Department of physics, NTNU
TFY4340 Mesoscopic Physics
Spring 2010

Exercise 4

Assistance: Tuesday February 16.

In the lectures, we used a simple 1D single–band nearest–neighbour tight–binding model to demonstrate the possibility of having electronic states localized near the crystal surface (which is zero–dimensional in this case). Within this model, we showed that if the dimensionless parameter $y \equiv \varepsilon_0/\gamma$ (positive for s–states and attractive potentials) is larger than 1, there is one or two such surface states, in addition to the usual band of delocalized states.

In this exercise, we will use *gaussian* states $|j\rangle$ and potentials V_j to verify that $y > 1$ is indeed possible. The gaussian form is not very realistic, but leaves all the relevant integrals tractable, since the product of two (or more) gaussians is a new gaussian, and we know that

$$\int_{-\infty}^{\infty} dx\, e^{-\lambda x^2} = \sqrt{\frac{\pi}{\lambda}}.$$

To be specific, choose

$$\begin{aligned} |j\rangle &= Ce^{-\kappa(x-ja)^2} \\ V_j &= -V_0 e^{-\beta(x-ja)^2} \end{aligned}$$

a) Show that with $C = (2\kappa/\pi)^{1/4}$ and $\kappa a^2/2 \gg 1$, the gaussian states are to a good approximation orthonormal, i.e., $\langle i|j\rangle \simeq \delta_{ij}$. (Hint: Complete the square in the exponent.)

b) Show that it is possible to achieve $y > 1$ within this model. More precisely, show that

$$y \simeq \exp\frac{a^2\kappa(\kappa-\beta)}{2\kappa+\beta},$$

which essentially implies that localized surface states are possible if the atomic orbitals $|j\rangle$ decay faster than the atomic potentials V_j. (Hint: Keep only the largest term(s) in ε_0 and γ.)