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Resonance states in scattering: some variational methods revisited

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Abstract. We have studied two variational methods of scattering, namely the Kohn method and the Harris modification of it and applied them to resonance. As a case study, we have considered a coulombic acceptor impurity potential in a zero-gap semiconductor like mercury telluride in which, on physical grounds, an impurity resonance is expected and also the free particle Hamiltonian has a fairly complex structure due to the strong spin orbit coupling.

The advantages and the limitations of the two methods are discussed with an emphasis on resonance.

We have made a significant improvement in the algorithms of both methods over their previous applications in the literature and have emphasised the role of the non-linear parameter which in effect has been used as a variational parameter in the theory.

1. Introduction

We are currently studying resonance impurity states in zero-gap semiconductors. The details of this study will be reported elsewhere (Joos *et al* 1978). We have employed methods of scattering theory, and in particular variational methods, to study the resonance states. We find that in the scattering literature although variational methods have occasionally been used to calculate resonance states, the pitfalls and possible improvements in the algorithm along the lines we have explored have not been properly discussed. We have decided to present our findings on two of the simplest variational methods in the hope that these will be of some interest and use to a wider section of physicists, many of whom, like the authors, may have felt the need for a simple yet reliable method to calculate such a delicate entity as a resonance state.

As is well known, a number of variational methods have been proposed in scattering theory. These are described in most standard references. We refer the reader to Joachain (1975) and to Truhlar *et al* (1974). We have explored two of these methods: (a) the Kohn method and (b) the Harris method which is a modification of the method of type (a). We have chosen these two methods because we find that they are the simplest to use and yet their physical content is appealing. The other variational methods based on the Feshbach projection formalism appear to us to be computationally involved. In some recently proposed variational methods based on the Rayleigh-Ritz principle, the resonance width (to be discussed later) is not calculable, as has been pointed out by Bransden (1977). These theories are therefore defective.

The problem under study is the resonance state due to an acceptor coulombic impurity in a zero-gap semiconductor, described by the Hamiltonian

$$H = H_0 + V(r) = (2m_0)^{-1}[(\gamma_1 + \frac{5}{2}\gamma)\mathbf{p}^2 - 2\gamma(\mathbf{p} \cdot \mathbf{J})^2] + V(r) \quad (1)$$

where m_0 is the free electron mass. J_x , J_y and J_z are 4×4 matrices corresponding to the angular momentum operator \mathbf{J} , having the value $J = \frac{3}{2}$; $\gamma = \frac{1}{5}(2\gamma_2 + 3\gamma_3)$. γ_1 , γ_2 and γ_3 are the band parameters of the host material. The complex structure of H_0 is due to the strong spin-orbit coupling and the symmetry induced degeneracy of the energy bands. The impurity potential $V(r)$ is taken to be spherically symmetrical. The calculations have been done for a screened coulomb potential

$$V(r) = \frac{e^2}{\epsilon_0} \frac{\exp(-r/b)}{r},$$

ϵ_0 being the bulk dielectric constant.

For a zero-gap semiconductor like mercury telluride (HgTe), the unperturbed Hamiltonian describes two degenerate bands—one conduction electron band and one hole band with small and large effective masses respectively (Gel'mont *et al*, 1976). An acceptor impurity has localised states in ordinary gap semiconductors. In a gap-less semiconductor, these states fall within the conduction band continuum and are expected to give rise to resonance states. The purpose of this paper is to show that a reliable calculation of these resonance states can be done by the Kohn-Harris variational methods.

2. Variational methods

Let us briefly recall the main features of scattering theory for our purpose. For the Schrödinger equation (in atomic units)

$$(-\nabla^2 + V(r))\psi_k = E_k\psi_k$$

with a spherically symmetric $V(r)$, $\psi_k(r)$ can be decomposed in partial waves

$$\psi_k(r) = \sum_l \frac{u_{l,k}(r)}{r} Y_l^m(\theta, \phi) \quad (2)$$

and the radial equation for $u_{k,l}(r)$ reads

$$(H - E)u_l(r) = 0$$

$$H = -\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2} + V(r). \quad (3)$$

A similar decomposition of equation (1) can be made, though the algebra is somewhat involved. This has been done by Gel'mont and D'yakonov (1972) and by Baldereschi and Lipari (1973). Due to the spin orbit coupling in the Hamiltonian (1), the lowest radial functions are now $u_0(r)$ and $u_2(r)$ satisfying the coupled equations

$$\begin{bmatrix} \frac{d^2}{dr^2} - V(r) + E & \mu \left(\frac{d^2}{dr^2} + \frac{3}{r} \frac{d}{dr} \right) \\ \mu \left(\frac{d^2}{dr^2} - \frac{3}{r} \frac{d}{dr} + \frac{3}{r^2} \right) & \frac{d^2}{dr^2} - \frac{6}{r^2} - V(r) + E \end{bmatrix} \begin{bmatrix} u_0(r) \\ u_2(r) \end{bmatrix} = 0 \quad (4)$$

where we have used for convenience the effective Rydberg units

$$R_0 = e^4 m_0 / 2 \hbar^2 \epsilon_0^2 \gamma_1 \quad a_0 = \hbar^2 \epsilon_0 \gamma_1 / e^2 m_0$$

ϵ_0 being the bulk dielectric constant of the medium. The band parameters have been condensed into $\mu = (6\gamma_3 + 4\gamma_2) / 5\gamma_1$.

The scattering solution of (3) has the boundary conditions that

$$u_l(0) = 0 \quad \text{and} \quad u_l(r) \rightarrow \sin kr + \lambda_l \cos kr, \quad r \rightarrow \infty. \quad (5)$$

$u_l(r)$ is asymptotically characterised by the phase shift δ_l , or more conveniently by $\lambda_l = \tan(\delta_l - p\pi/2)$. The corresponding boundary conditions for our problem of zero-gap semiconductors will be

$$\begin{bmatrix} u_0 \\ u_2 \end{bmatrix} \rightarrow 0, \quad r \rightarrow 0 \quad (6)$$

and

$$\begin{bmatrix} u_0 \\ u_2 \end{bmatrix} \rightarrow (\sin kr + \lambda \cos kr) \begin{bmatrix} 1 \\ \pm 1 \end{bmatrix}, \quad \begin{array}{l} + \text{ for electron} \\ - \text{ for hole} \end{array}$$

$$r \rightarrow \infty,$$

where λ is the tangent of the $l = 0$ phase shift and part of the $l = 2$ phase shift. The free particle kinematics are given by

$$E_{\pm}(k) = (1 \pm \mu)k^2.$$

When a phase shift passes and *increases* rapidly through $\frac{1}{2}\pi$ (modulo π), a resonance in scattering is said to occur. The scattering cross section σ having the familiar form

$$\sigma = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \sin^2 \delta_l$$

shows a peak due to a maximum in the l th partial wave contribution—in our case from u_0 and u_2 . The scattering state corresponding to this energy has a quasi-localised behaviour. The state has, of course, a finite lifetime and hence a finite width Γ given by

$$\Gamma = \left(\frac{d\delta}{dE} \right)_{E=E_R}^{-1}. \quad (7)$$

The positivity of Γ ($\Gamma > 0$), a consequence of causality, requires that δ_l should increase through $\pi/2$ at a true resonance. For a well-defined resonance we require $\Gamma \ll E_R$.

A variational method can be set up to solve for the scattering states of equation (3) as in a bound state problem but with the important difference that $u_l(r)$ does not vanish asymptotically but behaves as equation (5). It can be shown that the integral

$$J = (\mu |H - E|u) - k\lambda \quad (8)$$

where $(x) = \int_0^{\infty} x \, dr$ yields equation (3) with the boundary conditions (5), through its first order variation $\delta J = 0$.

Such a variational method usually makes use of trial functions of the form

$$u_t = \phi + S + \lambda C$$

$$\phi = \sum_{i=1}^N c_i \eta_i. \quad (9)$$

η_i is a basis set of localised functions with the c_i 's as the linear variational parameters, and asymptotically

$$S(r) \sim \sin kr; \quad C(r) \sim \cos kr \quad S(0) = C(0) = 0.$$

We shall first use the Kohn variational method and then the Harris method which is an interesting modification of the former. Since these methods are well known, we shall merely quote the essential steps.

2.1. The Kohn method

In this method the variational integral J is made stationary with respect to all the c_i 's and λ . $\partial J/\partial c_i = 0$ leads to

$$\sum_i (\eta_i | H - E | \eta_i) c_i = -(\eta_i | H - E | S + \lambda C), \quad i = 1, \dots, N. \quad (10)$$

The c_i 's can be written as

$$\sum_i (\eta_i | H - E | \eta_i) c_i^{S,C} = -(\eta_i | H - E | S), \quad i = 1, \dots, N.$$

It is convenient to write ϕ as

$$\phi = \phi_S + \lambda \phi_C$$

where

$$\phi_S = \sum_i c_i^S \eta_i, \quad \phi_C = \sum_i c_i^C \eta_i, \quad (11)$$

and after some algebra, $J(\lambda)$ can be expressed as

$$J(\lambda) = M_{00} + 2M_{10}\lambda + M_{11}\lambda^2$$

where

$$M_{00} = (S | H - E | \phi_S + S), \quad M_{10} = (C | H - E | \phi_S + S), \quad M_{11} = (C | H - E | \phi_C + C). \quad (12)$$

Next

$$\partial J/\partial \lambda = 0$$

leads to

$$\lambda_{\text{Kohn}} = -M_{10}/M_{11}. \quad (13)$$

In the Kohn method the integral $I = (u | H - E | u)$ is not put equal to zero. Consequently a second order correction to λ_{Kohn} can be made to give

$$[\lambda]_{\text{Kohn}} = \lambda_{\text{Kohn}} - k^{-1} I(\lambda_{\text{Kohn}}). \quad (14)$$

In fact the smallness of I in equation (14) can serve as a guideline for a reliable calculation which requires that J be stationary and $I \approx 0$.

The method can be applied to equation (4) with the boundary conditions (6) by considering the variational integral

$$J = (u_0, u_2 | \underline{H} - E | u_0, u_2) - 2(1 \pm \mu)k\lambda. \quad (15)$$

In arriving at equation (12) we utilised the symmetric property of the Hamiltonian

matrix such as

$$(\eta_i | H - E | \eta_i) = (\eta_i | H - E | \eta_i)$$

and

$$\left(\begin{array}{c} S \\ C \end{array} \middle| H - E \middle| \begin{array}{c} \eta_i \\ \eta_i \end{array} \right) = \left(\eta_i \middle| H - E \middle| \begin{array}{c} S \\ C \end{array} \right).$$

Because of the spin-orbit coupling term in the Hamiltonian of our problem this symmetry property no longer holds. Consequently all the relevant expressions will appear in symmetrised form. Equation (10), for instance, will now be

$$\sum_{i=1}^{2N} [(\chi_i | H - E | \chi_i) + (\chi_i | H - E | \chi_i)] c_i \\ = -[(\chi_i | \underline{H} - E | \underline{S} + \lambda \underline{C}) + (\underline{S} + \lambda \underline{C} | \underline{H} - E | \chi_i)], \quad i = 1, \dots, 2N. \quad (16)$$

where $\chi_{2i-1} = \eta_i^{(0)}$, $\chi_{2i} = \eta_i^{(1)}$, $\underline{S} = S_{(\pm 1)}$ and $\underline{C} = C_{(\pm 1)}$, N being the size of the set of η_i 's and $H - E$ the radial Hamiltonian. It should be noted that because of the two-component (spinor) nature of u_0 and u_2 , equation (16) is a $2N \otimes 2N$ matrix equation.

The Kohn method is simple and physically appealing. Unfortunately this method and the methods of its type have to contend with the appearance of some unphysical singularities, first noted by Schwartz (1961). Unlike the case of bound states, the scattering energy E scans a wide range in the process of calculation and E is likely to come close to an eigenvalue of H within the space spanned by the η_i 's. The unphysical singularities are related to the existence of these eigenvalues. We refer to Truhlar *et al* (1974) for a satisfactory and elaborate discussion of these singularities. Briefly, when E is equal to one of these eigenvalues, M_{10} and M_{11} develop poles of odd order. Because of these odd ordered poles, each of them passes through every value in the range $-\infty$ to ∞ in the vicinity of these eigenvalues. (This situation would not arise in a bound state problem where E is bounded from above.) Depending on the order in which M_{10} and M_{11} reach zero, λ will develop spurious singularities manifesting a resonance-like or an antiresonance-like behaviour. In the limit where the basis set is large enough to represent the exact solution, if the singularity is spurious, the zeroes of M_{10} and M_{11} coincide and the singularity disappears (except in the case of a real resonance). Besides, the existence of the eigenvalues poses another problem: the left hand side matrix of equation (10) will have a vanishing determinant and hence the matrix cannot be inverted. Therefore the variational calculation cannot be executed.

To avoid these difficulties, a non-linear parameter—in contrast to the linear parameters c_i —is introduced in the basis set $\{\eta_i\}$. In our calculation η_i has been taken as $\eta_i = (r/\alpha)^i \exp(-r/\alpha)$, $i = 1, \dots, N$, where α is the non-linear parameter. This parameter is then scanned to avoid the singularities. Specifically the algorithm of the Kohn method now proceeds as follows: for a given value of k , $\lambda(k)$ is calculated for several values of the non-linear parameter α , the singularities being avoided each time. A schematic plot of $\lambda(k)$ versus α is shown in figure 1. The singularities lie between the curves. α_S is selected from the smoothest plateau. The process is repeated for several values of k , resulting in a plot of $\alpha_S(k)$. This $\alpha_S(k)$ is then fed back into the basis set. Finally $\lambda(k)$ is calculated for various values of k . In the end, the singularities and the eigenvalues do limit the Kohn method. The number of eigenvalues increases as the basis set is increased and the matrix inversion becomes more and more difficult.

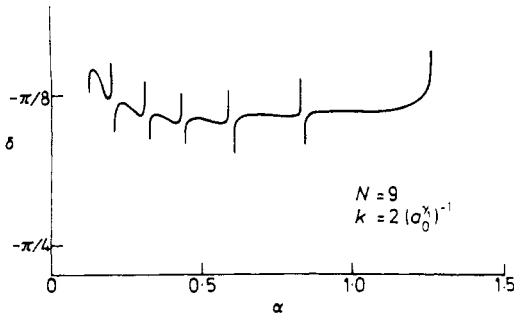


Figure 1. Typical plot of phase shift δ versus α , the non-linear parameter. k_μ 's lie about midway between the singularities.

2.2. The Harris method

Harris has introduced a modification of the Kohn method which avoids the spurious singularities and at the same time exploits the troublesome eigenvalues to advantage. We refer to Nesbet (1968) for a detailed account of this method. Harris noted that equation (10) can profitably be employed at the singular points where the matrix inversion fails, i.e. when $E = E_\mu$, one of the eigenvalues. let us consider ϕ_μ given by

$$\phi_\mu = \sum_i c_i^\mu \eta_i.$$

From equation (10) we obtain

$$\sum_i c_i^\mu \sum_j (\eta_j | H - E | \eta_j) c_j = - \sum_i c_i^\mu (\eta_i | H - E | S + \lambda C)$$

whence

$$(\phi_\mu | H - E | \phi) = -(\phi_\mu | H - E | S + \lambda C)$$

i.e.

$$(\phi | H - E | \phi_\mu) = -(\phi_\mu | H - E | S + \lambda C). \tag{17}$$

When $E = E_\mu$, the left hand side vanishes, giving rise to the difficulty of the matrix inversion in equation (10). But it can now be avoided if at the same time we require that

$$(\phi_\mu | H - E | S + \lambda C) = 0 \tag{18}$$

which immediately yields the phase shift

$$\lambda_{\text{Harris}} = - \frac{(\phi_\mu | H - E | S)}{(\phi_\mu | H - E | C)}. \tag{19}$$

It is interesting to note that λ_{Harris} is, as Nesbet has shown, actually the analytical limit of λ_{Kohn} (without the second order correction). The condition (18) therefore makes J stationary not only with respect to the inner wavefunction but with respect to λ as well.

The algorithm of the Harris method is then as follows: one calculates for a given α , the same non-linear parameter as in the Kohn method, a set of E_μ 's from the matrix

eigenvalue equation

$$\begin{aligned}
 (\tilde{H} + E_\mu \tilde{S}) \tilde{C}^\mu &= 0 \\
 \tilde{H}_{ij} &= (\eta_i | H | \eta_j) \\
 \tilde{S}_{ij} &= (\eta_i | \eta_j) \quad ; \quad i, j = 1, \dots, N.
 \end{aligned}
 \tag{20}$$

For each α , N values of λ are obtained corresponding to different k_μ 's. This procedure is repeated for a range of α , resulting in N curves for λ versus k . It is now seen that as the basis set N is increased a number of curves coalesce into one which does not move as N is increased further. This then implies that for a fixed k , a plot of λ versus α , as in figure 1, will have a plateau and stationary solutions with respect to α will obtain. It is to be noted that in our problem each of the λ_{Harris} versus k curves shows a resonance or rather a pseudo-resonance. When the convergence of the curves with respect to the basis set is reached we can conclude that a real resonance has been calculated. A plot of such an optimum resonance curve for a screened coulomb potential is shown in figure 2. The quantity of direct physical interest in our problem is the resonance energy E_R . As stated in the Introduction, we find that the convergence of E_r is somewhat faster than that of the phase shift δ . A plot of E_R versus α in figure 3 is presented and commented on in § 3.

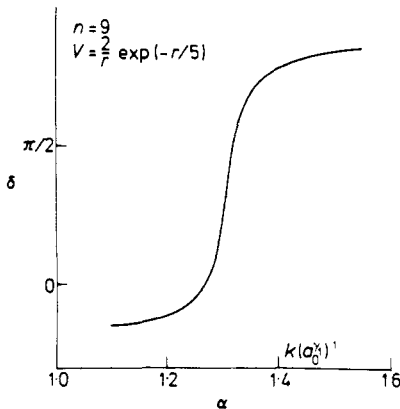


Figure 2. Phase shift δ as a function of k near a resonance (Harris method).

3. Results for a screened coulomb potential

With representative parameters for a typical zero-gap semiconductor, we take

$$V(r) = (2/r) \exp(-r/5).$$

The band parameters are $\mu = 1.1$ with

$$m_c^* = 0.029m_0, \quad m_v^* = 0.60m_0.$$

Figure 2 is a plot of the phase shift versus energy calculated in the Harris method for a basis set of size $N = 9$. The corresponding Kohn plot is close to it, giving approximately the same value of the resonance energy.

3.1. Resonance energy

Figure 3 is a plot of k_R versus α calculated in the Harris method for different values of N . As the figure indicates, convergence is reached in the range $0.3 \leq k\alpha \leq 0.9$ for $N = 8, 9$. When N is increased further, the plateau merely broadens horizontally. In fact we have extended the calculation to a more complex screened coulomb potential and have observed a similar trend (Joos *et al* 1978). The non-linear parameter α is intuitively related to the range of the potential. The reliable range of this parameter can conceivably be estimated at a theoretical level though we have not yet been able to explore it.

3.2. Resonance width

The resonance state has a finite life time because of its interaction with the continuum, and hence a finite width (cf the Breit–Wigner formula). The width indicates the strength of the resonance. In our calculation the width Γ of equation (7) has been obtained from the slope of the δ versus k curve at the resonance point. The widths in both the methods are found to be much smaller than E_R , indicating a sharp resonance. This is indeed in accord with the expectations on physical grounds as discussed in the Introduction.

4. Discussion

In this section we shall discuss two aspects of the calculation—the special role of the non-linear parameter and a comparative evaluation of the two variational methods.

4.1. Optimum use of α

An important highlight of our calculation is the optimum use of the non-linear parameter α which, in effect, has been used as a variational parameter. It appears that in the previous calculations with the Kohn method only a few values of α are scanned, mainly to keep away from the spurious singularities. In the few papers dealing with the Harris method we do not find an attempt to ensure that $\partial\lambda/\partial\alpha$ should also vanish, along with two other stationary conditions. We have made specific attempts to ensure this in both methods. Recalling equation (8) for J and equation (14) for $[\lambda]_{\text{Kohn}}$ we see that

$$\partial J/\partial\alpha = 0 \quad \Rightarrow \quad \partial[\lambda]_{\text{Kohn}}/\partial\alpha = 0. \quad (21)$$

In our calculation we have ensured that $\partial[\lambda]_{\text{Kohn}}/\partial\alpha$ should vanish. J is thus made stationary with respect to all the parameters, linear and non-linear. It can be argued that since in the Kohn method, with several values of α one normally obtains a plateau, a Kohn variational calculation would imply the vanishing of $\partial\lambda/\partial\alpha$, and $\partial J/\partial\alpha = 0$ would result. In previous variational calculations, however, only a few values of α have usually been considered, which would not result in a satisfactory plateau, and hence $\partial J/\partial\alpha$ cannot be regarded as vanishing with certainty. At the same time it should be emphasised that $\partial J/\partial\alpha = 0$ by itself *does not* necessarily ensure the full stationariness of J and hence a rapid convergence. Though $\partial J/\partial\alpha$ is vanishing for each plateau, the integral I may not necessarily be zero for each of them. We have searched and picked up that plateau for which $I \approx 0$. We believe that this full optimum use of α is a significant improvement over previous calculations of this type. It may be noted that

through optimising J with respect to α , the variational estimates for the phase shift and the wavefunctions satisfy the virial theorem of scattering theory (Demkov 1963, Heaton and Moiseiwitch 1971, McWhirter and Moiseiwitch 1974).

In the Harris method such an optimisation is less satisfactory. The reason is that, as we have noted, the Harris value is the analytical continuation of the Kohn phase shift. One can therefore obtain a Harris plateau. But I as such cannot be estimated in the Harris method. The optimisation procedure is thereby limited.

4.2. Comparison of the two methods

We shall finally make a few remarks on the relative merits of the two variational methods, with regard to their efficiency and accuracy in calculating resonance as well as non-resonance scattering. If the phase shift for a given energy is required, the Kohn method is more advantageous and satisfactory. In this method one has an explicit knowledge of I which should go to zero for an exact solution. The size of I therefore serves as an indication of the convergence being reached. The phase shift in the Kohn method can be variationally corrected and improved. Such an improvement cannot be done in the Harris method, where the only test of convergence is the convergence of λ to a fixed value as the basis set is increased toward completeness. There is a modified version of the Harris method due to Harris and Michels (1971) which can be variationally corrected. But in the latter method one has to calculate the free-free integrals, i.e. the integrals involving only the asymptotic wavefunctions. These integrals are often the most difficult to evaluate. A distinct advantage of the Harris method is that the free-free integrals need not be evaluated. The bulk of computation is accordingly greatly reduced. Furthermore since an explicit knowledge of ϕ is not needed in the Harris method, the difficulties with the singularities are avoided and, consequently, if the phase shift for a wide range of energy is required—as in our problem—the Harris method is expected to give good results with less computational labour.

There are also other reasons to believe that the Harris method is more advantageous specifically for the calculation of resonances. Let us consider two more computational difficulties with the Kohn method:

(a) The stationary value α_S of the non-linear parameter varies with the scattering energy. We have considered several plots like the one in figure 1, and have drawn a curve for $\alpha_S = \alpha_S(k)$. For reasons of computational cost we did not consider a large number of k -values. The curve was interpolated across the resonance k -value in a simpler manner, guaranteeing however that at a resonance the $\alpha_S(k)$ curve does not have a pronounced deviation from its projected path.

(b) One can improve the $\alpha_S(k)$ curve by taking more values of k , though at a computing cost. However, this by itself may not necessarily improve the final result. The reason is that a calculation with more k -values will amount to scanning extensively off resonance where the convergence is not very good, though it is good near a resonance. This can be attributed to the simplified nature of the trial functions used. For instance, off resonance the asymptotic part of the wavefunction may be more complicated, especially for a coulombic potential. These difficulties are either not encountered or are bypassed in the Harris method. The phase shift is now computed at E_μ 's, the eigenvalues obtained from equation (20) corresponding to the localised set η_i . Since a resonance is associated with a quasi-localised state embedded in the continuum, we expect on

physical grounds one of the E_μ 's to converge toward the resonance energy E_R . With a judicious choice of the localised set one can therefore hope to achieve a reasonably rapid convergence of E_μ to E_R .

In the Harris method we do not look for a stationary $\alpha_S(k)$ as such. As already stated, we scan over a reasonable interval of α . This leads directly to a set of $2N$ potential resonance curves, N being the size of the basis set. The convergence of these curves as N is increased determines the reliable E_R . The somewhat delicate problem with the $\alpha_S(k)$ curve is thus avoided.

In view of the discussion by Truhlar *et al* (1974), we have decided to limit our comparative study of the two methods mainly to resonance. We would like to make a remark on the use of the *linear* phase shift parameter λ_i in both the methods. At resonance δ_i increases through $\frac{1}{2}\pi$ (modulo π) and λ_i diverges. Since λ_i is a linear parameter in the method we have described, the study of resonance is a delicate problem. This difficulty with $\lambda \rightarrow \infty$ at resonance can of course be avoided with a more realistic choice of the asymptotic wavefunction, e.g. of the form $\sin(kr - \delta_i)$. δ_i is now a *non-linear* parameter in the theory. With such a trial function, however, the Kohn method may be virtually intractable. In the Harris method the phase shift can be calculated though with considerable labour.

We shall conclude with an observation on the minimum principle, if any, in our calculation. Unlike the bound state case, the variational calculation in scattering usually lacks a criterion for the minimum of the quantity being calculated, namely the phase shift. Establishing such a minimum principle for a general class of potentials seems to be a difficult task. We have however noted an interesting result in our calculation. The resonance energy is found to converge faster than the phase shift as N is increased to $N = 8, 9$ (figure 3). The convergence of the energy eigenvalue is

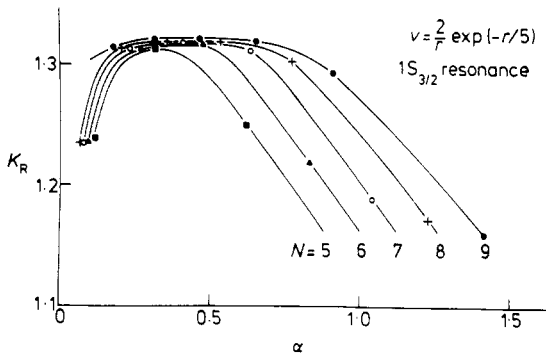


Figure 3. Dependence of momentum k_R at resonance on the size N of the basis set and the non-linear parameter α . The points on each curve correspond to the Harris values obtained for a given value of N .

somewhat reminiscent of the bound state problem. It is perhaps a fortunate consequence of our calculation being primarily directed at a resonance state for which the localised part of the wavefunction plays a more decisive role. The form of the wavefunction is thus simplified and the trial function becomes more accurate. However, the particular choice of the Hamiltonian (1) for a gap-less semiconductor and the optimum use of the non-linear parameter may also have contributed to the convergence.

Acknowledgments

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