be solved iteratively for $q = q(k)$. Other dispersion relations are easily obtained in the same fashion. We define

$$x = (ka)^2 = \delta(ka_0)^2 \qquad y = (qa)^2 = \delta(qa_0)^2 \qquad \delta \equiv (a/a_0)^2. \qquad \text{(B3)}$$

Equation (B1) then has the form

$$F(x) = G(y) + \delta H(y) \tag{B4}$$

where

$$F = \sum f^{(n)} = \sum a_n x^n \qquad G = \sum g^{(n)} = \sum b_n y^n \qquad H = \sum h^{(n)} = \sum c_n y^n. \tag{B5}$$

We choose (B4) such that $g^{(0)}(y) = y$, and look for $y = y(x)$ as a power series in x, and in the small parameter δ. The solution to nth order in δ is denoted y_n.

Iteration of (B4) is straightforward; y_0 is the solution of the (linear) equation

$$f^{(0)}(x) = g^{(0)}(y_0) = y_0.$$

Similarly, for y_1 we solve

$$y_1 = g^{(0)}(y_1) = -g^{(1)}(y_0) + f^{(0)} + f^{(1)} + \delta h^{(0)}(y_0).$$

For y_2

$$y_2 = g^{(0)}(y_2) = -g^{(1)}(y_1) - g^{(2)}(y_0) + f^{(0)} + f^{(1)} + f^{(2)} + \delta\left[h^{(0)}(y_1) + h^{(1)}(y_0)\right]$$

and so on.

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