The Rayleigh-Ritz Variational Procedure

$H|\varphi_n\rangle = E_n|\varphi_n\rangle$

Property of fundamental state $|\varphi_0\rangle$

$\forall|\psi\rangle$; $\quad \langle H\rangle = \dfrac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} \geqslant E_0 \hat{=}$ Fundamental State lowest energy.

$$|\psi\rangle = \sum_n c_n|\varphi_n\rangle$$

$$\langle\psi|H|\psi\rangle = \sum_{nn'} c_{n'}^* c_n \langle\varphi_{n'}|H|\varphi_n\rangle = \sum_n |c_n|^2 E_n \geqslant E_0 \sum_n |c_n|^2$$

$$\rightarrow \quad \frac{\langle\psi|H|\psi\rangle}{\sum_n |c_n|^2} \geqslant E_0$$

$$\text{or} \quad \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} \geqslant E_0$$

Rayleigh-Ritz procedure

Select $|\psi(\alpha)\rangle$ $\quad$ α are some variational parameters

$\rightarrow \langle H\rangle(\alpha)$; Minimize with respect to $\alpha \Rightarrow \alpha^*$

$\rightarrow \langle H\rangle(\alpha^*)$ is upper bound to E_0

Example

Harmonic oscillator

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \underbrace{\frac{1}{2}m\omega^2 x^2}_{\text{even with respect to } x}$$

$$\psi_\alpha(x) = e^{-\alpha x^2}$$

$$\langle \psi_\alpha | \psi_\alpha \rangle = \int_{-\infty}^{+\infty} e^{-2\alpha x^2} dx$$

$$\langle \psi_\alpha | H | \psi_\alpha \rangle = \int_{-\infty}^{+\infty} dx\, e^{-\alpha x^2} \left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2 \right) e^{-\alpha x^2}$$

$$= \left[\frac{\hbar^2}{2m}\alpha + \frac{1}{8}m\omega^2 \frac{1}{\alpha} \right] \int_{-\infty}^{+\infty} dx\, e^{-2\alpha x^2}$$

$$\langle H \rangle_\alpha = \frac{\hbar^2}{2m}\alpha + \frac{m\omega^2}{8}\frac{1}{\alpha}$$

$$\frac{\partial}{\partial \alpha}\langle H \rangle_\alpha = \frac{\hbar^2}{2m} - \frac{m\omega^2}{8}\frac{1}{\alpha^2} = 0 \Rightarrow \alpha^* = \frac{m\omega}{2\hbar}$$

$$\Rightarrow \langle H \rangle_{\alpha^*} = \frac{\hbar\omega}{2}$$

which is the exact solution

First excited state of harmonic oscillator E_1 ③

we select $\psi(x)$ orthogonal to wavefunction of fundamental state

Trial wavefunction $\psi_\alpha(x) = x\, e^{-\alpha x^2}$

$$\langle \psi_\alpha | \psi_\alpha \rangle = \int_{-\infty}^{+\infty} dx \; x^2 e^{-2\alpha x}$$

$$\langle \psi_\alpha | H | \psi_\alpha \rangle = \left[\frac{\hbar^2}{2m} 3\alpha + \frac{m\omega^2}{2} \frac{3}{4\alpha} \right] \int_{-\infty}^{+\infty} dx \; x^2 e^{-2\alpha x}$$

$$= \frac{3\hbar^2}{2m} \alpha + \frac{3}{8} m\omega^2 \frac{1}{\alpha}$$

$$\left. \frac{\partial}{\partial \alpha} \langle \psi_\alpha | H | \psi_\alpha \rangle \right]_{\alpha^*} = \frac{3\hbar^2}{2m} - \frac{3}{8} m\omega^2 \frac{1}{\alpha^{*2}} = 0$$

$$\alpha^* = \frac{1}{2} \frac{m\omega}{\hbar}$$

$$\rightarrow \frac{\langle \psi_{\alpha^*} | H | \psi_{\alpha^*} \rangle}{\langle \psi_{\alpha^*} | \psi_{\alpha^*} \rangle} = \frac{3}{2} \hbar\omega = \left(\frac{1}{2} + 1 \right) \hbar\omega$$

which is the correct value.

Suppose we would have selected as a trial wavefunction

$$\psi_a(x) = \frac{1}{x^2+a} \qquad a>0$$

$$\langle \psi_a | \psi_a \rangle = \int_{-\infty}^{+\infty} \frac{dx}{(x^2+a)^2} = \frac{\pi}{2a\sqrt{a}}$$

So $$\langle H \rangle (a) = \frac{\hbar^2}{4m}\frac{1}{a} + \frac{1}{2} m\omega^2 a$$

$$\frac{\partial}{\partial a}\langle H\rangle(a)\Big]_{a^*} = \frac{-\hbar^2}{4m}\frac{1}{a^{*2}} + \frac{1}{2}m\omega^2 = 0$$

$$a^* = \frac{1}{\sqrt{2}}\,\frac{\hbar}{m\omega}$$

and $$\frac{\langle H\rangle(a^*)}{\langle \psi_{a^*}|\psi_{a^*}\rangle} = \frac{1}{\sqrt{2}}\hbar\omega$$

This is $\sqrt{2}$ times larger than the actual value $\frac{\hbar\omega}{2}$

Error?

$$\frac{\frac{\langle H\rangle(a^*)}{\langle \psi_{a^*}|\psi_{a^*}\rangle} - \frac{\hbar\omega}{2}}{\frac{\hbar\omega}{2}} = \frac{\sqrt{2}-1}{2} \simeq \underline{\underline{20\%}}.$$

Triangular Well Problem

From S. Bandyopadhyay and M. Cahay
Introduction to Spintronics pp 509-512

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Example 2: The triangular well problem

The following two variational functions are used to describe the two lowest states in the two-dimensional electron gas formed at the interface of a HEMT. Close to the heterointerface, the conduction band in the semiconductor substrate is modeled as a triangular potential well [see Fig. 12.6]. The trial wavefunctions for the ground and first excited states are:

$$\xi_o(x) = (\frac{b_o^3}{2})^{\frac{1}{2}} x e^{\frac{-b_o x}{2}}, \tag{15.187}$$

$$\xi_1(x) = (\frac{3b_1^5}{2[b_o^2 + b_1^2 - b_o b_1]})^{\frac{1}{2}} x(1 - \frac{b_o + b_1}{6} x) e^{-\frac{b_1 x}{2}}, \tag{15.188}$$

where b_o and b_1 are two variational parameters, and $x = 0$ at the heterointerface.

Notice that both $\xi_o(x)$ and $\xi_1(x)$ are zero at $x = 0$, as they should be since neither wavefunction can penetrate the barrier at the heterointerface if it is very high. Since the potential energy increases linearly with distance into the substrate, the choice of exponentially decaying trial wavefunctions seems appropriate.

- Show that $\xi_o(x)$, $\xi_1(x)$ are an appropriate set of trial wavefunctions for the ground state and first excited states, i.e., $\xi_o(x)$ and $\xi_1(x)$ are both normalized, so that $\int_0^\infty |\xi_i(x)|^2 dx = 1$, and ξ_o and ξ_1 are orthogonal, meaning $\int_0^\infty \xi_o(x)\xi_1(x) dx = 0$.

Solution

Performing the integration over the probability in the ground state (magnitude of the square of the wavefunction), we get

$$\int_0^{+\infty} |\xi_o(x)|^2 dx = \int_0^{+\infty} (\frac{b_o^3}{2}) x^2 e^{-b_o x} dx = \frac{b_o^3}{2}\frac{2}{b_o^3} = 1. \tag{15.189}$$

So ξ_o is indeed normalized.

Similarly,

$$\int_0^{+\infty} |\xi_1(x)|^2 dx = \frac{3b_1^5}{2(b_o^2 + b_1^2 - b_o b_1)} [I_2 - I_3 + I_4], \tag{15.190}$$

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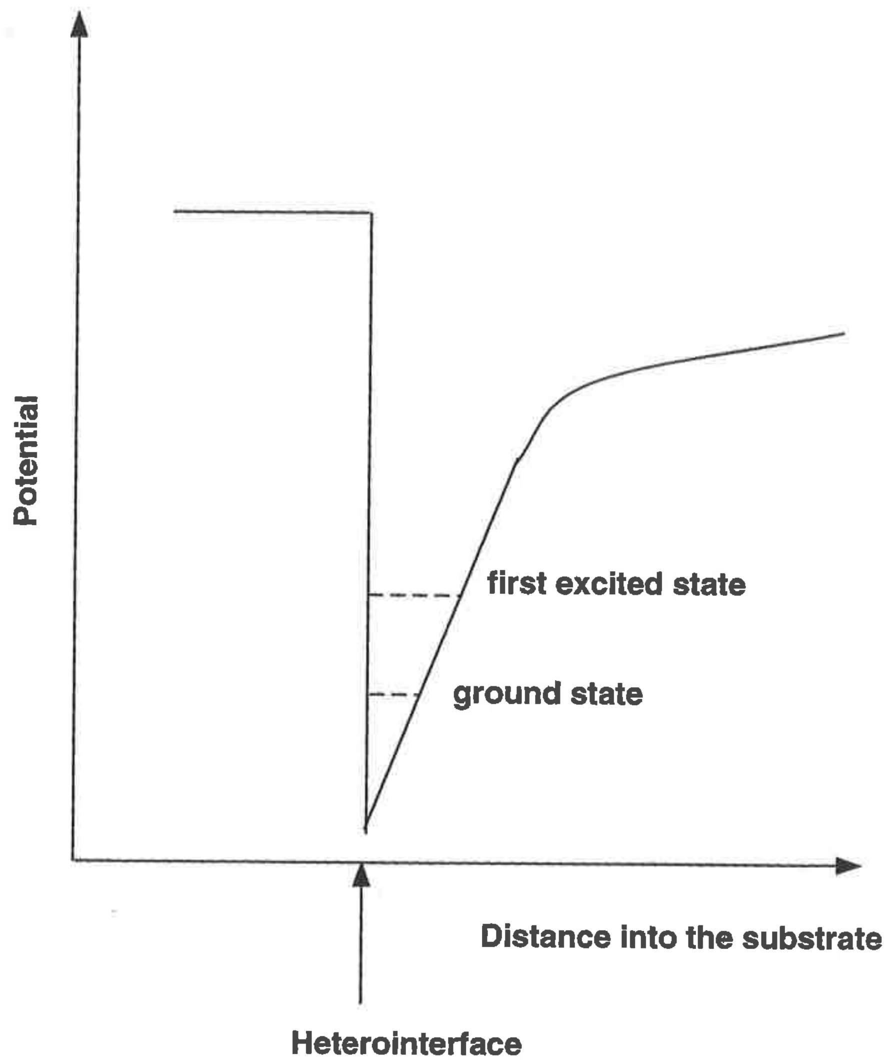

FIGURE 15.8
A triangular shape approximates the conduction band profile in the channel of a HEMT. The bound states and the wavefunctions of these states determine the channel carrier concentration and the threshold voltage.

where

$$I_2 = \int_0^{+\infty} x^2 e^{-b_1 x} dx, \tag{15.191}$$

$$I_3 = \frac{(b_o + b_1)}{3} \int_0^{+\infty} x^3 e^{-b_1 x} dx, \tag{15.192}$$

and

$$I_4 = (\frac{b_o + b_1}{6})^2 \int_0^{+\infty} x^4 e^{-b_1 x} dx. \tag{15.193}$$

We find

$$I_2 = \frac{2}{b_1^3}, \tag{15.194}$$

$$I_3 = \frac{2(b_o + b_1)}{b_1^4}, \tag{15.195}$$

and

$$I_4 = \frac{2}{3}\frac{(b_o + b_1)^2}{b_1^5}. \tag{15.196}$$

Hence

$$\int_0^{+\infty} |\xi_1(x)|^2 dx = \frac{3}{2}\frac{b_1^5}{[b_o^2 + b_1^2 - b_o b_1]}[\frac{2}{b_1^3} - \frac{2(b_o + b_1)}{b_1^4} + \frac{2(b_o + b_1)^2}{3b_1^5}]. \tag{15.197}$$

Simplifying

$$\int_0^{+\infty} |\xi_1(x)|^2 dx = \frac{3}{2}\frac{1}{[b_o^2 + b_1^2 - b_o b_1]}\frac{2}{3}[b_o^2 + b_1^2 - b_o b_1] = 1. \tag{15.198}$$

So $\xi_1(x)$ is also normalized.

To prove the orthogonality of ξ_o and ξ_1, we must show that the following integral is equal to zero

$$\int_0^{+\infty} \xi_o^*(x)\xi_1(x) dx = (\frac{b_o^3}{2})^{\frac{1}{2}}(\frac{3b_1^5}{2[b_o^2 + b_1^2 - b_o b_1]})^{\frac{1}{2}}(J_2 - J_3), \tag{15.199}$$

where

$$J_2 = \int_0^{+\infty} x^2 e^{-(\frac{b_o + b_1}{2})x} dx, \tag{15.200}$$

and

$$J_3 = (\frac{b_o + b_1}{6}) \int_0^{+\infty} x^3 e^{-(\frac{b_o + b_1}{2})x} dx. \tag{15.201}$$

We find

$$J_2 = J_3 = \frac{16}{(b_o + b_1)^3}. \tag{15.202}$$

Hence

$$\int_0^{+\infty} \xi_o(x)\xi_1(x) dx = 0, \tag{15.203}$$

and ξ_o, ξ_1 are indeed orthogonal.

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- Using the results above, calculate an upper bound for the energy of the ground state in a triangular well in which the potential is assumed to be equal to infinity for $x < 0$ and for which the potential energy is given by

$$E_c(x) = \beta x, \tag{15.204}$$

for $x > 0$.

This problem can actually be solved exactly but requires the use of Airy functions which are rather cumbersome to deal with. The exact result for the ground state energy is given by [19]

$$E_0 = 1.857(\frac{\beta^2\hbar^2}{m^*})^{1/3}. \tag{15.205}$$

Compare your answer obtained using the trial wavefunction with the exact value above.

Solution

The expectation value E_{min} appearing in the inequality (15.181) is easily calculated using MATHEMATICA [20] or other software tools such as MATLAB that allow symbolic manipulation. The minimum of E_{min} occurs for

$$b_{o,min} = (\frac{12\beta m^*}{\hbar^2})^{1/3}, \tag{15.206}$$

leading to an upper bound on the ground state energy

$$E_{min}(b_{0,min}) = 1.966(\frac{\beta^2\hbar^2}{m^*})^{1/3}, \tag{15.207}$$

which is only about 6% larger than the exact result.