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Two-Dimensional Electron Layers in External Fields: Analysis of the Effects of Non-Separability.

Samir Kumar Bhattacharya
Louisiana State University and Agricultural & Mechanical College

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TWO-DIMENSIONAL ELECTRON LAYERS IN EXTERNAL FIELDS: ANALYSIS OF THE EFFECTS OF NON-SEPARABILITY

The Louisiana State University and Agricultural and Mechanical Col. Ph.D. 1982

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TWO DIMENSIONAL ELECTRON LAYERS IN EXTERNAL FIELDS: ANALYSIS OF THE EFFECTS OF NON-SEPARABILITY

A Dissertation

Submitted to the Graduate Faculty of the Louisiana State University and Agricultural and Mechanical College in partial fulfillment of the requirements for the degree of Doctor of Philosophy

in

The Department of Physics and Astronomy

by

Samir Kumar Bhattacharya
B.Sc. (Hons), University of Calcutta, 1972
M.Sc., University of Delhi, 1975

December 1982
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This work is dedicated to my parents.
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ABSTRACT

Two-dimensional electron layers when placed in external electric and magnetic fields can display interesting features which arise solely due to the non-separability of electronic motions. Through simple, single electron Hamiltonians, we have studied in considerable detail the effects of the nonseparability on the eigenvalue structure of two distinct systems.

Intersubband cyclotron combined resonances in a quasi-two-dimensional space charge layer as found in metal-oxide-semiconductor sandwiches are studied using "triangular well" approximation. Two alternative basis sets have been pointed out which enable one to obtain analytical matrix elements of the Hamiltonian for all values of the magnitude and the angle of tilt of the applied magnetic field. Yet another basis set, constructed out of some variationally determined parameters, has been indicated which would facilitate the diagonalization of the Hamiltonian. The coupling between electronic motions normal and parallel to the layer has been found to give rise to deviations in the expected value of the Landau spacings as functions of the tilt angle of the magnetic field. Optical spectra for such systems show some features in qualitative agreement with experiments and other calculations. The system is a prototype
of nonseparable problems in two dimensions.

Surface state electrons on liquid helium when placed in perpendicular electric and magnetic fields can have a potential well with two minima for the electronic motion normal to the surface. Such double-minimum potential wells also arise for highly excited Rydberg states of atoms in crossed electric and magnetic fields and in certain molecular potential curves. We applied a WKB formalism, modified to treat cases when two of the classical turning points become very close together, to such double-minimum wells and calculated the energy splittings that arise when one is near "degeneracy", that is when either well, considered independently, can support a bound state at the same energy. We have also applied this formalism to many other potential curves considered previously in the literature to test its efficacy, for the first time to our knowledge, against other known methods.
A. Non-separable Problems

Non-separable problems in quantum mechanics are mostly associated with physical systems whose Hamiltonians fail to decouple into a sum of mutually commuting parts, each describing an independent dynamical mode of the system. A classic example, which continues to draw attention from physicists even today, is the case of an atom in a magnetic field. However, the question of non-separability may also arise in a problem due to a certain way of viewing the corresponding Hamiltonian. Thus, even in a single dimension, the motion of a particle in one of the wells of a double minimum potential (DMP) affects the motion in the other well, for they are actually coupled together because of possible tunneling through the intervening barrier (assumed to be of finite height and thickness). For a symmetric DMP, the eigenstates will therefore be only asymptotically degenerate and it is this coupling that is responsible for lifting the "degeneracy" of such a level and for consequent emergence of doublet structures around it. Numerous examples of actual physical systems having such DMPs can be found in the literature; for
specificity, we mention here the well known case of the ammonia molecule\(^1\), where such coupling gives rise to so-called inversion splitting.

Very often, non-separability of two (or more) otherwise independent dynamical modes of a system of interest can be, and is, introduced deliberately so as to study its effects on the character of the system as a function of some external parameter. Depending on the strength of the coupling so introduced, the effects may be as varied as the need for different theoretical approaches to understand them. Thus, to cite again the system of atoms in magnetic fields (B-fields), for low values of B, one gets the usual Zeeman levels while on the other hand, when the B-field is so large as to dominate the Coulomb field, the spectra one obtains are those of Landau levels perturbed by the "weak" Coulomb field. In between these two extremes, there lies a very interesting regime, the so-called strong field mixing (SFM) regime, where the atomic electron gets roughly equal (but opposite in sign) contribution to its energy from both the Coulomb and the magnetic field, and the resulting spectrum near the zero energy region is strikingly simple but characteristically different from the extreme cases just mentioned\(^2\). Likewise, for strong mixing of electric and Coulomb fields\(^3\) and also in a situation where all three fields were
present, equally striking resonance patterns near the ionization edge have been observed. Though seemingly complicated, partial understanding of these phenomena, particularly as regards the spacings of these resonances and the positions where they set in, have been achieved through simple semi-classical arguments. It is only recently that Rau has been able to point out non-separability of motions as a unifying element of these seemingly diverse phenomena. He has also pointed out other physical systems (than the atomic ones to which the attention has been restricted so far) where similar effects might arise, and so can be studied perhaps with certain advantages. These include two dimensional (2-D) electron gas layers in external fields.

B. Non-separable Motions in 2-D Electron Layers

In this dissertation, we analyze the effects of non-separable motions on the eigenvalue structure of so called two dimensional electron layers that are found in two different contexts. The first one, which is the subject matter of Chapter II, is the system of very thin space charge layers in metal-oxide-semiconductor (MOS) devices. When subjected to a magnetic field tilted with respect to the oxide-semiconductor interface, the carrier motion in two perpendicular directions gets coupled. This coupling, whose strength can be directly related to the
direction and the magnitude of the B-field, gives rise to otherwise forbidden transitions, viz., intersubband cyclotron combined resonances. The other system that we consider, which constitutes the content of Chapter III, is that of surface state electrons (SSE) on liquid helium. Such an electron is bound to the liquid surface by the combination of a short range repulsive potential barrier on the liquid side, and an attractive image Coulomb potential on the other. The SSE are essentially free to move in a plane parallel to the liquid surface. When placed in external electric and magnetic fields in certain orientations, the SSE find a double minimum potential for their motion normal to the liquid surface. The non-separability of motion in this case (due to tunneling) is of the same type as what gives rise to inversion splittings in molecules. This system is particularly interesting in that one can change the strength of the coupling a great deal by varying the external fields.

C. Motivation for Choosing These Systems

We choose these two dimensional electron gas systems, instead of atomic ones, for the study of non-separable motions for different reasons. Theoretically, these are often easier to handle, fewer variables being involved. Thus, when reduced to its simplest form, the potential terms in the Hamiltonian considered in Chapter II, are either linear or quadratic in position.
coordinates and still contain the non-separability essential for the phenomena under study. From the point of view of experiments, these systems are suitable because the electric and magnetic fields required for satisfying the SFM criteria are much weaker than the corresponding values for atoms and are readily accessible in the laboratory. Thus, for the He system, because of the "weak" image Coulomb potential, a few hundred V/cm or a few kGauss can drastically influence even the ground state energy, whereas in atoms the corresponding quantities are $\sim 2.57 \times 10^9$ V/cm and $\sim 2.35 \times 10^6$ kGauss, respectively.

The study of two dimensional electron gas systems is of considerable basic and applied interest. We also note that a complete theoretical understanding of SFM phenomena in atomic systems, requires, in general, a full knowledge of the quantum-mechanical aspects of non-separable motions in two dimensions. This, coupled with the fact that the electronic states in the He system are well approximated by the s-states of hydrogenic functions makes the systems we study prototypes of general non-separable problems in quantum mechanics. So, we hope, the knowledge gained through these might prove useful for understanding strong mixing effects in general besides those already encountered in atomic, molecular and condensed matter physics.
The following section presents short descriptions of the physical systems, along with a brief survey of relevant literature to provide a proper perspective for the problems tackled in greater detail in subsequent chapters.

D. Background and Brief Survey of Earlier Work

i. The MOS System

In the next chapter we consider the effects of the non-separable motions on the positions and amplitudes of intersubband cyclotron combined resonances observed in optical spectroscopy of 2-D electron layers in MOS capacitors. It is now well known that the strong electric field associated with the surface space charge layers in these devices quantizes the carrier motion normal (considered as the z-direction here) to the oxide-semiconductor interface (x-y plane) and groups them into energy levels called electric subbands. The existence of such subbands was first proposed by Schrieffer in 1957\textsuperscript{9} and subsequently, their 2-D character was confirmed experimentally by Fowler et al. in 1966\textsuperscript{10}. Since then, there has been an enormous growth of literature on this subject, and notably on n-channel Si-devices\textsuperscript{11}, to the study of which we also restrict ourselves.

The potential $V(z)$ that confines the electronic motion along the z-direction is determined by the electric field produced by the surface charge layer as well as electron
exchange and correlation effects which also depend on the areal density of carriers at the interface\textsuperscript{12}. Consequently, the subband structure can be determined only numerically through self-consistent calculations. But as a model\textsuperscript{13}, and a quite satisfactory one for low lying subband levels, a single particle "triangular well" potential \( V(z) = \infty \) for \( z \leq 0 \), \( e^{|z|} \) for \( z > 0 \) as in Fig. 1.1a is often used\textsuperscript{14} both for interpreting experimental results and for gaining theoretical understanding of the phenomena involved. Further, some systems are accurately described by this model, e.g., PbTe (Ref. 14a).

An additional magnetic field \( B \) along the \( z \)-direction further quantizes the electronic motion in the \( x-y \) plane into Landau orbits. In the absence of a coupling between the cyclotron motion and the \( \varepsilon \)-field dependent subband motion, the only transitions allowed in intersubband spectroscopy\textsuperscript{15} are those involving no change in the Landau quantum number \( N \) (\( \Delta N = 0 \)). If the \( B \)-field is tilted with respect to the \( z \)-axis, however, so that a component \( B_y \), parallel to the interface is also present, these two motions become coupled, thereby exciting \( \Delta N \neq 0 \) transitions, the so called intersubband cyclotron combined resonances in appropriate radiation fields. For a weak-\( B \)-field, a Born-Oppenheimer like separation with a subsequent application of perturbation technique, leads\textsuperscript{12} to a
Fig. 1.1 (a) Schematic potential diagram (corresponding to the triangular well approximation) for an electron in an n-channel MOS structure (shown in the inset). $z=0$ marks the oxide-semiconductor interface. (b) Potential diagram of the forces acting on an electron near a liquid helium surface.
positive diamagnetic shift to the subband energies and the appearance of substructure in the form of equally spaced Landau levels for the cyclotron motion with a spacing proportional to $B_z$ alone. In this picture, the $\Delta N = \pm 1$ combined resonances are expected to be positioned symmetrically on an energy scale about the $\Delta N = 0$ "main" transition. Though a similar pattern has been seen in spectroscopic investigation of 2-D layers of SSE on liquid He$^{16}$, an earlier attempt to locate the same in an MOS structure failed due to excessive "noise"$^{17}$. Ando$^{18}$, using a local density functional scheme, considered the effects of resonant screening and final state interaction on these resonances. He predicted no change in the positions of the $\Delta N = \pm 1$ resonances but a shift of the main resonance by a factor $(1 + \gamma)^{1/2}$, where $\gamma$ is the sum of inherently opposite, but nearly equal contributions due to these two effects. A recent experiment$^{19}$ observed an asymmetry in the position and amplitude of the $\Delta N = \pm 1$ resonances with respect to the main transition. Certain features of their observations, viz., the dependence of asymmetry on the magnitude and the angle of tilt of the B-field were somewhat unexpected in light of the earlier theoretical predictions. Although a detailed numerical calculation including some many body correction in an approximate fashion, has been carried out by Ando$^{20}$ and it
accounts for many features of the observations as arising
due to specific many body effects, our interest here is
to explore how much of the deviations from the Born-
Oppenheimer expectations are due to single particle
effects. To this end, a detailed analysis of the non-
separable motions due to the tilted B-field is necessary
and is attempted in the next chapter. It is perhaps not
inappropriate to note at this point that our treatment,
even in the framework of a single particle Hamiltonian,
leads to conclusions in qualitative agreement with those
obtained by Ando as well as with the experimental observa-
tions. Our findings thus point to possible contributions
due to the aspect of non-separability towards some of the
observed features in combined intersubband cyclotron
resonance patterns.

ii. The Helium System

Quasi 2-D electron layers on the surface of liquid
helium, when placed in perpendicular electric and mag-
netic fields, can have an asymmetric DMP for the electronic
motion normal to the surface (taken to be the z-direction
here). In Chapter III, we analyze the corresponding
eigenstates of motion in the coupled potential wells,
applying (for the first time to our knowledge) a version
of the WKB formalism modified\textsuperscript{21a} to treat cases when two
turning points lie very close together.

In recent years, the study of SSE on liquid helium
has been actively pursued\textsuperscript{22} for many reasons. The basic binding for the SSE is provided by the combination of a classical attractive image Coulomb potential (\(-Qe^2/z, z > 0\)) and a short range repulsive barrier (\(-1.0\text{eV}\)) to penetration into the liquid surface (assumed at \(z = 0\)) due to the Pauli exclusion principle. The resulting potential \(V(z)\) is sketched in Fig. 1.1b. Since liquid He has a permittivity slightly larger than 1, the effective charge \(Qe\) is low, \(Q\) being \(-7 \times 10^{-3}\). Given the other scale of energies determined by \(Q\), the barrier is to a first approximation infinitely high. The resulting energy spectrum is then hydrogenic, of course with the obvious modification in that now the binding energies are small (by a factor \(Q^2\)) and the "Bohr" radius is large (by a factor \(Q^{-1}\)). Also, there will be no \(l,m\) degeneracy associated with angular momentum. This hydrogenic model for the SSE on liquid He was proposed independently by Sommer\textsuperscript{23}, Cole and Cohen\textsuperscript{24} and Shikin\textsuperscript{25}. The origin of the image potential and the repulsive barrier is discussed in detail in Refs. 23 and 24. Theoretical treatments, that go beyond this hydrogenic model can also be found in the literature\textsuperscript{26}.

The nearly hydrogenic character of the energy spectrum was confirmed experimentally by Grimes and Brown in 1974\textsuperscript{27}. Exploiting the fact that the levels can be shifted by an applied electric field, they measured the
splittings between the ground state and the first two excited states by observing mm-wave absorption as the splittings were Stark tuned into resonance with the frequency of the incident radiation. Extrapolation to zero applied Stark tuning electric field yielded transition frequencies in reasonably good agreement with those predicted by the simple hydrogenic model. In subsequent studies, transitions through the seventh excited states have been observed. As stated earlier, this is also the first system where intersubband cyclotron combined resonances have been observed experimentally.

Because of the weak Coulomb field, strong field mixing regimes can be obtained for this system with external electric and magnetic fields that are readily accessible in laboratories. Simple WKB calculations confirm the expected characteristic energy patterns when either an electric or a magnetic field is strongly mixed with the Coulomb field. The novel DMP for the z-motion that results in a particular combination of both the fields, and its similarity with certain atomic problems, has been discussed only qualitatively before. Our analysis in Chapter III shows that by "tuning" the external fields, the depths as well as the shapes of these potential wells can be varied conveniently so that each well, considered independently, can support a bound state at
the same energy. The resultant coupling due to possible tunneling of the electron through the intervening barrier gives rise to a doublet of levels around that energy. This, therefore, resembles the problem of inversion splitting often encountered in the molecular physics literature. The advantage of the He system is that the shape of the "molecule" itself can be changed considerably by the experimenter. Unfortunately, no such experiment has been carried out as yet though we hope that in the near future this will be.

Though not of our direct interest here, we should perhaps mention very briefly the essential differences between the quasi 2-D electron gases in n-channel Si-MOS devices and on top of liquid He. The most significant of them is in the accessible range of areal densities. The typical values for the SSE on liquid He are in the range of $10^5$ to $10^9$ cm$^{-2}$ as contrasted to $10^{11}$ to $10^{13}$ cm$^{-2}$ for Si-MOS systems. For temperatures above a few milliKelvins, the SSE on He behave like a classical electron gas while an inversion layer in Si-MOS acts like a Fermi system at helium temperature. Consequently, different many body aspects are displayed by these two systems. In these regards, observation of Shubnikov-De Haas oscillations$^{30}$ in inversion layers and the first experimental confirmation of Wigner crystallization$^{31}$ and formation of "dimples"$^{32}$ in He systems may be
mentioned. Indeed both these systems offer a rich variety of interesting physical phenomena and many useful references are listed in a recently compiled bibliography by Ando, Fowler, and Stern.11.
A. Introduction

The origin of intersubband cyclotron combined resonance pattern in the absorption spectra of quasi 2-D electron layers in n-channel Si-MOS structures has already been discussed in Chapter I.D. We also noted the main features of recent experimental observations\(^{19}\) and their interpretation in terms of certain many body aspects of such systems put forward by Ando\(^{20}\) in a subsequent theoretical analysis. In this chapter, we study the absorption spectrum of such a system in a one-electron model using the "triangular well" approximation\(^{13}\). This is not to deny the importance of the many body aspects of the system, in fact they are known to be quite important, and more so for silicon structures\(^{18,33}\). However, use of such a model is quite common in the literature for many reasons. First, the model seems to be quite adequate for certain systems like PbTe\(^{14a}\). Secondly, because it serves as a common backdrop against which new many body effects can be viewed, the model continues to be used for this purpose\(^{14}\). The motivation for our study of the tilted magnetic field problem in this model is that it permits a thorough analysis of the corresponding (non-separable) Hamiltonian. We can thus delineate explicitly
relevant single particle contributions due to non-separable motions towards explaining the observed phenomena. Since we neglect many body aspects, we make no claim for a complete description of the system. The merit of our study, as we will see, is that we get results qualitatively similar to those hitherto attributed to many body effects. In this way our study points to another possible origin of some of the observed features of the combined resonances, viz., the non-separability of the subband and the cyclotron motions. Another important feature of the simple model is that it is a prototype of problems involving motions in more than one dimension (here two perpendicular directions) when the non-separability of the motions is essential for the phenomena under study. This is an aspect of general physics and relevant to many other areas of physics.

In Section B, we describe our model and formulate the problem. Section C describes some interesting characteristics of the Hamiltonian. We employ two alternative basis sets to obtain closed form and easily calculable matrix elements of the Hamiltonian. These are sketched in Section D. The details are given in Appendix A which is a published account of some of the results contained in this chapter. The results are discussed in Section E followed by a brief summary in Section F.
B. The Model

We consider the electron layer in an n-channel MOS device to be described by the triangular well model (see Fig. 1.1a) discussed earlier. The effective electric field \( \varepsilon \) along the normal (z-direction) to the oxide-semiconductor interface is then assumed proportional to the sum \( N_s \) of the areal number density of the charge carriers in the electron layer (assumed parallel to the x-y plane) and that in the depletion layer: \( \varepsilon = k N_s \). The constant of proportionality \( k \) is regarded as an adjustable parameter and can be chosen to reproduce the experimental value for the energy separation between the ground and the first excited subband. In this way, through the empirical choice of \( k \), the many body aspects may be thought to be included to some extent in our model. But, apart from that, we consider the system as one of a single electron moving in a triangular well. We emphasize once again that this is a simplified picture, for the actual effective potential for an electron may depart considerably over some ranges from the triangular one.\(^{33}\)

If a magnetic field is applied to such a system tilted with respect to the z axis by an angle \( \alpha \), let \( B_z \) and \( B_y \) be its components respectively perpendicular and parallel to the oxide-semiconductor interface. Choosing a gauge \( A = (z B_y - y B_z, 0, 0) \) as in Ref. 19 to describe this field, the Hamiltonian for this electron can be written as
\[ H = \frac{\hbar^2}{2m_t} + \frac{\hbar^2}{2m_\perp} + \frac{1}{2m_t} [p_x + \frac{e}{c} (z B_y - y B_z)]^2 + e\varepsilon z ; \]
\[ -\infty \leq y \leq \infty , \quad 0 \leq z \leq \infty , \]  
(2.1)

where \( m_t \) and \( m_\perp \) are the effective masses of the electron parallel and perpendicular to the interface respectively.

With \( H \) as given in Eq. (2.1) the \( x \)-part of the wave function is described by plane waves and translating \( y \) by \( \frac{e\varepsilon}{dB} \), the \( x \)-coordinate can be removed. This transformation is legitimate for all \( B_z \neq 0 \). Eq. (2.1) then becomes

\[ H = \left[ \frac{\hbar^2}{2m_t} + \frac{e^2 B^2_o}{2m_t c^2} \cos^2 \alpha y^2 \right] + \left[ \frac{\hbar^2}{2m_\perp} + \frac{e^2 B^2_o}{2m_\perp c^2} \sin^2 \alpha z^2 + e\varepsilon z \right] \]
\[ - \frac{e^2 B^2_o}{m_t c^2} \sin \alpha \cos \alpha yz , \]  
(2.2)

where now \( B_z \) and \( B_y \) are replaced by \( B_o \cos \alpha \) and \( B_o \sin \alpha \) respectively, \( B_o = (B^2_y + B^2_z)^{1/2} \) being the magnitude of the \( B \)-field. We wish to solve for the corresponding eigenvalues \( E \) from the Schrödinger equation

\[ H\psi(y,z) = E \psi(y,z) \]  
(2.3)

with the appropriate boundary conditions, viz.,

\[ \psi(y = \pm \infty, z) = 0, \quad \psi(y, z = \infty) = 0, \quad \text{and} \quad \psi(y, z = 0) = 0. \]  
(2.4)

The last condition is due to the infinite potential barrier at the oxide surface which confines the electronic motion in the semi-infinite plane for which \( z > 0 \).
Thereby, for $\alpha \neq 90^\circ$, the effect of the magnetic field is to quantize further the $y$-motion of the electron. Note that the last term, which denotes the coupling between the $y$ and $z$ motions, vanishes in either Faraday ($\alpha = 0^\circ$) or Voigt ($\alpha = 90^\circ$) geometry. Further, for $\alpha = 90^\circ$, the electron becomes free in the $y$ direction and is assumed to carry zero momentum in that direction in the subsequent discussions.

If the effect of the $B$-field is weak, a Born-Oppenheimer (B-O) type solution is possible wherein one starts with the undisturbed electric subbands and evaluates the $z^2$ and the $z$ terms in the magnetic part in terms of the unperturbed wave functions. One can then solve for the $y$-motion. Such a procedure leads to a positive correction

$$\Delta E_{B-O}^n = \frac{e^2 B_o^2}{2mc^2} \sin^2 \alpha (\langle z^2 \rangle_{nn} - \langle z \rangle_{nn}^2)$$

(2.5)

to the $n^{th}$ subband energy and the appearance of substructure in the form of equispaced Landau levels for the $y$ motion on each subband with spacing $\hbar \omega_z$ where $\omega_z = \omega \cos \alpha$ with $\omega = eB_o/m_e c$. Some recent experimental results\(^{14a}\), however, showed substantial departure from the expected $\cos \alpha$ dependence for the Landau spacings, particularly for large $\alpha$. This calls for a more thorough analysis of the coupling term than what can be accomplished in the simple B-O type of separation of the $y$ and the $z$ motions.
C. Some Interesting Features of the Hamiltonian

The Hamiltonians in Eqs. (2.1) and (2.2) have two interesting features which we discuss briefly in the following.

i) The Hamiltonian in Eq. (2.1) reduces to that in Eq. (2.2) also for the parametric choice \( \langle p_x \rangle = 0 \). While this choice does not affect the eigenvalue structure for all \( \alpha \neq 90^\circ \), (because of the admissible translation in \( y \)), it does not give the true ground state energy when \( \alpha = 90^\circ \). The value of \( \langle p_x \rangle \) which minimizes the energy in this case is seen from Eq. (2.1) to be \( -eB_y\langle z \rangle /c \), and then the appropriate Hamiltonian becomes

\[
H = \frac{p_y^2}{2m_y} + \frac{p_z^2}{2m_z} + ecz + \frac{e^2 B_o^2}{2m_e c^2} \sin^2 \alpha (z - \langle z \rangle)^2 .
\] (2.6)

For \( \alpha = 90^\circ \), the difference between the two Hamiltonians given by Eqs. (2.2) and (2.6) is due to the presence of the \( \langle z \rangle \) term in the latter. We however, attempt in this chapter to solve for the Hamiltonian given by Eq. (2.2), after noting that this is singular at \( \alpha = 90^\circ \), and that its eigenvalues have a jump discontinuity at \( \alpha = 90^\circ \), the magnitude of the "jump" being equal to the difference in the eigenvalues of the Hamiltonian (2.2) from the corresponding ones of the Hamiltonian (2.6). A comparison with Eq. (2.5) immediately shows the magnitude of this difference is roughly equal to \( e^2 B_o^2 \langle z \rangle^2 / 2m_e c^2 \).
ii) It is possible to find a set of transformations $T$ which decouples the Schrödinger equation (2.3) at the level of the potential energy but makes the boundary conditions (b.c.) in (2.4) non-separable, thus retaining the complexity of the problem. Consider, e.g., the linear transformation

$$
T = e^{\gamma z \frac{\partial}{\partial y} - \delta y \frac{\partial}{\partial z}}
$$

(2.7)

where $\gamma$ and $\delta$ are hitherto undetermined parameters. Under $T$, Eq. (2.3) transforms as

$$
\tilde{H} \tilde{\psi} = E \tilde{\psi}
$$

(2.8)

where

$$
\tilde{H} = T H T^{-1}
$$

(2.9)

and

$$
\tilde{\psi} = T \psi.
$$

(2.10)

Two specific choices (say, choice A and choice B) can be made for the values of $\gamma$ and $\delta$ for which the corresponding $H$ (say $\tilde{H}_A$ and $\tilde{H}_B$, respectively) do not contain any cross terms in $y$ and $z$ variables, namely terms proportional to $\frac{\partial^2}{\partial y \partial z}$ and $yz$. These are the following:

Choice A: $\gamma_1 = -\frac{m_t \sin \alpha \cos \alpha}{m_t \sin^2 \alpha + m_\perp \cos^2 \alpha}$

$$
\delta_1 = m_t \tan \alpha / m_\perp
$$

(2.11)

Choice B: $\gamma_2 = -\gamma_1$, $\delta_2 = -\cot \alpha$.

(2.12)
Clearly, the transformation $T$ becomes singular for $\alpha = 90^\circ$ and $\alpha = 0^\circ$ for choices A and B, respectively. The corresponding Hamiltonians are

$$ H_A = -\frac{\hbar^2}{2m_t} \Delta_1 \frac{\partial^2}{\partial y^2} + \frac{e^2_B}{2m_Tc^2} \cos^2 \frac{\alpha}{2} y^2 - e\frac{m_t}{m_k} \tan \alpha \gamma $$

$$ - \frac{\hbar^2}{2m_k} \frac{1}{\Delta_1} \frac{\partial^2}{\partial z^2} + e\gamma \Delta_1 z, \quad \alpha \neq 90^\circ $$

and

$$ H_B = -\frac{\hbar^2}{2m_t} \Delta_2 \frac{\partial^2}{\partial y^2} + e\gamma \cot \alpha \gamma - \frac{\hbar^2}{2m_k} \frac{1}{\Delta_2} \frac{\partial^2}{\partial z^2} + \frac{e^2_B}{2m_Tc^2} \sin^2 \alpha z^2 $$

$$ + e\gamma \Delta_2 z, \quad \alpha \neq 0^\circ $$

where $\Delta_i = 1 + \gamma_i \delta_i$ ($i = 1, 2$) and lies within the range $0 < \Delta_i < 1$. Even though the Hamiltonians $H_A$ and $H_B$ contain no coupling term like the $yz$ term as in Eq. (2.2), the Schrödinger equation (2.8) can not be decoupled, for now the boundary conditions are coupled. This can be seen more clearly if we note that the transformation $T$ in Eq. (2.7) is equivalent to a mapping of the $y,z$ coordinates onto another set $\xi, \eta$ given by

$$ \begin{pmatrix} \xi \\ \eta \end{pmatrix} = \begin{pmatrix} 1 + \gamma_i \delta_i & \gamma_i \\ \delta_i & 1 \end{pmatrix} \begin{pmatrix} y \\ z \end{pmatrix}. $$

Note that this corresponds to an area preserving, but nonorthogonal transformation of the coordinate system.

The resulting Hamiltonians, for the same values of $\gamma_i, \delta_i$ as in Eqs. (2.11) and (2.12), are of the same form as given.
by Eqs. (2.13) and (2.14), respectively, with \( y \) and \( z \) now replaced by \( \xi \) and \( \eta \). The b.c. for \( \psi \) in Eq. (2.3) that it must vanish for all \( z \leq 0 \) now becomes coupled and requires that the wave function, expressed in terms of \( \xi \) and \( \eta \) must vanish on the semi-infinite plane for which \( \eta \leq \left( \frac{\delta_1}{\Delta_1} \right) \xi \).

Because of this restriction, the Hamiltonian \( \tilde{H}_A \) is bounded from below, inspite of the presence of the third term in Eq. (2.13), which is linear in \( y \) (or \( \xi \)). Besides, \( \tilde{H}_A \) and \( \tilde{H}_B \) must ensure that they are positive definite, to conform with the same property of the original Hamiltonian in Eq. (2.2).

Non-separable problems wherein the coupling is present only at the level of the boundary conditions are relatively rare and the standard prescription\(^{34}\) for tackling them calls for finding transformations which transfer the non-separability to the Hamiltonian level, whereupon one can employ well known techniques. For the present problem, this implies starting with \( \tilde{H}_A \) or \( \tilde{H}_B \) and then obtaining \( H \) as in Eq. (2.2) by the use of the inverse transformation \( T^{-1} \).

Our discussion in this section is motivated by the interesting feature of \( H \) which qualifies it as a nice textbook like example of problems involving non-separable boundary conditions. Further work along the lines of solving the problem with the Hamiltonian itself in separable form (in Eqs. (2.13) and (2.14)) but with the coupling contained entirely in the boundary conditions was finally abandoned.
in favor of other approaches given in the next sections. However, the question remains intriguing because, once again, one can envisage other problems in physics of the same structure and it appears an attractive possibility to keep the Hamiltonians separable and somehow incorporate directly the coupled boundary conditions.

D. Choice of the Basis Sets for Diagonalization

We first note that if the coupling due to the yz term in the Hamiltonian H in Eq. (2.2) is neglected, the y and the z parts of H decouple, the corresponding wave functions being described by the well known harmonic oscillator and Weber functions, respectively. However, Weber functions are, in general, more cumbersome to handle. Depending on whether the electric field or the magnetic one dominates the subband structure (z-motion), either Airy functions Ai(z) or harmonic oscillator wave functions U(z) (of odd order, since the wave function must vanish at z = 0 for all y) provide us with two suitable alternative choices of the basis functions to diagonalize H. We define a parameter

\[ \theta = \left( \frac{e^2 \epsilon^2 \hbar^2}{2m^*} \right)^{1/3} \frac{\hbar \omega_o}{\omega_o^*} ; \quad \omega_o^* = \frac{eB_o}{m^* c} \]  

(2.17)

which gives a measure of the strength of the \( \epsilon \)-field relative to the B-field. \( \theta \approx 0.57 \) implies, for example, a situation where the energy separation between the ground electric subband and the next higher one equals the Landau
spacing for \( \alpha = 0^\circ \). It may be interesting to note that \( \Theta \) as defined above, can also be written as the ratio \( \frac{m_e l_B^2}{m_t l_e^2} \), where \( l_B \) and \( l_e \) are the characteristic lengths associated with the magnetic and the electric fields and are given by \( (\hbar/2m_e \omega_o)^{\frac{1}{2}} \) and \( (\hbar^2/2m_e e \epsilon)^{\frac{1}{3}} \), respectively.

Although \( \Theta \approx 0.57 \) may suggest that a strongly mixed regime is achieved, we should note at this point that unlike all the SFM phenomena studied so far in the context of atomic systems, the \( z \)-motions due to the \( \epsilon \) and \( B \)-field in this case do not compete with each other, rather their effects are similar in the sense that they both try to push the electron toward the oxide-semiconductor interface. This is a pointer to there being possibly no strikingly different energy spectrum at any energy, since no "zero energy" regime can be achieved.

In most of the space charge layers in MOS devices studied so far \( \Theta \) is large. However, a situation where the \( B \)-field dominates the \( z \)-quantization (i.e., \( \Theta \) small and \( \alpha \) large) has also been reported. For \( \Theta \) large, the appropriate basis is the set of product functions \( U_N(y)A_{in}(z) \); \( n,N (= 0, 1, 2, ...) \) being the subband index and the Landau quantum number, respectively. Similarly, for \( \Theta \) small and \( \alpha \) large, the corresponding basis is \( U_N(y)U_{2n+1}(z) \).

The matrix elements in these two basis sets have been derived in closed form in Appendix A, where we have also obtained an expression required for calculating the
optical absorption spectrum of this system corresponding to a weak, z-polarized radiation (see Eqs. 6 through 27 in Appendix A). Somewhat complicated matrix elements like \( \langle z \rangle_{nm}', \langle z^2 \rangle_{nm} \) in terms of the Airy functions and \( \langle z \rangle_{nm} \) in terms of the oscillator functions have been derived in Appendices B and C, respectively. Any of the large matrices given by Eqs. (11), (16), or (23) of Appendix A can be diagonalized for appropriate values of the parameters to obtain energy eigenvalues \( E_{\mu} \) and the corresponding eigenfunctions \( \psi_{\mu} \).

E. Results and Discussions

For calculations of the energy levels and the corresponding wave functions the matrices given by Eqs. (A.11) and (A.16) have been diagonalized. Twenty Landau levels and 15 subband levels were included in the basis. For effective masses we used values appropriate to the silicon (100) surface, viz., \( m_t = 0.1905m \), \( m_\perp = 0.916m \), \( m \) being the free electron mass. Most of the calculations were performed using 0 or 0 as defined in Eqs. (2.17) and (A.15) as parameters and the energies expressed in units of \( \hbar \omega_0 \) and \( \hbar \omega_z \), respectively. \( E_n^N(a) \) denotes energy levels on the \( n^{th} \) subband and the \( N^{th} \) Landau level; \( n, N = 0, 1, 2, \ldots \). \( E_{10}^N(a) \) denotes the energy corresponding to the transition from the ground (\( n=0 \)) subband level to the first excited subband involving no change in the Landau quantum number. \( E_{10}^{AN}(a) \) corresponds to similar transitions involving a simultaneous
change $\Delta N(\neq 0)$ in the Landau index. We should emphasize
that the wave function belonging to $E_n^\alpha(\alpha)$ may contain as
much or even more of the original $|n,N+1>$ character than
of the $|n,N>$ function, especially at large tilt angles.

Figure 2.1 shows the difference of the ground state
energy $E_0^\alpha(\alpha)$ from the unperturbed ground subband energy
$\beta_0^\alpha (\beta_n$ being the negative of the $n^{th}$ zero of the Airy
functions) as a function of the tilt angle $\alpha$ for various
values of $\theta$. Except at regions very close to $90^\circ$, the
curves approximate the expected "cos$\alpha$ + diamagnetic shift"
type of behavior. Because of their large diamagnetic
shifts, curves corresponding to lower $\theta$ lie above the
others. The minimum of each curve and the steep rise
beyond it is believed to be caused by the smoothing out
of the singularity at $\alpha = 90^\circ$ due to an inadequate basis
set. This is however expected, since the eigenvalue spectra
Corresponding to the $y$-parts of the Hamiltonians $H_{01}$ and $H_{02}$
in Eqs. (A.6) and (A.18) change from discrete (for $\alpha < 90^\circ$)
to continuous character as $\alpha$ equals $90^\circ$. Consequently, an
infinite number of bound state wave functions $U_{n}(y)$ are
needed to describe the $y$-part of the wave function at
$\alpha = 90^\circ$, when the $y$-motion of the electron becomes free. In
spite of this, the very close proximity of the eigenvalue
minima to the point $\alpha = 90^\circ$, as can be seen from the
figure, implies that except for a very narrow range of $\alpha$
near $90^\circ$, the basis sets chosen for diagonalizing $H$ are
adequate. We note that the energy values at $\alpha = 90^\circ$ are
Fig. 2.1. Plots of ground state energy $E^0_0(\alpha)$ relative to ground unperturbed electric subband level $\beta_0 \theta$ as a function of the tilt angle $\alpha$. The ordinate is expressed in units of $\hbar \omega_0$. 
higher than the true ground state energies by about 
\[ \frac{1}{2} m_w^2 \omega_0^2 \sin^2 a \langle z^2 \rangle_{\infty}. \]
One can obtain reasonably accurate estimates of the ground state energies by extrapolating to 90° the portion of each curve just to the left of the corresponding minimum.

Figure (2.2) shows \( E_{10}(\alpha) - E_{10}(\alpha = 0) \), i.e., the change in the main transition energy as a function of the tilt angle for different values of \( \theta \). The origin of the sharp features near \( \alpha = 90^\circ \) region is explained in the previous paragraph. Except for \( \theta = 0.57 \), all the other curves approximate the Born-Oppenheimer values 
\[ \frac{1}{2} m_w^2 \omega_0^2 \sin^2 a (\langle z^2 \rangle_{\perp} - \langle z^2 \rangle_{\parallel} + \langle z^2 \rangle_{\perp}). \]
The additional structure for \( \theta = 0.57 \) is due to strong mutual interaction among the unperturbed states brought about by the coupling term whose strength as a function of \( \alpha \) has a maximum at \( \alpha = 45^\circ \).

In Fig. 2.3 the inverse of the quantity \( E_{10}^{10} - E_{10}(\alpha = 0^\circ) \) is plotted against \( \alpha \) for several \( \theta \). The ordinate is equivalent to the cyclotron mass normalized with respect to \( m_t \), that is, \( m_c/m_t \). If the effect of finite \( B_y \) is neglected, the ratio \( m_c/m_t \) is expected to follow a \((\cos \alpha)^{-1}\) type of behavior (the dashed curve in the figure) as a function of \( \alpha \). Finite values of \( m_c/m_t \) at \( \alpha = 90^\circ \) reflect the diamagnetic shift in Voigt geometry when \( \langle p_x \rangle \) is assumed to be zero. What is interesting is the departure of the curves from the \((\cos \alpha)^{-1}\) type of behavior even for tilt angles much less than the ones where the sharp
Fig. 2.2. Shift of the main resonance energies from the values corresponding to the Faraday geometry plotted as a function of the tilt angle $\alpha$. The additional structure for $\theta \sim 0.57$ is due to strong mutual interaction among the unperturbed states brought about by the coupling term.
Fig. 2.3. Effective cyclotron mass normalized with respect to $m_t : m_c/m_t$ corresponding to transitions from $|n = 0, N = 0\rangle$ state to $|n = 1, N = 1\rangle$ state. $(m_c/m_t)$ is equivalent to $\{E_{10}^{\pm}(\alpha) - E_{10}(\alpha=0)\}^{-1}$. Note the deviation from the $(\cos \alpha)^{-1}$ curve given by the dashed line.
features are located. As we can see, this departure becomes more prominent at large tilt angles for all $\theta$, but for small $\theta$, this sets in even at moderate tilt angles.

Figure 2.4 displays the details of Figs. 2.1-2.3 from $\alpha = 85^\circ$ to $\alpha = 90^\circ$ range. This shows more clearly the characteristic angles of tilt where the sharp feature of each plot is located. As mentioned before, this angle is extremely close to $90^\circ$ if $\theta$ is large while it moves very slightly to the left as $\theta$ is decreased. This figure then gives some idea about the range of tilt angles over which our calculations can be trusted. For most experiments, $\theta$ is greater than 1.0 and a very conservative estimate for this range is $0 \leq \alpha \leq 85^\circ$. As commented upon earlier, the upper limit of this range is determined by the ability of the basis functions to represent free particle like behavior as the tilt angle approaches $90^\circ$. An improved basis function can be found, however, which does just that. We have constructed an orthonormal basis of the type $U_N(\nu y)U_{2n+1}(\lambda z)$ where $\nu$ and $\lambda$ are two variational parameters which minimize the ground state energy. Details about this procedure are given in Appendix D.

Figure 2.5 shows curves similar to Fig. 2.2 But now we envisage experimental situations wherein the $z$-component of the magnetic field, $B_z$, is kept fixed while the tilt angle is changed. This implies $B_y$ is changed and is given by $B_z \tan \alpha$. Different values of $\theta_z$ denote different
Fig. 2.4. Details of the figures 2.1-2.3 from $\alpha = 85^\circ$ to $\alpha = 90^\circ$ range.
Fig. 2.5. Shift of the main resonance energy from the corresponding quantity in Faraday geometry is plotted against different values of the tilt angle $\alpha$ for different values of $\theta_z$. The ordinate is expressed in units of $\hbar \omega_z$. $B_y$ is related to $\alpha$ and is given by $B_z \tan \alpha$. 
relative strengths of the $\varepsilon$-field to $B_z$; the ordinate now is plotted in units of $\hbar \omega_z$. Here also, as in the case of the plots in Fig. 2.2, the curves agree reasonably with the Born-Oppenheimer values, particularly for large $\theta$. For small $\theta$, Born-Oppenheimer values underestimate the actual ones, since for small $\theta$, the argument that the $y$ motion has little or no effect on the $z$-quantization is not valid.

Table 2.1 displays the energies corresponding to transitions from the ground to the first excited subband with a simultaneous change $\Delta N = (0, \pm 1)$ in the Landau quantum number $N$ for a fixed $B_z$ ($= 3.5 T$), two different electric fields corresponding to $N_s = 1.0 \times 10^{12} \text{ cm}^{-2}$ and $N_s = 0.5 \times 10^{12} \text{ cm}^{-2}$, and for various values of $B_y$. For these calculations, $\theta_z$ have been determined after fixing the constant of proportionality between the $\varepsilon$-field and $N_s$ by translating $13.683 \text{ meV}$, the energy separation $E_{10}$ to an $N_s$ value of $1.05 \times 10^{12} \text{ cm}^{-2}$, as obtained from Ref. 19. The unperturbed Landau spacings $\hbar \omega_z$ for $B_z = 3.5 T$ is $2.127 \text{ meV}$. The energies in this table are expressed in meV's. The last two columns show the energy differences $|E_{10} - E_{10''}|$, which are the same as the energy separations between the first two Landau levels on $n = 0$ and $n = 1$ subbands respectively. Note that all the transitions, the main one ($\Delta N = 0$) as well as the combined ones ($\Delta N = \pm 1$) shift to higher energies as $B_y$ is increased from 0. We also note the dependence of the Landau separations on $B_y$ and the subband index. For both subbands, they are smaller than the
expected $\hbar \omega_z = 2.127$ meV, though the differences are rather small until $B_y \approx 10$ T. That the Landau separation on the first excited subband is smaller than that on the ground subband, as can be seen from a comparison of columns 5 and 6, implies asymmetric positioning of the $\Delta N = \pm 1$ transitions. This is in accord with the experimental findings of Beinvogl and Koch\textsuperscript{19}, though their other observations, viz., the shift of the main resonance to the lower energy side and almost stationary positions for the combined resonances ($\Delta N = \pm 1$) with increasing $B_y$ are in serious disagreement with our calculations. However, a rigorous comparison of our results with the results in Ref. 19 is not possible because most of the interpretations of the latter where the different transition frequencies are obtained by normalizing the resonance peaks to a common $N_s$ value assuming only a $N_s^{2/3}$ dependence for all the energies, is affected by the $N_s$ (or $\varepsilon$-field) dependence of the transition energies as is evident from the Table 2.1 (or, so far as the main transition is concerned, from Fig. 2.5). Ando\textsuperscript{20}, in his calculations has found agreement with the experiment so far as the shift of the main resonance relative to the combined ones is concerned. He has attributed this shift to many body effects like resonant screening and final state interactions. He has also found the combined resonances to show diamagnetic shifts which are in qualitative agreement
TABLE 2.1

<table>
<thead>
<tr>
<th>$B_y$ (in T)</th>
<th>Transition energies $E^{\Delta N}<em>{10}$ corresponding to $E^{AN}</em>{10}$</th>
<th>$E^0_{10} - E^{-1}_{10}$</th>
<th>$E^1_{10} - E^0_{10}$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\Delta N=-1$</td>
<td>$\Delta N=0$</td>
<td>$\Delta N=+1$</td>
</tr>
<tr>
<td>0</td>
<td>11.118</td>
<td>13.245</td>
<td>15.372</td>
</tr>
<tr>
<td></td>
<td>(6.217)</td>
<td>(8.344)</td>
<td>(10.471)</td>
</tr>
<tr>
<td>2</td>
<td>11.130</td>
<td>13.255</td>
<td>15.379</td>
</tr>
<tr>
<td></td>
<td>(6.237)</td>
<td>(8.360)</td>
<td>(10.480)</td>
</tr>
<tr>
<td>4</td>
<td>11.164</td>
<td>13.285</td>
<td>15.401</td>
</tr>
<tr>
<td></td>
<td>(6.298)</td>
<td>(8.409)</td>
<td>(10.508)</td>
</tr>
<tr>
<td>6</td>
<td>11.121</td>
<td>13.335</td>
<td>15.439</td>
</tr>
<tr>
<td></td>
<td>(6.400)</td>
<td>(8.492)</td>
<td>(10.562)</td>
</tr>
<tr>
<td>8</td>
<td>11.302</td>
<td>13.405</td>
<td>15.492</td>
</tr>
<tr>
<td></td>
<td>(6.543)</td>
<td>(8.612)</td>
<td>(10.644)</td>
</tr>
<tr>
<td>10</td>
<td>11.406</td>
<td>13.497</td>
<td>15.563</td>
</tr>
<tr>
<td></td>
<td>(6.728)</td>
<td>(8.764)</td>
<td>(10.767)</td>
</tr>
<tr>
<td>20</td>
<td>12.228</td>
<td>14.277</td>
<td>16.228</td>
</tr>
</tbody>
</table>

Values of the transition energies (in meV) at which the various $\Delta N$ resonances appear as a function of $B_y$; $B_z = 3.5T$ and $N_s = 1.0 \times 10^{12} \text{ cm}^{-2}$. Figures in parentheses correspond to $N_s = 0.5 \times 10^{12} \text{ cm}^{-2}$. 

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with our results. In view of these, we feel that more experiments, preferably of a frequency sweep type, will be desirable.

Figures 2.6-2.8 show examples of the optical absorption spectra corresponding to a weak z-polarized radiation. For these a common $\theta_z$ value corresponding to $B_z = 5$ T and $E_{10} (\alpha = 0) = 28.0$ meV has been assumed, but the angles of tilt $\alpha$ of the B-field are taken to be $70^\circ$, $75^\circ$, and $80^\circ$ respectively for the Figs. 2.6-2.8. $B_y$ for each figure is thus given by $B_z \tan \alpha$. An unperturbed energy separation of 28.0 meV between the ground and the first excited subbands is typical of n-type silicon inversion layers and corresponds roughly to a carrier density $N_s \approx 2.1 \times 10^{12}$ cm$^{-2}$. The first four Landau levels on the $n = 0$ subband are assumed to be occupied. Phenomenological width parameters $\Gamma$ have been assumed whose values are shown in the figures. $\hbar \omega_z$ for $B_z = 5$ T is about 3.04 meV. In all the figures, several combined resonances ($\Delta N \neq 0$) are distinctly visible in addition to the main transition ($\Delta N = 0$). For $\alpha = 70^\circ$ (Fig. 2.6), $\Delta N = \pm 1$ resonances are seen to be placed about 3 meV on either side of the main resonance located at $\pm 28.2$ meV. Combined resonances $\Delta N = \pm 2$ are also visible. As the tilt angle is increased to $75^\circ$, we can see from Fig. 2.7 the enhancement of the amplitudes of the combined resonances relative to the amplitude of the main transition. Note the amplitude asymmetry of the $\Delta N = \pm 1$ resonances in both Figs. 2.6 and 2.7. All the resonances move toward the
Fig. 2.6. Calculated optical absorption spectrum in an inversion layer on the Si(100) surface in a tilted magnetic field. Tilt angle \( \alpha = 70^\circ \); \( B_z = 5T, B_y = B_z \tan 70^\circ \); \( N_s \sim 2.1 \times 10^{12} \) cm\(^{-2} \) is assumed to correspond to \( E_{10} (\alpha = 0^\circ) = 28.0 \) meV (taken from Ref. 20).
Fig. 2.7. Same as in Fig. 2.6 but with tilt angle $\alpha = 75^\circ$. 

$\Gamma = 1.00 \text{ meV}$
$\Gamma = 0.75 \text{ meV}$
$\Gamma = 0.50 \text{ meV}$
Fig. 2.8. Same as in the previous figure but now with $\alpha = 80^\circ$. Note that the amplitude of the $\Delta N = +1$ resonance is even higher than the "main" resonance $\Delta N = 0$ (at ~ 28.9 meV).
higher energy side due to the diamagnetic shift as the tilt angle is increased. As the tilt angle is increased further to 80°, we can see the great modification in the spectrum from Fig. 2.8. Now the amplitude of the "main" transition at \( \sim 28.9 \text{ meV} \) is even smaller than that of the \( N = +1 \) resonance, which is located at \( \sim 31.8 \text{ meV} \). The \( N = -1 \) transition occurs at \( \hbar \omega \sim 26.0 \text{ meV} \). Though these spectra have been calculated for parameter values appropriate to an inversion layer, similar effects are expected to show up, in fact more strongly, for the lower values of \( E_{10} \) corresponding to accumulation layers. The asymmetry of the \( \Delta N = +1 \) combined resonances and their enhancement relative to the main transition with increasing \( B_y \) essentially agree with experiments. No serious conclusion should be made concerning resonances involving \( \Delta N > 1 \) because for such resonances, particularly for accumulation layers, our simple triangular well model will be grossly inadequate. However, considering the simplified nature of our model, it is satisfying to note that the amplitude asymmetry for the combined resonances, observed in Ref. 19 and calculated in Ref. 20, owes its origin, at least partly, to the single electron aspects of the system.

F. Summary

We have calculated the energy levels and the intersub-
band cyclotron combined resonance spectrum of an effectively 2-D space charge layer in a tilted magnetic field using a simple non-relativistic model Hamiltonian. The coupling between two perpendicular motions introduced by the magnetic field has been taken fully into account. Two alternative basis sets have been pointed out in which the matrix elements of the full Hamiltonian can be obtained in closed form. These two choices enable one to solve for the Hamiltonian exactly for arbitrary strengths of the magnetic field relative to the electric one for a wide range of tilt angles. This range is expected to be extended by diagonalizing the Hamiltonian in yet another basis as pointed out in Appendix D which describes a simple variational method for obtaining the eigenvalue spectrum to a reasonably good accuracy.

Asymmetry in amplitude and positioning of the combined resonances relative to the main one are in qualitative agreement with some recent experiment of Beinvogl and Koch and with the calculations of Ando. These point to possible (though small) contributions from the single electron aspects of the problem to the observed phenomena. Our calculations show, also in qualitative agreement with the calculations of Ando, diamagnetic shifts of the combined resonances as the component of the B-field parallel to the surface is increased. Since the experimental
results do not show this shift, it remains unexplained.

Landau spacings on different subbands are found not to be determined by the normal component of the B-field alone as expected in a naive picture. Instead, they are found to depend also on the parallel component of the B-field, the relative strength of the electric to the magnetic field, and on the subband index. The Landau spacings are reduced for both the ground and the higher subbands, the reduction being slightly more for the higher subband. However, deviations from the expected values are not appreciable unless the ratio of the parallel to the perpendicular component of the magnetic field is quite large.

We end this chapter with a couple of remarks on the general features of such problems. The first concerns the fact that the Hamiltonian we have used may be considered as a prototype of non-separable problems in two dimensions. This Hamiltonian is very interesting in that the non-separability is due to the restriction of the coordinate space to a semi-infinite plane. Thus we have shown how through a set of successive linear transformations of the coordinate variables, the coupling can be pushed from the level of the potential energy to the level of the boundary conditions.
Secondly, electron layers on a liquid helium surface also appear to be a promising system with which to study the effects of tilted magnetic fields. Though somewhat different (an image Coulomb potential, instead of a linear electric potential, is the holding potential along the normal direction), such systems are more clean since the electron density is low; the lower density means there are not large many body corrections of the inversion layers and it is more suitably described by a single particle model. Despite being the first system where combined intersubband cyclotron resonances were reported to be observed by Zipfel et al.\textsuperscript{16}, any detailed spectroscopic investigation of the space charge layer for different values of the parameters have not been reported in the literature. In this system, as well as in other space charge layers, more experiments, preferably of the frequency sweep type, will be highly desirable.
CHAPTER III
COUPLED MOTIONS IN ONE DIMENSION—DOUBLE MINIMUM POTENTIALS

A. Introduction:

In Chapter I.D we have discussed the basic binding potential for the SSE on a medium of very low dielectric constant like liquid $\text{He}^4$ and the resulting nearly hydrogenic spectrum due to quantization of their motion normal to the liquid surface. Because of the behavior as an almost free 2-D gas, SSE are of interest for a variety of reasons, some of which have been already mentioned in Chapter I. A major one of these is that they represent analogs of the three-dimensional gas in a metal but with the added convenience that the number density can be readily varied over many orders of magnitude by changing the value of an external electric field that clamps the electrons to the surface of the liquid. In this manner, for instance, the first experimental observation of Wigner crystallization of an electron gas has been demonstrated in this system$^{31}$. Other recent experiments on "dimples" and lattices formed by these dimples$^{32}$ are examples of the interesting phenomena displayed by such electron layers. Our interest in this chapter is not the condensed matter aspects in the two dimensions of the layer but rather the atomic-like aspects of the system in the other perpendicular direction normal
to the surface (the z-direction in what follows). In most of the experiments an additional clamping electric field $\varepsilon$ has been applied to the z-direction. This added potential $\varepsilon z$ shifts the hydrogenic energy levels (due to the image Coulomb potential which, however, is not symmetric with respect to $z$, thus allowing for linear Stark shifts) and the resulting values are referred to as "electric subbands". The motion parallel to the surface is considered free in absence of other applied fields so that each of the subbands is infinitely degenerate. Many such subbands have been experimentally observed and their energy positions satisfactorily accounted for via simple single electron models. As mentioned in the previous chapter, there have also been experiments in which additional magnetic fields tilted at an arbitrary angle to the surface have been applied. Theoretical studies of strong field mixing phenomena involving the image Coulomb potential and an equally "strong" electric or magnetic field exemplifies the advantage of studying such systems, as analogs of similar problems involving actual atomic systems.

When placed in perpendicular electric and magnetic fields of appropriate strengths and orientations, the SSE can have a potential well with two minima for the z-motion. Such double-minimum potentials also arise for highly excited Rydberg states of atoms in crossed
electric and magnetic fields and in certain molecular potential curves. The electronic motions in the two potential wells become coupled due to possible "penetration" through the intervening barrier. When either well, considered independently, can support a bound state at the same energy, the coupling due to tunneling lifts the degeneracy giving rise to a doublet structure. This phenomenon closely resembles what causes "inversion splitting" in a molecule like NH₃ except that now the potential wells are asymmetric and that their shapes can be varied at will a great deal by changing the external fields. We develop and apply a WKB formalism to calculate such splittings for various widths of the potential barriers. For very thin barriers, two of the classical turning points for the electrons lie very close together, necessitating a modification of the usual WKB formalism. We apply this (for the first time, to our knowledge) to the problem of SSE on liquid He in crossed fields. We also apply this to many other test potentials to compare explicitly the efficacy of the modified WKB version with the usual one, as well as with results obtained otherwise.

Section B describes briefly the usual WKB formalism appropriate to a general asymmetric DMP for eigenenergies corresponding to four classical turning points, and the modifications therein necessary in cases when two of the
turning points become very close. These formalisms are applied in Section C for several potentials encountered in the molecular physics literature. These are, respectively, (i) an asymmetric double harmonic potential, (ii) a Morse potential with a Gaussian hump and (iii) a symmetric anharmonic oscillator potential. In Section D, we analyze the eigenstates of motion of the SSE in the coupled potential well, for different values of the applied electric and magnetic fields, corresponding to cases when the couplings due to tunneling can be either "weak" or "strong". A very close analog of this problem is that of the motion of an atomic electron in a certain slice of the potential when the atom is subjected to external fields of appropriate strengths in similar orientations. We present some sample calculations for this situation also in Section D. Section E summarizes this chapter.

B. The WKB Formalism for Double Minimum Potentials:
   i. General Considerations

   The WKB method as well as showing the correspondence between classical and quantum mechanics, provides useful approximations to the solutions of the one-dimensional Schrödinger equation. Attention has however been largely restricted to cases of quantization in a simple potential well, because there is frequently no analog of the Bohr
quantization condition in more complicated situations. In this section, we outline the method of obtaining such quantization conditions for any general double minimum potential which satisfies the so-called semi-classicality conditions. The method based on the usual WKB formalism fails, however, when two (or more) of the classical turning points are located very close together. Based on the work of Miller and Good, we derive a modified version of the WKB formalism which takes into account the close proximity of two of the turning points across a potential barrier. An added advantage of this method is that it can be applied uniformly for energies both below and above the barrier maximum under certain conditions.

ii. The Formalism

Consider a particle of mass \( m \) moving in a one-dimensional potential \( V(z) \) and let \( z_j \) \((j = 1, 2, 3, ...)\) be the classical turning points corresponding to an energy \( E \). The usual WKB approach proceeds by writing the approximate solution \( \psi_j(z) \) of the corresponding time independent Schrödinger equation as

\[
\psi_j(z) = A_j \, k^{-\frac{1}{2}} \exp \left( i \int_{z_j}^z k(z) \, dz \right) + B_j \, k^{-\frac{1}{2}} \exp \left( -i \int_{z_j}^z k(z) \, dz \right)
\]

(3.1)
in the classically "allowed" regions \((E > V(z))\) and as

\[
\psi_j(z) = C_j \kappa^{-\frac{1}{2}} \exp \left( - \int_{z_j}^{z} \kappa(z) dz \right) + D_j \kappa^{-\frac{1}{2}} \exp \left( \int_{z_j}^{z} \kappa(z) dz \right)
\]

(3.2)
in the "forbidden" regions \((E < V(z))\), where

\[
k(z) = \left[ 2m (E - V(z))/\hbar^2 \right]^{\frac{1}{2}} = i\kappa(z)
\]

(3.3)
with \(\kappa(z)\) taken to be positive. The above representations are valid in the "semiclassical regions" (assumed to be separated by \(z_j\), \(j = 1,2,3,...\)) such that

\[
\left| \frac{d}{dz} \left( \frac{1}{\kappa(z)} \right) \right| \ll 1.
\]

(3.4)

Clearly, these solutions diverge as \(z\) approaches \(z_j\).

However, one circumvents this problem of matching the coefficients \(C_j, D_j\) and \(A_j, B_j\) on either side of a turning point \(z_j\) by comparing the Eqs. (3.1) and (3.2) with the asymptotic forms of the exact quantal solutions to appropriate model problems. Usually, one employs the linear approximation, wherein the actual potential in the neighborhood of \(z_j\) is replaced by a linear form which coincides locally with \(V(z)\). The solutions, in this case, are Airy functions and the corresponding connection formulae obtained can be written \(^{39}\) in the matrix form as

\[
\begin{pmatrix}
C_j \\
D_j
\end{pmatrix} = M_1 \begin{pmatrix}
A_j \\
B_j
\end{pmatrix}
\]

(3.5)
if the potential barrier is to the right of \( z_j \), and as

\[
\begin{pmatrix}
A_j \\
B_j
\end{pmatrix} = M_2 \begin{pmatrix}
C_j \\
D_j
\end{pmatrix}
\]

(3.6)

otherwise. Here,

\[
M_1 \equiv \begin{pmatrix}
\theta^* / 2 & \theta / 2 \\
\theta & \theta^*
\end{pmatrix}, \quad \text{and} \quad M_2 = \begin{pmatrix}
\theta / 2 & \theta^* \\
\theta^* / 2 & \theta
\end{pmatrix}
\]

(3.7)

with \( \theta = e^{i\pi/4} \). A simpler type of coefficient change arises merely from a change of the lower integration limits, or phase reference points in Eqs. (3.1) and (3.2). Thus, if two points \( z_j, z_{j+1} \) lie in the same semiclassical segment, say, e.g., in a classically allowed region, the same wave function \( \psi \) can be written in terms of either \( A_j, B_j \) or \( A_{j+1}, B_{j+1} \), respectively in the form of the Eq. (3.1). This implies a relation of the form

\[
\begin{pmatrix}
A_{j+1} \\
B_{j+1}
\end{pmatrix} = L(\rho) \begin{pmatrix}
A_j \\
B_j
\end{pmatrix}
\]

(3.8)

where

\[
L(\rho) \equiv \begin{pmatrix}
e^{i\rho} & 0 \\
0 & e^{-i\rho}
\end{pmatrix}
\]

(3.9)

with

\[
\rho = \int_{z_j}^{z_{j+1}} k(z) dz.
\]

(3.10)

A similar relation exists between coefficients \((C_j, D_j)\) and \((C_{j+1}, D_{j+1})\). With the help of Eqs. (3.5) - (3.10), the amplitudes of a WKB function at any semiclassical
region can be written in terms of those in a different region. Quantization conditions are usually obtained by imposing proper boundary conditions on these amplitudes.

iii. The Quantization Conditions

As remarked earlier, the connection matrices that relate the amplitudes of the WKB wavefunction in some semiclassical region to those in a different one depend on the model potential chosen to approximate the actual one in the intervening region. Thus, for instance, \( M_1 \), \( M_2 \) as given in Eqs. (3.7) correspond to the so called linear approximation. It is clear then that, at least in principle, different model potentials can be used to obtain different connection matrices and thus correspondingly different quantization conditions. The relative merit of such models will depend obviously on how closely these can mock the actual potential and also, for practical reasons, on the ease with which these yield to actual calculations. We sketch below the method of obtaining the WKB quantization condition corresponding first, to the linear approximation, and, subsequently as an improvement, a quadratic approximation.

(a) Linear Approximation:

Let \( z_j \) (j = 1,2,3,4) be the four real turning points corresponding to a DMP \( V(z) \) and energy \( E \) as shown in Fig. (3.1). We first write a pair of solutions in the
Fig. 3.1. Example of an asymmetric double minimum potential. $z_1$, $z_2$, $z_3$, and $z_4$ are the four classical turning points corresponding to energy $E$. When $z_2$, $z_3$ become very close together the usual WKB formalism needs to be modified. This is also the potential in Eq. (3.39). The relevant parameters are given along with the Table (3.2).
form of Eqs. (3.1) and (3.2) on either side of \( z_j \).

Using Eqs. (3.5) - (3.10), we can write

\[
\begin{pmatrix}
C_4 \\
D_4
\end{pmatrix} = M_1 \mathcal{L}(\sigma) M_2 \begin{pmatrix}
C_3 \\
D_3
\end{pmatrix},
\]

(3.11)
as well as

\[
\begin{pmatrix}
C_1 \\
D_1
\end{pmatrix} = M_2^{-1} \mathcal{L}^{-1}(\lambda) M_2^{-1} \mathcal{L}^{-1}(i\phi) \begin{pmatrix}
C_3 \\
D_3
\end{pmatrix},
\]

(3.12)

where \( \lambda, \sigma \) are the so-called WKB integrals over the potential wells

\[
\lambda = \int_{z_1}^{z_2} k(z) \, dz \quad \sigma = \int_{z_3}^{z_4} k(z) \, dz
\]

(3.13)

and \( \phi \) is the barrier integral

\[
\phi = \int_{z_2}^{z_3} \kappa(z) \, dz.
\]

(3.14)

Finiteness of the wavefunctions as \( z \to \pm \infty \) imply \( D_4 \) and \( C_1 \) must vanish. These b.c. when applied to Eqs. (3.11) and (3.12) give us

\[
\frac{C_3}{D_3} = 2 \cot \sigma
\]

(3.16)

and

\[
\frac{C_3}{D_3} = \frac{1}{2} \tan \lambda \exp(-2\phi)
\]

(3.17)

respectively. Equating the rhs's of the above we get the required eigenvalue condition, viz.,
\[ \cot \lambda \cot \sigma = \left( \frac{1}{4} \right) \exp (-2\phi) . \quad (3.18) \]

The phase integrals \( \lambda \) and \( \sigma \) receive extra contributions in specific situations such as when, e.g., the potential function has an infinitely high barrier at \( z < 0 \), so that \( z_1 = 0 \). In this case, one starts with the solution (3.1) with \( A_1 = -B_1 \) and obtains the usual modification wherein \( \lambda \) is replaced by \( \lambda = \frac{\pi}{4} \). The quantization condition for the individual wells follows, of course, when the tunneling through the barrier is negligible, that is, \( \phi \rightarrow 0 \), so that

\[ \lambda = \left( n_{\lambda} + \frac{1}{2} \right) \pi ; \quad \sigma = \left( n_{\sigma} + \frac{1}{2} \right) \pi , \quad (3.19) \]

\( n_{\lambda} \) and \( n_{\sigma} \) being the appropriate quantum numbers for the two wells. For certain situations, Eq. (3.18) can be simplified. Thus for an asymptotically degenerate energy level \( E_0 \) satisfying both the Eqs. (3.19), the resulting doublet of energy levels upon lifting of the degeneracy are at \( E_0 \pm \delta \) where \( \delta \) can be obtained by expanding \( \lambda \) and \( \sigma \) about \( E = E_0 \) and keeping only the leading term on the rhs. This gives

\[ \delta \approx \frac{1}{2} \exp (-\phi) \left[ \left( \frac{d\lambda}{dE} \right)_0 \left( \frac{d\sigma}{dE} \right)_0 \right]^{-\frac{1}{2}} , \quad (3.20) \]

where the subscript zero implies that the respective quantities are evaluated at \( E_0 \). Also if an energy \( E_1 \) satisfies, say the first of the Eqs. (3.19) but is well
separated from the solutions to the second equation, similar expansions lead to a correction \( \delta_1 \) to \( E_1 \), given by

\[
\delta_1 = -\frac{1}{4} \tan \sigma(E_1) \exp(-2\varphi(E_1)) \left(\frac{d\sigma}{dE}\right)^{-1}_{E_1}
\] (3.21)

A parallel expression can be written down for \( \delta_2 \), the correction to the energy \( E_2 \) satisfying \( \sigma(E_2) = (n + \frac{1}{2})\pi \).

(b) **Quadratic Approximation:**

Though the previous WKB treatment, based on the linear approximation of \( V(z) \) near any turning point \( z_j \) suffices for many purposes, it can be improved upon, particularly when the barrier width becomes very small, that is when \( z_2 \) and \( z_3 \) in Fig. 3.1 get very close together. In this case, a better approximation is achieved by mapping \( V(z) \) onto a parabolic form in a region that includes, besides the point \( z_0 \) when the barrier maximum \( V_{\text{max}} \) is assumed to be located, the turning points \( z_2 \) and \( z_3 \) as well. Miller and Good, using as basis functions the solutions of a model comparison problem with a quadratic barrier, obtained WKB-type solutions to the Schrödinger equation in that region whose asymptotic forms are similar to those in Eq. (3.1). Another advantage of this method is that it can be applied uniformly for energies both below and above the barrier maximum, provided that the real turning points \( z_2 \) and \( z_3 \) for \( E < V_{\text{max}} \) go over unambiguously to a pair of complex (conjugate) turning points \( z_+ \) (with \( \text{Im} z_+ \) assumed
positive) as \( E \) becomes greater than \( V_{\text{max}} \). To be specific, they have established the following asymptotic behaviour of a pair of linearly independent solutions \( \phi_\pm \) (which can be written in terms of the well known Weber functions) of the model comparison equation:

\[
\left( \frac{2}{\pi} \right)^{\frac{1}{4}} \left( \frac{|W|}{2e} \right)^{\frac{i}{2}} \Gamma \left( \frac{iW}{2} + \frac{1}{2} \right) \cosh \left( \frac{W\pi}{2} \right) e^\frac{W\pi}{4} k^{-\frac{1}{2}}(z) \exp \left( \pm i \text{Re} \int k(z) dz \right) \\
\frac{1}{2} \left( \frac{1}{2} \right) + i k^{-\frac{1}{2}}(z) \exp \left( \pm i \text{Re} \int k(z) dz \right) \\
e^\frac{i\pi}{2} k^{-\frac{1}{2}}(z) \exp \left( \pm i \text{Re} \int k(z) dz \right) \\
\frac{W\pi}{2} e^\frac{z}{2} k^{-\frac{1}{2}}(z) \exp \left( \pm i \text{Re} \int k(z) dz \right), \tag{3.22}
\]

where \( \text{Re} \) indicates that the real part of the integral is to be used, and with

\[
W = -\frac{2\phi}{\pi}, \tag{3.23}
\]

\[
\phi = \begin{cases} 
\frac{z^3}{3} \int k(z) dz & \text{if } E \leq V_{\text{max}} \\
\int_{z_2}^{z} k(z) dz & \text{if } E > V_{\text{max}}
\end{cases} \tag{3.24}
\]

In doing the \( \phi \) integration for \( E > V_{\text{max}} \), that branch of \( k(z) \) is to be chosen which renders \( \phi \) negative. Obviously, the asymptotic behavior of a linear superposition of the base functions \( \phi_\pm \) will also be similar to that in Eq. (3.1).
Thus, if we write the WKB wavefunctions in terms of 
\((A_2, B_2)\) and \((A_3, B_3)\) in the form of Eq. (3.1) in the semi-
classical regions to the left of \(z_2\) and to the right of 
\(z_3\), respectively, then, asymptotic expansions of a function 
of the type \(f \phi^+ + g \phi^-\) (\(f, g\) two arbitrary constants) via Eq.
(3.22) leads to the following matrix relation between the 
corresponding amplitudes:

\[
\begin{pmatrix}
A_3 \\
B_3
\end{pmatrix}
= \mathbf{M}_3
\begin{pmatrix}
A_2 \\
B_2
\end{pmatrix}
\tag{3.25}
\]

with

\[
\mathbf{M}_3 = 
\begin{pmatrix}
[1 + e^{2\phi}]^{1/2} e^{-i\mu} e^{i\phi} e^{i\nu} \\
[1 + e^{2\phi}]^{1/2} e^{i\mu}
\end{pmatrix},
\tag{3.26}
\]

\[
\nu = \begin{cases} 
0 & \text{if } E < V_{\text{max}} \\
\int k(z)dz & \text{if } E > V_{\text{max}}
\end{cases}
\tag{3.27}
\]

and

\[
\mu = \mu \left( \frac{2\phi}{\pi} \right) = \arg \Gamma \left( \frac{1}{2} - \frac{\phi}{\pi} \right) - \frac{\phi}{\pi} \left( 1 - \ln \left| \frac{\phi}{\pi} \right| \right) = -\mu \left( \frac{2\phi}{\pi} \right).
\tag{3.28}
\]

\(\mu(x)\) can be calculated easily using an algorithm and it 
can be seen that \(\mu\) is positive for positive \(x\).

The corresponding eigenvalue conditions can now be 
easily obtained following the same procedure as in the 
previous section. Thus writing the wavefunctions in the 
form of Eqs. (3.1) and (3.2) on either side of the turning 
points \(z_1\) and \(z_4\) (where we assume the linear approximation
to be valid) but only in the form of Eq. (3.1) on the l.h.s. of $z_2$ and on the r.h.s. of $z_3$, we get

$$\begin{pmatrix} C_4 \\ D_4 \end{pmatrix} = M_1 L(\sigma) M_3 \begin{pmatrix} A_2 \\ B_2 \end{pmatrix}, \quad (3.29)$$

as well as

$$\begin{pmatrix} C_1 \\ D_1 \end{pmatrix} = M^{-1} \begin{pmatrix} 1 \\ 2 \end{pmatrix} L^{-1}(\lambda) \begin{pmatrix} A_2 \\ B_2 \end{pmatrix}. \quad (3.30)$$

As before, the b.c. i.e. $D_4 = 0 = C_1$ leads to the following equations:

$$\frac{A_2}{B_2} = i \frac{e^{i(\sigma+\nu)} + e^{2\phi} e^{-i(\sigma-\mu)}}{e^{-i(\sigma+\nu)} + e^{2\phi} e^{i(\sigma-\mu)}} = -i \frac{e^{i\lambda}}{e^{-i\lambda}}, \quad (3.31)$$

which reduces to

$$(1 + e^{2\phi}) \cos(\lambda+\sigma-\mu) = -e^{\phi} \cos(\lambda-\sigma+\nu). \quad (3.32)$$

The above equation can be simplified in specific circumstances. Thus for $E >> V_{\text{max}}$, we have $\phi << 0$ and the roots are given by the simple quantization formula

$$\lambda + \sigma - \mu = \int_{z_1}^{z_4} k(z) dz - \mu = \left(n + \frac{1}{2}\right) \pi, \quad (3.33)$$

which is analogous to the usual WKB-condition $\lambda + \sigma = \left(n + \frac{1}{2}\right) \pi$ except for a small (positive) level shift due to the phase correction $\mu$. Similarly, when $E < V_{\text{max}}$, $\nu = 0$ and Eq. (3.32) can be cast into a form similar to Eq. (3.18), viz.,
where
\[
\tilde{\lambda} = \lambda - \frac{1}{2} \mu \left( -\frac{2\phi}{\pi} \right), \quad \tilde{\sigma} = \sigma - \frac{1}{2} \mu \left( -\frac{2\phi}{\pi} \right)
\]  

The equivalents of Eqs. (3.19) are now given by
\[
\tilde{\lambda} = (n^z + \frac{1}{2}) \pi, \quad \tilde{\sigma} = (n_z + \frac{1}{2}) \pi,
\]  

which imply a small (negative) shift of the corresponding "isolated" energies given by Eq. (3.19) due to \(\mu\). Similarly, the Eq. (3.20) is now replaced by
\[
\delta_m \approx \left\{ \frac{(1 + e^{\frac{\phi}{2\rho}}) e^\frac{\phi}{2} - e^{\frac{\phi}{2}}}{(1 + e^{\frac{\phi}{2\rho}}) e^\frac{\phi}{2} + e^{\frac{\phi}{2}}} \right\}^{\frac{1}{2}} \left( \frac{d\tilde{\lambda}}{dE} \right)_o \left( \frac{d\tilde{\sigma}}{dE} \right)_o^{-1}.
\]  

iv. Remarks

We end this section with a couple of remarks. The first is directed towards the fact that semi-classical methods often complement other usual approximation schemes. Thus, basic understanding of strong field mixing phenomena can readily be obtained via this method while, for instance, a perturbation technique fails due to the lack of any "small" part of the Hamiltonian. For double minimum potentials, for energies close to the barrier maximum, the motions of a particle in the two wells are strongly coupled to each other and the method outlined above may be adequate for many purposes. Also, systems exhibiting either strong field
mixing phenomena or strongly coupled motions in double minimum potentials are usually associated with energy regimes that typically involve high density of states and large quantum numbers. Semiclassical methods are known to work well in such situations. Secondly, we have shown that the problem of finding the eigenvalues for such potentials reduces to a single analytical equation, the solution of which requires at most the numerical quadrature for a number of semiclassical phase integrals. These quadratures take the place of the matrix diagonalizations in numerical solutions of the Schrödinger equation employed in more direct approaches to the problem.

C. Application:

In the following, we apply the above WKB formalisms to three different double minimum potentials. Our motivation for choosing these potentials are essentially two-fold. First, all these potentials have been treated before, so that the eigenvalues for these potentials obtained through the WKB formalisms can be tested explicitly against those obtained by other methods. Also, one of these potentials, viz., the double well anharmonic oscillator potential, has been drawing continued attention from theoreticians as a test case for various approximation schemes. Secondly, all these potentials are often encountered in the molecular physics literature and are
quite similar to the DMP for the SSE on liquid He in crossed fields that we consider in the next section. The shape of the latter can be easily controlled by external fields, and may thus prove to be a "clay model", on which experiments can be performed. The results can be tested against predictions which pertain to systems other than the immediate one of the quasi two dimensional electron gas.

i. Asymmetric Double Harmonic Oscillator

Rackovsky\(^{35}\) considered the asymmetric double harmonic oscillator potential

\[
V(z) = \begin{cases} 
\frac{1}{2} m \omega^2 (z + a)^2, & z < 0 \\
V_1 + \frac{1}{2} m \omega^2 (z - a')^2, & z > 0 
\end{cases}
\] (3.38)

and obtained the doublet splittings around the energies \((n + \frac{1}{2}) \hbar \omega\) for \(n = 0,1\) through a perturbative extension of the usual WKB method applicable for a symmetric DMP\(^{42}\). The result in effect is the same as can be obtained through the use of Eq. (3.20). He also calculated the same quantities by matching at \(z = 0\) the harmonic oscillator type wavefunctions centered at \(-a\) and \(a'\), respectively. We have calculated the tunneling frequencies using Eq. (3.18). The relevant integrals \(\lambda, \sigma\) and \(\phi\) are straightforward to obtain and are also given in Ref. 35. The results are displayed in Table (3.1) along with the values obtained by Rackovsky for comparison. The quantum numbers
Table 3.1

<table>
<thead>
<tr>
<th>$V_1$ (cm$^{-1}$)</th>
<th>HO</th>
<th>WKB (a)</th>
<th>WKB (b)</th>
</tr>
</thead>
<tbody>
<tr>
<td>n=0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>20.0</td>
<td>6.13x10$^{12}$</td>
<td>5.40x10$^{12}$</td>
<td>5.46x10$^{12}$</td>
</tr>
<tr>
<td>40.0</td>
<td>5.61</td>
<td>4.89</td>
<td>4.95</td>
</tr>
<tr>
<td>60.0</td>
<td>5.14</td>
<td>4.43</td>
<td>4.49</td>
</tr>
<tr>
<td>80.0</td>
<td>4.72</td>
<td>4.03</td>
<td>4.09</td>
</tr>
<tr>
<td>100.0</td>
<td>4.34</td>
<td>3.68</td>
<td>3.73</td>
</tr>
<tr>
<td>n=1</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>20.0</td>
<td>2.85x10$^{13}$</td>
<td>2.41x10$^{13}$</td>
<td>3.10x10$^{13}$</td>
</tr>
<tr>
<td>40.0</td>
<td>2.79</td>
<td>2.35</td>
<td>3.04</td>
</tr>
<tr>
<td>60.0</td>
<td>2.74</td>
<td>2.30</td>
<td>2.98</td>
</tr>
<tr>
<td>80.0</td>
<td>2.68</td>
<td>2.25</td>
<td>2.92</td>
</tr>
<tr>
<td>100.0</td>
<td>2.63</td>
<td>2.20</td>
<td>2.86</td>
</tr>
</tbody>
</table>

Tunneling frequencies (in s$^{-1}$) for the potential in Eq. (3.38) for different values of $V_1$. Here $\omega = 10^{15}$ s$^{-1}$, $m = 1.64 \times 10^{-24}$ g, $a + a' = 0.4$ Å, taken from Ref. 35. Values in the second and the third columns are also taken from Ref. 35 and have been calculated using harmonic oscillator and WKB type wavefunctions respectively. The last column shows our result from the usual WKB formalism.
n = 0,1 imply the energy positions \( E_n = (n + \frac{1}{2}) \hbar \omega \) where the doublets appear. While we note that our calculations essentially agree with Rackovsky's for \( n = 0 \), this is not so for \( n = 1 \). The reason for this discrepancy is that the higher member of the \( n = 1 \) doublet lies above the barrier maximum. Through the use of an equation (like Eq. (3.20)) that gives the tunneling frequency directly, Rackovsky has failed to notice this. This serves to illustrate that caution should be exercised while using an equation of the type (3.20), particularly for energies just below the barrier maximum.

ii. Morse Potential with a Gaussian Hump

This is an example of an asymmetric double minimum potential which is a Morse potential with a Gaussian near the minimum:

\[
V(z) = D_e \{1 - \exp [-B(z-z_a)]\}^2 + A \exp \{-C(z-z_o)^2\}.
\]

(3.39)

This is shown in Fig. (3.1) and the Table (3.2) shows the appropriate parameter values. Wicke and Harris\textsuperscript{36} calculated several eigenvalues for this potential using three different numerical techniques. We report here our calculations for the energies \( E^{(0)}, E^{(m)} \) corresponding to four real turning points and obtained respectively through the use of the usual (Eq. (3.18)) and modified (Eq. (3.34)) versions of the WKB formalism. The necessary integrals \( \lambda, \sigma \) and \( \phi \) have
**TABLE 3.2**

<table>
<thead>
<tr>
<th>n</th>
<th>$E^{(a)}$ (cm$^{-1}$)</th>
<th>$E^{(m)}$ (cm$^{-1}$)</th>
<th>$E^{(o)}$ (cm$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>3207.9</td>
<td>3201.1</td>
<td>3205.3</td>
</tr>
<tr>
<td>2</td>
<td>4244.2</td>
<td>4234.9</td>
<td>4227.3</td>
</tr>
<tr>
<td>3</td>
<td>5158.9</td>
<td>5147.9</td>
<td>5144.3</td>
</tr>
<tr>
<td>4</td>
<td>6140.8</td>
<td>6071.6</td>
<td>6064.2</td>
</tr>
<tr>
<td>5</td>
<td>7122.6</td>
<td>7103.2</td>
<td>7092.7</td>
</tr>
<tr>
<td>6</td>
<td>7642.7</td>
<td>7625.0</td>
<td>7614.6</td>
</tr>
<tr>
<td>7</td>
<td>8960.0</td>
<td>8932.5</td>
<td>8911.5</td>
</tr>
<tr>
<td>8</td>
<td>9146.2</td>
<td>9105.7</td>
<td>9095.7</td>
</tr>
<tr>
<td>9</td>
<td>10247</td>
<td>10227</td>
<td>10208</td>
</tr>
</tbody>
</table>

Usual and modified WKB results for the eigenenergies of an asymmetric DMP (Eq. (3.39)) and also considered in Ref. 36. $D_e = 31250$ cm$^{-1}$, $B = (8\pi^2 \text{ cm}\chi/h)^{\frac{1}{2}} \times 10^{-8}$, $m = 5.000 \text{ g/mole}$, $\chi = 8$ cm$^{-1}$, $z_e = 1.5 \text{ A}^0$, $A = 10^4$ cm$^{-1}$, $C = 200 \text{ A}^{0.2}$, $z_o = 1.6 \text{ A}^0$. (from Ref. 36).

- **a:** numerically obtained values from Ref. 36.
- **m:** modified WKB result.
- **o:** ordinary WKB result.

Only those eigenvalues that correspond to four real turning points are shown.
been evaluated numerically using Gaussian quadrature. The results are displayed in Table (3.2) along with the "exact" values obtained from Ref. 36. First, we note that $E^{(m)}$ is always less than $E^{(o)}$. Secondly, $E^{(m)}$ shows marked improvement over $E^{(a)}$ for all the quantum numbers except $n = 1$. This is perhaps due to the fact that in this case, the turning points $z_3$ and $z_4$ across the second well are very close together, instead of the points $z_2$ and $z_3$ across the barrier being so, as is assumed in the derivation of Eq. (3.34).

The modified WKB procedure, besides being able to provide more accurate results, may prove to be advantageous for yet another reason. As is noted in Ref. 36, in certain types of iterative numerical method such as the one based on the work of Numerov \textsuperscript{43} and Cooley \textsuperscript{44}, the rate of convergence to any desired eigenvalue depends strongly upon the initial estimates or guesses of the same. Since the same integrals $\lambda$, $\sigma$ and $\phi$ are required in both the usual and the modified WKB formalism, the little extra work in evaluating the function $\psi$ and in solving Eq. (3.34) instead of Eq. (3.18) may often be desirable considering the possible reduction in computer time in an exact numerical integration that uses the modified WKB results as its input.
iii. **Double Minimum Anharmonic Oscillator Potentials**

An anharmonic oscillator potential with two minima has been the subject of many investigations for both pedagogic\(^{41b,c}\) and practical\(^{37,45}\) reasons. Here we consider, in somewhat greater detail than in the previous example, the WKB results for a symmetric potential \(V(z)\) given by

\[
V(z) = -az^2 + bz^4 ; \quad a, b > 0
\]  

(3.40)

which, through a simple scale transformation, can also be written as

\[
V(z) = -dz^2 + z^4 ; \quad d > 0
\]  

(3.41)

Ezawa *et al.*\(^{37}\), using a numerical integration technique originally due to Milne\(^{46}\), accurately obtained a few of the eigenvalues of the Schrödinger equation with the above potential. The same potential, in the form of Eq. (3.40), has been used earlier by Sommorjai and Hornig\(^{45}\). Their calculations, while not as accurate as those due to Ezawa *et al.*, were based on the diagonalization of the appropriate Hamiltonian in a basis set of 20 harmonic oscillator type functions. We present the relevant WKB results, now for energies both below and above the barrier maximum (at zero), and compare these with the previous calculations in order to provide a better perspective on such approximation methods.

We consider the potential in the form of Eq. (3.41) and also assume \(2m = \hbar^2 = 1\). The values of \(a\) and \(b\) are specified
in Table 3.3. The potential minima (\(= -d^2/4\)) are located at \(=(d/2)^k\). For an energy \(E\) such that \(-d^2/4 < E \leq 0\), the four real turning points \(z_1, z_2, z_3, z_4\) (with \(z_1 < z_2 < z_3 < z_4\)) are given respectively, by

\[
\begin{align*}
  z_1 &= -\frac{1}{\sqrt{2}} (d + \sqrt{d^2 + 4E})^{1/2} \\
  z_2 &= \frac{1}{\sqrt{2}} (d - \sqrt{d^2 + 4E})^{1/2} \\
  z_3 &= -\frac{z_2}{2}; z_4 &= -\frac{z_1}{2}.
\end{align*}
\]

(3.42)

For energies above the barrier maximum, i.e., for \(E > 0\), \(z_1\) and \(z_4\) are still given by the above but \(z_2\) and \(z_3\) go over to a pair of complex conjugate roots \(z_\pm\) with \(z_\pm = \pm i z_3\), with \(z_3\) as given in the above equation.

The integrals \(\lambda (= \sigma, \text{due to symmetry})\), \(\phi\) and \(\nu\) as defined in Section B can be easily obtained\(^{47}\) for both positive and negative energies. These are:

\[
\lambda = \sigma = \begin{cases} 
\frac{1}{3} z_4 \left( z_4^2 + z_3^2 \right) \left[ 1 - \frac{z_3^2}{z_4^2} \right] - 2 z_3^2 K \left( 1 - \frac{z_3^2}{z_4^2} \right) & \text{if } E < 0 \\
\frac{1}{3} \left( z_4^2 + |z_+|^2 \right) \left[ |z_+|^2 K \left( 1 + |z_+|^2/z_4^2 \right)^{-1} \right] + \left( z_4^2 - |z_+|^2 \right) E \left( 1 + \left( \frac{|z_+|^2}{z_4^2} \right)^{-1} \right) & \text{if } E > 0 
\end{cases} 
\]

(3.43)
TABLE 3.3

<table>
<thead>
<tr>
<th>n</th>
<th>$E^{(0)}$</th>
<th>$E^{(m)}$</th>
<th>$E^{(a)}$</th>
<th>$E^{(a)} - E^{(0)}$</th>
<th>$E^{(a)} - E^{(m)}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>-4.3683</td>
<td>-4.4094</td>
<td>-4.4368</td>
<td>-0.0685</td>
<td>-0.0274</td>
</tr>
<tr>
<td>1</td>
<td>-4.2833</td>
<td>-4.3282</td>
<td>-4.3498</td>
<td>-0.0665</td>
<td>-0.0216</td>
</tr>
<tr>
<td>2</td>
<td>-0.0119</td>
<td>0.0608</td>
<td>0.0242</td>
<td>0.0361</td>
<td>-0.0366</td>
</tr>
<tr>
<td>3</td>
<td>1.7587</td>
<td>1.5825</td>
<td>1.5671</td>
<td>-0.1916</td>
<td>-0.0154</td>
</tr>
<tr>
<td>4</td>
<td>4.7478</td>
<td>4.8432</td>
<td>4.8312</td>
<td>0.0834</td>
<td>-0.0120</td>
</tr>
<tr>
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<td>8.2758</td>
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<tr>
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<td>12.203</td>
<td>0.022</td>
<td>-0.003</td>
</tr>
<tr>
<td>7</td>
<td>16.460</td>
<td>16.479</td>
<td>16.478</td>
<td>0.018</td>
<td>-0.001</td>
</tr>
</tbody>
</table>

First eight eigenvalues of the symmetric double minimum potential (Ref. 37) corresponding to an anharmonic oscillator. $a = 2.56$ and $b = 0.32$ in Eq. (3.40).

o: usual WKB method (Eqs. (3.18) and (3.19)).

m: modified WKB method (Eqs. (3.33) and (3.34)).

a: numerically obtained values (Ref. 37).
\[
\phi = \begin{cases}
\frac{2}{3} \frac{z}{4} \left[ (z_{3}^{2} + z_{3}^{2}) K \left( \frac{z_{3}^{2}}{z_{4}^{2}} \right) - (z_{4}^{2} - z_{3}^{2}) K \left( \frac{z_{3}^{2}}{z_{4}^{2}} \right) \right] & \text{if } E \leq 0 \\
- \frac{2}{3} \left( z_{4}^{2} + |z_{+}|^{2} \right)^{1/2} \left[ z_{4}^{2} K \left( \frac{1 + z_{4}^{2}/|z_{+}|^{2}}{1 - z_{4}^{2}/|z_{+}|^{2}} \right) \right] & \text{if } E > 0
\end{cases}
\]

(3.44)

and \( \nu = 0 \) for both \( E < 0 \) and \( E \geq 0 \). Here \( K \) and \( E \) are the complete elliptic integrals of the first and second kind respectively and are defined as in Ref. (40). These can be obtained accurately and quite conveniently using a well known algorithm. \( \mu = \mu(-2\psi/\pi) \) can be calculated as mentioned before. The results are shown in Table 3.3. A comparison of the WKB results with the values obtained by Ezawa et al. clearly shows the marked improvement of the modified WKB values over those due to the usual WKB method. As expected, the WKB results improve with increasing quantum number with the exception of the \( n = 2 \) level. Here, the modified WKB value is at least of the correct sign, unlike the usual one, but is numerically inaccurate, perhaps due to the very close proximity of two (complex) turning points.

D. Surface State Electrons on Liquid Helium in External Fields: Eigenstates of Motion in Coupled Potential Wells:

i. General
We have briefly discussed in Chapter I the origin of the nearly hydrogenic spectrum for the surface state electrons on liquid He\(^4\) corresponding to the quantization of the electronic motion normal to the liquid surface (the z-direction in what follows). In the absence of other fields, we consider the electronic motion parallel to the surface (assumed to be the x-y plane) to be completely free. When placed in crossed electric and magnetic fields, the electrons can find for their z-motion an asymmetric double minimum potential. By changing the external fields, it is possible to obtain energy eigenvalues which are asymptotically degenerate, i.e., the two wells, considered independently, can support a bound state at the same energy. However, the motions in the two wells are actually coupled, due to possible tunneling through the intervening barrier. This results in a lifting of the "degeneracy", giving rise to a doublet of energy levels. This phenomenon has been discussed only qualitatively before\(^6\). We report here more detailed and accurate calculations on such doublet spacings using the WKB methods developed in Section B of this chapter.

\[\text{ii. The Potential}\]

Since liquid He\(^4\) has a permittivity \(\varepsilon = 1.0572\) which is only slightly larger than unity, the surface state electrons are bound by a weak attractive image potential,
a one-dimensional Coulomb potential

\[ V_{im}(z) = -Qe^2 / z, \quad z > 0 \quad (3.46) \]

with

\[ Q = \frac{1}{4} \frac{\varepsilon - 1}{\varepsilon + 1} \approx 6.955 \times 10^{-3} \quad (3.47) \]

where \( z = 0 \) marks the surface of the liquid and \( Qe \) is the effective charge of the one-dimensional Coulomb potential. For \( z < 0 \) the liquid represents a barrier (of height \( \approx 1 \text{ eV} \)) to the electrons and given the other scale of energies set in the problem by \( Q \), the barrier is to a first approximation infinitely high so that the boundary condition can be taken to be that the electronic wave function vanishes at \( z = 0 \). More careful treatments that go beyond this approximation are available in the literature\textsuperscript{26,27} but we restrict ourselves to the initial approximation since it is known to be quite accurate in practice. The \( z \)-motion then is quantized into energy levels \( -mQ^2e^4/2n^2\hbar^2 \), \( n = 1, 2, \ldots \). Note the exact correspondence to the s-wave radial problem of the hydrogen atom. We choose as units of energy and distance the effective "Rydberg" (\( \tilde{R}_Y \)) and the effective "Bohr" radius (\( \tilde{a}_O \)), respectively:

\[ \tilde{R}_Y = Q^2 R_Y \approx 0.7 \text{ meV} ; \quad \tilde{a}_O = Q^{-1} a_o \approx 143 a_o \quad , \quad (3.48) \]

\( R_Y \) and \( a_o \) being the usual Rydberg and Bohr radius, respectively.

Now suppose an electric field \( \varepsilon \) is applied along \( -\hat{z} \) and a magnetic field \( B \) along the liquid surface, say in the \( x \)-direction. Adopting a gauge \( \hat{A} = (0, -Bz, 0) \) to describe
the B-field, the complete Hamiltonian for a SSE takes the form

$$H = \frac{p_x^2}{2m} + \frac{p_z^2}{2m} + \frac{1}{2m} \left( p_y - \frac{eB}{c} \right)^2 - \frac{Qe^2}{z} - e\varepsilon z, \; z > 0.$$  

(3.49)

Our interest is in the z-motion but some remarks are in order regarding the other dimensions. $p_x$ completely separates out of the problem, is a conserved quantum number and represents a remaining degeneracy of every level. $p_y$ too is conserved because it commutes with $H$. The problem, therefore, reduces to a one-dimensional one with a combination of an image potential, a linear potential and a harmonic oscillator well centered at $z = cp_y/eB$. Such a combination has the generic form of a double-minimum potential. In our calculations, we restrict ourselves to the parametric value $p_y = 0$ when the potential takes the forms shown in Fig. 3.2. We note that minimizing the energy with respect to $p_y$, the minimum lies at $<p_y> = \hbar \omega_c <z>$ where $\omega_c = eB/mc$ is the cyclotron frequency. Since $\varepsilon$ and $B$ are unspecified our results for $(<p_y> = 0, \varepsilon, B)$ can be mapped on to those where $<p_y>$ has been minimized by the replacement $\varepsilon - \hbar \omega_c^2 <z>/e + \varepsilon$ and an overall re-definition of the zero of the energy scale by $\hbar \omega_c^2 <z>^2$.

The problem we consider is, therefore,

$$V(z) = \begin{cases} \infty & z \leq 0 \\ -\frac{Qe^2}{z} - e\varepsilon z + \frac{e^2B^2}{2mc^2} z^2 & z > 0 \end{cases}.$$  

(3.50)
Fig. 3.2. Plots of the potential $V(z)$ in Eq. (3.50) for two different values of $\epsilon$ and $B$. $\hbar \omega_c$ ($= \sqrt{eB/m_c}$) is the cyclotron frequency corresponding to the magnetic field $B$. 
This potential has the following notable features:

(a) Even in the absence of external fields (ε=\(E=0\)), \(V(z)\) is not invariant under the transformation \(z \rightarrow -z\). This implies a linear Stark shift of the levels in the presence of an ε field. Such Stark shifted levels are the so-called electric subbands.

(b) The "critical" values \(\epsilon_c\) and \(B_c\) for the electric and the magnetic fields, for which the magnitudes of the \(z\) and \(z^2\) terms in Eq. (3.50), each equals 1 Ry at \(z = a_o\) are respectively -855 \(V/cm\) and -55 kGauss only. These values give a measure of the strengths of the external fields which are on par with the basic binding due to the Coulomb field and are to be compared with the values of \(2.57 \times 10^9\) \(V/cm\) and \(2.35 \times 10^6\) kGauss respectively for the corresponding quantities for a hydrogen atom (\(Q=1\)). Thus strong field mixing regimes can be easily attained for such a system with laboratory values of ε and B fields.

(c) As is evident from Fig. 3.2, the potential resembles, to some extent, the potential curves often encountered in the molecular physics literature such as the ones discussed in the previous section. However, the shape of this potential depends a great deal on the external parameters like ε and B.

The above features point out that this system can perhaps be studied with some advantage as analogs of the other problems in atomic and molecular physics.

iii. Calculation of the Doublet Spacings

We have applied the results derived in Section B to obtain the doublet spacings \(\Lambda^{(o)} = 2\delta\) (we use the same notation as in Section B) around an asymptotically degenerate eigenenergy \(E_o\), for sample values of ε and B. Because of
the infinitely high potential barrier at $z = 0$, $z_1$ is also zero and the wave function must vanish there, thus necessitating the modification of replacing $\lambda$ by $\lambda - \frac{\pi}{4}$ in the relevant equations. We, however, have replaced $\lambda$ by $\lambda - \frac{\pi}{2}$ to obtain the well known hydrogenic energy levels in the inner well in the absence of $\epsilon$ and $B$ fields. $E_0$ is chosen to be the ground state in the inner minimum: $n_{\lambda} = 0$. The values of $\epsilon$ and $B$ are "tuned" iteratively so as to bring levels in the outer minimum to coincide with $E_0$. The usual WKB integrals, as well as the integrals $\left(\frac{d\lambda}{dE}\right)_0$ and $\left(\frac{d\sigma}{dE}\right)_0$ have been derived in Appendix E in closed analytical form in terms of complete elliptic integrals of first, second and third kinds whose arguments involve the zeroes of $k^2(z)$. The integrals have been evaluated conveniently and quite accurately using a standard algorithm.

Table 3.4 gives the doublet spacings $\Delta$ obtained from Eq. (3.20) for sample values of small and large $n_0$. A representative potential curve is shown in Fig. 3.2 for which $\epsilon = 85$ V/cm and $B = 5$ kGauss. Since the barrier width is quite appreciable here, use of Eq. (3.20) is justified. The spacings are roughly of the order of $\mu$eV and the doublet structure may not be fully resolved in an experimental investigation. Table 3.5 presents results for another situation where the parameters are chosen so as to make the barrier at $E_0$ very thin (see the graph for $\epsilon = 225$ V/cm and $B = 9$ kGauss in Fig. 3.2). The splittings are, therefore, much larger. The doublet separations now
Doublet splittings $\Delta^{(0)} (=2\delta)$ obtained by the usual WKB method (Eq. (3.20)). The asymptotically degenerate eigenvalues $E_0$ (satisfying (Eqs. (3.19)) with $n^\lambda = 0$ and $n^c$ as given above) for the potential in Eq. (3.50) are obtained by "tuning" $\varepsilon$ and $B$ fields. $\hbar\omega_C$ ($=\hbar eB/mc$) is the cyclotron energy.
TABLE 3.5

<table>
<thead>
<tr>
<th>$\varepsilon$</th>
<th>$B$</th>
<th>$n_o$</th>
<th>$\omega_o$</th>
<th>$\Delta^{(0)}$</th>
<th>$\Delta^{(m)}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>(V/cm)</td>
<td>(kGauss)</td>
<td></td>
<td>(\mu eV)</td>
<td>(\mu eV)</td>
<td>(\mu eV)</td>
</tr>
<tr>
<td>224.84</td>
<td>8.8886</td>
<td>9</td>
<td>102.9</td>
<td>64.21</td>
<td>56.79</td>
</tr>
<tr>
<td>225.17</td>
<td>9.1131</td>
<td>8</td>
<td>105.5</td>
<td>64.39</td>
<td>57.09</td>
</tr>
<tr>
<td>225.56</td>
<td>9.3655</td>
<td>7</td>
<td>108.4</td>
<td>64.52</td>
<td>57.38</td>
</tr>
<tr>
<td>226.04</td>
<td>9.6527</td>
<td>6</td>
<td>111.7</td>
<td>64.58</td>
<td>57.64</td>
</tr>
<tr>
<td>226.63</td>
<td>9.9850</td>
<td>5</td>
<td>115.6</td>
<td>64.54</td>
<td>57.82</td>
</tr>
</tbody>
</table>

Same as in Table 3.4, but now $E_0 (= -0.7443$ meV) is kept fixed, and modified WKB values $\Delta^{(m)}$ (Eq. (3.37)) are also displayed for comparison with $\Delta^{(0)}$. 
are well within the range of experimental accuracy and the field strengths are quite reasonable for an experimental observation of this phenomenon. The sensitive dependence on tunneling which is further, very sensitive to the width of the barrier, makes this phenomenon extremely sensitive to the values of ε and B. We also compare in Table 3.5 the doublet spacings given by the simpler expression (3.20) with those obtained from the more accurate Eq. (3.37) where, however, we have assumed \( \frac{d \mu}{dE} \bigg|_0 = 0 \). To our knowledge, these may be the first actual numerical comparison of these alternative expressions.

iv. An Analogous System: Rydberg Atoms in Crossed Fields

The potential in Eq. (3.50) also arises in the study of highly excited Rydberg states of atoms in external static fields. Most studied cases of strong field mixing phenomena in such systems, as discussed already in Chapter I, typically involve the Coulomb field and either an electric or a magnetic field. But a situation where crossed electric and magnetic fields are present due to a motional Stark effect has been studied experimentally\(^4\) and theoretically\(^49\). The more general instance of arbitrary ε and B leading to double-minimum potentials has only been discussed qualitatively\(^50\). We note that an electric field in the z-direction and a magnetic field in the x-direction gives a potential for an atom with nuclear
charge $Q$ which takes the following form for a certain slice ($x = y = 0$) of the coordinates:

$$V(z) = -\frac{Qe^2}{|z|} - ecz + \frac{e^2B^2}{2mc^2} z^2. \quad (3.51)$$

This potential is, therefore, very similar to (3.50) except that for $z < 0$ it is a steeply-rising potential instead of a barrier at $z = 0$. Figure 3.3 gives an example for certain values of $\epsilon$ and $B$ for a hydrogenic atom ($Q=1$). Since it would be of interest to excite atomic levels which fall in the range of energies where there can be substantial localization in the outer valley, we present sample calculations applicable to this model as well. The results are shown in Table 3.6. Note the rapid variation in the doublet spacing with $n_0$. We should, however, remember that in an actual potential, the $z$-motion of the electron is coupled to motion in the other dimensions as well and as a result, each energy level corresponding to the potential above may be shifted and broadened.

E. Summary:

Two dimensional layers of surface state electrons on liquid helium, when placed in crossed electric and magnetic fields, can have a potential with two minima for the electronic motion normal to the liquid surface. We have analyzed the electronic motion in such coupled potential wells. In particular, employing the WKB formalism, we have calculated the energy splittings that arise
Fig. 3.3. Example of the potential in Eq. (3.51).
<table>
<thead>
<tr>
<th>$\varepsilon$ (V/cm)</th>
<th>$B$ (kGauss)</th>
<th>$n_o$</th>
<th>$\gamma \omega_c$ (meV)</th>
<th>$\Delta (0)$ (meV)</th>
<th>$\Delta (m)$ (meV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>6812.9</td>
<td>54.642</td>
<td>0</td>
<td>0.633</td>
<td>4.12</td>
<td>4.13</td>
</tr>
<tr>
<td>6662.8</td>
<td>51.329</td>
<td>5</td>
<td>0.594</td>
<td>35.75</td>
<td>35.53</td>
</tr>
<tr>
<td>6557.5</td>
<td>48.897</td>
<td>10</td>
<td>0.566</td>
<td>70.84</td>
<td>69.08</td>
</tr>
<tr>
<td>6478.1</td>
<td>46.980</td>
<td>15</td>
<td>0.544</td>
<td>100.8</td>
<td>95.54</td>
</tr>
<tr>
<td>6415.7</td>
<td>45.408</td>
<td>20</td>
<td>0.526</td>
<td>124.8</td>
<td>114.5</td>
</tr>
</tbody>
</table>

Similar to Table 3.5, but now the results correspond to the atomic potential (Eq. (3.51)). $E_0 ( = -56.076 \text{ meV})$ corresponds to the $n_\lambda = 17 \text{ Rydberg level in } \varepsilon \text{ and } B$: $\lambda (E_0) = (n_\lambda - \frac{1}{2}) \times 2\pi$. Note the rapid increase in $\Delta$'s with increase in $n_o$. 
because of the coupling. In the limit of "strong" coupling, the usual WKB method does not suffice. Based on the work of Miller and Good \cite{21a}, we have developed a modified version of WKB formalism for such double minimum potentials and have applied it, for the first time to our knowledge, to this problem as well as a variety of sample potentials. The result is encouraging.
CHAPTER IV
CONCLUSIONS

In the framework of single particle Hamiltonians, we have analyzed in considerable detail the influence of non-separable motions on the eigenvalue structures of two distinct physical systems. Both of these involve quasi two dimensional layers of electrons, and external fields that cause the non-separable motions. We have considered a wide range of magnitude of such fields, and consequently, a corresponding wide range of the strength of the coupling between the motions.

In the case of the first system, viz., the space charge layers on a Si(100) surface, an external magnetic field tilted with respect to the surface couples the electronic motions in two perpendicular directions. This coupling itself is responsible for the recently observed phenomenon of intersubband cyclotron combined resonances. Certain features of these resonances, viz., the asymmetry in amplitudes and positions of the combined resonances with respect to the main one have been hitherto attributed to specific many body aspects of the system. Since our calculations also show qualitatively similar features, single particle effects due to the non-separability of motions may, at least partly, account for the experimental observations. Any attempt at a complete
understanding of this phenomenon should therefore include, besides the appropriate many body corrections, the aspects of non-separable motions borne out by our calculations. A major one of these, we believe, is the fact that the Landau separation on each electric subband is determined not just by the normal component of the magnetic field alone, as expected in a naive picture, but also by its component parallel to the surface and by the respective subband index.

The model Hamiltonian we have used for this problem is interesting also for a couple of other reasons. First, viewed as a function of the parameter \( \alpha \), the angle of tilt of the magnetic field, the Hamiltonian shows a jump discontinuity of definite magnitude at \( \alpha = 90^\circ \), a configuration corresponding to the Voigt geometry. Secondly, through a linear transformation, the Hamiltonian itself can be obtained in a separable form, but with the coupling contained entirely in the boundary conditions. It is conceivable that there may be other problems in physics with a similar structure for their corresponding Hamiltonians. It might be an attractive possibility to approach these problems by keeping the Hamiltonians separable, but somehow incorporating the coupled boundary conditions. This, we feel, deserves further attention in the future.
Electronic motions in coupled potential wells have been analyzed in the case of the second system, viz., the two dimensional sheets of surface state electrons that exist just outside the surface of liquid helium. A novel double minimum potential for the electronic motion normal to the liquid surface can be formed by applying electric and magnetic fields in specific orientations. The resulting coupling between the electronic motions in the individual potential wells can be changed drastically by varying the external fields. This problem is a close analog of the problems pertaining to the vibrational levels of molecules as well as to the problem of an atomic system in similar external fields. We have shown how by "tuning" the external fields, asymptotically degenerate energy levels can be obtained inspite of the asymmetry of the potential involved. By employing semiclassical techniques, we have calculated the resultant splittings of such energy levels caused by the coupling due to barrier penetration, in the limits when the strength of this coupling is either small or large. For cases when the coupling strengths, that is, the barrier penetration probabilities are large, one needs to modify the usual WKB formalism to take into account the close proximity of the turning points across the potential barrier. Based on the work of Miller and Good, we have done so and obtained
the relevant quantization conditions for a general asymmetric double minimum potential. We have applied this method, perhaps for the first time, to this problem. In order to compare its utility against those due to other methods, we have also applied this formalism to many other sample potentials considered in the literature before. We find the results to be encouraging.

The obvious extensions of the work presented here will be to study the He system in the presence of a tilted magnetic field. This system will have a large number of parameters. For example, for parameter values such as to form a single potential well for the electronic motion along the normal direction, this problem will be parallel to the one we have considered for the Si-system. Also, when there is a double minimum potential for this motion, it will be interesting to see the interplay between the coupled motions in the normal direction with the added coupling, due to the tilt of the magnetic field, that will tend to scatter the electron into a plane parallel to the liquid surface. The modified version of the WKB formalism should prove to be useful for various problems concerning barrier penetration in the strong coupling limit, when other methods such as the perturbation technique or the usual WKB method become inadequate.
These problems include, besides those already mentioned, the problems of field ionization of weakly bound particles, like Rydberg electrons or negative ions. Some of these will be tackled by us in the near future.
REFERENCES


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references therein.


30. Ref. 10. Also see, for instance, S. Kawaji, Surf. Sci. 73, 46 (1977).


34. Philip M. Morse and Herman Feshbach, Methods of Theoretical Physics, Part II (McGraw Hill, New York 1953), §9.6.


42. Ref. 38, p. 183.


47. I. S. Gradshteyn and I. W. Ryzhik, Tables of Integrals, Series and Products (Academic, New York, 1965), §3.155. (Note that Eq. 3.155.5 is in error, the 2 within {} should be replaced by 1).

48. Ref. 40, §17.6-17.7. Note that the arguments used here are what are called $k^2 = \sin^2 \alpha$ in Ref. 40.


53. Ref. 47, p. 845.

APPENDIX A

TWO-DIMENSIONAL SPACE CHARGE LAYER IN
A TILTED MAGNETIC FIELD
Two-dimensional space-charge layer in a tilted magnetic field

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Combined intersubband cyclotron resonances in a quasi-two-dimensional space-charge layer with a magnetic field tilted with respect to the surface are studied through a simple single-electron model. Two alternative basis sets have been pointed out which enable one to obtain analytical matrix elements of the Hamiltonian for all values of the magnitude and the angle of tilt of the magnetic field. The effect of the coupling between electronic motions normal and parallel to the layer has been investigated in detail and is found to give rise to deviations in the expected values of the Landau spacings as functions of the tilt angle of the \( B \) field. Optical spectra for such systems show some features in qualitative agreement with experiments and other calculations. The system is a prototype of nonseparable problems in two dimensions.

I. INTRODUCTION

In recent years, the study of two-dimensional space-charge layers (as can be found in metal-oxide—semiconductor sandwiches) under a tilted magnetic field has been of increasing theoretical and experimental interest.\(^1\) Following a report\(^2\) on combined intersubband cyclotron resonances, Ando\(^1\) performed a detailed numerical calculation with a large basis set that includes many-body corrections which account for many features of the observations. We present here a simple one-electron model for a two-dimensional space-charge layer under a tilted magnetic field. This is not to say that many-body effects are unimportant; in fact, they are important, particularly in the silicon system which is the system most extensively studied.\(^1,2\) However, use of a model potential,\(^4\) in which the electron in the space-charge layer is assumed to be held in the \( z \) direction (normal to the interface) by a "triangular" potential well due to the applied electric field, is not uncommon in the literature.\(^3,5\) This is because the model seems to be quite adequate for certain systems like PbTe (Ref. 3) and, because it serves as a common backdrop against which new many-body effects can be viewed, the model continues to be used for this purpose.\(^5\) The motivation for our study of the tilted magnetic field problem in this model is that it seems desirable to be able to explore which and how much of the observed phenomena can arise out of the single-particle description. Such a complete study of single-particle effects will serve to point out more clearly features which are due solely to many-body aspects of the problem. Since we neglect many-body aspects, we make no claim for a complete description of a space-charge layer in a tilted field. The merit of our study, as we will see, is that we get results qualitatively similar to those hitherto attributed to many-body effects. In this way, our study points to another possible origin of some of the observed features of the combined resonances, namely the coupling between the motions parallel and perpendicular to the interface induced by the tilted magnetic field. A further and important feature of the simple model is that it is a prototype of problems involving motions in more than one dimension (here two perpendicular directions) when the nonseparability of the motions is essential for the phenomena under study. Being simple enough, this prototype may serve to give insights into the general quantum mechanical problem of nonseparable motions.

The electric field normal to the oxide-semiconductor interface (\( x-y \) plane) groups the electrons into quantized energy levels called electric subbands. An additional magnetic field along the \( z \) direction further quantizes the electronic motion in the \( x-y \) plane. Since there is no coupling between the cyclotron motion in the \( x-y \) plane and the subband motion along the \( z \) direction, such a problem is trivial. A more interesting case results when the \( B \) field is tilted from the normal so that a component \( B_y \) is present as well. As shown in Sec. II, the Hamiltonian, when reduced to its simplest form, contains a term coupling the \( y \) and \( z \)
motions. Because of this coupling between the cyclotron and subband motions, transitions between energy levels involving a simultaneous change in the subband index as well as the Landau quantum number become possible under an external radiation field. These are the combined intersubband cyclotron resonances. Depending on the strength of the magnetic field relative to the electric one and on the angle of tilt of the $B$ field, the coupling can modify the optical spectrum considerably. In most of the experiments done so far, particularly on Si-MOSFET (metal-oxide—semiconductor field-effect transistor) devices, the quantization of the $z$ motion has been dominated by the electric field. However, situations where even the $z$ motion is governed mainly by the $B$ field have appeared recently in the literature. Thus the model Hamiltonian we consider proves to be even more interesting in that it contains a nontrivial coupling between two competing modes (the $y$ and $z$ motions) and such systems may prove to be a fertile ground where one may expect to find features due to the strong mixing phenomenon as has been suggested in the literature. This provides a further motivation for investigating such systems. The Hamiltonian as given in Sec. II represents a simple (in that all the dependences are either linear or quadratic in the coordinate variables) prototype of two-dimensional nonseparable systems.

We employ two alternative basis sets to diagonalize the Hamiltonian. The matrix elements obtained are in closed form and easily calculable. Section II describes briefly the model Hamiltonian and the methods for calculating the energy levels as well as the optical spectrum for a weak $z$-polarized radiation. Section III then proceeds to describe the numerical results and their discussions. Section IV contains a summary and conclusions.

II. CALCULATION OF ENERGY LEVELS AND OPTICAL SPECTRUM

As our model for the space-charge layer in metal-oxide—semiconductor (MOS) devices, we consider it to be effectively a two-dimensional electron gas. Each electron describes free motion in the $x$-$y$ plane (assumed parallel to the oxide-semiconductor interface) but is held in the $z$ direction (normal to the interface) by an infinite potential barrier at $z=0$ on the oxide side and a linear electric field potential $eze$ on the other side. The electronic subband levels are then considered to be the quantized energy levels in such a triangular potential well. The strength of the electric field is proportional to the sum $N_e$ of the number density of the space-charge layer and that in the depletion layer: $e=kn$. The constant of proportionality $k$ is regarded as an adjustable parameter and can be chosen to reproduce the experimental value for the energy separation of the ground and the first excited subband. In this way, through the empirical choice of $k$, the many-body aspects may be thought to be included to some extent in our model. But, apart from that, we consider the system as one of a single electron moving in a triangular potential well. This approximation is reasonably justified for inversion layers as well as for low-doped semiconductors (quasi-accumulation-layers). We do emphasize, however, that this is an oversimplification, because the actual effective potential for an electron, especially in an excited state or in accumulation layers, departs considerably over some ranges from the triangular one.

If a magnetic field is applied to such a system tilted with respect to the normal to the interface by an angle $\alpha$, let $B_z$ and $B_y$ be its components perpendicular and parallel to the surface, respectively. Choosing a gauge $\mathbf{A}=(zB_y - yB_z,0,0)$ as in Ref. 2 to describe this field, the Hamiltonian for the electron can be written as

$$H = \frac{p_y^2}{2m_l} + \frac{p_z^2}{2m_l} + \frac{1}{2m_f} \left[ p_x + \frac{e}{c} (zB_y - yB_z) \right]^2 + eze,$$

$$-\infty \leq y \leq \infty, \ 0 \leq z \leq \infty \quad (1)$$

where $m_f$ and $m_l$ are the effective masses of the electron parallel and perpendicular to the interface, respectively. With $H$ as given in Eq. (1) the $x$ part of the wave function is described by plane waves and translating $y$ by $cp_x/eB_z$, the $x$ coordinate can be removed. This transformation is legitimate for all $B_z \neq 0$. Equation (1) then becomes

$$H = \left[ \frac{p_y^2}{2m_l} + \frac{e^2B_y^2}{2m_l c^2} y^2 \right] + \left[ \frac{p_z^2}{2m_l} + eze + \frac{e^2B_y^2}{2m_l c^2} z^2 \right]$$

$$-\frac{e^2B_yB_z}{m_l c^2} yz \quad (2a)$$
One obtains the same Hamiltonian as above for the parametric choice \( \langle p_z \rangle = 0 \). We note that while this choice of \( \langle p_z \rangle \) does not affect the eigenvalue structure when \( B_z \) is nonzero (because of the admissible translation in \( y \)), it does not give the true ground-state energy when \( B_z = 0 \). The value of \( \langle p_z \rangle \) which minimizes the energy in this case is seen from Eq. (1) to be \( -eB_y/c(z) \) and then the appropriate Hamiltonian becomes

\[
H = \frac{p_y^2}{2m_l} + \frac{p_z^2}{2m_i} + eiz + \frac{e^2B_y^2}{2m_i c^2}(z - \langle z \rangle)^2.
\]

(2b)

For \( B_z = 0 \), the difference between the two Hamiltonians given by Eqs. (2a) and (2b) is due to the presence of the \( \langle z \rangle \) terms in the latter. We, however, attempt in this paper to solve for the Hamiltonian given by Eq. (2a), after noting that this is singular at \( B_z = 0 \), and that its eigenvalues have a jump discontinuity at \( B_z = 0 \), the magnitude of the \"jump\" being equal to the difference in the eigenvalues of the Hamiltonian (2a) from the corresponding ones of the Hamiltonian (2b).

Thereby, for \( B_z \neq 0 \), the effect of the magnetic field is to quantize further the \( y \) motion of the electron. Note that the last term, which denotes the coupling between the \( y \) and \( z \) motions, vanishes in either Faraday (\( \alpha = 0^\circ \)) or Voigt (\( \alpha = 90^\circ \)) geometry. Further, for \( \alpha = 90^\circ \), \( B_z \) is zero and the electron becomes free in the \( y \) direction and is assumed to carry zero momentum in that direction in the subsequent discussions.

If the effect of the \( B \) field is weak, a Born-Oppenheimer- (BO-) type solution is possible wherein one starts with the undisturbed electric subbands and evaluates the \( x^2 \) and the \( z \) terms in the magnetic part in terms of the undisturbed wave functions. One can then solve for the \( y \) motion. Such a procedure leads to a positive correction

\[
\Delta E_{BO}^n = \langle e^2B_y^2/2m_i c^2 \rangle (z^2)_{an} - \langle z \rangle_{an}^2
\]

(3)

to the \( n \)th subband energy and the appearance of substructure in the form of equally spaced Landau levels for \( y \) motion on each subband with spacing \( \hbar \omega_y \) where \( \omega_y = eB_y/m_i c \). It may be interesting to note that when \( B_y = 0 \), the BO-type approach leads to the same correction when applied to the Hamiltonian (2b) but to a different and larger correction when applied to the Hamiltonian (2a). The difference between these, viz., \( (e^2B_y^2/2m_i c^2)\langle z \rangle_{an}^2 \) is roughly equal to the magnitude of the \"jump\" at the singular point \( B_y = 0 \) for the Hamiltonian (2a), as mentioned before. We will return to this point again in Sec. III. With regard to the Landau substructure formed on each subband, the experimental results,2,3 however, showed substantial departure from the expected pattern of equispaced Landau levels, particularly at large tilt angles. As an example, the Landau-level spacings were not given solely in terms of \( B_x \). We regard this as a crucial point. Within an adiabatic separation of \( y \) and \( z \) motions, the Landau-level spacing is unequivocally a function of \( B_y \) alone. However, proper treatment of the coupling between the two motions can, even within a single particle description, account for additional dependences of the spacings on \( B_x \) as well.

Note that if the coupling is neglected, the \( y \) and \( z \) part of the wave functions are described by the well-known harmonic oscillator and Weber functions, respectively. However, Weber functions are, in general, more cumbersome to handle. Depending on whether the electric field or the magnetic one dominates the subband structure, however, either Airy functions or harmonic oscillator wave functions (of odd order, since the wave function must vanish at \( z = 0 \) for all \( y \)) provide us with two suitable alternative choices of the basis functions to diagonalize \( H \). We define a parameter

\[
\Theta = (e^2\hbar^2/2m_i c^2)^{1/3}/\hbar \omega_y, \quad \omega_y = eB_0/m_i c ,
\]

(4)

\[
B_0 = (B_y^2 + B_z^2)^{1/2},
\]

which gives a measure of the strength of the \( \epsilon \) field relative to the \( B \) field. \( \Theta \sim 0.57 \) implies a situation where the energy separation between the ground electric subband and the next higher one equals the Landau separation for \( \alpha = 0^\circ \). It may be interesting to note that \( \Theta \), as defined above, can also be written as the ratio \( m_1 l_b^2/m_1 l_E^2 \), where \( l_b \) and \( l_E \) are the characteristic lengths associated with the magnetic and the electric fields and are equal to \( (\hbar^2/m_1 \omega_y)^{1/2} \) and \( (\hbar^2/2m_i e \epsilon)^{1/2} \), respectively. In most of the space-charge layers studied so far, \( \Theta \) is large. However, a situation where the \( B \) field dominates the \( z \) quantization (i.e., \( \Theta \) small and \( \alpha \) large) has also been reported.3 Accordingly, we proceed to obtain the matrix elements of \( H \) in two alternative basis sets.

(i) Electric field dominating the \( z \) quantization. We
write

\[ H = H_0 + H' , \]

where

\[ H_{01} = \left[ -\frac{\hbar^2}{2m_1} \frac{d^2}{dy^2} + \frac{e^2B^2}{2m_1c^2}y^2 \right] + \left[ -\frac{\hbar^2}{2m_1} \frac{d^2}{dz^2} + e\beta \right], \]  

and

\[ H' = \frac{e^2B^2}{2m_1c^2}z^2 - \frac{e^2B_bB_y}{m_1c^2}yz . \]

The orthonormal basis is provided by the eigenfunctions \(|nN\rangle\) of \(H_{01}\), which satisfy

\[ H_{01}|nN\rangle = \epsilon_{nN}|nN\rangle, \]

where \(e_{nN} = (N + \frac{1}{2})\hbar \left[ \frac{eB_z}{m_1c} + \beta_n \left( \frac{e^2\hbar^2}{2m_1} \right)^{1/3} \right], \) \(\beta_n\) being the negative of the \(n\)th zero of the Airy function and \(n,N = 0,1,2, \ldots\). The wave functions are written as

\[ \langle y,z|nN\rangle = U_N(y)A_i(z), \]

where \(U_N\) and \(A_i\) are the usual harmonic-oscillator wave function and the Airy function, respectively, and are assumed to be properly normalized. In this basis, the matrix elements of the full Hamiltonian can now be written\(^\text{9}\) in dimensionless form (after being scaled to \(\hbar\omega_0\)) as

\[ \langle n'N'|H|nN\rangle/\hbar\omega_0 = [\beta_n n + (N + \frac{1}{2}) \cos \alpha] \delta_{nn'} + \left[ \frac{l_E}{2l_B} \right]^2 \sin^2 \alpha \left[ \frac{z^2}{l_E^2} \right] \delta_{NN'} - \left[ \frac{l_E}{2l_B} \right] \sin \alpha \cos \alpha \left[ \frac{\pi}{l_E^2} \right] \langle nN|nN\rangle , \]

where \(B_x = B_0 \cos \alpha, B_y = B_0 \sin \alpha, \)

\[ \left[ \frac{y \cos \frac{1}{2} \alpha}{l_B} \right]_{nn'} = (N')^{1/2} \delta_{N,N'-1} + (N'+1)^{1/2} \delta_{N,N'+1}, \]

\[ \left[ \frac{x}{l_E} \right]_{nn'} = \frac{1}{2} \beta_n \quad \text{if } n = n', \]

\[ \left[ \frac{x}{l_E} \right]_{nn'} = \frac{1}{2} \beta_n \quad \text{if } n = -n', \]

and

\[ \left[ \frac{\left[ \frac{z^2}{l_E^2} \right]}{nN'} = \frac{1}{2} \beta_n \quad \text{if } n = n', \]

\[ \left[ \frac{\left[ \frac{z^2}{l_E^2} \right]}{nN'} = \frac{-24}{(\beta_n - \beta_n)^4} \quad \text{if } n \neq n'. \]

Notice that the last term in (11) represents the coupling of the \(y\) and \(z\) motions with the ratio \(l_E/2l_B\) appearing as the coupling constant. The matrix given by (11) can be cast into another form, convenient for situations where the \(z\) component of the magnetic field, \(B_z\), is kept fixed while the tilt angle is changed so that \(B_y\) is now given by \(B_x \tan \alpha\). As in (4), defining

\[ \Theta_\alpha = \left( \frac{\epsilon^2\hbar^2}{2m_1l_x} \right)^{1/3}, \]

the matrix elements of \(H\) after being scaled to \(\hbar\omega_0\) are now given by

\[ \langle n'N'|H|nN\rangle/\hbar\omega_0 = [\beta_n \Theta_\alpha + (N + \frac{1}{2})] \delta_{nn'} \delta_{NN'} + \left[ \frac{l_E}{2l_B} \right]^2 \tan^2 \alpha \cos \alpha \left[ \frac{z^2}{l_E^2} \right] \delta_{NN'}, \]

\[ \left[ \frac{l_E}{2l_B} \right] \tan \alpha \cos \frac{1}{2} \alpha \left[ \frac{z}{l_E} \right]_{nn'} \left[ \frac{y \cos \frac{1}{2} \alpha}{l_B} \right]_{NN'}, \]

where

\[ y \cos \frac{1}{2} \alpha \left[ \frac{y \cos \frac{1}{2} \alpha}{l_B} \right]_{nn'} \left[ \frac{y \cos \frac{1}{2} \alpha}{l_B} \right]_{NN'}. \]

(16)
Magnetic field dominating the subband structure (Θ small and θ large). As before, we write
\[ H = H_0 + H'_2, \]
where
\[ H_0 = \left[ -\frac{\hbar^2}{2m_l} \frac{d^2}{dy^2} + \frac{e^2B_y^2}{2m_l c^2} y^2 \right] \]
\[ + \left[ -\frac{\hbar^2}{2m_l} \frac{d^2}{dz^2} + \frac{e^2B_y^2}{2m_l c^2} z^2 \right], \]
and
\[ H'_2 = e\varepsilon z - \frac{e^2B_y B_z}{m_l c^2} y z. \]
The basis is provided by the orthonormal eigenfunctions of \( H_0 \),
\[ \langle y, z | \rho P \rangle = U_\rho(y)U_{2P+1}(z), \quad P = 0, 1, 2, \ldots \]
which satisfy
\[ H_0 | \rho P \rangle = \epsilon^2_{\rho P} | \rho P \rangle, \]
where
\[ \epsilon^2_{\rho P} = (p + \frac{1}{2}) \left( \frac{\hbar e B_y}{m_l c} \right) \]
and \( U_\rho \) and \( U_{2P+1} \) are the usual harmonic-oscillator wave functions. Note the occurrence of only the odd functions for the \( z \) motion because of the boundary conditions at \( z = 0 \).

The integral \( \int_0^\infty U_{2P+1}(z)U_{2P'+1}(z)dz \) can easily be calculated and the matrix elements of \( H \) are obtained as (when scaled to \( \hbar \omega_0 \))
\[ \langle \rho' P' | H | \rho P \rangle = \left( p + \frac{1}{2} \right) \cos \alpha + \left[ 2P + \frac{3}{2} \right] \left( \frac{m_l}{m_1} \right)^{1/2} \sin \alpha \delta_{\rho \rho'} \delta_{PP'} + \left[ \frac{2}{\sin \alpha} \right]^{1/2} \left( \frac{l_{B}}{l_{E}} \right)^{3/4} \left( \frac{m_l}{m_1} \right)^{3/4} \delta_{\rho \rho'} I_{PP'}, \]

where \( (y \cos^{1/2} \alpha / l_B)_{\rho P} \) is given by Eq. (12) and
\[ I_{PP'} = \frac{2}{\sqrt{\pi}} \frac{2^{2P+P'}\Gamma(P + \frac{1}{2})\Gamma(P' + \frac{1}{2})}{\sqrt{(2P + 1)(2P' + 1)} \Gamma(P - P' + \frac{1}{2})\Gamma(P' - P + \frac{1}{2})}. \]

Note the presence of the \( \sin \alpha \) term in the denominator of the second term in (23) which, as expected, implies that this basis is not suitable for small tilt angles. Any of the large symmetric matrices given by (11), (16), or (23) can be diagonalized for appropriate values of the parameters to obtain energy eigenvalues \( E_\rho \) and the corresponding eigenfunctions \( \psi_\rho \).

In order to see what information can be obtained regarding the strengths of various transitions from the ground to an excited subband in the presence of a magnetic field, we have calculated the optical-absorption spectrum of the system under a weak \( z \)-polarized radiation, using linear response and the dipole approximation. Following Ando, \( \sigma_\omega(\omega) \) for which a phenomenological width parameter \( \Gamma \) has been assumed. \( f_{\mu \nu} \) is the oscillator strength between states \( \mu \) and \( v \), given by
\[ f_{\mu \nu} = \frac{2m_l}{\hbar^2} (E_\mu - E_\nu) | \langle \Psi_\mu | z | \Psi_\nu \rangle |^2, \]

and satisfies the sum rule
\[ \sum_\mu f_{\mu \nu} = 1. \]
nances occur when the incident photon energy \( h\omega \) equals the energy differences between the unoccupied levels and the occupied levels. A main modification, due to the many-body aspects, is expected to shift this energy, particularly for transitions with a large amplitude, through the depolarization effect.\(^1\)

III. RESULTS AND DISCUSSION

For calculations of energy levels and the corresponding wave functions the matrices given by Eqs. (11) and (16) have been diagonalized. Twenty Landau levels and 15 subband levels are included in the basis. For effective masses we used values appropriate to the silicon (100) surface, viz., \( m_1 = 0.1905 m_0 \), \( m_2 = 0.915 m_0 \), \( m \) being the free-electron mass. Most of the calculations were performed using \( \Theta \) or \( \Theta_1 \) as defined in Eqs. (4) and (15) as parameters and the energies expressed in units of \( \hbar \omega_0 \) and \( \hbar \omega_x \), respectively. \( E_{n}^{N}(\alpha) \) denotes energy levels on the \( n \)th \((n=0,1,2,\ldots)\) subband and \( N \)th \((N=0,1,2,\ldots)\) Landau level. \( E_{10}^{N}(\alpha) \) denotes the energy corresponding to the transition from the ground \((n=0)\) to the first \((n=1)\) excited subband level involving no change in the Landau quantum number, while \( E_{N}^{N}(\alpha) \) corresponds to similar transitions involving a simultaneous change \( \Delta N (\neq 0) \) in the Landau index. We should emphasize that the wave function belonging to \( E_{n}^{N}(\alpha) \) may contain as much or even more of the original \(|n,N\pm 1)\) character than of the \(|nN)\) function, especially at large tilt angles.

Figure 1 shows the difference of the ground-state energy \( E_{0}^{0}(\alpha) \) from the unperturbed ground subband energy \( \beta_0\Theta \) as a function of the tilt angle \( \alpha \). The ordinate is expressed in units of \( \hbar \omega_0 \).

Magnetic ground-state energies at \( \alpha=90^\circ \) by extrapolating to 90° the portion of each curve just to the left of the minimum.

Figure 2 shows \( E_{10}^{N}(\alpha)-E_{10}^{N}(\alpha=0) \), i.e., the difference between the main transition energy in the presence of a magnetic field and that when the \( B \) field is absent (or normal to the interface) as a function of the tilt angle \( \alpha \) and for several values of \( \Theta \). Note again the sharp rise near \( \alpha=90^\circ \) whose origin is explained in the above paragraph. For angles below which the sharp rise takes place, the curves can be well approximated by the Born-Oppenheimer value

\[
\left( \frac{e^2}{2m_e c^2} \right) B_x^2 \left( \langle z^2 \rangle_{11} - \langle z^2 \rangle_{00} - \langle z \rangle_{11}^2 + \langle z \rangle_{00}^2 \right).
\]

In Fig. 3 the inverse of the quantity \( E_{10}^{N}(\alpha=0) \) is plotted as a function of tilt angle

\[
E_{10}^{N}(\alpha=0) = \frac{1}{E_{10}^{N}(\alpha=0)}.
\]
FIG. 3. Effective cyclotron mass normalized with respect to $m_i$: $m_c/m_i$, corresponding to transitions from $|n=0,N=0\rangle$ state to $|n=1,N=1\rangle$ state. $m_c/m_i$ is equivalent to $[E_{i0}(\alpha)-E_{f0}(\alpha=0)]^{-1}$. Note the deviation from the $(\cos \alpha)^{-1}$ curve given by the dashed line.

$\alpha$ for different values of $\Theta$. The ordinate is equivalent to the cyclotron mass normalized with respect to $m_i$; that is, $m_c/m_i$. If the effect of finite $B_y$ is neglected, the ratio $m_c/m_i$ is expected to follow a $(\cos \alpha)^{-1}$ type of behavior with respect to variations in $\alpha$. Finite values of $m_c/m_i$ at $\alpha=90^\circ$ reflect the diamagnetic shift in the Voigt geometry when $(\rho_x)$ is assumed to be zero. What is interesting is the departure of the curves from the $(\cos \alpha)^{-1}$ type of behavior even for tilt angles much less than the ones where the sharp features are located. As can be noted from the figure, this departure becomes more and more prominent at large tilt angles for all $\Theta$, but for small $\Theta$, this departure sets in even at moderate tilt angles. The feature near $\alpha=90^\circ$ has the same origin as in Fig. 1 discussed above.

Figure 4 displays the details of the Figs. 1—3 from $\alpha=85^\circ$ to $\alpha=90^\circ$ range. From this the characteristic angle of tilt where the sharp feature of each plot is located can be seen easily. It is also seen that generally for large $\Theta$ this angle is extremely close to $90^\circ$ while as $\Theta$ is decreased, the characteristic angle moves towards smaller values. This figure then gives some idea about this range of the tilt angles over which our calculations can be trusted. For most experiments, $\Theta$ is greater than 1.0 and a conservative estimate for the range is $0 < \alpha < 85^\circ$.

Figure 5 shows curves similar to Fig. 2, but
now we envisage experimental situations wherein the z component of the magnetic field, $B_z$, is kept fixed while the tilt angle $\alpha$ is changed. This implies $B_y$ is changed and is given by $B_y \sin \alpha$. Different values of $\Theta_2$ denote different relative strengths of the $e$ field to $B_z$; the ordinate now is plotted in units of $\hbar \omega_z$. Here also, as in the case of the plots in Fig. 2, the curves are very well approximated by the corresponding Born-Oppenheimer values particularly for large $\Theta_2$. For small $\Theta_2$, Born-Oppenheimer values underestimate the actual ones, since for small $\Theta_2$, such an argument that the $y$ motion has little or no effect on the $z$ quantization is not valid.

Table I displays the energies corresponding to transitions from the ground to the first excited subband with a simultaneous change $\Delta N (=0, \pm 1)$ in Landau quantum number for a fixed $B_z (=3.5$ T), two different electric fields corresponding to $N_x=1.0 \times 10^{12}$ cm$^{-2}$ and $N_x=0.5 \times 10^{12}$ cm$^{-2}$, and for various values of $B_y$. For these calculations, $\Theta_2$ have been determined after fixing the constant of proportionality between the $e$ field and $N_x$ by translating $13.683$ meV, the energy separation between the ground and the first excited electric subband, to an $N_x$ value of $1.05 \times 10^{12}$ cm$^{-2}$, as obtained from Ref. 2. The unperturbed Landau spacing $\hbar \omega_z$ for $B_z=3.5$ T is $2.127$ meV. The energies are expressed in meV's. The last two columns show the energy differences between the first two Landau levels on $n=0$ and $n=1$ subbands, respectively, which are the same as the energy separations of the combined resonances $\Delta N = \pm 1$ from the main ($\Delta N = 0$) one, respectively. We first note that all the transitions, the main one ($\Delta N = 0$) as well as the combined ones ($\Delta N = \pm 1$), shift to higher energies as $B_y$ is increased from 0. We also note the $B_y$ and subband-dependent Landau separations. For both subbands, they are smaller than the expected $\hbar \omega_z \sim 2.127$ meV, though the differences are rather small until $B_y \sim 10$ T. That the Landau separation on the first excited subband is smaller than that on the ground subband, as can be noted from a comparison of columns 5 and 6, implies asymmetric positioning of the $\Delta N = 0$ transition with respect to the $\Delta N = \pm 1$ transitions. This is in accord with the experimental findings of Beinvogl and Koch, though their other observations, viz., the shift of the main ($\Delta N = 0$) resonance to the lower energy side and almost stationary positions for the combined resonances ($\Delta N = \pm 1$) with increasing $B_y$ are in serious

<table>
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<th>$B_y$ (T)</th>
<th>$\Delta N = -1$</th>
<th>$\Delta N = 0$</th>
<th>$\Delta N = 1$</th>
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disagreement with our calculations. However, a rigorous comparison of our calculations with the results in Ref. 2 is not possible because much of the interpretations of the latter, where the different transition frequencies and spacings are calculated by placing the resonance peaks to a common $N_n$ value, assuming only a $N_n^{1/3}$ dependence for all the energies is affected by the $N_n$ (or $\epsilon$ field) dependence of the transition energies as is evident from the Table I (or, so far as the main transition is concerned, from Fig. 5). Ando, in his calculations based on a local-density-functional formalism, has found agreement with the experiment so far as the shift of the main resonance relative to the combined ones is concerned. This effect has been attributed to excitonlike and depolarization effects. He has also found the combined resonances to show diamagnetic shifts which is in qualitative agreement with our results. In view of these, we feel that more experiments, preferably of a frequency-sweep type, will be desirable.

Figure 6 is presented as a representative example of the optical absorption spectra corresponding to a weak $z$ polarized radiation. We have taken a $\Theta_z$ value corresponding to $B_z = 5$ T and $E_{10}(\alpha = 0) = 28.0$ meV. The angle of tilt $\alpha$ of the $B$ field is taken to be 75°. This implies $B_y = B_z \tan 75^\circ = 18.7$ T. An unperturbed energy separation of 28.0 meV between the ground and the first electric subband level is typical of $n$-type silicon inversion layers and corresponds roughly to a carrier density $N_n = 2.1 \times 10^{12}$ cm$^{-2}$. The first four Landau levels on the ground subband ($n = 0$) are assumed to be occupied. Phenomenological width parameters $\Gamma$ have been assumed whose values are shown in the figure. $\hbar \omega_0$ for $B_z = 5$ T is about 3.04 meV. Several combined resonances ($\Delta N \neq 0$) are distinctly visible in addition to the main transition ($\Delta N = 0$) and are roughly equally spaced with respect to each other. The $\Delta N = \pm 1$ resonances can be seen to be placed about 3 meV away on either side of the main resonance ($\Delta N = 0$) which is located at $-28.5$ meV. Combined resonances $\Delta N = \pm 2$ are also visible. Note the amplitude asymmetry of the $\Delta N = \pm 1$ resonances. We have other calculations at other tilt angles which show how the positions, amplitudes, and amplitude asymmetries vary with $\alpha$ but choose not to present them here because they are substantially similar to the results in Ref. 1.

Though these spectra have been calculated for parameter values appropriate to an inversion layer, similar effects are expected to show up, in fact more strongly, for the lower values of $E_{10}$ corresponding to accumulation layers. The asymmetry in amplitude of the combined resonances $\Delta N = \pm 1$ and their enhancement relative to that of the main transition with increasing $B_y$ essentially agree with experiments. No serious conclusion should be made concerning resonances involving $\Delta N > 1$ because for such resonances, particularly for accumulation layers, our simple triangular well model will be grossly inadequate. However, considering the simplified nature of our model, it is satisfying to note that the amplitude asymmetry for the combined resonances, observed in Ref. 2 and calculated with detailed many-body effects in Ref. 1, owes its origin, at least partly, to the single-electron aspects of the system. The magnetic coupling between the motions parallel and perpendicular to the layer can itself lead to such effects.

IV. CONCLUSIONS

We have calculated the energy levels and the intersubband optical spectrum of an effectively two-dimensional space-charge layer in a tilted magnetic field using a simple nonrelativistic model Hamiltonian. The coupling between two perpendicular motions introduced by the tilted magnetic field has been taken fully into account. Two alternative basis sets have been pointed out in which the matrix elements for the Hamiltonian can be obtained in closed form and are easily calculable. These two choices enable one to solve for the Hamiltoni-
an exactly for arbitrary strengths of the magnetic field relative to the electric one for a wide range of tilt angles.

Asymmetry in amplitude and positioning of the combined resonances relative to the main one are in qualitative agreement with some recent experiments of Beinvogl and Koch and with the calculations of Ando. These point out to possible (though small) contributions from the single-electron aspects of the problem to the observed phenomena. Our calculations show, also in qualitative agreement with the calculations of Ando, diamagnetic shifts of the combined resonances as the component of the \( B \) field parallel to the surface is increased. Since the experimental results do not show this shift, it remains unexplained.

Landau spacings on different subbands are found not to be determined by the normal component of the \( B \) field alone as expected in a naive picture. Instead, they depend also on the parallel component of the \( B \) field, the relative strength of the electric to the magnetic field and on the subband index. Landau spacings are reduced for both the ground and the higher subband, the reduction being slightly more for the higher subband. However, deviations from the expected values are not appreciable unless the ratio of the parallel to the perpendicular component of the magnetic field is quite large.

We end with a couple of remarks on the general features of such problems. The first concerns the fact that the Hamiltonian we have used may be considered a prototype of nonseparable problems in two dimensions. The magnetic part itself is very interesting in that the nonseparability is due to the restriction of the coordinate space to a semi-infinite plane. The coupling term makes such problems more interesting exactly where usually they are more difficult to solve, viz., in the nonperturbative regime. Such a feature is not unique to this Hamiltonian; rather it belongs to a general class of interesting physical problems.\(^{15}\)

Secondly, electron layers on a liquid-helium surface also appear to be a promising system with which to study the effects of tilted magnetic fields. Though somewhat different (because of the image Coulomb potential), such systems are more clean since the electron density is low. Despite being the first system where intersubband combined resonances were reported to be observed by Zipfel et al.\(^{16}\) any detailed spectroscopic investigation of the space-charge layer for different values of the appropriate parameters has not been reported in the literature. Since the lower density electron layer on liquid helium does not have the large many-body corrections of inversion layers, it is more suitably described by a single-particle model. In this system, as well as in other space-charge layers, more experiments, particularly of the frequency-sweep type, will be highly desirable.

ACKNOWLEDGMENTS

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\(^{7}\)A. R. P. Rau, in Abstracts of III International Conference on Electronic Properties of Two-Dimensional Systems, Yamada, Japan, 1979 (unpublished); Comments
6This study would be of direct interest for experiments where $B_z$ is held fixed and $B_y$ varied independently.
APPENDIX B

DERIVATION OF THE MATRIX ELEMENTS $<z>_{nm}$ AND $<z^2>_{nm}$ IN THE BASIS OF THE UNPERTURBED ELECTRIC SUBBAND WAVEFUNCTIONS

In the triangular well model, the unperturbed electric subband wavefunctions $\psi_n(z)$ and the corresponding eigenvalues $E_n$ satisfy the Schrödinger equation

$$\left(-\frac{\hbar^2}{2m_L} \frac{d^2}{dz^2} + e \varepsilon z\right) \psi_n(z) = E_n \psi_n(z) \quad (B.1)$$

with the boundary conditions

$$\psi_n(z) = 0 \quad \text{at} \quad z = 0; \quad \psi_n(z) \xrightarrow{z \to \infty} 0 \quad (B.2)$$

Through a change of the variable $z$:

$$\xi = \gamma (z - E_n/e \varepsilon); \quad \gamma = (\hbar^2/2m_L e \varepsilon)^{-1/3} \quad (B.3)$$

Eq. (B.1) can be transformed to

$$\frac{d^2}{d\xi^2} \psi_n(\xi) = \xi \psi_n(\xi) \quad (B.4)$$

Together with the boundary conditions in (B.2), the solutions for the normalized wavefunctions are the well known Airy functions

$$\psi_n(z) = N_n \text{Ai}[\gamma(z + \delta_n)] \quad (B.5)$$

where $N_n$ is the normalization constant (assumed real) satisfying

$$n_n^2 \int_0^\infty \text{Ai}^2[\gamma(z + \delta_n)] \, dz = 1 \quad (B.6)$$
and

\[ \gamma_n = -\gamma E_n / e^\varepsilon = -\beta_n , \]  \hspace{1cm} (B.7)

\(-\beta_n (\beta_n > 0)\) being a zero of the Airy function. Eq. (B.7) ensures that \( \psi_n (z = 0) = 0 \) and, in turn, gives the subband energies

\[ E_n = \beta_n \left( e^{2 \varepsilon \hbar^2/2m_\alpha} \right)^{1/3} . \]  \hspace{1cm} (B.8)

The key formulae we use for the desired matrix elements are given by

\[
\int \mathrm{Ai}[\gamma(z+\delta_n)] \, \mathrm{Bi}[\gamma(z+\delta_m)] \, \mathrm{d}z \equiv I_{nm}
\]

\[
\begin{cases}
(z+\delta_n) \, \mathrm{Ai}[\gamma(z+\delta_n)] \, \mathrm{Bi}[\gamma(z+\delta_m)] \\
- \mathrm{Ai}[\gamma(z+\delta_n)] \, \mathrm{Bi}[\gamma(z+\delta_m)]/\gamma & \text{if } n = m \\
(\gamma^2(\delta_n-\delta_m))^{-1} \cdot \left( \mathrm{Ai}'[\gamma(z+\delta_n)] \, \mathrm{Bi}[\gamma(z+\delta_m)] \\
- \mathrm{Ai}[\gamma(z+\delta_n)] \, \mathrm{Bi}'[\gamma(z+\delta_m)] \right) , \text{ if } n \neq m ;
\end{cases}
\]  \hspace{1cm} (B.9a)

where primes denote differentiation with respect to the \( \text{w.r.t.} \) argument. The above is true for any function \( \mathrm{Ai}, \mathrm{Bi} \) satisfying Eq. (B.4) and can be verified directly by taking derivatives on both sides of \( I_{nm} \, \text{w.r.t. } z \). Since, the required matrix elements

\[ <z>_{nm} = N_n N_m \int_0^\infty \mathrm{Ai}[\gamma(z+\delta_n)] \, z \, \mathrm{Ai}[\gamma(z+\delta_m)] \, \mathrm{d}z \]  \hspace{1cm} (B.10)

and

\[ <z^2>_{nm} = N_n N_m \int_0^\infty \mathrm{Ai}[\gamma(z+\delta_n)] \, z^2 \, \mathrm{Ai}[\gamma(z+\delta_m)] \, \mathrm{d}z \]  \hspace{1cm} (B.11)
involve only the functions $A_i$, we accordingly modify Eqs. (B.9) and write

$$ \int A_i^n A_i^m \, dz \equiv I_{nm} \equiv \begin{cases} (z+\delta_n^2) A_i^n - A_i^n /\gamma ; & \text{if } n = m \quad (B.12a) \\ [\gamma^2 (\delta_n - \delta_m)]^{-1} \cdot (A_i^n A_i^m - A_i^n A_i^m) & \text{if } n \neq m \end{cases} $$

where, for brevity, we have introduced the notation

$$ A_i^n \equiv A_i[\gamma(z+\delta_n)] . \quad (B.13) $$

Before we proceed to evaluate $<z>_{nm}$ and $<z^2>_{nm}$, we note the following properties:

Property (i): $A_i^n = 0$ at $z = 0$, and $A_i^n, A_i^n \to 0$ exponentially as $z \to \infty$.

Property (ii): (by virtue of Eq. (B.4) that is satisfied by $A_i^n$), second or higher derivatives of these functions can always be eliminated in favor of the functions themselves or their first derivatives.

Using Eqs. (B.12a) and (B.14) in Eq. (B.6), we get the normalization constant as

$$ N_n = \gamma^\frac{\delta}{A_i} (-\beta_n) . \quad (B.15) $$

A. To Obtain $<z>_{nm}$:

Differentiating the left hand side of $I_{nm}$ in Eq. (B.12) twice w.r.t. say $\delta_n$, and rearranging terms, we get
\[ \int A_{i_n} z A_{i_m} \, dz = J_{nm} = \frac{1}{\gamma^3} \frac{d^2 I_{nm}}{d\delta_n^2} - \delta_n I_{nm}. \]  

(B.16)

Using the r.h.s.'s of Eqs. (B.12), and Eq. (B.4), we obtain:

\[ J_{nn} = \frac{1}{3} \left[ \left( z^2 - z\delta_n - 2\delta_n^2 \right) A_{i_n}^2 + \gamma^2 \cdot A_{i_n} A_{i_n} + \gamma^{-1} (2\delta_n - z) \right] \]

and for \( n \neq m; \)

\[ J_{nm} = -\frac{\delta_n + \delta_m + 2z}{\gamma^3 (\delta_n - \delta_m)^2} A_{i_n} A_{i_m} + \left( \frac{z}{\gamma^2 (\delta_n - \delta_m)} + \frac{2}{\gamma^5 (\delta_n - \delta_m)^3} \right) x A_{i_n} A_{i_m} \]

(B.18)

Therefore, for \( n = m, \)

\[ <z>_{nn} = N_n N_n \left[ J_{nn} \right]_{z=0} = -\frac{2}{3} \delta_n, \]  

(B.19)

and for \( n \neq m, \)

\[ <z>_{nm} = N_n N_m \left[ J_{nm} \right]_{z=0} = -\frac{2}{\gamma^3 (\delta_n - \delta_m)^2}. \]  

(B.20)

In obtaining the above, we have used Eqs. (B.14) and (B.15).

Using (B.7) and (B.3), we can therefore write

\[ <z>_{nm} = \begin{cases} 
\frac{2}{3} \beta_n \cdot (\kappa^2/2m_\gamma \epsilon \epsilon)^{\frac{1}{3}} & \text{if } n = m \\
\frac{-2}{(\beta_n - \beta_m)^2} \cdot (\kappa^2/2m_\gamma \epsilon \epsilon)^{\frac{1}{3}} & \text{if } n \neq m.
\end{cases} \]  

(B.21)
B. To Obtain \( <z^2>_{nm} \):

As before, differentiating the l.h.s. of \( J_{nm} \) in Eq. (B.16) twice w.r.t. say \( \delta_n \), and rearranging terms, we get

\[
\int A_i z^2 A_i m \, dz = L_{nm} = \frac{1}{\gamma^3} \frac{d^2 J_{nm}}{d\delta_n^2} - \delta_n J_{nm} \quad \text{(B.21)}
\]

so that,

\[
<z^2>_{nm} = N_n N_m \left[ \frac{1}{\gamma^3} \frac{d^2 J_{nm}}{d\delta_n^2} - \delta_n J_{nm} \right] \bigg|_{z=0} \bigg|_{z=\infty} \quad \text{(B.22)}
\]

Depending on whether \( n = m \) or \( n \neq m \), the term in the square bracket can be evaluated from Eqs. (B.17) and (B.18) respectively. Repeated use of Eq. (B.4) reduces all the terms to a bilinear form involving \( A_i \) and \( A_i \), of which, because of the limits and the properties given in Eq.(B.14), only the term proportional to \( A_i A_i m \), evaluated at \( z = 0 \), contributes to \( <z^2>_{nm} \). Since this calculation is straightforward and proceeds as outlined above, we only display the result, which is:

\[
<z^2>_{nm} = \begin{cases}
\frac{8}{15} \beta_n^2 \left( \frac{\mu^2}{2m_e \epsilon c} \right)^{2/3} & \text{if } n = m \\
-\frac{24}{(\beta_n - \beta_m)^4} \left( \frac{\mu^2}{2m_e \epsilon c} \right)^{2/3} & \text{if } n \neq m .
\end{cases}
\quad \text{(B.23)}
\]
APPENDIX C

DERIVATION OF THE MATRIX ELEMENT $<z>_{pp'}$ IN THE BASIS OF "HALF A HARMONIC OSCILLATOR" WAVE FUNCTIONS

The solutions to the Schrödinger Eq.

$$i\frac{\hbar^2}{2m}\frac{d^2\psi}{dz^2} + \frac{1}{2}m_t\omega_o^2\sin^2\alpha z^2 = E\psi(z) \quad (C.1)$$

with the boundary conditions

$$\psi(z = 0) = 0 ; \quad \psi(z \rightarrow 0 , z \rightarrow \infty) \quad (C.2)$$

are the well known harmonic oscillator wave functions of odd order:

$$\psi(z) = U_{2P+1}(z) = N_{2P+1}\gamma^\frac{1}{2}e^{-\gamma z^2}H_{2P+1}(\gamma z) \quad (C.3)$$

where $P = 0,1,2, \ldots$, $H_{2P+1}(\gamma z)$ are the Hermite polynomials,

$$\gamma = \left(\frac{\sqrt{\alpha}m_t\omega_o}{\hbar}\sin\frac{\alpha}{\hbar}\right)^{\frac{1}{2}} \quad (C.4)$$

and

$$N_{2P+1} = [2^{2P} (2P+1)!]^{-\frac{1}{2}} (\pi)^{-\frac{1}{2}} \quad (C.5)$$

is the normalization constant.

We wish to evaluate

$$<z>_{pp'} = \int_0^\infty U_{2P+1}(z) z U_{2P'+1}(z) dz \quad (C.6)$$

Using (C.3) and changing the variable to $z_1 = \gamma z$, Eq. (C.6) can be written as

$$<z>_{pp'} = N_{2P+1}N_{2P'+1}(\gamma)^{-1}\int_0^\infty e^{-z_1^2}H_{2P+1}(z_1) z_1 H_{2P'+1}(z_1) dz_1 \quad (C.7)$$

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or

\[ \langle z \rangle_{pp'} = N_{2P+1} N_{2P'+1} (\gamma)^{-1} (-)^{P+P'} 2^{2P+2P'+2} \frac{p!p'}{1} \]

\[ \int_0^\infty \frac{-z^2}{z_1^3} \frac{L_p^b(z_1^2)}{L_p^b(z_1^2)} \frac{L_p'^b(z_1^2)}{L_p'^b(z_1^2)} dz_1 \]

(C.8)

where we have used the relationship\(^{52}\)

\[ H_{2P+1}(X) H_{2P'+1}(X) = (-)^{P+P'} 2^{2P+1} p! p'! X^2 \frac{1}{L_p(X^2)} \frac{1}{L_p'(X^2)} \]

(C.9)

\(L_p^b, L_p'^b\), being the associated Laguerre polynomials. To evaluate the integral above, we first change the variable from \(z_1\) to \(z_2\) via

\[ z_1^2 = z_2 \]

(C.10)

and subsequently use the formula\(^{53}\)

\[ \int_0^\infty \frac{-z^3}{z_3} \frac{L_p^b(z_3)}{L_p^b(z_3)} \frac{L_p'^b(z_3)}{L_p'^b(z_3)} dz_3 = (-)^{P+P'} \frac{\Gamma(P+\frac{3}{2})}{\Gamma(P+1)} \frac{\Gamma(P'+\frac{3}{2})}{\Gamma(P'+1)} \]

\(C.11\)

which gives

\[ \langle z \rangle_{pp'} = N_{2P+1} N_{2P'+1} (\gamma)^{-1} 2^{2P+2P'+1} \frac{\Gamma(P+\frac{3}{2})}{\Gamma(P-P'+\frac{3}{2})} \frac{\Gamma(P'+\frac{3}{2})}{\Gamma(P'-P+\frac{3}{2})} \]

(C.12)
Finally, using Eqs. (C.4) and (C.5) we obtain

\[
\langle \varphi^p \varphi^{p'} \rangle = \frac{2}{\sqrt{\pi}} \frac{2^{2P+P'}}{\sqrt{(2P+1)! \cdot (2P'+1)!}} \frac{\Gamma(P+\frac{3}{2}) \Gamma(P'+\frac{3}{2})}{\Gamma(P-P'+\frac{1}{2}) \Gamma(P'+P+\frac{1}{2})} \left( \frac{\hbar}{\sqrt{m_\perp m_\chi \omega_0 \sin \alpha}} \right)^{\frac{1}{2}}.
\]

(C.13)
The attempt to solve for the Schrödinger Eq. (2.3) through the Rayleigh-Ritz variational method is motivated by the fact that a simple oscillator like trial function $\phi_o(z) = \lambda ze^{-\frac{1}{2}\lambda^2 z^2}$ with a single parameter $\lambda$ reproduces the ground electric subband energy in the triangular well model to within a surprising $0.3\%$ accuracy. For the next excited subband state, a function orthogonal to $\phi_o$, but containing the same parameter $\lambda$, estimates the corresponding energy to $-2\%$ accuracy. Further, the expectation value of the Hamiltonian can be easily calculated in simple but non-trivial oscillator like trial wavefunctions and as we shall see, the variational parameters thus obtained can be used with some advantage to construct an orthonormal basis which may extend the region of validity of our calculations in Chapter II beyond $\alpha = 85^\circ$.

We choose the normalized trial function for the ground state of the Hamiltonian (2.3) to be:

$$\psi_t = N_1 \phi_t(z) N_2 \chi_t(y) \quad \text{(D.1)}$$

with

$$\phi_t(z) = \lambda z e^{-\frac{1}{2}\lambda^2 z^2} \quad \text{(D.2)}$$

and

$$\chi_t(y) = (1 + C \mu y) e^{-\frac{1}{2}\mu y^2} \quad \text{(D.3)}$$

where $\lambda, \mu$ and $C$ are the variational parameters. The
parameter \( C \) is deliberately introduced to include the coupling in the \( y \) and the \( z \) motions (due to the last term in Eq. (2.2)). \( N_1 \) and \( N_2 \) are the normalization constants for \( \phi_t(z) \) and \( \chi_t(y) \) respectively, so that

\[
N_1^2 \int_{0}^{\infty} |\phi_t(z)|^2 \, dz = 1, \quad \text{(D.4)}
\]

and

\[
N_2^2 \int_{-\infty}^{\infty} |\chi_t(y)|^2 \, dy = 1. \quad \text{(D.5)}
\]

Substitution of Eqs. (D.2) and (D.3) in Eqs. (D.4) and (D.5) immediately gives \( N_1 \) and \( N_2 \):

\[
N_1^2 = \frac{4\lambda}{\sqrt{\pi}}, \quad \text{(D.6)}
\]

\[
N_2^2 = \frac{\mu}{(\sqrt{\pi}(1 + \frac{1}{2} C^2))}. \quad \text{(D.7)}
\]

The expectation value \( E_{t}^{(o)} \) of \( H \) as in Eq. (2.2) in the state \( \psi_{t}^{(o)} \) can be calculated in a straight forward manner (all the integrals involved are expressible in terms of Gamma functions), and the result, when scaled to \( \hbar \omega_o \), is:

\[
E_{t}^{(o)}/\hbar \omega_o = \frac{1}{4} \cdot \frac{1 + \frac{3}{2} C^2}{1 + \frac{1}{2} C^2} \cdot \left( \frac{\mu^2}{\lambda^2} + \frac{\cos^2 \alpha}{\mu^2} \right)
\]

\[
+ \frac{3}{4} \left[ \frac{m_t}{m_k} \lambda^2 + \frac{\sin^2 \alpha}{\lambda^2} + \frac{2}{3} \sqrt{\frac{2}{\pi}} \frac{m_t}{m_k} \left( \frac{q_B}{\sqrt{E}} \right)^3 \cdot \frac{1}{\lambda} \right]
\]

\[- \frac{2G}{1 + \frac{1}{2} C^2} \cdot \frac{\sin \alpha \cos \alpha}{\sqrt{\pi}} \cdot \frac{1}{\lambda \mu}, \quad \text{(D.8)}
\]

where the symbols are kept the same as in Chapter II. The partial derivative of the r.h.s. of the above Eq. w.r.t. \( \mu, \lambda \) and \( C \) when equated to zero, provide us with three algebraic equations necessary to solve for the parameters.
\( \mu_0', \lambda_0', C_0 \) (say) which minimize \( E_t^{(0)} \). These are, respectively

\[
(1 + \frac{3}{2} C^2) \left( \mu^2 - \frac{\cos \alpha}{\mu^2} \right) + \frac{4C}{\lambda \mu} \frac{\sin \alpha \cos \alpha}{\sqrt{\pi}} = 0 , \tag{D.9}
\]

\[
(1 + \frac{1}{2} C^2) \left( \frac{m_1}{m_\ell} \right)^2 - \frac{\sin^2 \alpha}{\lambda^2} - \frac{4}{3} \sqrt{\frac{2}{\pi}} \frac{m_1}{m_\ell} \frac{B}{E} \left( \frac{\lambda B}{E} \right)^3 \frac{1}{\lambda} + \frac{4C}{3 \lambda \mu} \frac{\sin \alpha \cos \alpha}{\sqrt{\pi}} = 0 , \tag{D.10}
\]

and,

\[
C \left( \mu^2 + \frac{\cos^2 \alpha}{\mu^2} \right) - \frac{4(1 - \frac{1}{2} C^2)}{\lambda \mu} \frac{\sin \alpha \cos \alpha}{\sqrt{\pi}} = 0 . \tag{D.11}
\]

Eq. (D.11) can be used to eliminate \( C \) from Eqs. (D.9) and (D.10). This leaves us finally with two coupled nonlinear algebraic equations in \( \lambda \) and \( \mu \) to be solved. We have solved these numerically for different tilt angles \( \alpha \), starting progressively from \( \alpha=0 \). An iteration scheme was used in which, for any tilt angle \( \alpha \), the solutions \( \lambda_0, \mu_0 \) from the previous tilt angle were used as input. For \( \alpha=0^\circ \), a physically acceptable solution for \( C \) from Eq. (D.11) is seen to be \( C = 0 \), which, in turn, decouples Eqs. (D.9) and (D.10). The respective solutions \( \lambda_0 \) and \( \mu_0 \) for \( \alpha=0^\circ \) are thus used as input to the calculation for the next tilt angle \( \alpha (= 5^\circ) \) greater than zero.

Figure D.1 shows sample results for the ground state eigenvalues for various tilt angles within the range \( 0 \leq \alpha \leq 85^\circ \), for two different values of \( \theta \). As expected, the variational estimates are higher than the corresponding "exact" results.
Fig. D.1. Ratio of the variational estimates of the ground state energy $E_t^{(o)}$ w.r.t. $E_o^0$ obtained through diagonalization of (A.11) plotted as functions of tilt angle $\alpha$. 

TILT ANGLE $\alpha$ IN DEGREE
obtained through diagonalization of the matrix (Eq. (A.11)). A comparison of the respective curves shows that the variational estimates are accurate to within \( \pm 5\% \). In Table D.1, we display the ratios of the variational parameters \( \mu \) w.r.t. the corresponding expected values \( \mu_0 \) \( (=\sqrt{\cos \alpha}) \) in the absence of any coupling between the \( y \) and the \( z \)-motions. We note that \( \mu \) decreases, and more rapidly so, as \( \alpha \) increases. This is expected for, as we have discussed in Chapter II, as \( \alpha \) approaches \( 90^\circ \), the \( y \) spectrum becomes that of a free particle, requiring more spreading out of the oscillator like wave functions to represent that situation. This points to the fact that these parameters \( \mu_0 \) and \( \lambda_0 \) can be used to construct an orthonormal basis similar to the one in Eq. (2.32) in which the Hamiltonian is expected to converge more rapidly, particularly for large \( \alpha \). Such a procedure is then expected to extend the region of validity of our calculations in Chapter II beyond \( \alpha = 85^\circ \). We should, however, keep in mind that the success in this will be limited, for, in principle, an infinite number of oscillator like functions are required to represent a free particle wave function, which represents the \( y \) motion at \( \alpha = 90^\circ \).

Since most of the required calculations proceed in the same fashion as in Chapter II, we show here only the final result for the matrix element of the Hamiltonian in such a basis. The basis functions are
### TABLE D.1

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<th>α (deg)</th>
<th>$\nu/\nu_0$ for $E_{10}$ ($\alpha=0^\circ$)/$\sqrt{\mu_0} = \varepsilon/3$</th>
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<tr>
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<td>0.6515</td>
</tr>
</tbody>
</table>

Ratio of variationally determined value of $\mu$ w.r.t. $\nu_0$ as functions of $\alpha$ and for different relative strengths of the electric to the magnetic field.
\[ <y, z | p, P>_v = U_p^\dagger (\mu y) U_{2P+1} (\lambda z), \quad p, P = 0, 1, 2, \ldots \]  

(D.12)

where \( \mu, \lambda \) are obtained from Eqs. (C.9) - (C.11) and

\( U_p, U_{2P+1} \) are harmonic oscillator like wave functions normalized over the range \((-\infty, \infty)\) and \((0, \infty)\) respectively. The matrix elements of \( H \) in Eq. (2.2) in this basis, when scaled to \( \hbar \omega_o \), are then given by

\[
\langle P' P' | H | P P \rangle / \hbar \omega_o = \delta_{p, P'} \left[ \frac{1}{4} \left( \mu^2 + \frac{\cos^2 \alpha}{\mu^2} \right) (2p+1) \delta_{P, P'} + \frac{1}{4} \left( \frac{\sin^2 \alpha}{\lambda^2} - \mu^2 \right) \right] \\
+ \frac{1}{4} \left( \frac{\sin^2 \alpha}{\lambda^2} - \frac{m_t}{m_\lambda} \lambda^2 \right) \left[ \sqrt{2p(p+1)} \delta_{p', P+2} + \sqrt{2p(p-1)} \delta_{p', P-2} \right] \\
+ \frac{1}{4} \left( \frac{\sin^2 \alpha}{\lambda^2} - \frac{m_t}{m_\lambda} \lambda^2 \right) \left[ \sqrt{2p(p+2)} \delta_{p', P+1} + \sqrt{2p(p-2)} \delta_{p', P-1} \right] \\
- \frac{\sin \alpha \cos \alpha}{\lambda \mu} \cdot \left[ \frac{1}{2} \delta_{p', P+1} + \sqrt{2} \delta_{p', P-1} \right] \right] \]  

(D.13)

where \( I_{p, P'} \) is defined in Eq. (A.24). As expected, the above expression reduces to Eq. (A.23) when \( \lambda \) and \( \mu \) are
chosen to satisfy Eq. (A.21).
APPENDIX E

EVALUATION OF THE INTEGRALS REQUIRED IN CHAPTER III.D.

We wish to evaluate the usual WKB integrals $\lambda, \sigma$ and $\phi$ as defined in Eqs. (3.13) and (3.14) as well as the integrals $(d\lambda/dE)_0$ and $(d\sigma/dE)_0$, that are associated with the local level spacings around some energy $E_0$ in the wells of the potential $V(z)$ in Eq. (3.50). $k^2(z)$ as defined in Eq. (3.3) for this energy is assumed to have four real zeroes $z_i^*(i = 1,2,3,4)$. Because of the infinitely high potential barrier at $z = 0$, $z_1$ is zero for all energies. The other three (non-zero) turning points, $z_2$, $z_3$ and $z_4$ ($z_2 < z_3 < z_4$) are given by the roots of the cubic equation $zk^2(z) = 0$. It is convenient to scale the distances and energies to the effective "Bohr" radius $\tilde{a}_0 (= \hbar^2/mQe^2)$ and the effective "Rydberg" $\tilde{R}_y (= mQ^2e^4/2\hbar^2)$ respectively, so that each of the integrals $\lambda, \sigma$ and $\phi$ can be written in terms of dimensionless variables in the form

$$I = \int_{z'}^{z''} [z^{-1} A(z-z_2)(z-z_3)(z-z_4)]^{1/2} \, dz , \quad (E.1)$$

where $z', z''$ denote the appropriate turning points for the respective integral and $A = \pm B^2/B_c^2$, $B_c$ being the "critical" magnetic field ($= m^2Q^2c^3e/\hbar^3$) defined in Chapter III.D. The sign of $A$ is chosen such that $I$ is positive. The integrals $(d\lambda/dE)_0$ and $(d\sigma/dE)_0$ are of the form
\[ J = (2 \tilde{R}_y)^{-1} \int_{z'}^z z^4 [A(z-z_2)(z-z_3)(z-z_4)]^{-\frac{1}{2}} \, dz . \tag{E.2} \]

After a little algebra, \( I \) in Eq. (E.1) can be cast in the form:

\[ I = A\gamma_0[y]^{z''}_z + \gamma_1[I_0]^{z''}_z + \gamma_2[I_1]^{z''}_z + \gamma_3[I']^{z''}_z, \tag{E.3} \]

where

\[ \gamma_0 = (2A)^{-1}, \quad \gamma_1 = -\frac{3}{4} z_2 z_3 z_4 \]
\[ \gamma_2 = -\frac{1}{8} \left( z_2 + z_3 + z_4 \right)^2 + \frac{1}{2} \left( z_2 z_3 + z_3 z_4 + z_4 z_2 \right) \]
\[ \gamma_3 = -\frac{1}{4A} \left( z_2 + z_3 + z_4 \right) \tag{E.4} \]

\[ y^2 = A(z-z_2)(z-z_3)(z-z_4) \tag{E.5} \]

\[ I_n = \int \frac{z^n}{y} \, dz . \tag{E.6} \]

and

\[ I' = A[I_2 - 4\gamma (z_2 + z_3 + z_4) I_1] . \tag{E.7} \]

By changing the variable of integration from \( z \) to \( \xi \) via the Legendre transformation

\[ z = \frac{a \sin^2 \xi + b}{c \sin^2 \xi + d} ; \quad 0 \leq \xi \leq \pi/2 \tag{E.8} \]

the limits \( z' \) and \( z'' \) for each of the integrals \( \lambda, \sigma \) and \( \phi \) turn out to be 0 and \( \pi/2 \) respectively, and the "normal" integrals \( I_n \) and \( I' \) can be written in terms of complete elliptic integrals \( K, E \) and \( \Pi \). The result is

\[ [y]^{z''}_z = 0 \tag{E.9a} \]
\[ [I_\circ]^z_2 = 2 \xi \kappa(k^2) \quad \text{(E.9b)} \]

\[ [I_1]^z_2 = 2 \xi \left[ \frac{a}{c} \kappa(k^2) - \frac{1}{cd} \Pi\left(-\frac{c}{d}, k^2\right) \right] \quad \text{(E.9c)} \]

\[ [I']^z_2 = \frac{A\xi}{cd} \left[ (-2ab + \frac{b1}{c+d} - \frac{a1}{c+k^2d}) \kappa(k^2) + \frac{1^2}{(c+d)(c+k^2d)} \right] \quad \text{(E.9d)} \]

The various parameters involved in Eqs. (E.9) depend on the sign of A as well as on the limits of integration and are given in Table E.1. With the help of this table, and Eqs. (E.4) and (E.9), the integrals \( \lambda, \sigma \) and \( \phi \) can be obtained from Eq. (E.3).

The integrals \( J \) corresponding to \( \frac{d\lambda}{dE} \) and \( \frac{d\sigma}{dE} \) are simply given in terms of \([I_1]^z_2\), and can be evaluated immediately with the help of Eq. (E.9c) and the Table E.1.
<table>
<thead>
<tr>
<th>Integrals Involved</th>
<th>Sign of A</th>
<th>Integration Intervals</th>
<th>( \kappa^2 )</th>
<th>( a, b, c, d )</th>
<th>( \tau )</th>
<th>( \xi )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \lambda, \left( \frac{d\lambda}{dE} \right)_0 )</td>
<td>-</td>
<td>( z' = 0 = z_1 ) ( z'' = z_2 )</td>
<td>( \frac{z_2(z_4 - z_3)}{z_3(z_4 - z_2)} )</td>
<td>( a = z_2 z_4 ) ( b = 0 ) ( c = z_2 ) ( d = z_4 - z_2 )</td>
<td>( z_2 z_4 (z_4 - z_2) )</td>
<td></td>
</tr>
<tr>
<td>( \sigma, \left( \frac{d\sigma}{dE} \right)_0 )</td>
<td>-</td>
<td>( z' = z_3 ) ( z'' = z_4 )</td>
<td>( \frac{z_2(z_4 - z_3)}{z_3(z_4 - z_2)} )</td>
<td>( a = z_2 (z_4 - z_3) ) ( b = z_3 (z_4 - z_2) ) ( c = z_4 - z_3 ) ( d = z_3 - z_2 )</td>
<td>( (z_4 - z_3) (z_4 - z_2) ) ( (z_3 - z_2) )</td>
<td></td>
</tr>
<tr>
<td>( \phi )</td>
<td>+</td>
<td>( z' = z_2 ) ( z'' = z_3 )</td>
<td>( \frac{z_2(z_4 - z_3)}{z_3(z_4 - z_2)} &lt; 1 )</td>
<td>( a = 0 ) ( b = -z_2 z_3 ) ( c = z_3 - z_2 ) ( d = z_3 )</td>
<td>( z_2 (z_4 - z_3) )</td>
<td></td>
</tr>
</tbody>
</table>

Parameters required to evaluate the integrals in Eq. (E.9).
APPENDIX F
SOME USEFUL CONSTANTS

Listed in the table below are some useful constants along with their usual symbols and the values.

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>$e$ (Electronic charge)</td>
<td>$-4.8032 \times 10^{-10}$</td>
<td>esu</td>
</tr>
<tr>
<td>$m$ (Electron rest mass)</td>
<td>$9.1095 \times 10^{-28}$</td>
<td>gms</td>
</tr>
<tr>
<td>$h$ (Planck's constant)</td>
<td>$6.624 \times 10^{-27}$</td>
<td>erg. sec.</td>
</tr>
<tr>
<td>$c$ (Speed of light)</td>
<td>$2.9979 \times 10^{10}$</td>
<td>cm/sec</td>
</tr>
<tr>
<td>$a_0$ (Bohr radius)</td>
<td>$0.5292$</td>
<td>A°</td>
</tr>
<tr>
<td>$R_y$ (1 Rydberg)</td>
<td>$13.6058$</td>
<td>eV</td>
</tr>
<tr>
<td>$A^0$ (1 Angstrom)</td>
<td>$10^{-8}$</td>
<td>cm</td>
</tr>
</tbody>
</table>

SOME USEFUL CONSTANTS
VITA

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Candidate: Samir Kumar Bhattacharva

Major Field: Physics

Title of Thesis: Two Dimensional Electron Layers in External Fields: Analysis of the Effects of Non-separability

Approved:

[Signatures of Major Professor and Chairman, Dean of the Graduate School]

EXAMINING COMMITTEE:

[Signatures of committee members]

Date of Examination:

July 16, 1982