Solution to Problem 1.5

We begin by considering the following diagram: 1.5a. Note that the “shallow” trap levels are not shown. We assume that the temperature is high enough that these traps are fully ionized. Note the import of the last statement. Temperature - the energy stored as heat in the solid - ionizes the traps. From this principle you can get an idea of the “freeze-out” temperature of the impurity. If $E_i$ is the separation of the trap energy from the relevant band edge, freeze out occurs at thermal energies ($kT/q$) less than the trap energy.

For the situation illustrated above, The shallow trapping is dominantly donor-like and the Fermi energy is above mid-gap ($E_i$). The Fermi energy is, thus, well above $E_{DA}$ and $E_{DD}$.
- the acceptor and donor deep states. This means (using our Fermi “book-keeping rules”
that the acceptor state is charged negatively and the donor is uncharged (sunk in the Fermi
sea, and flooded with electrons, keeping it neutral.) The position of the Fermi level is set
by the shallow dopants (donors in this case). We slide the Fermi level along by changing
the net densities of shallow traps - \( N_d - N_a \).

The first part of this problem is actually easy. But is complicated by poor wording and,
possible, a conceptual error. You find trap charge state just as you evaluate band occu-
pancy:

\[
\text{occupancy} = \int_{E_{gap}} D(E)P(E)dE
\]

where \( D(E) \) is the density of trap states and \( P(E) \) is the probability of trap charging. For
the discrete-energy trap, the density function is particularly nice. Its just a Dirac delta:

\[
D(E) = N_t \delta(E - E_t)
\]

The charge probability functions are also pretty easy: for a charged donor, the electron
does not occupy the state, and the charging probability is \( 1 - F_D(E) \), where \( F_D(E) \) is the
Fermi-Dirac distribution. The resulting integration yields the following equations for the
fraction of charged states:

\[
N_{tD}^+ = \frac{N_t}{1 + \exp\left(\frac{q}{kT}\left((\phi_f - \phi_i) - (\phi_{tD} - \phi_i)\right)\right)}
\]

and

\[
N_{ta}^+ = \frac{N_t}{1 + \exp\left(\frac{q}{kT}\left((\phi_{tA} - \phi_i) - (\phi_f - \phi_i)\right)\right)}
\]

The probability that a trap is unoccupied is the joint probability:

\[
\frac{N_o}{N_t} = \left(1 - \frac{N_{tD}^+}{N_t}\right) \times \left(1 - \frac{N_{tA}^-}{N_t}\right)
\]

These expressions are easily evaluated, as shown in the plots below:

Note that, in this case, the trap energies are sufficiently separate that a large number of
totally unoccupied traps are observed. Also note, we haven’t solved the harder problem:
solve for \( \phi_b \) as a function of the net densities of shallow traps - \( N_d - N_a \). An outline for
doing this from the charge neutrality equation was given in class. The problem only calls
for the results presented here.

1.5b Deep defects alter the band mobile occupancies just like deep dopants. Its just that
they needn’t be charged at room temperature. One must solve the charge neutrality
equations to find the precise density of charged deep traps.
1.5c. Let us propose the following “thought” experiment. Start with a very low density of
deep traps as described in the problem. The Fermi level will be near mid gap, but only the
acceptor side of the trap is occupied. This makes the material p-type. Now, in our minds at least, we increase the density of deep traps. The material becomes more p-type and the Fermi level lowers. If we continue adding deep traps, the donors start to charge, adding electrons to the conduction band. Eventually, the Fermi level reaches the point midway between the donor and acceptor trap energies. Lowering the Fermi level more would discharge the charged acceptors and charge more donors. But this would argue that the Fermi level would raise. But then, the acceptor states would re-charge and the donors discharge... Oops, this is a contradiction. So what happens is this. Adding more deep states lowers the Fermi level to the point midway between the acceptor and donor levels and then the Fermi level “gets stuck” there.

1.5c. The shallow dopant dominates setting the Fermi level above mid-gap. Thus, there are $2 \times 10^{17}$ electrons in the conduction band. As the Fermi level is well above the acceptor energy, all the shallow acceptors are charged, yielding $5 \times 10^{16}$ holes. This overwhelms the intrinsic mobile charge as well. The total mobile charge is electron-like, of an amount equal to $1.5 \times 10^{17}$ charges. This yields a bulk potential which is:

$$\phi_b = 0.0259 \ln \left( \frac{1.5 \times 10^{17}}{1.45 \times 10^{10}} \right) = 0.42 \text{V}$$

above midgap.