

CHAPTER VI

DISCUSSIONS

We have constructed several potentials of Li and Na which include the polarization correction. The energy levels produced by each of constructed potentials are given and compared with the experimental values in chapter V .

The Na potential has been constructed following the procedure given by Dumrongrak. The reasons for us to consider again this potential are as follows.

First, we find that there exists some errors in Dumrongrak's calculation.

Second, it is possible to get better accuracy using the new HP-97 calculator available at the Physics Department.

In order to see the mistakes in Dumrongrak's work, it is necessary to examine his calculation. He tested his constructed Na potential quantum mechanically by solving the ground state wave function of the Na free atom. The procedure employed to solve the wave function was given by Hartree (1955, 1957). In this procedure, one had to solve the second order differential (Schrodinger) equation numerically. The asymptotic radial wave function (for $\rho \rightarrow 0$) for the ground state, s state, used in Dumrongrak's calculation was in the form ρ^{l+1} ; but this asymptotic form does not hold for the s state. Another mistake occurred because he did not reset a new table of solving a wave function when he varied the integration intervals in both outward and inward integrations. This mistake led to an error in the ground state energy. The ground

state energy reproduced from his potential should be different from that given in his thesis. However, the procedure employed to construct the potential is still useful.

We have first tested our constructed Na potential quantum mechanically. Small corrections to the errors made by Dumrongsak have been made. The details of these corrections are given in section 5.4.2. Though the quantum mechanical method can give reasonable results, it takes too much time to determine each energy level. Instead, the relation between the quantum defect and the potential given recently by Jaffé and Reinhardt (1977) is used to determine the energy levels. It is found that a slight improvement upon the Prokofjew's result can be obtained. For instance, the predicted ground state energy is within a few tenth percent. It can be seen that both predicted ground state energies computed quantum mechanically and semiclassically (QDM) are better than those obtained by using the Prokofjew's potential.

In the case of Li, the results obtained are not as good as that obtained when using the Seitz' Li potential. For instance, our ground state energy, $2s$, is lower (greater in magnitude) than the experimental result. This may be due to the fact that in considering $Q(\rho)$ for ρ less than ρ_{\min} of $1s$ state, we have used the boundary condition $Q(\rho) = Z\rho$. The assumption may not be very good for the case of Li because the Li nucleus has only three positive charges which cause the $1s$ state to be loosely bound. As a result, the nucleus would produce attractive field stronger than expected.

The polarization correction term is inserted into both potentials. It is found that all the inner energy levels reproduced from the potentials with the polarization term are not better than the potentials

without polarization. This may be due to the sudden cut off of the polarization at ρ_{min} of the f states. We cannot continue the polarization correction because no analytical integration expression which includes the polarization term for some finite limits is available. However, the insertion of the polarization term gives better outer energy levels, the f states, for both metals. We expect that if the integration formula were available we may obtain more accurate energy levels and may penetrate closer to the nucleus. Consequently, the matching without data cannot be performed.

For both types of atoms, we give special attention to the potential which can reproduce the better ground state energy level because the ground state is needed for calculating the cohesive energy. Other physical quantities of the atom such as Knight shift, lattice constant, thermal expansion coefficient, compressibility, etc., can be determined if the effective potential is known. If the potential is in an analytical form, it is easy to use it for solving the Schrodinger equation. This is the reason why we have created the Li potential in an analytical form even though this potential cannot reproduce energy levels as accurate as the Seitz's potential does.

Further work may be done on

- a) Calculating energy levels of Na and Li atoms quantum mechanically i.e. finding out the energy levels by solving wave functions instead of using the QDM.
- b) Constructing a new potential with polarization by using polarization of the form (Hartree, 1955)

$$Q(\rho) = \frac{\delta}{\rho^2 + a^2}$$

where a is a constant.

The new polarization increases less rapidly as ρ decreases, and it does not have a singularity at $\rho = 0$. Using this correction, we may find better energy levels between s and f levels.

- c) Constructing effective potentials of other alkali atoms. For these cases, the relativistic effect may dominate the polarization term; so we must solve the quantization condition which will include the term $1/\rho$, the relativistic term.