P.G. Sem - III

MPHYCC11

Condensed Matter Physics

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# The augmented-plane wave (APW) method:

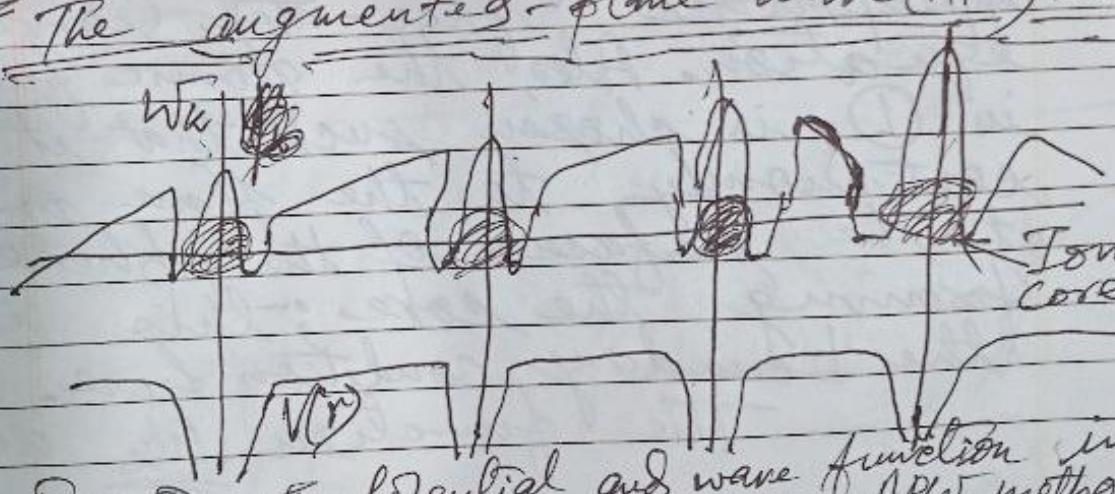


Fig. (21) The potential and wave function in the APW method.

The APW method (Slater, 1937) uses the results of the cellular method, but is so formulated as to avoid its shortcomings. Since the effective crystal potential was found to be constant in most of the open spaces between the cores, the APW method begins by assuming such a potential (Fig. 2), which is referred to as the muffin-tin potential. The potential is that of a free ion at the core, and is strictly constant outside the core. The wave function for the wave vector $\vec{k}$ is now taken to be

$$\psi_{\vec{k}} = \begin{cases} \frac{1}{V^{1/2}} e^{i\vec{k}\cdot\vec{r}}, & r > r_s, \\ \text{atomic function}, & r < r_s, \end{cases} \quad \rightarrow (1)$$

where $r_s$ is the core radius. Outside the core the function is a plane wave because the potential is constant there. Inside the core the function is atom-like, and is found by solving the appropriate free-atom Schrödinger equation. Also, the atomic function in (1) is chosen such that it joins continuously to the plane wave at the surface of the sphere forming the core; this is the boundary condition here.

The function $\psi_{\vec{k}}$ does not

have the Bloch form, but this can be remedied by forming the linear combination

$$\psi_k = \sum_G a_{k+G} w_{k+G}, \longrightarrow (2)$$

where the sum is over the reciprocal lattice vectors, which has the proper form. The best linear combination (1) is that which makes the energy as low as possible. The coefficients $a_{k+G}$ are determined by requiring that $\psi_k$ minimize the energy. In practice the series in (2) converges quite rapidly, and only four or five terms — or even less — suffice to give the desired accuracy. Thus the APW method is a sound one for calculating the band structure.