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On the Friedel Phase Shift Sum Rule for a Charged Dislocation

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Friedel's phase shift sum rule [1],

$$Z = \frac{2}{\pi}\sum_{l=0}^{\infty}(2l+1)\delta_l(k_F)\,, \tag{1}$$

is widespreadly used in self-consistent studies of electron-screened impurity ions in quantum electron gases (see, e. g., [2-4] and references therein). In (1), Ze is the surplus charge of the static point-like ion immersed into a three-dimensional gas of screening electrons with the Fermi wave number k_F, and $\delta_l(k_F)$ denotes the phase shift suffered by the electronic partial wave with orbital momentum l. The rule rests on the fact that as a consequence of the electron time delay in elastic scattering off the spherically symmetric potential of the ion there is induced electron density or positive hole around the defect depending on the sign of its charge.

It has been concluded by Seeger and Stehle that for a cylindrically symmetric scattering potential associated with a charged core of a straight dislocation line in a metal the analog of the Friedel sum rule (1) looks as follows [5,6]:

$$\frac{Q}{e} = -\frac{2}{\pi^2}\int_0^{k_F} dk_z \sum_{n=-\infty}^{\infty}\eta_n(k_\perp)\,, \tag{2}$$

$$k_\perp = \sqrt{k_F^2 - k_z^2}\,.$$

Here and elsewhere, the z-axis of the cylindrical coordinate frame (ρ,φ,z) runs along the dislocation line, Q is the charge accumulated by unit length of the electrically active dislocation core, the components of the electron wave vector perpendicular and parallel to the dislocation line are denoted by $k_\perp$ and k_z, respectively, and $\eta_n(k_\perp)$ is the phase shift of the *n-th* cylindrical partial wave ($n = 0, \pm 1, \pm 2, \ldots$).

In the present contribution, our main objective is to examine the structure of the sum rule (2) within the framework of the first-order Born (B1) approximation. We also demonstrate how the obtained B1 rule can be utilized in a self-consistent study of the screening length operating around an acceptor-type dislocation [7-9] in a degenerately doped *n*-type semiconductor.

Let us begin our analysis by noting that due to axial symmetry of the dislocation scattering potential, $U = U(\rho)$, the wave function of the conduction band electron, $\Psi = \Psi(\rho,\varphi,z)$, can be presented in factorized form [10]

$$\Psi(\rho,\varphi,z) = \psi(z)\sum_{n=-\infty}^{\infty} R_n(\rho)e^{in\varphi} ,$$

in which $\psi(z) = e^{ik_z z}$ describes a free motion along the dislocation line and $R_n(\rho)$ satisfies the radial Schroedinger equation

$$\frac{d^2}{d\rho^2}R_n(\rho) + \frac{1}{\rho}\frac{d}{d\rho}R_n(\rho) + \left(k_\perp^2 - \frac{n^2}{\rho^2} - U(\rho)\right)R_n(\rho) = 0 .$$

In the far-field region, $\rho \to \infty$, the radial function $R_n(\rho)$ is described by asymptotic expression [10]

$$R_n(\rho) \approx \text{const}\frac{1}{\sqrt{k_\perp\rho}}\cos\left[k_\perp\rho - \frac{n\pi}{2} - \frac{\pi}{4} + \eta_n(k_\perp)\right],$$

where the scattering phase shifts have to fulfill the sum rule (2).

So long as $U(\rho)$ can be treated as a weak perturbation [9] for the electronic motion, one can expand the η_n into multiple-scattering Born [4, 10] series,

$$\eta_n = \sum_{N=1}^{\infty}\eta_n^{BN} = \eta_n^{B1} + \eta_n^{B2} + \ldots$$

where the phase shift in the B1 approximation is given by [10]

$$\eta_n^{B1}(k_\perp) = -\frac{\pi m}{\hbar^2}\int_0^\infty d\rho\rho U(\rho)[J_n(k_\perp\rho)]^2 , \tag{3}$$

m denotes the effective mass of the scattered electron, and $J_n(x)$ is the Bessel function. By substituting Eq. (3) into Eq. (2), one can see that at the level of the B1 description the sum rule for the scattering phase shifts obtains the following preliminary form:

$$\frac{Q}{e} = \frac{2}{\pi}\frac{m}{\hbar^2}\int_0^{k_F} dk_z \sum_{n=-\infty}^{\infty}\int_0^\infty d\rho\rho U(\rho)\left[J_n(k_\perp\rho)\right]^2 . \tag{4}$$

From now on, our attention will be focused exclusively on the case of a negatively charged (acceptor type) edge dislocation causing an upward band bending in a degenerately doped *n*-type material with free electron concentration $n = k_F^3 / 3\pi^2$. In such a case the linear charge Q can be presented as [7-9]

$$Q = \frac{f}{c} e \,, \tag{5}$$

where c is the atomic-scale distance between the acceptor centres along the dislocation line, f is the statistical filling factor of these centres. Using Eq. (5) and the summation formula [11]

$$\sum_{n=-\infty}^{\infty} J_n^2(x) = 1 \,,$$

we may now reorganize the sum rule (4) into a compact adimentional form,

$$\frac{f}{f_0} = \frac{2}{\pi} \frac{m}{\hbar^2} I \,, \tag{6}$$

in which the radial (Jost-Pais) integral

$$I = \int_0^{\infty} d\rho \rho U(\rho) \tag{7}$$

is supposed to be convergent [12], and the value of the characteristic filling factor is controlled by the Fermi gas concentration, $f_0 = ck_F \sim cn^{1/3}$.

For purposes of qualitative discussion, the formula (6) can be rewritten as an order-of-magnitude relation

$$\frac{f}{f_0} \sim \frac{ma^2}{\hbar^2} U_0 \,,$$

where *a* is the influence range (screening length) of the dislocation scattering field characterized by its Coulomb energy scale, U_0. This relation shows in it's own physically transparent way that in weakly interacting electron-dislocation systems [9] the screening length *a* is obliged to display a linear dependence on the Planck's constant, $a = a(\hbar) \propto \hbar$.

Our next objective is to show in more detail how the sum rule (6) can be utilized for describing the fundamentals of self-consistent dislocation line screening from the standpoint of the Friedel-adjustment procedure. For this purpose we perform a one-parameter model potential [2-4] calculation where the perturbing potential $U(\rho)$ is constructed according to the following scenario:

$$U(\rho) = U_0 S(\rho / a) \,, \tag{8}$$

$$U_0 = \frac{2eQ}{\varepsilon} = \frac{2fe^2}{\varepsilon c} \,. \tag{9}$$

In this model, the energy scale U_0 has the familiar structure [7-9], ε is the dielectric constant of the host medium, and the *S*-function is some screening function [2-4] decaying sufficiently fast in the far-field region $1 << \rho / a \to \infty$. The screening length *a* residing in (8) acts as an open parameter [2-4].

By substituting the interaction (8) into (7) and introducing a new integration variable via $\rho = ua$, one arrives at the following radial integral,

$$I = 2\frac{fe^2}{\varepsilon c}a^2\int_0^\infty duuS(u)\,.$$

By placing this I into the sum rule (6), one concludes that the self-consistently determined a obeys the relation

$$\frac{1}{f_0} = \frac{4}{\pi}\frac{a^2}{ca_B}\int_0^\infty duuS(u)\,, \tag{10}$$

in which the length scale $a_B = \varepsilon\hbar^2 / me^2$ is recognized as the electronic Bohr radius.

As can be seen from Eq. (10), the value of the Friedel adjusted screening length is sensitive to the shape of the *S*-function. To clarify this point, let us choose the screening function either in the smoothly varying form [7-9],

$$S(\rho / a) = K_0(\rho / a)$$

or in the cut-off form,

$$S(\rho / a) = \begin{cases} 2, & \rho / a \le 1, \\ 0, & \rho / a > 1, \end{cases}$$

where $K_0(x)$ is a zero-order modified Bessel function. In both cases the corresponding screening integrals have the same value,

$$\int_0^\infty duuK_0(u) = 2\int_0^1 duu = 1\,,$$

and Eq. (10) delivers for the screening length a the fundamental structure of the Thomas – Fermi theory [7-9],

$$a = (\pi ca_B / 4f_0)^{1/2} = (\pi a_B / 4k_F)^{1/2} \equiv \lambda_{TF}\,.$$

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On the Friedel Phase Shift Sum Rule for a Charged Dislocation

The Friedel phase shift sum rule for an electrically active dislocation line is studied on the basis of the first-order Born-approximation of the scattering theory. A model potential calculation is presented for describing from the standpoint of Friedel's adju-stment procedure the self-consistent screening of a negatively charged acceptor-type edge dislocation in a degenerately doped *n*-type semiconductor.

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Լիցքավորված դիսլոկացիայի համար Ֆրիդելի գումարման կանոնի մասին

Ֆրիդելի գումարման կանոնը լիցքավորված դիսլոկացիայի համար հետազոտվում է բախումների քվանտային տեսության Բորնի առաջին մոտավորության հիման վրա: *n*-տիպի այլասերված կիսահաղորդչում բացասական լիցք կրող եզրային դիսլոկացիայի էկրանավորման խնդիրը դիտարկվում է Ֆրիդելի ինքնահամաձայնեցման ընթացակարգի տեսանկյունից:

**Л. Б. Овакимян, член-корреспондент НАН РА Г. Г. Матевосян,
Г. Б. Нерсисян, К. А. Саргсян**

О правиле сумм Фриделя для заряженной дислокации

Правило сумм Фриделя для электрически активной дислокации в кристалле исследуется на основе первого борновского приближения квантовой теории столкновений. Экранирование отрицательно заряженной краевой дислокации в вырожденном полупроводнике *n*-типа анализируется с точки зрения фриделевской процедуры самосогласования.

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