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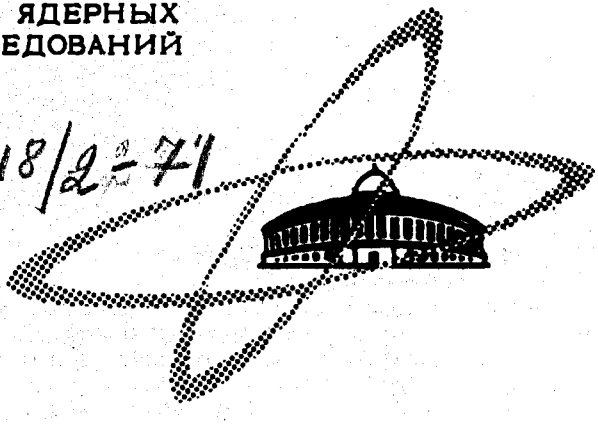

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GENERALIZED FRIEDEL SUM RULE AND DENSITY OF STATES IN DISORDERED SYSTEMS

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GENERALIZED FRIEDEL SUM RULE AND DENSITY OF STATES IN DISORDERED SYSTEMS

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For non-interacting electrons, moving in an extended system of non-overlapping muffin-tin (mt)-potentials, Lloyd[1] using separable pseudo-potentials has shown, that the integrated density of states $N(E)$ may be expressed in a form, which involves only the phase shifts η_L^n and the positions $\vec{R}_L^n$ of the scatterers. In the following a simple derivation of the Lloyd formula is given using a generalization of the Friedel sum rule.

Let us consider a non-spherically symmetric potential. Using the generalized partial wave method, discussed by Demkov and Rudakov[2] the asymptotic behaviour of scattering states $\phi_\lambda(\vec{r})$ with generalized phase shifts η_λ is given by

$$\phi_\lambda(\vec{r} \to \infty) \to A_\lambda(\vec{n}) \frac{1}{r} e^{i(\kappa r + \eta_\lambda)} + \text{c.c.}, \quad \vec{n} = \frac{\vec{r}}{r}, \quad \kappa = \sqrt{E}. \qquad (1)$$

From this one obtains (completely analogous to the spherically symmetric case[3]) the number of electrons localized by the potential (Friedel sum rule)

$$Z = \frac{2}{\pi} \sum_\lambda \eta_\lambda(\kappa_F) \qquad (2)$$

and the asymptotic behaviour of the radial density of these electrons (Friedel oscillations)

$$n(r\to\infty)\to\frac{1}{2\pi^2 r^3}\sum_{\lambda} I_\lambda(\kappa_F)\sin\eta_\lambda(\kappa_F)\cos[2\kappa_F r+\eta_\lambda(\kappa_F)] \qquad (3)$$

with $I_\lambda(\kappa)=\int d\Omega A^*_\lambda(\vec{n})A_\lambda(-\vec{n})$ as the expectation value of the inversion operator. From equation (2) follows immediately the change of the integrated density of states

$$N(E)-N^0(E)=\frac{2}{\pi V}\sum_{\lambda}\eta_\lambda(\kappa) \qquad (4)$$

due to an extended potential with phase shifts η_λ, the number of which is in this case proportional to the volume V of the system. Owing to the connection of the phase shifts with the eigenvalues $-\kappa^{-1}\,tg\,\eta_\lambda$ of the K-matrix, equation (4) can be written as

$$N(E)-N^0(E)=-\frac{2}{\pi V}Tr\ arctg\,\kappa K=-\frac{2}{\pi V}Im\ Tr\ ln(1+i\kappa K). \qquad (5)$$

For a system of non-overlapping mt-potentials, the K-matrix of the whole system can be obtained from a scheme, given by us /4/, how to calculate the phase shifts η_λ of such a system:

$$K^{nn'}_{LL'}=\sum_{n'',L''}(M^{-1})^{nn''}_{LL''}\left(-\frac{1}{\kappa}tg\,\eta^{n''}_{L''}\right)J^{n''n'}_{L''L'},\quad M^{nn'}_{LL'}=\delta_{nn'}\delta_{LL'}+tg\eta^{n}_{L}N^{nn'}_{LL'}. \qquad (6)$$

The matrices N and J in (4) contain only the structure $\vec{R}_n$; each mt-potential has non-vanishing phase shifts η^n_L only for a finite set of angular momenta L. From equations (5) and (6) immediately follows the Lloyd-formula

$$N(E)-N^0(E)=-\frac{2}{\pi V}Im\ ln\ det\,\|\delta_{nn'}\delta_{LL'}+tg\eta^n_L(N^{nn'}_{LL'}-iJ^{nn'}_{LL'})\|. \qquad (7)$$

Instead of the position representation the usual L-representation of the K-matrix is obtained by a suitable transformation of the eigenvalue equation as in /5/. Namely, with the splitting

$$J^{nn'}_{LL'} = \sum_{\mathfrak{L}} J^{n0}_{L\mathfrak{L}} J^{0n'}_{\mathfrak{L}L'} , \qquad (8)$$

which uses only the completeness of the spherical harmonics (that is, $\mathfrak{L}$ is in contradistinction to L unlimited), it turns out:

$$K_{\mathfrak{L}\mathfrak{L}'} = \sum_{\substack{n,n' \\ L,L'}} J^{0n}_{\mathfrak{L}L} (M^{-1})^{nn'}_{LL'} \left(-\frac{1}{\kappa} tg\, \eta^{n'}_{L'}\right) J^{n'0}_{L'\mathfrak{L}'} . \qquad (9)$$

$K_{\mathfrak{L}\mathfrak{L}'}$ contains in difference to $K^{nn'}_{LL'}$ also the scattering states with vanishing phase shifts η_λ .

According to Klima, McGill and Ziman /6/ and /7/x/ the large influence of the short range order in amorphous covalent semiconductors on their density of states can be described in a good approximation, assuming the system to consist of randomly arranged, rigid clusters of atoms and neglecting the multiple scattering between these clusters. In this approximation the K-matrix (6) of the whole system involves only the cluster-K-matrices K^I, from which via (5) follows

$$N(E) - N^0(E) \approx -\frac{2}{\pi V} \sum_I Im\, Tr\, ln\,(1 + i\kappa K^I) = -\frac{2}{\pi V} \sum_{I,\lambda} \eta^I_\lambda . \qquad (10)$$

The equivalence with /6,7/ is seen, if one changes as in equation (9) from the position-representation of K^I to its L-representation; the denotations Δ and G, used in /6/, correspond to J and N.

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