Theory of band tails in heavily doped semiconductors

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The random distribution of impurities in a semiconductor host lattice introduces potential fluctuations that allow energy levels within the forbidden energy gap. This statistical effect distorts the unperturbed density of states of the pure semiconductor, and, at high doping concentrations, substantial band tails appear. The changes in the density-of-states function are particularly important in determining the number of free carriers in a heavily doped semiconductor. Together with many-particle interactions, band tailing constitutes one of the most significant heavy-doping effects. Although the band-tailing phenomenon has been studied for many years, only a one-dimensional analytical model, which assumes a Gaussian white-noise probability distribution of the potential fluctuation, exists. In this paper the different classes of theories that describe this band tailing of the density of states in heavily doped semiconductors are reviewed in detail.

CONTENTS

I. INTRODUCTION

The aim of this work is to review the principal theoretical developments in the theory of band tails, particularly in heavy doped semiconductors.

By doping a pure semiconductor, one creates a slightly different material. Since the band structure characterizes a material, the change induced by doping is also reflected as a deformation of the band structure. This altering of the band structure is caused by different physical mechanisms, which we shall briefly discuss. In heavily doped semiconductors, a large number of impurities is inserted into the host lattice. Each impurity ion locally introduces a distinct level in the band gap. At high densities these local levels interact to form a band. At high n (p)-type doping concentrations, this impurity band merges with the conduction (valence) band. The conduction electrons together with the donor electrons form an interacting Fermi gas (Berggren and Sernelius, 1985). The interactions of electrons both among themselves and with the positive impurity ions change the parabolic $E_0(k)$ relation of the noninteracting Fermi gas [or equivalently the density of states (DOS) of the unperturbed semiconductor] considerably. These effects may be viewed as a rigid shift of the conduction band towards the valence band (band-gap narrowing) and a distortion of the DOS. In addition to this distortion, the fact that the impurities are randomly distributed in space causes the DOS to tail. Since both the many-body effects and the random distribution of impurities are responsible for this bandtailing effect, one should be very cautious in the interpretation of experiments showing tails. However, band tailing that is observed in heavily-doped-semiconductor photoluminescence spectra is fundamentally different from the exponential band tails resulting from purely random effects. These follow from the lifetime broadening caused by the electron-electron interaction (Sernelius, 1986). The electron-electron band tail (Berggren and Sernelius, 1981) is relatively small and terminates somewhere in the forbidden energy zone. The tails caused by electron-impurity interactions are more pronounced, as demonstrated by Klauder (1961) using a one-dimensional multiple-scattering (Born) approximation with δ-function impurity potentials; by Wolff (1962) via many-body perturbation theory; by Serre and Ghazali (1983), who have applied a numerical extension of Klauder's method to three dimensions with screened Coulomb impurity potentials; by John (1987) studying polaron and exciton interactions; and by Gold, Serre, and Ghazali (1988) using a two-dimensional analog. It is also worth mentioning that stress in heavily doped semiconductors may also lead to tailing (Sernelius, 1983). In this review, we focus mainly on the statistical fluctuations in impurity distributions, which we call the "band-tail problem." We neglect many-body effects and treat the band-tail problem in a one-electron picture (except in Sec. V).

Before overwhelming the reader with the mathematical aspects of the different theories, we shall sketch the physics of the band-tail problem as described by Halperin (1973). Let us first consider a dilute system of attractive impurities distributed in some random fashion, as spatially shown in Fig. 1. Let E_1 be the energy of the ground state of an isolated impurity. If the system is sufficiently dilute, so that the overlap of the wave function is generally small, then there will be a band of states close to the energy E_1. In order to generate a local state with an energy well below E_1, it is necessary to have two or more impurities close enough together. Let E_2 be the energy of an electron in the ground state of a pair of impurities that are spatially as close together as possible. For energies between E_1 and E_2, an energy level can occur bound to a pair of impurities separated by the appropriate distance for that energy; the DOS should be roughly given by the probability of finding a pair of the correct separation (Lifshitz, 1964). For energies below E_2, it is necessary to consider a cluster of three impurities, etc. In summary, for the dilute case, if one knows the probability distribution of the impurities, it is relatively straightforward to calculate the DOS in the tail of the impurity band.

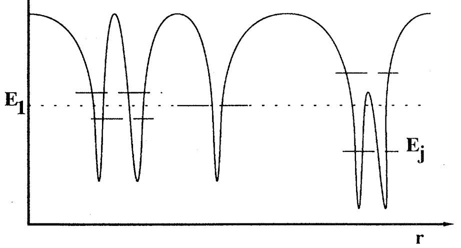

FIG. 1. Schematic drawing of the potential $V(\mathbf{x})$ (solid curve) and low-lying energy levels (dashed line) for a dilute system of attractive impurities.

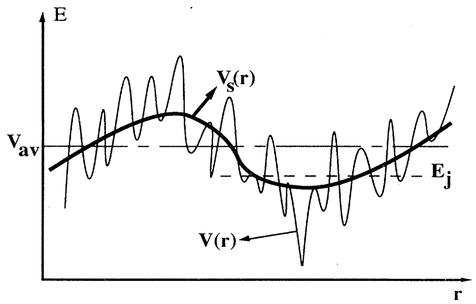

FIG. 2. Sketch of the potential $V(\mathbf{r})$ (solid thin line) for the case of a large number of impurities. The solid bold line represents the smoothed potential $V_s(\mathbf{r})$, and the dashed line is a low-lying energy level E_j, while the straight line $V_{\rm av}$ denotes the average potential of the system.

A more complicated situation occurs when there are many impurities within the range of a wave function, so that the fluctuation producing the low-lying energy states arises from a large number of impurities, rather than a small cluster, and the position of any one impurity is not very important. This situation is sketched in Fig. 2. We wish to find a state with energy E below the average potential of the system $V_{\rm ac}$. The wave function must be large in some local potential fluctuation with $V(\mathbf{r})<E$, and small in all regions with $V(\mathbf{r})>E$, in order for its average potential energy to be less than E. The necessary potential fluctuation may be produced by a local excess density of attractive impurities or a smaller-than-average local density of repulsive impurities. If $V(\mathbf{r})$ arises from thermal fluctuations in a crystalline lattice, the potential well may be produced by a larger-than-average local compression or dilation. In any case, the calculation of the DOS is a calculation of the probability of finding a potential fluctuation of the required magnitude. In the energy-band picture, the random position of impurities in the host of a pure crystal breaks the translational invariance of the lattice and thus causes levels in the forbidden band. The description of these levels, distributed over energy, as drawn in Fig. 3, belongs to the more general theory of disordered systems or to the theory of localized states in amorphous materials (Ziman, 1969, 1990; Thouless, 1970; John and Grein, 1990). However, we confine ourselves to heavily doped semiconductors. This restriction has some interesting distinguishing features. First, the framework of the effective-mass approximation remains applicable; since the characteristic energies determining the "tail region" are much smaller than the

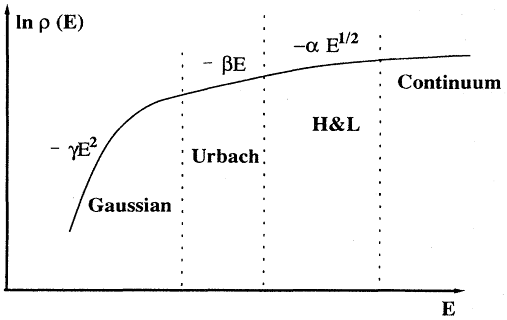

FIG. 3. Schematic of the energy E dependence of the DOS $\rho(E)$, showing the four different regions. The Gaussian and continuum regions are contracted, while the Urbach region is expanded relative to the Halperin-Lax region. For a heavily doped semiconductor, the Urbach region is simply a transition region between the Halperin-Lax and the Gaussian regions in which the $\ln\rho(E)$ has a point of inflection and thus looks linear.

band gap E_g. Throughout this article, m denotes the effective mass. Second, since many-body effects, which polarize the electron medium and screen the ions, are omitted, the impurity potential is of the Coulomb type, i.e., long-range.

Long-range potential correlations exclude a simple exponential bandtailing, as first empirically proposed by Urbach (1953). The theory of the Urbach tail was recently thoroughly studied by John *et al.* (1988) and physically explained in their review article (Cohen *et al.*, 1988). They demonstrated by field theory (see Sec. IX) that an exponential tail occurs for systems with rapidly decaying short-range correlations (as in *a*-Si), but that this behavior is not universal and may not be observed in heavily doped semiconductors. The fact that Urbach tails may not appear in heavily doped semiconductors was noted earlier by Sritrakool *et al.* (1986) using a path-integral method. However, the short-range correlation does not seem a necessary condition for exponential bandtails. By postulating the existence of a dilute concentration of charged defects, Lewis and Movaghar (1990) and Silver *et al.* (1989) claim by numerical simulations that the Coulomb interaction leads effectively to an exponential band tail.

This review is organized as follows. The second section briefly sketches the importance of band-tail effects in heavily doped semiconductors. In Sec. III, some general definitions and properties of the DOS are presented. An important special random system, which can be solved exactly, will be discussed in Sec. IV, before we examine the various methods that describe "tailed distributions." Section V describes a generalized semiclassical approach, which models the majority carriers in a heavily doped semiconductor excellently. When many-body effects are excluded and when a parabolic unperturbed DOS is assumed, the semiclassical model reduces to Kane's model (Kane, 1963). We discuss briefly possible descriptions including both the statistical and the many-body effects. Due to the semiclassical treatment of the kinetic energy, this simple model fails in the deep-tail region. In Secs. VI and VII, we examine the Halperin and Lax minimum counting method and the Efros optimal-fluctuation model. The underlying principles of these two theories are related, and both are called fluctuation models (Kane, 1985). In Sec. VIII, we illustrate the application of the elegant Feynman path-integral formalism to bandtailing. A functional-integral method related to the n-replica method in field theory (Cardy, 1978; Edwards, 1979; Brézin and Parisi, 1980; John *et al.*, 1988; John and Grein, 1990) is introduced in Sec. IX. Section X compares the discussed theories and offers some conclusions.

II. IMPORTANCE OF BAND TAILS FOR PROPERTIES OF HEAVILY DOPED SEMICONDUCTORS AND SEMICONDUCTOR DEVICES

Before examining band-tail theories in detail, we should like briefly to illustrate the importance of band tails in heavily doped semiconductors. In disordered materials, the prominent observation is the exponential Urbach tail. The Urbach theory, the appearance of band tails in amorphous materials, and experimental techniques are discussed in the recent review of John and Grein (1990). Since agreement between theory and experiments in heavily doped semiconductors is still not satisfactory in every case, Takeshima (1983; 1983b; 1984; 1985; 1986; 1989) has devoted much effort to explaining band-tail experiments with approximate or semiempirical Green's-function models.

Recent developments in molecular-beam epitaxy and metal-organic chemical-vapor deposition make it possible to study one-dimensional random structures. Superlattices with random well width (Brennan, 1990; Yamamoto, *et al.*, 1990) can be grown (as shown in Fig. 5 in Sec. IV). The more quantum wells are created, the better the structure will mimic a random one-dimensional chain (see Sec. IV). Spatial disorder is intentionally introduced in crystalline semiconductors in order to enhance the photoluminescence. Due to the relaxation of conservation of momentum (the k-selective rule) for recombination through localized states, disordered semiconductors are expected to radiate photoluminescence as intense as that from single-crystal semiconductors. Yamamoto *et al.* (1990) found that the photoluminescence intensity $I_{\rm PL}$ of a random superlattice can be modeled as a function of temperature T by an Urbach-like expression,

$$I_{\rm PL} \sim [1 + A\exp(T/T_0)]^{-1} ,$$

where T_0 is a characteristic temperature corresponding to the energy depth of localized states and A is a tunneling factor.

Compositional fluctuations in semiconductor alloys, together with lattice strain, may be responsible for recombination of carriers localized in band-tail states, as observed in photoluminescence spectra by Reihlen *et al.*

(1990) in $GaP_{1-x}Sb_x$. Tamor (1986) reported the first observation of multiple trapping in the crystalline semiconductor $Pb_{1-x}Sr_xS$ by measuring the transient photoconductivity.

The optical characterization of band tails and the underlying recombination mechanisms are the subject of intensive research (Domanevskii *et al.,* 1988; Quang, 1989). Recently, Liebler and Haug (1990) have proposed a theory for the band-tail absorption saturation. This plays an important role in nonlinear optical switching devices because they operate in the band-tail region (Haug, 1988). Glaser *et al.* (1986) and Glaser and McCombe (1988) have shown that far-infrared measurements in the n-inversion layer in the Si MOSFET provide direct evidence for screening of localized states as well as for the existence of long band tails and impurity bands. In addition, Hafez *et al.* (1990) have demonstrated the importance of band tails in MOSFET circuits at low temperatures, where the Fermi level lies close to the band edge and thus directly probes bandtail effects. We should like to mention the importance of band tails on the operation of semiconductor lasers, sketched in Fig. 4 and thoroughly examined by Yamamoto (1983) and Yamamoto *et al.* (1983). From capacitance measurements on abrupt symmetrical diodes, band-gap narrowing and information about band tailing can be extracted (Van Mieghem *et al.,* 1990a; 1990b). Finally, band tails can cause significant deterioration of the current gap of bipolar transistors, especially at lower temperatures (Van Mieghem, *et al.,* 1992).

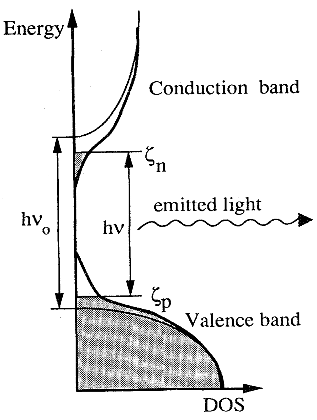

FIG. 4. Schematic of the laser operation at $T=0$ K in GaAs which is a result of population inversion (Pankove, 1971; Sze, 1981). $\zeta_{n,p}$ is the quasi-Fermi level for the electrons (holes). The narrow line denotes the unperturbed DOS, while the heavy line depicts the DOS modified by heavy-doping effects: both valence and conduction band are shifted towards each other (band-gap narrowing) and the DOS is distorted, showing bandtails. These heavy-doping effects result in a different emitted spectrum.

III. PROPERTIES

A. Definitions

The DOS, $\rho(E)$, gives the number of energy eigenstates in the interval $[E,E+dE]$ and can be represented as

$$\rho(E)=\frac{1}{V_0}\sum_\alpha \delta(E-E_\alpha)\ , \tag{3.1}$$

where $\delta(x)$ denotes the Dirac function, E_α is an energy eigenvalue belonging to the eigenfunction $\phi_\alpha(\mathbf{r})$ of some particular Hamiltonian, and V_0 is the macroscopic volume. Because $\rho(E)$ is a (real positive) *nonanalytic* function of the real variable E, it is convenient to introduce the system's Green's function (Fetter and Walecka, 1971; Economou, 1979),

$$G(\mathbf{r}',\mathbf{r},E)=\sum_\alpha \frac{\phi_\alpha(\mathbf{r})\phi_\alpha^*(\mathbf{r}')}{E-E_\alpha}\ . \tag{3.2}$$

Using the identity for $\eta\rightarrow 0^+$,

$$\frac{1}{E-E_\alpha\mp i\eta}=P\left[\frac{1}{E-E_\alpha}\right]\pm i\pi\delta(E-E_\alpha)\ , \tag{3.3}$$

and integrating over $\mathbf{r}$, we find

$$\rho(E)=\frac{1}{V_0}\left[\pm\frac{1}{\pi}\mathrm{Im}[\mathrm{Tr}G^{\pm}(\mathbf{r}',\mathbf{r},E)]\right]\ , \tag{3.4}$$

where $G^{\pm}(\mathbf{r}',\mathbf{r},E)=G(\mathbf{r}',\mathbf{r},E\mp i\eta)$. If we define a local DOS at a position $\mathbf{r}$ as

$$\rho(E,\mathbf{r})=\sum_\alpha \phi_\alpha(\mathbf{r})\phi_\alpha^*(\mathbf{r})\delta(E-E_\alpha)\ , \tag{3.5}$$

then we may establish the following relations:

$$\rho(E)=\frac{1}{V_0}\int d\mathbf{r}\rho(E,\mathbf{r}), \tag{3.6}$$

$$\begin{aligned}\rho(E,\mathbf{r})&=\mp\frac{1}{\pi}\mathrm{Im}[G^{\pm}(\mathbf{r},\mathbf{r},E)],\\ G(\mathbf{r},\mathbf{r},E)&=\int_{-\infty}^{\infty}\frac{\rho(\zeta,\mathbf{r})}{E-\zeta}d\zeta\ .\end{aligned} \tag{3.7}$$

When the Hamiltonian is translationally invariant, i.e., when $G(\mathbf{r}',\mathbf{r},E)\equiv G(\mathbf{r}'-\mathbf{r},E)$, the $\mathbf{k}$ representation is often useful,

$$G(\mathbf{k},E)=\int d\mathbf{r}\,G(\mathbf{r},E)e^{i\mathbf{k}\cdot\mathbf{r}}\ . \tag{3.8}$$

For any random system, we average $G(\mathbf{r}',\mathbf{r},E)$ over the ensemble of possible potentials, assuming an infinite volume for the system. The result $\langle G(\mathbf{r}',\mathbf{r},E)\rangle_V$ depends only on the difference $\mathbf{r}'-\mathbf{r}$, meaning that $\langle G(\mathbf{r}',\mathbf{r},E)\rangle_V\equiv G_v(\mathbf{r}'-\mathbf{r},E)$ is translationally invariant.

B. The exact variational principle

An interesting property of the DOS is that there exists an exact variational principle (Lloyd and Best, 1975), which states that the exact DOS is that function which maximizes the pressure $P(E)$ of the fermion system,

$$P(E)=\int_{-\infty}^{E} N(E')dE' , \tag{3.9}$$

where $N(E)$ is the integrated (or cumulative) DOS,

$$N(E)=\int_{-\infty}^{E} \rho(E')dE' . \tag{3.10}$$

In order to prove this principle, we note that the ground-state energy of a many-particle system at $T=0$, E_{ground}, is given by

$$E_{\text{ground}}=V_0\int^{\mu} E\rho(E)dE .$$

E_{ground} may be estimated variationally, which implies that a variational principle involving $\rho(E)$ exists. Suppose we use trial many-fermion wave functions with variational parameter(s) λ in a system with a fixed number of particles N_0. Then the true ground-state energy, for a fixed Fermi level μ, is a lower bound of the functional

$$F(E,\lambda)=V_0\int^{\mu} E\rho(E,\lambda)dE+\beta\left[\int^{\mu}\rho(E,\lambda)dE-N_0\right] ,$$

where β is a Lagrange multiplier. This condition implies (by integrating F by parts) that

$$P(\mu)\geq \max_{\lambda}\int^{\mu} N(E',\lambda)dE' .$$

Another derivation based on the convexity theorem [i.e., if $f(x)$ is convex, or $f''(x)>0$, then $\langle f(x)\rangle \geq f(\langle x\rangle)$ where $\langle \cdots \rangle$ is an expectation value] is given by Lloyd and Best (1975).

C. Free electrons

The expressions in d dimensions are derived from the Green's-function expression which, in this case, reads

$$G^0(\mathbf{k},E)=\left[E-\frac{\hbar^2k^2}{2m}-i\eta\right]^{-1} . \tag{3.11}$$

Applying the definitions from Sec. II A, we obtain

$$\begin{aligned}
\rho_1(E)&=\frac{\sqrt{m}}{\sqrt{2}\pi\hbar}\frac{1}{\sqrt{E}}\theta(E) ,\\
\rho_2(E)&=\frac{m}{2\pi\hbar^2}\theta(E) ,\\
\rho_3(E)&=\frac{m^{3/2}}{\sqrt{2}\pi\hbar^3}\sqrt{E}\,\theta(E) ,
\end{aligned} \tag{3.12}$$

where $\theta(x)$ is Heaviside's step function. If not explicitly mentioned, the spin correction ($\times 2$) is not included.

D. Crystal electrons

Crystal electrons are described by the well-known Bloch theorem. Assuming that a crystal property in a macroscopically large volume differs negligibly from its infinite-volume limit, definition (3.1) may be rearranged as (Ashcroft and Mermin, 1981, p. 37)

$$\begin{aligned}
\rho(E)&=\lim_{V_0\to\infty}\frac{1}{V_0}\sum_{\mathbf{k}}\delta(E-E_k)\\
&=\int_{\text{any primitive cell}}\frac{d\mathbf{k}}{8\pi^3}\delta(E-E(\mathbf{k})) .
\end{aligned} \tag{3.13}$$

According to Bloch's theorem, an alternative representation of the DOS of a particular band n can be constructed (Ashcroft and Mermin, 1981, p. 144 and Madelung, 1981, p. 66). Ignoring spin correction, we have

$$\rho_n(E)dE=\frac{1}{V_0}\times\left\{\begin{matrix}\text{number of allowed wave vectors in band } n\\ \text{in the energy range from } E \text{ to } E+dE\end{matrix}\right\} .$$

The number of allowed wave vectors in band n in this energy range is just the volume of a k-space primitive cell, with $E\leq E_n(\mathbf{k})\leq E+dE$, divided by the volume per allowed wave vector, $\Delta\mathbf{k}=8\pi^3/V_0$. Thus

$$\rho_n(E)dE=\int_{E\leq E_n(\mathbf{k})\leq E+dE}\frac{d\mathbf{k}}{8\pi^3} . \tag{3.14}$$

This volume integral is more elegantly expressed as a surface integral. If $S_n(E)$ denotes a surface of constant energy $E_n(\mathbf{k})=E$, then

$$\rho_n(E)dE=\int_{S_n(E)}\frac{dS}{8\pi^3}\delta n(\mathbf{k}) , \tag{3.15}$$

where $\delta n(\mathbf{k})$ is the infinitesimal vector at $\mathbf{k}$, starting perpendicular to the constant energy surface $S_n(\mathbf{E})$ and ending on $S_n(E+dE)$. Since the k gradient of $E_n(\mathbf{k})$, $\nabla_{\mathbf{k}}E_n(\mathbf{k})$, is also a vector normal to $S_n(E)$, whose magnitude equals the rate of change of $E_n(\mathbf{k})$ in the normal direction, i.e., $dE=|\nabla_{\mathbf{k}}E_n(\mathbf{k})|\cdot\delta n(\mathbf{k})$, we find an explicit relation between the DOS and the band structure,

$$\rho_n(E)=\int_{S_n(E)}\frac{dS}{8\pi^3}\frac{1}{|\nabla_{\mathbf{k}}E_n(\mathbf{k})|} . \tag{3.16}$$

IV. A PARTICLE IN A ONE-DIMENSIONAL RANDOM POTENTIAL

A. Statement of the problem

The problem (Halperin, 1965) consists in evaluating the energy DOS of a particle moving in one dimension in the interval $[0,L]$ and subjected to the Hamiltonian

$$H=-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x)\ , \tag{4.1}$$

where V is a random potential described by a Gaussian statistical distribution with the expectation values

$$\langle V(x)\rangle=0\ , \tag{4.2}$$

$$\langle V(x)\cdot V(x')\rangle=\tfrac{1}{2}D\delta(x-x')\ , \tag{4.3}$$

where D is a constant. The wave functions are assumed to satisfy boundary conditions[1] of the form

$$\Psi'(0)=a\cdot\Psi(0)\ \text{ and }\ \Psi'(L)=b\cdot\Psi(L) \tag{4.4}$$

for arbitrary real constants a and b.

B. Statistical properties of the potential V

For what follows, it is instructive to recall briefly some statistical quantities (Wang and Uhlenbeck, 1945). Consider a random process $y(t)$ over a very long time T. Taking $y(t)=0$ outside the time interval T, one can develop the resulting function in a Fourier integral:

$$y(t)=\int_{-\infty}^{\infty}A(f)e^{2\pi ift}df\ , \tag{4.5}$$

where $A(f)=A^*(-f)$ since $y(t)$ is real. From Parzeval's theory (Titchmarsh, 1967) we have

$$\int_{-\infty}^{\infty}y^2(t)dt=\int_{-\infty}^{\infty}|A(f)|^2df\ . \tag{4.6}$$

Using the fact that $|A(f)|^2$ is an even function of f and the definition of $y(t)$, one can write this relation (for $T\rightarrow\infty$) as

$$\begin{aligned}\langle y^2(t)\rangle&=\lim_{T\rightarrow\infty}\frac{1}{T}\int_{-T/2}^{T/2}y^2(t)dt\\&=\lim_{T\rightarrow\infty}\frac{1}{T}\int_{-\infty}^{\infty}y^2(t)dt=\int_0^{\infty}G(f)df\ ,\end{aligned} \tag{4.7}$$

where

$$G(f)=\lim_{T\rightarrow\infty}\frac{2}{T}|A(f)|^2 \tag{4.8}$$

is the spectral density. Analogously,

$$\begin{aligned}\langle y(t)\cdot y(t+\tau)\rangle&=\lim_{T\rightarrow\infty}\frac{1}{T}\int_{-\infty}^{\infty}y(t)y(t+\tau)dt\\&=\lim_{T\rightarrow\infty}\frac{1}{T}\int_{-\infty}^{\infty}|A(f)|^2e^{2\pi ift}df\end{aligned} \tag{4.9}$$

or, employing the fact that $|A(f)|^2$ is an even function of f,

$$\begin{aligned}\langle y(t)\cdot y(t+\tau)\rangle&=\int_0^{\infty}G(f)\cos(2\pi f\tau)df\ ,\\G(f)&=4\int_0^{\infty}\langle y(t)y(t+\tau)\rangle\cos(2\pi f\tau)d\tau\ .\end{aligned} \tag{4.10}$$

Finally, let us define the normalized correlation function as

$$C(\tau)=\frac{\langle y(t)\cdot y(t+\tau)\rangle}{\langle y^2(t)\rangle} \tag{4.11}$$

and the normalized spectrum as

$$S(f)=\frac{G(f)}{\int_0^{\infty}G(f)df}\ . \tag{4.12}$$

For an almost pure random process, $C(\tau)$ drops very rapidly from 1 to 0, and consequently $S(f)$ remains constant except for very high frequencies f. This spectrum is called a white spectrum; of course the $S(f)=$constant for all f, which corresponds to a pure random process, is a limiting case which will never occur in practice. The potential V is thus described as white Gaussian noise. A physical interpretation of V, which will be used below, is the potential arising in the high-density limit as a set of δ-function potentials of fixed magnitude, distributed at random on the line $[0,L]$. In this limit, the fluctuations about the average potential tend to a Gaussian-white-noise distribution with $D=2nv_0^2$, where v_0 denotes the potential strength and n is the expected number of scatterers per unit length.

C. Some general features of a random process

Since Markoff processes constitute a very important class, we shall examine them, restricting ourselves to stationary processes. A Markoff process can be defined by stating that the conditional probability P_n that y lies in the interval (y_n,y_n+dy_n) at time t_n, given that y is equal to $y_1,y_2,\dots,y_{n-1}$ at the times $t_1,t_2,\dots,t_{n-1}$ (where $t_i<t_j$ for $i<j$), depends *only* on the value of y at the previous time t_{n-1} (besides, of course, the obvious dependence on y_nt_n):

$$P_n(y_1t_1;y_2t_2;\dots;y_{n-1}t_{n-1}|y_nt_n)=P_2(y_{n-1}t_{n-1}|y_nt_n)\ . \tag{4.13}$$

The conditional probability P_2 (we omit the subscript hereafter) of a Markoff process fulfills the Smoluchowski equation,

$$P(x|y,t+\Delta t)=\int dz\,P(x|z,t)P(z|y,\Delta t)\ , \tag{4.14}$$

for all values of $\Delta t\geq 0$. This equation follows from the definition of a Markoff process. The moments of the change in space coordinate in a small time Δt are given by

$$M_n(z,\Delta t)=\int dy\,(y-z)^nP(z|y,\Delta t)\ . \tag{4.15}$$

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[1] The importance of the boundary conditions and the averaging of the Schrödinger equations is discussed in detail by Klauder (1961, pp. 66–75).

Consider now the physically interesting processes for which the space coordinate can only change with small amounts in small times. Or, assume that, for $\Delta t \to 0$, only the first and second moments become proportional to Δt, so that the following limits exist:

$$A(z)=\lim_{\Delta t\to 0}\frac{M_1(z,\Delta t)}{\Delta t},\qquad B(z)=\lim_{\Delta t\to 0}\frac{M_2(z,\Delta t)}{\Delta t}. \tag{4.16}$$

Combining Eqs. (4.14) and (4.16), we can derive the general Fokker-Planck equation for P (Wang and Uhlenbeck, 1945),

$$\frac{\partial P}{\partial t}=-\frac{\partial}{\partial y}[A(y)P]+\frac{1}{2}[B(y)P]. \tag{4.17}$$

Let us concentrate on Gaussian distributions. A characteristic property of a Gaussian distribution $F(t)$ is that it is completely described by its first and second moment, or equivalently

$$\begin{aligned}&\langle F(t_1)\cdot F(t_2)\cdots F(t_{2n+1})\rangle=0,\\&\langle F(t_1)\cdot F(t_2)\cdots F(t_{2n})\rangle\\&\quad=\sum_{\text{all pairs}}\langle F(t_i)\cdot F(t_j)\rangle\langle F(t_k)\cdot F(t_l)\rangle\cdots.\end{aligned} \tag{4.18}$$

Furthermore, the relation between a Gaussian process and a Markoff process is given by a theorem due to Doob (1.53): *A one-dimensional Gaussian process will be Markoffian only if the correlation function* $C(\tau)=\exp(-\beta\tau)$ *so that the spectrum* $S(f)\sim(\beta^2+\omega^2)^{-1}$.

D. Solution of the problem

The considerations of the preceding section suggest the following methodology. If we can reformulate the problem in terms of a variable $y(t)$ which constitutes a Markoff process, a Fokker-Planck equation can be derived. Since we are dealing with a Gaussian random process, this equation completely describes the process. The resulting problem is then to extract information about the density of eigenvalues from the probability distribution P.

Guided by the form of the Langevin equation (Wang and Uhlenbeck, 1945), we transform the Schrödinger equation with Hamiltonian (4.1) to

$$\frac{dz}{dx}+z^2+\lambda=2v(x), \tag{4.19}$$

where

$$v(x)=\frac{m}{\hbar^2}V(x),\qquad \lambda=\frac{2m}{\hbar^2}E, \tag{4.20}$$

and

$$z(x)=\frac{\Psi'(x)}{\Psi(x)}. \tag{4.21}$$

If we now assume that z has the Markoff property, we readily find $A(z)$ as

$$A(z)=-(z^2+\lambda), \tag{4.22}$$

while for $B(z)$ we consider

$$\Delta z^2=\left[-(z^2+\lambda)\Delta x+2\int_x^{x+\Delta x}du\, v(u)\right]^2,$$

which reads after averaging

$$\langle\Delta z^2\rangle=[(z^2+\lambda)\Delta x]^2+4\int_x^{x+\Delta x}\int_u^{u+\Delta u}du\,dy\langle v(u)v(y)\rangle.$$

Employing Eq. (4.3), we find

$$\langle\Delta z^2\rangle=[(z^2+\lambda)\Delta x]^2+2D^*\cdot\Delta x$$

such that, with Eq. (4.16),

$$B(z)=2D^*, \tag{4.23}$$

where

$$D^*=\left[\frac{m}{\hbar^2}\right]^2 D. \tag{4.24}$$

Hence we obtain the Fokker-Planck equation

$$\frac{\partial P}{\partial x}=\frac{\partial}{\partial z}(z^2+\lambda)P+D^*\frac{\partial^2 P}{\partial z^2}. \tag{4.25}$$

Unfortunately, $z(x)$ is not Markoffian, as is readily verified from Doob's theorem. However, Halperin (1965) introduces a second stochastic variable U_1 and shows, by rather complicated reasoning, that (z,U_1) constitute a two-dimensional Markoff process. If only the DOS is concerned, the two-dimensional Fokker-Planck equation found by Halperin reduces to Eq. (4.25).

The method for extracting the DOS from the probability distribution P is due to Frisch and Lloyd (1960)[2,3] (although inspired by Rice, 1944). Because of the clarifying ideas, we outline their method.[4] They considered a simplified version of our problem (Fig. 5), with

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[2] A detailed comparison between the results of Frisch and Lloyd and Klauder's diagrammatic method is presented by Klauder (1961).

[3] Another method that treats nearly the same problem was given earlier by Schmidt (1957).

[4] Recent studies on the dynamic properties of the 1D random walk (Aslangul *et al.*, 1991; Bouchaud *et al.*, 1991) use the result (4.51), which can be computed through other approaches such as a Dyson-Schmidt technique (Ziman, 1990) and the replica method.

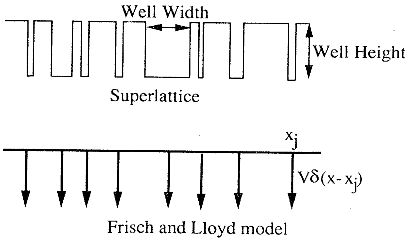

FIG. 5. Schematic drawing of the random superlattice. In the limit of zero barrier width and infinite barrier height, we get the theoretical structure considered by Frisch and Lloyd (1960).

$$V(x)=V\sum_{j=-\infty}^{\infty}\delta(x-x_j) \tag{4.26}$$

and $\omega=(\ldots,x_{-1},x_0,x_1,\ldots)$ a sequence of randomly distributed x_j on an infinite line assuming a Poisson distribution. If n is the expected number of scatterers, Eq. (4.26) describes a Gaussian potential when $n\to\infty$ and $V\to 0$, while nV remains finite, as already explained in Sec. IV. Each sequence ω is treated as a single point in an infinite-dimensional configuration space Ω, and the sequences ω are the "random variable."

For each ω let $E_1(L,\omega)\le E_2(L,\omega)\le\cdots$ denote the eigenvalues of the Schrödinger equation with Hamiltonian (4.2) and with (4.26) for a finite interval $[0,L]$. Define then

$$N_L(E,\omega)=\frac{1}{L}[\text{number of } E_m(L,\omega) \text{ satisfying } E_m(L,\omega)\le E] \; . \tag{4.27}$$

The intregrated DOS $N(E)$ [Eq. (3.10)] equals

$$N(E)=\lim_{L\to\infty}N_L(E,\omega) \; . \tag{4.28}$$

It can be proven that this limit exists and that it is independent of ω, and, consequently, that probability is not involved in this limiting case.

From the Sturm-Liouville eigenvalue theorems (Morse and Feshbach, 1978, p. 719), it follows that the number of eigenstates equals the number of zeros $v_L(E,\omega)$ of the wave function $\Psi(x;E,\omega)$ in the interval $[0,L]$ within a possible error of ± 1 such that

$$N(E)=\lim_{L\to\infty}v_L(E,\omega) \; , \tag{4.29}$$

and this limit is independent both of probability and of the boundary conditions $\Psi(0;E,\omega)=\xi_0$ and $\Psi'(0;E,\omega)=\eta_0$. The problem is thus reduced to finding the average number of zeros per unit length of real solutions of the Schrödinger equation. Finally, we introduce the dimensionless quantity

$$v_0=-\frac{m^*}{\hbar^2}V>0 \; . \tag{4.30}$$

Let us further reformulate the problem to a time variable t as in Sec. IV.2. Rewriting the Schrödinger equation in state space as in the theory of linear systems, with $\xi(t)=\Psi(x)$ and $\eta(t)=\Psi'(x)$, we have

$$\begin{aligned}\xi'(t)&=\eta(t),\\ \eta'(t)&=-\left[\lambda+2v_0\sum_{j=-\infty}^{\infty}\delta(t-t_j)\right]\xi(t) \; .\end{aligned} \tag{4.31}$$

We interpret $\delta(t-t_j)$ as a hit at time t_j. At each hit, the particle coordinate is unchanged (continuity of Ψ),

$$\lim_{\varepsilon\to 0}\xi(t_j+\varepsilon)=\lim_{\varepsilon\to 0}\xi(t_j-\varepsilon) \; , \tag{4.32}$$

but the particle momentum receives an increment proportional to the displacement,

$$\lim_{\varepsilon\to 0}[\eta(t_j+\varepsilon)-\eta(t_j-\varepsilon)]=-2v_0\xi(t_j) \tag{4.33}$$

[obtained by integrating Eq. (4.31) from $t_j-\varepsilon$ to $t_j+\varepsilon$ for small ε]. Between the hits, the process evolves as a linear system

$$\begin{aligned}\xi'(t)&=\eta(t) \; ,\\ \eta'(t)&=-\lambda\xi(t)\end{aligned} \tag{4.34}$$

($t\neq t_j$) describing elliptical motion

$$\begin{aligned}\xi(t)&=\frac{A}{\sqrt{\lambda}}\cos\theta(t) \; ,\\ \eta(t)&=A\sin\theta(t) \; .\end{aligned} \tag{4.35}$$

The zeros of Ψ are now determined by the η-axis crossings. The effect of the hits is to speed up the angular motion $\theta(t)$, because

$$\theta'(t)=-\sqrt{\lambda}-\frac{2v_0}{A^2}\sum_{j=-\infty}^{\infty}\delta(t-t_j) \; .$$

Since we are only interested in the η-axis crossings, we may treat the angular part separately. Accordingly, we introduce the variable $z=\eta/\xi$ so that
(a) Equations (4.32) and (4.34) become

$$\lim_{\varepsilon\to 0}z(t_j+\varepsilon)=\lim_{\varepsilon\to 0}z(t_j-\varepsilon)-2v_0 \; . \tag{4.36}$$

(b) Equation (4.34) becomes

$$z'(t)=-(z^2+\lambda) \; . \tag{4.37}$$

In a Poisson process, the times of the hits occurring after a certain time τ are statistically independent of the times of the hits occurring before τ. Hence the conditional probability distribution of $z(t,\omega)$, give all values $[z(t,\omega), -\infty<t<\tau\}$, is the same as the conditional probability distribution of $z(t,\omega)$ given only $z(\tau,\omega)$. Consequently, in view of Eq. (4.13), the random variables $z(t,\omega)$ constitute a Markov process. The probability distribution of $z(t,\omega)$ is found by reasoning on a Poisson process.

Assume that the probability distribution of $z(t,\omega)$ has the density

$$P\{z(t,\omega)\leq\xi\}=\int_{-\infty}^{\xi}T(z,t)dz \quad \text{for all real } \xi \ , \tag{4.38}$$

where, of course, for all real t,

$$\begin{gathered} T(z,t)\geq 0 \ , \\ \int_{-\infty}^{\infty}T(z,t)dz=1 \ , \end{gathered} \tag{4.39}$$

and recall the characteristics of a Poisson process:

(a) $P\{$the time interval $(t,t+dt)$ contains no hit$\}=1-n\cdot dt+o(dt)$,

(b) $P\{$the time interval $(t,t+dt)$ contains exactly 1 hit$\}=n\cdot dt+o(dt)$

(c) $P\{$the time interval $(t,t+dt)$ contains more than 1 hit$\}=o(dt)$

Then $T(z,t)\delta z$ is the fraction of z points that lie in an interval $(z,z+\delta z)$ at time t. A continuity equation can be derived by considering the z points that lie in $(z,z+\delta z)$ at time $t+dt$:

(a) Those which were in $(z',z'+\delta z')$ at time t and received no hit during $(t,t+dt)$ (with probability $1-n\cdot dt$). These are easily found by Eq. (4.37) to yield

$$\begin{gathered} z'=z-dz=z+(z^2+\lambda)\cdot dt \ , \\ \delta z'=(dz'/dz)\delta z=(1+2z\cdot dt)\delta z \ . \end{gathered}$$

(b) Those which were in $(z'',z''+\delta z'')$ at time t and received exactly one hit during $(t,t+dt)$ (with probability $n\cdot dt$). With Eq. (4.36) these yield

$$z''=z+2v_0 \quad \text{and} \quad \delta z''=\delta z \ .$$

Apart from a negligible proportion that reaches $(z,z+\delta z)$ after being hit more than once during $t+dt$, the conservation of z points requires

$$T(z,t+dt)\delta z=(1-n\cdot dt)T(z',t)\delta z'+n\cdot dt T(z'',t)\delta z'' \ .$$

From this we find, after some manipulation,

$$\frac{\partial T(z,t)}{\partial x}=\frac{\partial}{\partial z}(z^2+\lambda)T(z,t)+n[T(z+2v_0,t)-T(z,t)] \ . \tag{4.40}$$

This equation must be compared with (4.25).

Frisch and Lloyd showed that every solution of Eq. (4.40), whatever the initial distribution $T(z,0)$, tends to a limiting density $T(z)=\lim_{t\to\infty}T(z,t)$. The stationary density $T(z)$ is the unique solution of

$$\frac{d}{dz}(z^2+\lambda)T(z)+n[T(z+2v_0)-T(z)]=0 \tag{4.41}$$

or, by integrating,

$$(z^2+\lambda)T(z)+n\int_{z}^{z+v_0}T(u)du=c \ , \tag{4.42}$$

where c is the integration constant. This equation asserts that the flux of z points is constant, hence c equals this flux. The expected η-axis crossing ($\Psi=\xi=0$ or $z=\infty$) rate $N(E)$ equals the flux at $z=\infty$, but since this flux is independent of z, we have that $c=N(E)$. Rewriting Eq. (4.42) gives

$$T(z)=\frac{1}{z^2+\lambda}\left[N(E)-n\int_{z}^{z+v_0}T(u)du\right] \tag{4.43}$$

or, since the integral vanishes as $z\to\pm\infty$, it follows that

$$N(E)=\lim_{z\to\pm\infty}z^2\cdot T(z) \ . \tag{4.44}$$

This result enables us to proceed with the solution of our initial problem.

As explained above, the link between a Poisson and a Gaussian process is the limiting case, where the number of scatterers $n\to\infty$ but their intensity v_0 approaches zero, while the overall interaction nv_0 remains finite. Thus expanding $T(z+2v_0)$ in Eq. (4.41) to second order in v_0 yields

$$2nv_0^2\frac{d^2T(z)}{dz^2}+\frac{d}{dz}(z^2+\lambda+2nv_0)T(x)=0 \ , \tag{4.45}$$

which obeys Eq. (4.25) with $D^*=2nv_0^2$. In the case of a Gaussian process, higher orders than 2 need not be included. On the other hand, if we consider only a first order in v_0, we easily obtain from Eq. (4.43)

$$T(z)=\frac{N(E)}{z^2+\lambda+2nv_0} \ .$$

But using the normalization condition (4.39) gives

$$N(E)=\frac{1}{\pi}\sqrt{\lambda+2nv_0} \ ,$$

so that, if $\lambda\leq-2nv_0$, $T(z)$ is not everywhere positive as required by Eq. (4.39). This justifies the second-order expansion. Invoking Eq. (4.43), we find that Eq. (4.45) becomes

$$\frac{dT(t)}{dt}+(t^2+2b)T(t)=a^2N(E) \ , \tag{4.46}$$

where

$$\begin{gathered} t=az \ , \\ b=\left[\frac{\hbar^2}{mD^2}\right]^{1/3}(E-n|V|) \ , \\ a=\left[\frac{\hbar^2}{m}\right]^{2/3}D^{-1/3} \ . \end{gathered} \tag{4.47}$$

Since Eq. (4.47) is a linear first-order differential equation, an analytical solution is always possible, which is easily found to be

$$T(t)=a^2N(E)\exp\left[-\frac{1}{3}t^2-2bt\right] \times\int_{-\infty}^{t}\exp(\tfrac{1}{3}u^3+2bu)du \ , \tag{4.48}$$

where the lower limit ($t\to-\infty$) is needed to render finite results for $T(t)$ as $t\to-\infty$. Finally, the cumulative DOS is found using the normalization (4.39) of $T(z)$ and Eq. (4.47),

$$aN(E)=\left[\int_{-\infty}^{\infty}dz\,\exp(-\tfrac{1}{3}z^3-2bz)\times\int_{-\infty}^{z}\exp(\tfrac{1}{3}u^3+2bu)du\right]^{-1}. \qquad (4.49)$$

After changing the variables ($u=z-t$) and evaluating a Gaussian integral, we find that Eq. (4.49) becomes

$$N(E)=\left[a\sqrt{\pi}\int_0^{\infty}du\,u^{-1/2}\exp(-\tfrac{1}{12}u^3-2bu)\right]^{-1}. \qquad (4.50)$$

By Fourier transforming and recalling the properties of a probability distribution (4.39), Halperin (1965) derived a more elegant form of Eq. (4.50) in terms of Airy functions,

$$N(E)=\frac{1}{a\pi^2}\frac{1}{[Ai(-2b)]^2+[Bi(-2b)]^2}. \qquad (4.51)$$

This function is drawn in Fig. 6. The energy is lowered by the average potential nV of the impurities. By referring the energy to this average, we can further neglect the shift. From either Eq. (4.50) or Eq. (4.51), we may establish the asymptotic expressions

$$\begin{aligned} N(E)&\sim\frac{1}{a\pi}\sqrt{2b} \quad \text{for } E\gg 0\,, \\ N(E)&\sim\frac{\sqrt{|2b|}}{a\pi}\exp(-\tfrac{1}{4}|2b|^{3/2}) \quad \text{for } E\ll 0\,. \end{aligned} \qquad (4.52)$$

The first result is just the free-carrier cumulative DOS (in one dimension). The second relation is a typical result of a tailed distribution caused by random effects. The DOS derived from the latter

$$\rho(E)=\frac{dN(E)}{dE}\sim\frac{8E}{\pi D}\exp\left[-\frac{16}{3D}\sqrt{\hbar^2/2m}\,E^{3/2}\right] \qquad (4.53)$$

will be taken as a reference to check the various other approximate methods.

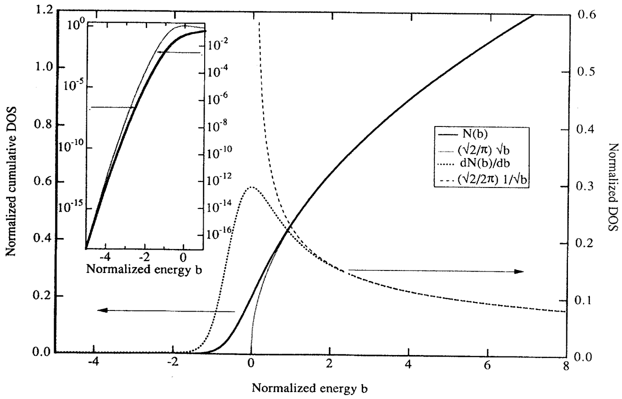

FIG. 6. Both $N(b)$ and $\rho(b)$ with their respective positive b asymptotes as a function of normalized energy $b=(\hbar^2/mD^2)^{1/3}(E-n|V|)$. Notice that the number of carriers in the tail (at $T=0$ K) equals $N(0)=0.20096/a$. The tails (negative b asymptotes) are shown in the inserted graph. The names of the axes are omitted for clarity but are identical to those of the larger graph.

E. Conclusion

The problem of a particle in a one-dimensional random potential has been discussed in detail because it elucidates the solution method for random stochastical processes. Since this problem is only a limiting case and is simplified to one dimension, the complexity already involved predicts that, for the realistic problem, only approximate models are feasible.

The same problem as that considered by Frisch and Lloyd (1960) was also solved by Borland (1961). Since his method is less physically inspired and his final expression (involving the dilogarithmic function) is an approximation, we do not discuss his results, but merely mention the agreement of his results with the numerical (Monte Carlo) results of Lax and Philips (1958) [which was also the reference of comparison in the work of Frisch and Lloyd (1960)].

The reduction of the DOS to Eq. (4.50) or (4.51) is a rather remarkable accomplishment. An extension of the presented methods to more dimensions seems impossible because there is no Markov property when the parameter is d dimensional (with $d>1$) and there is no mathematical evidence to generalize Eq. (4.29). Nevertheless, there are three-dimensional models involving disorder (or random processes) which have been solved exactly (Lloyd, 1969). The Lloyd model is a simple, single-band, tight-binding model in which the single-site energies are independent random variables having an identical Lorentzian probability distribution of half-width Γ about vanishing average value. The DOS is

$$\rho(E)=\int dE'\rho_0(E')\frac{1}{\pi}\frac{\Gamma}{(E-E')^2+\Gamma^2}\,, \qquad (4.54)$$

where $\rho_0(E)$ is the DOS in the periodic case ($\Gamma=0$). The tails introduced by disorder are clearly not exponential. However, since the Hamiltonian containing the random elements is somewhat artificial, and the probability distribution for selecting these elements is limited to a Lorentz distribution, the resulting DOS of this model is of less interest in heavily doped semiconductors.

V. THE GENERALIZED SEMICLASSICAL MODEL

A. Introduction

A detailed description that rigorously combines both many-body and statistical fluctuation effects must be exceedingly complicated, if it exists. A theory (Serre, Ghazali, and Hugon, 1981) that partially includes many-body effects with statistical effects has been developed, but this requires extensive numerical calculations and a number of approximations. A totally different approach would be the introduction of many-body effects into a

Feynman path integral because, in the absence of many-body effects, an exact path-integral formula (8.5) exists. However, it is known that the path-integral method is not the best one to describe many-fermion systems. Alternatively, one could try to generalize the replica method (Sec. IX) to interacting systems.

The discouraging difficulties that arise in first-principle models suggest approximate techniques. We should like to demonstrate that a combination of the electron medium and the statistical fluctuations can be formulated in a semiclassical framework. Because band-tail effects as well as many-body effects only significantly alter the DOS at high doping concentrations, a semiclassical approach (Davydov, 1976) looks highly suitable, covering the high-density limit exactly (Sa-yakanit and Glyde, 1980). The major advantages of the generalized semiclassical DOS are its simple physical interpretation and the explicit use of an arbitrary energy-versus-wave-vector relation, $E(k)$, necessary to include many-body effects and to deal with a nonparabolic unperturbed DOS (such as the DOS of $\mathrm{InSb}_x\mathrm{As}_{1-x}$). The expression for the DOS can be written as a closed analytical formula. Moreover, the semiclassical model is the only existing simple formula that covers the whole energy range. The analyticity of our approach makes it possible to approach DOS expressions in different geometrical dimensions.

In materials science, one is mainly interested in estimations of the expected band-gap narrowing. In order to make quick estimations of the band tailing effect, an analytical closed formula is presented. All numerical results are calculated for n-type GaAs.

B. The generalized semiclassical DOS

1. A semiclassical approach

Kane (1963), Bonch-Bruevich (1963,1965), Keldysh and Proshko (1964), Bagaev *et al.* (1964–1965), and Shlovskii and Efros (1984) have applied a semiclassical method to the calculation of the DOS in heavily doped semiconductors. Our approach generalizes their results to different dimensions, interacting Fermi liquids, and arbitrary initially unperturbed densities of state.

The semiclassical approach assumes basically one approximation: the classical description of the electron wave packet. The potential fluctuations caused by charged impurities are assumed to be smooth in the sense that they change little over the electron wavelength. The electron only "feels" the potential of the point where it is located. Thus this approximation considers electrons with energies sufficiently higher than the averaged potential V_{av} in Fig. 7 such that the actual potential $V(\mathbf{r})$ can be replaced by the smoothed, slowly varying potential $V_s(\mathbf{r})$. Let $\rho_0(E)$ denote the DOS in the crystal not perturbed by impurities. The energy E is measured from the bottom of the band in the noninteracting electron system, which will be represented by the subscript n while the interacting electron system will be denoted by the subscript i.

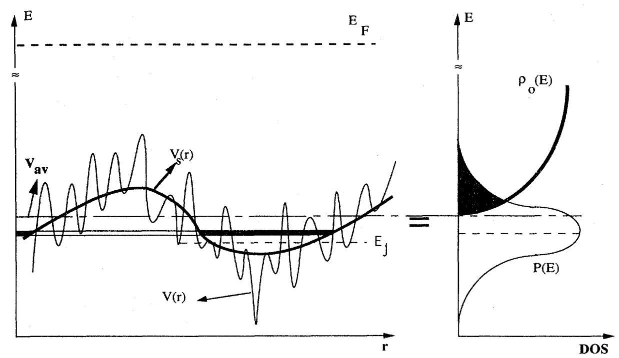

FIG. 7. Sketch of the semiclassical method: all states with energy above the smoothed potential $V_s(r)$ are counted. This summation of states within the shaded infinitesimal-energy strip in coordinate space is equivalent to the shaded area (a convolution) of the right-hand-side plot.

From Fig. 7 and Kane (1963) and Schlovskii and Efros (1984), we obtain a semiclassical expression for the DOS,

$$\rho(E)=\int_{-\infty}^{E-\rho_0^{-1}(0)}\rho_0(E-V)P(V)dV$$
$$=\int_{\rho_0^{-1}(0)}^{\infty}\rho_0(v)P(E-v)dv\ , \tag{5.1}$$

where $P(V)$ is the distribution function for the potential energy $V(\mathbf{r})$ to be determined and where $x=\rho_0^{-1}(y)$ is the inverse DOS function or solution of $y=\rho_0(x)$. This notation is required for interacting electron systems, where the DOS shifts down to lower energies due to many-body interactions, Hence, $\rho_{0i}^{-1}(0)<0$ in contrast to $\rho_{0n}^{-1}(0)=0$, by definition as the reference energy. Introducing the definition of the convolution of two functions $g(t)$ and $f(t)$ as

$$g(t)^*f(t)=\int_{-\infty}^{\infty}f(t-\tau)g(\tau)d\tau\ ,$$

we observe that our generalized result can be written as

$$\rho(E)=\rho_0(E)\cdot\theta(\rho_0(E))^*P(E)\ ,$$

where $\theta(E)$ denotes Heaviside's step function. At this point, we note a formal resemblance to the exactly solvable Lloyd model (4.54), which clearly obeys $\rho(E)=\rho_0(E)^*P(E)$ with

$$P(E)=\frac{1}{\pi}\frac{\Gamma}{E^2+\Gamma^2}\ .$$

Figure 7 illustrates that in the semiclassical approach all energies above $V_s(r)$ contribute to the DOS. The actual energy levels E_j are discrete and their spacing increases as the potential well narrows, which actually occurs at lower energies. As the semiclassical approach ignores this quantum-mechanical effect, the semiclassical DOS overestimates the number of electrons in the deep tails, but gains accuracy for increasing energies and finally becomes exact in the high-density limit. For degenerate semiconductors, most of the physics will be included if the electron can be regarded as classical. Energy states deep under the unperturbed energy band surely do need a quantum-mechanical description (see Secs. VI–IX). Because these deep-lying energy states are not properly taken into account in a semiclassical approach, the model will describe only majority carriers (with Fermi level above the unperturbed band edge) sufficiently well.

Let us now assume that the energy-versus-wave-vector relation is isotropic in k space: $E(\mathbf{k})=E(|\mathbf{k}|)=E(k)$. Using Eq. (3.16) for a different geometrical dimension d, $\rho_{0;kd}(k)$ yields

$$\rho_{0;k3}(k)=\frac{k^2}{\pi^2 E'(k)} , \tag{5.2a}$$

$$\rho_{0;k2}(k)=\frac{k}{2\pi E'(k)} , \tag{5.2b}$$

$$\rho_{0;k1}(k)=\frac{1}{\pi E'(k)} , \tag{5.2c}$$

where $E'(k)$ denotes the k derivative of $E(k)$. Observe that

$$\rho_{0,k}(k)=\rho_0(E(k)) . \tag{5.3}$$

A replacement of the independent variable V by $E-E(k)$ in Eq. (5.1) yields

$$\rho(E)=\int_0^\infty \rho_0(E(k))P(E-E(k))E'(k)dk , \tag{5.4}$$

since the lowest energy $\rho_0^{-1}(0)$ corresponds to $k=0$. Applying Eqs. (5.2) and (5.3) finally gives $\rho_d(E)$ in different dimensions,

$$\rho_3(E)=\frac{1}{\pi^2}\int_0^\infty k^2 P(E-E(k))dk , \tag{5.5a}$$

$$\rho_2(E)=\frac{1}{2\pi}\int_0^\infty kP(E-E(k))dk, \tag{5.5b}$$

$$\rho_1(E)=\frac{1}{\pi}\int_0^\infty P(E-E(k))dk . \tag{5.5c}$$

From these relations we conclude that if the distribution function $P(V)$ and the $E(k)$ relation of electrons in an unperturbed crystal are known, the DOS for majority carriers can be calculated.

2. The distribution function $P(V)$ of the potential energy V in an interacting Fermi system

An analytical, exact expression for $P(V)$ exists only on the condition that the potential at a certain point $\mathbf{r}$ can be written as a superposition of the influences of all impurities in a system with volume V_0. For, if the probability $p(\mathbf{r}_i)$ having an impurity at an arbitrary point $\mathbf{r}_i$ is constant and, hence, equals V_0^{-1} and if the potential energy $V(\mathbf{r},\{\mathbf{r}_i\})$ at $\mathbf{r}$, caused by a configuration of N impurities at positions $\{\mathbf{r}_i\}$, can be written as a superposition,

$$V(\mathbf{r},\{\mathbf{r}_i\})=\sum_{i=1}^{N} v(\mathbf{r}-\mathbf{r}_i) , \tag{5.6}$$

where $v(\mathbf{r})$ is an arbitrary well-behaved function, then an exact expression for the probability distribution function $P(V)$ can be derived (see Appendix A), yielding

$$P(V)=\frac{1}{2\pi}\int_{-\infty}^{\infty}\exp\left[iVt+n\int d\mathbf{R}(e^{-iv(\mathbf{R})t}-1)\right]dt . \tag{5.7}$$

The superposition (5.6) implies a superposition of the charge densities, indicating that the Poisson equation must be linear, which generally is not the case in an electron medium. As long as the potential fluctuations are small, linear-response theory (Fetter and Walecka, 1971; Mahan, 1986) applies, providing a general expression for the potential induced by an impurity charge $Ze\delta(\mathbf{r})$ in an electron medium:

$$v(\mathbf{r})=Z\int\frac{d\mathbf{q}}{(2\pi)^d}e^{i\mathbf{q}\cdot\mathbf{r}}\frac{v_q}{\varepsilon(q)} , \tag{5.8}$$

where $v_q=e^2/\varepsilon q^2$ is the Fourier transform of the bare Coulomb potential and $\varepsilon(q)$ denotes the static dielectric function. With an explicit expression for $E(k)$,

$$E(\mathbf{k})=\frac{\hbar^2k^2}{2m}+\hbar\Sigma(\mathbf{k},E) , \tag{5.9}$$

where $\hbar\Sigma(\mathbf{k},E)$ denotes the system's self-energy due to many-body interactions, all quantities needed to calculate Eq. (5.5) are defined. In this general form, as both the self-energy $\hbar\Sigma(\mathbf{k},E)$ and the dielectric function $\varepsilon(\mathbf{q})$ depend on the number of electrons and thus on $\rho(E)$, Eqs. (5.5) and (5.7)–(5.9) represent a coupled system of equations.

The assumption of linearity is, of course, an approximation, but a very good one for heavily doped but noncompensated[5] semiconductors, and it becomes exact in the high-density limit. Thus the proposed model based on the semiclassical approach and the requirement of linearity exactly describes band-tailing and many-body interactions in the high-density limit. In the following, we shall illustrate the proposed model for a 3D noninteracting and interacting system. A 2D noninteracting system is calculated in Van Mieghem *et al.* (1991).

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[5] Compensated heavily doped semiconductors suffer from large potential fluctuations (Shklovskii and Efros, 1984), which inhibit linearization.

C. A noninteracting Fermi system in three dimensions: the Kane DOS

As an alternative to Eq. (5.8) and in order to follow the original derivation of Kane (1963), the Coulomb potential can be retained from the Poisson equation,

$$\Delta V(\mathbf{r}) = -\frac{e\gamma(\mathbf{r})}{\varepsilon} .$$

The charge density equals

$$\gamma(\mathbf{r}) = e\{n_{\mathrm{el}}(E_F) - n_{\mathrm{el}}[E_F + V(\mathbf{r})] + N_D(\mathbf{r})\} ,$$

where $n_{\mathrm{el}}(E_F)$ denotes the average electron concentration corresponding to a Fermi level E_F, $n_{\mathrm{el}}[E_F + V(\mathbf{r})]$ the electron concentration at $\mathbf{r}$, and $N_D(\mathbf{r})$ the density of fixed impurity charges. The permittivity ε has been assumed constant. As shown above, the classical description of the electron requires $|V(\mathbf{r})| \ll E_F$ such that the Poisson's equation can be linearized with

$$n_{\mathrm{el}}[E_F + V(\mathbf{r})] = n_{\mathrm{el}}(E_F) + \left.\frac{dn_{\mathrm{el}}[E_F + V(\mathbf{r})]}{dE_F}\right|_{V=0} V(\mathbf{r}) .$$

yielding

$$\Delta V(\mathbf{r}) = \kappa^2 V(\mathbf{r}) - \frac{e^2 N_D(\mathbf{r})}{\varepsilon} , \tag{5.10}$$

where κ denotes an inverse screening length,

$$\kappa^2 = \left.\frac{e^2}{\varepsilon}\frac{dn_{\mathrm{el}}(E_F)}{dE_F}\right|_{V=0} . \tag{5.11}$$

Worked out further,

$$\kappa^2 = \frac{e^2}{\varepsilon}\int_{-\infty}^{\infty} \rho(E)\frac{df_{FD}(E - E_F)}{dE_F} dE , \tag{5.12}$$

where $f_{FD}(x) = [1 + \exp(x/k_B T)]^{-1}$ is the Fermi-Dirac distribution function. The solution of Eq. (5.10) is written (Economou, 1979, Sec. 1.2)

$$V(\mathbf{r}) = -\int K(\mathbf{r} - \mathbf{r}')N_D(\mathbf{r}')d\mathbf{r}' \tag{5.13}$$

with

$$K(\mathbf{r}) = \frac{e^2}{4\pi\varepsilon r}\exp(-\kappa r) . \tag{5.14}$$

A configuration of N impurities (single positive charges in n-type material) at positions $\{\mathbf{r}_i\}$, for which $N_D(\mathbf{r}) = \sum_{i=1}^{N}\delta(\mathbf{r} - \mathbf{r}_i)$, causes a potential $V(\mathbf{r}, \{\mathbf{r}_i\}) = \sum_{i=1}^{N}K(\mathbf{r} - \mathbf{r}_i)$ which is of the form (5.6). Although Eq. (5.12) reveals that κ has to be solved self-consistently, this self-consistent procedure is shown (Van Mieghem *et al.* 1991) to be needlessly sophisticated compared to the approximations already made. Due to lattice vibrations (for $T > 0$ K), the impurity positions are perturbed from their fixed zero-temperature equilibrium positions $\{\mathbf{r}_i\}$. This introduces a supplementary temperature dependence of the tailed DOS, which can be included in Eq. (5.13) if the position distribution function $w(\mathbf{r}, T)$ is known, yielding $N_D(\mathbf{r}) = \sum_{i=1}^{N} w(\mathbf{r} - \mathbf{r}_i, T)$. In the following, these lattice vibrations are neglected. When we investigate many-body effects, only the zero-temperature case is treated because temperature effects complicate both ion-electron interactions (phonons) and electron-electron interactions[6] considerably.

Despite the fact that all quantities in Eq. (5.1) are calculated, complications due to the divergence of Eq. (5.7) using (5.14) arise. Indeed, all semi-invariants [Eq. (A8)] of order $m > 2$ diverge, due to the $1/r$ dependence of the potential (5.14). However, Kane argued that one should use an $1/(r + r_0)$ dependence (for which all semi-invariants rapidly converge) because, first, an electron can never approach the impurity nucleus arbitrarily close ($r \to 0$) and, second, the semiclassical theory is not valid for deep energy tails. The influence range of the potential should be limited to a certain r_0. Thus the semiclassical Kane formula (5.15) is limited by divergences to the first two semi-invariants. In view of Eq. (A7), this means that Eq. (5.15) can only be used in the high-density limit. The Kane expression, which is clearly a high-density-limit asymptotic form [see also Eq. (8.49)] reads

$$\rho_n(E) = \frac{m^{3/2}}{\pi^{5/2}\hbar^3 \cdot \sigma_n}\int_{-\infty}^{E} \sqrt{E - V} \times \exp\left[-\left[\frac{V}{\sqrt{2}\sigma_n}\right]^2\right] dV , \tag{5.15}$$

where

$$\sigma_n = \frac{e^2}{\varepsilon}\sqrt{n/8\pi\kappa_n} ,$$

$$\kappa_n = \left[\frac{m^{3/2}e^2}{2\sqrt{2}\pi^2\hbar^3 k_B T\varepsilon}\int_0^{\infty}\sqrt{E}\,\mathrm{sech}^2\left[\frac{E - E_{F_{0n}}}{2k_B T}\right] dE\right]^{1/2} \tag{5.16}$$

It can also be written, as suggested by Kane, in terms of a function $y(x)$ (Fig. 8),

$$\rho(E) = \frac{(2m)^{3/2}}{2\pi^2\hbar^3}(\sqrt{2}\sigma_n)^{1/2} y\left[\frac{E}{\sqrt{2}\sigma_n}\right] \tag{5.17}$$

and

$$y(x) = \frac{1}{\sqrt{\pi}}\int_{-\infty}^{x}\sqrt{x - \xi}\exp(-\xi^2)d\xi . \tag{5.18a}$$

This function can be written in terms of the parabolic cylinder function $D_{-a-1/2}(z)$, which offers useful

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[6] To the best of the author's knowledge, there exists no rigorous calculation of the temperature-dependent band-gap-narrowing problem.

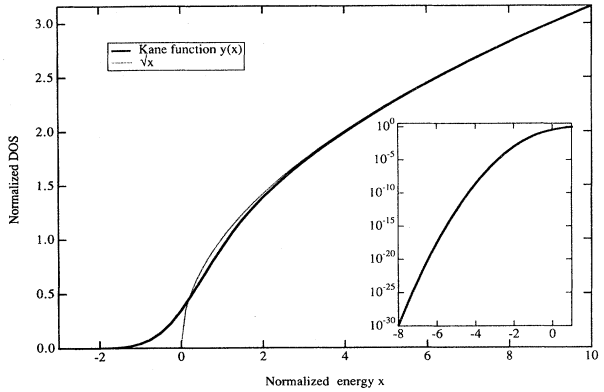

FIG. 8. The Kane function $y(x)$ and $\sqrt{x}$. The asymptotic properties of $y(x)$ are

$$y(x)\sim\sqrt{x}\,,\quad x\gg 0\,,$$

$$y(x)\sim\exp(-x^2),\quad x\ll 0\,,$$

and

$$y(0)=\frac{1}{2\sqrt{\pi}}\Gamma(\tfrac{3}{4})=0.345\,683\,6\,,$$

$$Y(0)=\int_{-\infty}^{0} y(x)dx=\frac{1}{12\sqrt{\pi}}\Gamma(\tfrac{1}{4})=0.170\,460\,9\,.$$

The axis annotation of the inserted graph is identical to that of the large plot.

mathematical relations (Abramowitz, 1968 and Sec. VIII.D),

$$D_{-a-1/2}(z)=\frac{1}{\Gamma(1/2+a)}\exp\left[-\frac{z^2}{4}\right]\times\int_0^{\infty}\exp\left[-\frac{s^2}{2}-zs\right]s^{a-1/2}ds$$

as

$$y(x)=2^{-5/4}\exp\left[-\frac{x^2}{2}\right]D_{-3/2}(-\sqrt{2}x)\,. \tag{5.18b}$$

Finally, we should like to mention that Eq. (5.15) can also be obtained by Green's-function diagram techniques (Efros, 1971).

D. The interacting Fermi liquid in three dimensions

The calculation will be demonstrated for the simplest expression of the self-energy. We confine ourselves to exchange effects because they dominate in the high-density limit. We neglect the influence of correlation and describe the exchange effect by the simple Hartree model at $T=0$ K (Ashcroft and Mermin, 1981, p. 334),

$$\hbar\Sigma(\mathbf{k})=-\frac{e^2}{2\pi^2\varepsilon}k_F F\left[\frac{|\mathbf{k}|}{k_F}\right] \tag{5.19}$$

where

$$F(x)=\frac{1}{2}+\frac{1-x^2}{4x}\ln\left|\frac{1+x}{1-x}\right|\,. \tag{5.20}$$

Further, we choose the Thomas-Fermi dielectric function (Mahan, 1986),

$$\varepsilon(q)=1+\frac{\kappa^2}{q^2}\,, \tag{5.21}$$

yielding for Eq. (5.8) the screened potential (5.14). At this point, we have the same problem as for a noninteracting system, namely, that Eq. (5.7) diverges for the screened Coulomb potential (5.11) because all semi-invariants (A8) of order higher than 2 diverge. Restricting ourselves to the high-density limit, however, we find that $P(V)$ reduces to a Gaussian (A7) which requires only the knowledge of κ. We still have to determine the *interacting* inverse screening length κ_i (at $T=0$ K). If the $E(k)$ relation is isotropic, the number of carriers at zero temperature equals

$$n_{\mathrm{el}}=\frac{1}{3\pi^2}k_F^3\,. \tag{5.22}$$

Plugging the Hartree 3D expression for the exchange (5.19) into Eq. (5.9), we find, since $F(1)=0.5$,

$$E_F=\frac{\hbar^2}{2m}k_F^2-\frac{e^2}{4\pi^2\varepsilon}k_F\,.$$

Solving this equation for k_F results in

$$k_F=\frac{1}{\pi a_B}+\left[\left[\frac{1}{\pi a_B}\right]^2+\frac{2\hbar^2}{m}E_F\right]^{1/2}\,. \tag{5.23}$$

Substituting Eq. (5.23) into (5.22) and using (5.12) not self-consistently, we find the zero-temperature inverse screening length for the interacting system,

$$\kappa_i=\frac{2k_F}{\sqrt{\pi a_B k_1-1}}\,. \tag{5.24}$$

Finally, we can compute (5.5a) combining Eqs. (A7) and (5.9) with (5.19) as

$$\rho_{3i}(E)=\frac{k_F^3}{\pi^2\sqrt{2\pi}\sigma_i}\int_0^{\infty}dx\,x^2\exp\left[-\frac{1}{2}\left[\frac{E}{\sigma_i}-\sqrt{\kappa_i/8\pi n}\,k_F[k_F a_B x^2-\frac{4}{\pi}F(x)]\right]^2\right]\,, \tag{5.25}$$

where the root mean square of the potential fluctuation energy in the interacting system σ_{3i} reads

$$\sigma_i = \frac{e^2}{\varepsilon}\sqrt{n/8\pi\kappa_i} \ .$$

Although it looks impressive, Eq. (5.25) is actually a relatively simple, closed analytical expression that includes many-body interactions through the function $F(x)$ [Eq. (5.20)] and statistical effects through Eq. (A7). A comparison of Eq. (5.25) with the noninteracting DOS and free-electron DOS, drawn in Fig. 9, shows the supplementary downward Fermi-level shift due to the Hartree-Fock electron exchange energy, $\Delta E_{\mathrm{ex}} = (3e^2/16\pi^2\varepsilon)k_F$. In addition to the low-energy band tail, a strong nonparabolic behavior around the Fermi level is observed. At high energies, all DOS functions tend to the free-electron DOS.

E. Discussion

The derivation above shows the importance of the inverse screening length as a link between the electron medium and the impurity that introduces the potential fluctuation. One could ask if there exist methodologies that rigorously describe both many-body interactions and statistical effects. Apart from the semiclassical approach, Serre *et al.* (1981) suggested a numerical approach. Their method consists in calculating the DOS in a sufficiently large number of subvolumes, each containing a particular impurity concentration N, yielding $\rho_N(E)$. Secondly, a distribution function $P(N)$ for the probability of having a local concentration N is derived, given the mean value N_{av} of N. By averaging the sets of $\rho_N(E)$ with $P(N)$, one finds the average DOS. Serre *et al.* (1981) assumed a Poisson distribution for $P(N)$ and included only electron-impurity contributions. Since this method is actually a straightforward numerical execution of the definition "averaging over impurity fluctuations," no special physical understanding is gained. Moreover, the calculated band tail strongly depends on the assumed probability distribution. As far as we know, there does not exist a more accurate analytical description including many-body effects than the semiclassical model.

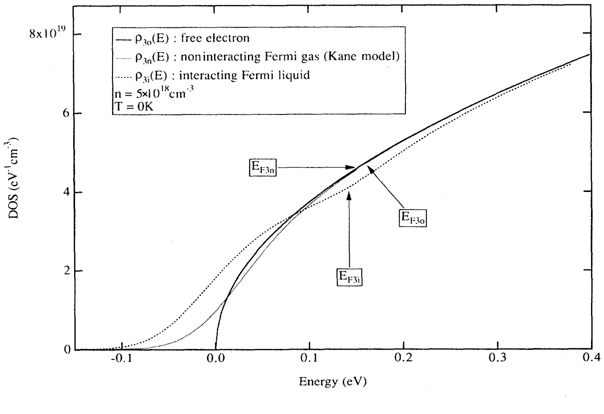

FIG. 9. A comparison between the DOS and the corresponding Fermi levels for the unperturbed [$\rho_{30}(E)$: free electron], the noninteracting [$\rho_{3n}(E)$: Kane DOS] and the interacting [$\rho_{3i}(E)$] electron systems for $n = 5\times10^{18}$ cm^{-3} in GaAs. The Hartree exchange shift equals $\Delta E_{\mathrm{ex}} = 13.8$ meV and agrees with $E_{F3n} - E_{3Fi}$.

The semiclassical approach yields a simple expression for the estimation of the equivalent band-gap narrowing due to band tailing in noninteracting systems (Van Mieghem *et al.*, 1991):

$$\Delta E_F \approx \frac{e^2}{\varepsilon k^2}\frac{1}{\sqrt{\pi}}\int_0^\infty dt \int_0^{\sqrt{2}\sigma t} \rho_0(u)du \exp(-t^2) \ . \quad (5.26)$$

Equation (5.26) is calculated for GaAs in 3D and shown in Fig. 10. Values of band-gap narrowing in the literature (Abram, Rees, and Wilson, 1978) indicate that the maximum Fermi-level shift due to band tailing (at $T = 0$ K) equals approximately one seventh of the band-gap narrowing due to many-body interactions. Usually the band-tail effect is neglected because its impact is smaller than that of band-gap narrowing. However, the majority carrier band tailing in heavily doped devices (Van Mieghem *et al.*, 1992) is too significant to neglect. In addition, Arnaudov *et al.* (1977) have demonstrated the necessity of considering band tailing in the analysis of the Burstein-Moss effect. In GaAs heavily doped with tellurium, they found experimentally an effective narrowing of the band gap nicely agreeing with Eq. (5.26) and due to Gaussian impurity fluctuations. In the high-density limit where the theory is valid, band-gap narrowing due to band tailing barely depends on temperature, a feature that seems to characterize the total energy shift due to heavy-doping effects (Abram *et al.*, 1978). Estimations of the band-tailing effect in InSb$_x$As$_{1-x}$, which exhibits a strong nonparabolicity, are discussed in Dobbelaere *et al.* (1991).

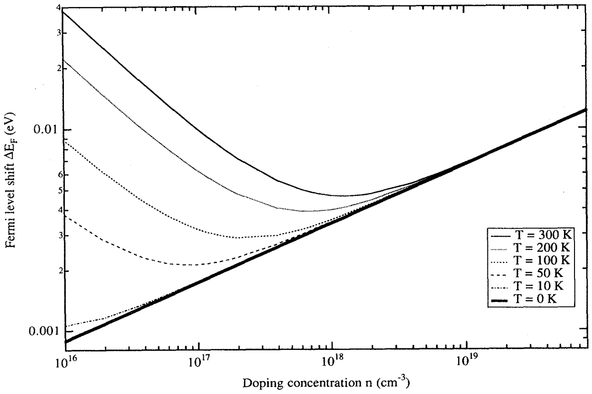

FIG. 10. The ΔE_{F3} in GaAs vs doping concentration for different temperatures. It should be stressed that ΔE_{F3} is only valid at the high-density region ($n_3 > a_B^{-3}$), as clearly demonstrated by extrapolations to low-doping regions.

VI. THE WAVE-MECHANICAL MODEL OF HALPERIN AND LAX

The inability of the previous semiclassical method to describe deep tail states forces us to use a quantum-mechanical picture. The most famous model, based on quantum-mechanical principles, was given by Halperin and Lax (1966). Since then, a variety of other models have been derived, which differ more in mathematical ingenuity than in physical relevance.

A. Principle of the minimum counting method

The crucial assumption in this model is the following ansatz: *At any given energy E in the low-energy tail a particular shape of the potential fluctuation is assumed that is most likely (or least unlikely) to produce a bound state of the required energy (and consequently one particular shape for the wave function); large deviations from this shape are very unlikely to occur.* Thus whenever an eigenstate $|j\rangle$ has energy $E_j \approx E$, we find

$$\Psi_j(\mathbf{x}) \approx f(\mathbf{x}-\mathbf{x}_j) , \tag{6.1}$$

where f is a fixed function (for each given E) and $\mathbf{x}_j$ is a position variable that may be anywhere in the system and will be different for each eigenstate. The reasoning behind this assumption is the following: potential fluctuations much wider in space than the optimal size are unlikely, because it is more improbable to have a potential fluctuation of given magnitude over a large region than over a small one. Potential fluctuations much narrower than the ideal one become unlikely because it is then difficult to overcome the large kinetic energy resulting from the localization of the wave function.

For the present, let us assume that the function f is known. [It is no restriction to choose f to be real and properly normalized and to require that f reach its maximum when its argument is zero.] If we use the function $f(\mathbf{x}-\mathbf{y})$, with $\mathbf{y}$ a free parameter, in a variational estimate of the energy E_j, we find

$$E(y) = \langle f(\mathbf{x}-\mathbf{y})|H|f(\mathbf{x}-\mathbf{y})\rangle , \tag{6.2}$$

where the one-electron Hamiltonian is $H = T + V(\mathbf{x})$ such that Eq. (6.2) can be written as the sum of two terms:

$$E(\mathbf{y}) = \theta + V_s(\mathbf{y}) , \tag{6.3}$$

where

$$\theta = -\int f(\mathbf{x}-\mathbf{y}) \frac{\hbar^2\nabla^2}{2m} f(\mathbf{x}-\mathbf{y}) d^3x , \tag{6.4}$$

$$V_s(\mathbf{y}) = \int f(\mathbf{x}-\mathbf{y})^2 V(\mathbf{x}) d^3x . \tag{6.5}$$

The kinetic energy θ is independent of the choice of $\mathbf{y}$ because the operator T is translationally invariant ($\nabla_{\mathbf{x}} = \nabla_{\mathbf{x}+\mathbf{z}}$ for each constant vector $\mathbf{z}$). On the other hand, the potential energy $V_s(\mathbf{y})$ is an average of the potential $V(\mathbf{x})$ in a region about $\mathbf{x}=\mathbf{y}$ (see Fig. 2). When we vary $\mathbf{y}$ throughout the system, $V_s(y)$ will fluctuate about the average potential V_{av} of the system and at various places in the crystal $V_s(\mathbf{y})$ will exhibit an unusually large negative fluctuation. These places correspond to regions of very low $V(\mathbf{x})$, and hence to places where we expect to find a low-energy eigenstate $\Psi_j(\mathbf{x})$. Since a variational estimate of the ground-state energy of a system always overestimates this energy, we expect that in a region of negative potential fluctuation

$$E(\mathbf{y}) \geq E_j ,$$

where E_j denotes the true energy of the local low-energy eigenstate. Consequently the best estimate of E_j is obtained by choosing $\mathbf{y}$ so that $E(\mathbf{y})$ is a local minimum. Even though $E(\mathbf{y})|_{\min}$ may be considerably greater than E_j, in general, we expect $E(\mathbf{y})$ to be a good approximation to E_j if the assumption (6.1) holds.

This physical reasoning establishes a close correspondence between local minima in $E(\mathbf{y})$ and the true energy eigenstates in the vicinity of E; hence the number of these eigenstates with energy E is approximately equal to the number of local minima in $E(y)$ with value E, or

$$\rho(E) \approx n_f(E) , \tag{6.6}$$

where $n_f(E)dE$ is the number of local minima in $E(\mathbf{y})$ per unit volume [or equivalently, as shown by Halperin and Lax, the number of points where $\nabla E(\mathbf{y})=0$, in short notation $\{\nabla E(\mathbf{y}_j)=0\}$] such that at the minimum $E \leq E(\mathbf{y}) \leq E + dE$.

Due to the variational principle and regardless of the choice of f, the energies of all the eigenstates in the low-energy tail are overestimated, such that $n_f(E)$ underestimates the true DOS $\rho(E)$. Clearly, the best choice of f, for any given energy E, is that which maximizes $n_f(E)$. Now, Eq. (6.6) may be written as

$$n_f(E) = \frac{1}{V_0} \int_{V_0} d\mathbf{y} \left\langle \sum_j^{\{\nabla E(\mathbf{y}_i)=0\}} \delta(\mathbf{y}-\mathbf{y}_j)\delta(E-E(\mathbf{y})) \right\rangle \tag{6.7}$$

When the indicated average over all potential configurations has been taken, the quantity between $\langle \cdots \rangle$ becomes independent of $\mathbf{y}$, and the $\mathbf{y}$ integration merely yields a factor of V_0. Since $\nabla E(\mathbf{y}) = \nabla V_s(\mathbf{y})$, we may write

$$n_f(E) = \left\langle \delta(E-E(\mathbf{y})) \sum_j^{\{\nabla V_s(\mathbf{y}_i)=0\}} \delta(\mathbf{y}-\mathbf{y}_j) \right\rangle . \tag{6.8}$$

A change of the variable $\mathbf{y}$ to the variable $\nabla V_s(\mathbf{y})$, according to the transformation properties of the Dirac delta function, gives

$$n_f(E) = \langle \delta(E-\theta-V_s(\mathbf{y}))\delta(\nabla V_s(\mathbf{y}))|\det\nabla\nabla V_s(\mathbf{y})| \rangle , \tag{6.9}$$

where $|\det\nabla\nabla V_s(\mathbf{y})|)$ arises as the Jacobian of the transformation. In what follows, the absolute values will be dropped, since almost all the critical points $\mathbf{y}_j$ have positive second derivatives; the probability of having another kind of extremum close to a local minimum is quite negligible in the low-energy region.

Notice that Eq. (6.9) may also be interpreted as

$$n_f(E)=P(E-\theta)\cdot p(0|E-\theta)\cdot\chi(E-\theta,0)\ , \tag{6.10}$$

where $P(\lambda)$ is the probability density for $V_s(\mathbf{y})$ to take on the value λ at an arbitrary point $\mathbf{y}$; $p(\Lambda|\lambda)$ is the conditional probability density for $\nabla V_s(y)$ to take on the value Λ when it is specified that $V_s(\mathbf{y})=\lambda$; and $\chi(\lambda,\Lambda)$ is the conditional expectation value of $\det\nabla\nabla V_s(\mathbf{y})$ when it is specified that both $V_s(\mathbf{y})=\lambda$ and $\nabla V_s(\mathbf{y})=\Lambda$. A crude estimate of $p'=p(0|E-\theta)\cdot\chi(E-\theta,0)$ is L^{-3}, where L is the average distance between local minima of V_s and linked to a characteristic correlation range for the smoothed potential V_s. In fact, p' is somewhat larger than this, essentially because it is more likely for $V_s(\mathbf{y})$ to have an unusually large negative excursion if $\mathbf{y}$ is close to a local minimum than if it is far from the nearest local minimum. Nonetheless, p' is a relatively slowly varying function of the wave function f and energy E. In contrast, P is a rapidly varying function of E in the low-energy tail and will be quite sensitive to the choice of f, since at sufficiently high doping concentration the random variable $V_s(\mathbf{y})$ obeys Gaussian statistics, which constitutes an exponential behavior of its arguments. Thus, in practice, maximizing $n_f(E)$ with respect to f is equivalent to maximizing P, and the rapid variation of the DOS in the tail will be dominated by P.

In order to proceed further, we must characterize the potential $V(x)$. Generally, $V(\mathbf{x})$ is the sum of the individual impurity potentials,

$$V(\mathbf{x})=\int v_b(\mathbf{x}-\mathbf{z})n_b(\mathbf{z})d\mathbf{z}\ , \tag{6.11}$$

where b denotes the type of impurity, $v_b(\mathbf{x}-\mathbf{z})$ is the potential at $\mathbf{x}$ resulting from a b-type impurity at $\mathbf{z}$, and $n_b(\mathbf{z})$ is the density of impurities at point $\mathbf{z}$. Since the impurity positions are usually not known, $n_b(\mathbf{z})$ is replaced by its average n. Neglecting the explicit dependence on impurity type, the autocorrelation functions $\langle V(\mathbf{x})V(\mathbf{x}')\rangle$ and $\langle V_s(\mathbf{y})V_s(\mathbf{y}')\rangle$ are then defined as

$$\langle V(\mathbf{x})V(\mathbf{x}')\rangle=W(\mathbf{x}-\mathbf{x}')=n\int v(\mathbf{x}-\mathbf{z})v(\mathbf{x}'-\mathbf{z})d\mathbf{z} \tag{6.12}$$

and

$$\langle V_s(\mathbf{y})V_s(\mathbf{y}')\rangle=G(\mathbf{y}-\mathbf{y}')=\int f^2(\mathbf{x}-\mathbf{y})f^2(\mathbf{x}'-\mathbf{y}')W(\mathbf{x}-\mathbf{x}')d\mathbf{x}\,d\mathbf{x}'\ . \tag{6.13}$$

The principles of Halperin and Lax's method have been outlined, and in the next section we confine ourselves to the important case of the high-density limit, for which an analytic form of $\rho(E)$ can be derived.

B. The high-density limit

From Eq. (6.5) and the assumed properties of f, one deduces that the impurities that contribute heavily to $V_s(\mathbf{y})$ are those which fall in a sphere about $\mathbf{y}$ whose radius is roughly the width of the wave function f. When the impurity concentration is high enough that there are many impurities in this region, the central-limit theorem indicates that Gaussian statistics apply (see Appendix A). The statistical properties of $V_s(\mathbf{y})$ in the Gaussian case are completely determined by the autocorrelation function $\langle V_s(\mathbf{y})V_s(\mathbf{y}')\rangle$, if we take $\langle V_s(\mathbf{y})\rangle=V_{\rm av}=0$ (Sec. IV.C),

$$P(\lambda)=\frac{1}{\sqrt{2\pi}\sigma}\exp\left[-\frac{\lambda^2}{2\sigma^2}\right] \tag{6.14}$$

with variance

$$\sigma^2=\langle V_s(\mathbf{y})^2\rangle=G(0)\ . \tag{6.15}$$

In order to determine $p(\Lambda|\lambda)$, we notice that

$$\langle V_s(\mathbf{y})\nabla V_s(\mathbf{y})\rangle=\nabla_{\mathbf{y}'}G(\mathbf{y}-\mathbf{y}')|_{\mathbf{y}=\mathbf{y}'}=0$$

because G is an even function and hence $\nabla G(0)=0$. But since Gaussian variables (of zero mean) are completely described by their second moments, uncorrelated variables [such as $V_s(\mathbf{y})$ and $\nabla V_s(\mathbf{y})$] are statistically independent. Thus the conditional distribution $p(\Lambda|\lambda)$ is independent of λ and reduces to the ordinary probability distribution of $\nabla V_s(\mathbf{y})$.

The covariances of the derivatives $\nabla V_s(\mathbf{y})$ among themselves are

$$\langle\nabla V_s(\mathbf{y})\nabla V_s(\mathbf{y})\rangle=\nabla_{\mathbf{y}}\nabla_{\mathbf{y}'}G(\mathbf{y}-\mathbf{y}')|_{\mathbf{y}=\mathbf{y}'}=-\nabla\nabla G(0)\ , \tag{6.16}$$

and the coordinate axes can always be chosen so as to diagonalize the matrix of second derivatives of G (i.e., the Hessian) with

$$\operatorname{diag}[-\nabla\nabla G(0)]=\operatorname{diag}[\sigma_1^2,\sigma_2^2,\sigma_3^2]\ , \tag{6.17}$$

and consequently the three components of $\nabla V_s(\mathbf{y})$ are uncoupled or uncorrelated, and $p(\Lambda|\lambda)$ is just the product of three Gaussians,

$$p(\Lambda|\lambda)=\frac{1}{(2\pi)^{3/2}\sigma_1\sigma_2\sigma_3}\times\exp\left[-\left[\frac{\Lambda_1}{\sqrt{2}\sigma_1}\right]^2-\left[\frac{\Lambda_2}{\sqrt{2}\sigma_2}\right]^2-\left[\frac{\Lambda_3}{\sqrt{2}\sigma_3}\right]^2\right]\ . \tag{6.18}$$

Finally, $\chi(\lambda,\Lambda)$ must be determined. Since the derivation is rather cumbersome and not very important, we merely give the exact result and refer the reader for the details to Halperin and Lax (1966):

$$\chi(E-\theta,0)=-(E-\theta)^3\left[\frac{\sigma_1\sigma_2\sigma_3}{\sigma^3}\right]^2\left[1-3\left[\frac{\sigma}{E-\theta}\right]^2\right] . \tag{6.19}$$

Combining Eqs. (6.14), (6.18), and (6.19), with (6.10), we have

$$n_{f3}(E)=(\theta-E)^3\left[\frac{\sigma_1\sigma_2\sigma_3}{(2\pi)^2\sigma^7}\right]\left[1-3\left[\frac{\sigma}{E-\theta}\right]^2\right] \times\exp\left[-\frac{(\theta-E)^2}{2\sigma^2}\right] , \tag{6.20}$$

while the one-dimensional expression can be derived analogously,

$$n_{f1}(E)=(\theta-E)\left[\frac{\sigma_1}{(2\pi)\sigma^3}\right]\exp\left[-\frac{(\theta-E)^2}{2\sigma^2}\right] . \tag{6.21}$$

As discussed above, the true DOS is best approximated by choosing f to maximize $n_f(E)$. Since the pre-exponential factor varies slowly with respect to f, we restrict the maximization of $n_f(E)$ to the minimization of the argument of the exponential, yielding $\min_f(\Gamma)$ where

$$\Gamma=\frac{(\theta-E)^2}{\sigma^2}=\frac{\left[E-\int f(\mathbf{x})Tf(\mathbf{x})d^3x\right]^2}{\int f^2(\mathbf{x})f^2(\mathbf{x}')W(\mathbf{x}-\mathbf{x}')d\mathbf{x}\,d\mathbf{x}'} . \tag{6.22}$$

In order to make this expression homogeneous in f, we multiply E by the normalization integral $\int f(\mathbf{x})^2d\mathbf{x}=1$, to obtain

$$\Gamma=\frac{\left[\int f(\mathbf{x})[Ef(\mathbf{x})-Tf(\mathbf{x})]d^3x\right]^2}{\int f^2(\mathbf{x})f^2(\mathbf{x}')W(\mathbf{x}-\mathbf{x}')d\mathbf{x}\,d\mathbf{x}'} . \tag{6.23}$$

It is now easily verified that putting $f(\mathbf{x})=\alpha g(\mathbf{x})$ does not alter Γ for any arbitrary constant α. Hence Γ may be minimized by fixing the denominator at an arbitrary value, say α, while minimizing the numerator,

$$\begin{aligned}&\min_f\left[I_1=\int f(\mathbf{x})[Ef(\mathbf{x})-Tf(\mathbf{x})]d^3x\right] ,\\&I_2=\int f^2(\mathbf{x})f^2(\mathbf{x}')W(\mathbf{x}-\mathbf{x}')d\mathbf{x}\,d\mathbf{x}'=\alpha .\end{aligned} \tag{6.24}$$

Introducing the Lagrange multiplier μ, we have to minimize the functional $F=I_1+\mu(I_2-\alpha)$ or

$$F=\int f(\mathbf{x})\left[Ef(\mathbf{x})-Tf(\mathbf{x})+\mu f(\mathbf{x})\int f^2(\mathbf{x}')W(\mathbf{x}-\mathbf{x}')d\mathbf{x}'\right]d^3x-\alpha\mu ,$$

which is clearly minimal with respect to f, if

$$Ef(\mathbf{x})-Tf(\mathbf{x})+\mu f(\mathbf{x})\int f^2(\mathbf{x}')W(\mathbf{x}-\mathbf{x}')d\mathbf{x}'=0 . \tag{6.25}$$

Condition (6.25) looks like the famous self-consistent Hartree equation; the only difference is that E is specified and that μ is considered as the eigenvalue to be found. Although it is physically obvious that there exists a minimum value for Eq. (6.22), it has not yet been proved that the solution f of Eq. (6.25) is unique.

Despite the lack of an analytical expression for f, we are able to represent the DOS as [see Eqs. (6.21) and (6.22)]

$$n_f(E)=A(E)\exp[-B(E)] , \tag{6.26}$$

where $B(E)=\Gamma_{\min}$. Furthermore, the kinetic energy θ of an eigenstate increases as the well depth increases or the ratio of θ to the total energy E, θ/E, decreases monotonically for energies deeper in the tail; hence $\Gamma/E^2=(\theta-E)^2/E^2$ decreases monotonically as $E\to-\infty$ for any fixed f. Now, let f_i be the best f at energy E_j. If $E_2<E_1$, then $B(E_2)\equiv\Gamma(f_2,E_2)\le\Gamma(f_1,E_2)$ and thus

$$\frac{B(E_2)}{E_2^2}\le\frac{\Gamma(f_1,E_2)}{E_2^2} .$$

Combined with the previous result for any fixed f, $\Gamma(f_1,E_2)/E_2^2\le\Gamma(f,E_1)/E_1^2$, this gives

$$\frac{\Gamma(f_1,E_2)}{E_2^2}\le\frac{\Gamma(f_1,E_1)}{E_1^2}\equiv\frac{B(E_1)}{E_1^2},$$

which means that $B(E)/E^2$ decreases monotonically as $E\to-\infty$. Consequently the DOS falls off less rapidly than a Gaussian, illustrating the failure of the semiclassical approach when $E\to-\infty$.

C. A comparison of the method with an exact result

As discussed in Sec. IV, the DOS of a particle in a "white-Gaussian-noise" potential in one dimension can be calculated exactly. In order to test the Halperin-Lax theory, we take [see Eq. (4.3)]

$$\langle V(x)V(x')\rangle=W(x-x')=\tfrac{1}{2}D\delta(x-x') . \tag{6.27}$$

Equation (6.25) reads

$$-\frac{\hbar^2}{2m}f'(x)-\frac{1}{2}\mu Df^3(x)=Ef(x) , \tag{6.28}$$

where $f(x)$ is subjected to the following boundary conditions:

$$\begin{aligned}&f(x)=f'(x)=0 \quad\text{for } x\to\infty ,\\&f'(0)=0 ,\\&\int_{-\infty}^{\infty}f(x)^2dx=1 .\end{aligned} \tag{6.29}$$

The solution can be expressed in analytical form,

$$f(x)=\sqrt{\beta/2}\,\mathrm{sech}\beta x\ , \tag{6.30}$$

$$\mu=\frac{4}{\xi D}\ , \tag{6.31}$$

where

$$\beta=\sqrt{-2mE/\hbar^2}\ . \tag{6.32}$$

In order to find the DOS (6.21), we need to calculate three parameters:

$$\sigma^2=\langle V_s(\mathbf{y})^2\rangle=\xi\int_{-\infty}^{\infty} f^4(x)dx=\frac{D\beta}{6}\ , \tag{6.33}$$

$$\sigma_1^2=\langle V_s'(\mathbf{y})^2\rangle=\xi\int_{-\infty}^{\infty}\left[\frac{d[f^2(x)]}{dx}\right]^2 dx=\frac{2D\beta^3}{15}\ , \tag{6.34}$$

$$\theta=-\frac{\hbar^2}{2m}\int_{-\infty}^{\infty} f(x)f'(x)dx=\frac{\beta^2\hbar^2}{6m}\ . \tag{6.35}$$

After putting these expressions into Eq. (6.21), we obtain

$$n_{f1}(E)=\frac{1}{\sqrt{5}}\frac{8E}{\pi D}\exp\left[-\frac{16}{3D}\sqrt{\hbar^2/2m}\,E^{3/2}\right]\ . \tag{6.36}$$

This result (6.36) differs only by a factor $\sqrt{5}$ from the exact asymptotic form (4.53), which shows a remarkably good agreement. By applying a sophisticated mathematical technique, based on functional integration, Zittartz and Langer (1966) showed that their method reproduces the exact asymptotic result in the case of a "white-Gaussian-noise" potential in one dimension. They demonstrate that the shape of the wave function itself must change with local changes in the shape of the potential fluctuation if the pre-exponential factor is to be determined exactly.

D. The DOS in heavily doped semiconductors

As shown in Sec. V, the impurity potential in heavily doped material is well described by a screened Coulomb potential (5.24): $v(\mathbf{x}-\mathbf{z})=K(\mathbf{x}-\mathbf{z})$. The autocorrelation function then reads

$$\langle V(\mathbf{x})V(\mathbf{x}')\rangle=W(\mathbf{x}-\mathbf{x}')=\xi e^{-\kappa|\mathbf{x}-\mathbf{x}'|}\ , \tag{6.37}$$

where

$$\xi=n\frac{2\pi}{\kappa}\left[\frac{e^2}{4\pi\varepsilon}\right]^2=\sigma_n^2\ . \tag{6.38}$$

The use of a screened Coulomb potential is justified in weakly compensated materials. If the compensation ratio increases, the superposition of $K(\mathbf{r})$ functions is not valid and we enter the region of "nonlinear" screening.[7]

The differential equation (6.25) can only be solved numerically. By dimensional arguments and Eq. (6.26), $n_f(E)$ must have the form

$$n_f(E)=\frac{E_\kappa^3\kappa^3}{\xi^2}a(\nu)\exp\left[-\frac{E_\kappa^2}{2\xi}b(\nu)\right]\ , \tag{6.39}$$

where

$$E_\kappa=\frac{\hbar^2\kappa^2}{2m} \tag{6.40}$$

and

$$\nu=(-E)/E_\kappa>0 \tag{6.41}$$

and $a(\nu)$ and $b(\nu)$ are dimensionless functions.

The results [e.g., $a(\nu)$ and $b(\nu)$] are given in table form in Halperin and Lax (1966) and are therefore less convenient than analytic forms. It is interesting to note that $d\log b(\nu)/d\log(\nu)$ varies smoothly from $\frac{1}{2}$ to 2 as ν increases. The validity regions for $\rho(E)$ are also discussed and various inequalities are given, but the main conclusions is that, deep enough in the tail, the use of minimum counting methods should be quite valid. On the other hand, if E is too far into the low-energy tail, Gaussian statistics are certainly not valid and Eq. (6.39) will be incorrect. This complicates calculations substantially.

Analytical approximate expressions for $a(\nu)$ and $b(\nu)$ are proposed by Chaiyasith, Kokpol, and Sa-yakanit (1983). They have improved the method of Eymard and Duraffourg (1973) by choosing a more appropriate trial wave function in the potential fluctuation, which optimizes $b(\nu)$.

VII. THE OPTIMAL-FLUCTUATION METHOD

The interesting feature of the optimal-fluctuation method is its ability to estimate the range of applicability of Gaussian statistics and to yield results deep in the low-energy tail where Gaussian statistics are valid. As a drawback, the optimal-fluctuation method does not permit the evaluation of the pre-exponential factor in the DOS, although it suffices to determine the leading term in the exponential, i.e., $\ln[\rho(E)/\rho(0)]$ or $E_\kappa^2/2\xi\, b(\nu)$ in Eq. (6.39). In practice, however, just this quantity is measured.

A. Outline of the method

The idea of the method, which is closely related to that of Halperin and Lax, is as follows. The characteristic size of the wave function is supposed to greatly exceed the average separation between impurities in a fluctuation. Quantum-mechanical averaging then smears out the discrete impurity charge, and the fluctuation varies as a smooth function of coordinates $z(\mathbf{r})$, which represents the deviation of the impurity concentration $n(\mathbf{r})$ from its average value n. The determination of the DOS requires

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[7] For compensated materials, the fluctuations of the impurity density are no longer small compared to the Fermi level. Hence the Thomas-Fermi approximation does not apply. The resulting Poisson equation is clearly nonlinear (see Sec. V).

a summation over the contributions of all impurity configurations that contain an electron state of energy E. In the low-energy tail, these configurations have vanishingly small probabilities, and the sum is dominated by the most probable configuration. Let a probability of a fluctuation $z(\mathbf{r})$ be written as $\exp(-\Omega\{z\})$. If z_E^* is the most probable fluctuation among those which contribute to energy level E, then we can expect that, as E increases, the DOS will fall off as $\exp(-\Omega\{z_E^*\})$. In seeking z_E^*, it is assumed sufficient to consider only those fluctuations in which E is the lowest energy level, since the probability of a fluctuation in which this level corresponds to an excited state is certainly lower. In what follows, we consider only uncorrelated impurity distributions. Ideas concerning correlated impurity distributions can be found in the work of Efros (Schlovskii and Efros, 1984, part 2).

B. The fundamental equations

In order to find the probability of a fluctuation $z(\mathbf{r})$, we consider a volume element ΔV_0 small enough that we may regard the impurity concentration within ΔV_0 as constant, but still containing a large number of impurities, $N \equiv n(\mathbf{r})\cdot\Delta V_0 \gg 1$. To count the number of states, we assume that the impurities can be located only at the lattice sites, whose concentration p is large, $p \gg n(\mathbf{r})$. The number of sites in the volume, $P = p\Delta V_0$, can accommodate N impurities in $\Gamma_{\Delta V_0}$ different ways, where

$$\Gamma_{\Delta V_0} = \frac{P!}{N!(P-N)!} . \tag{7.1}$$

The entropy in the volume ΔV_0 is given by

$$S_{\Delta V_0} \equiv \ln(\Gamma_{\Delta V_0}) . \tag{7.2}$$

Invoking Stirling's asymptotic formula for large x, $\ln x! \approx x \ln x - x$, and the fact that $P \gg N$, we find

$$\begin{aligned} S_{\Delta V_0} &\approx P \ln P - N \ln N - (P-N)\ln(P-N) \\ &\approx N \ln P - N \ln N + (P-N)\{N/P + o(N/P)\} \\ &\approx N \ln \frac{Pe}{N} . \end{aligned} \tag{7.3}$$

The entropy density is defined by

$$\sigma(\mathbf{r}) \equiv \frac{S_{\Delta V_0}}{\Delta V_0} = n(\mathbf{r}) \ln \frac{pe}{n(\mathbf{r})} . \tag{7.4}$$

Finally, the total entropy of the crystal volume is given by

$$S = \int_{V_0} d^3r\, \sigma(\mathbf{r}) . \tag{7.5}$$

Let us find the entropy of a fluctuation $z(\mathbf{r})$ in a volume V which constitutes a minor fraction of V_0, while in the rest of the volume one has $z(\mathbf{r}) \ll n$. From the conservation of the particle number, $\int_{V_0} d^3r\, z(\mathbf{r}) = 0$, we obtain

$$\int_{V_0 - V} d^3r\, z(\mathbf{r}) = -\int_V d^3r\, z(\mathbf{r}) . \tag{7.6}$$

The entropy of such a fluctuation is

$$S = \int_{V_0 - V} d^3r\, \sigma(\mathbf{r}) + \int_V d^3r\, \sigma(\mathbf{r}) . \tag{7.7}$$

Since we have measured $z(\mathbf{r}) \ll n$ in the volume $V_0 - V$, we can expand $\sigma(\mathbf{r}) = f[n(\mathbf{r})]$ as $f[n(\mathbf{r})] = f[n + z(\mathbf{r})] \approx f[n] + f'[n]\cdot z(\mathbf{r})$, so that Eq. (7.7) becomes

$$\begin{aligned} S = &\int_V d^3r (n + z(\mathbf{r})) \ln \frac{pe}{n + z(\mathbf{r})} + (V_0 - V) n \ln \frac{pe}{n} \\ &+ f'[n] \int_{V_0 - V} d^3r\, z(\mathbf{r}) . \end{aligned} \tag{7.8}$$

Transforming Eq. (7.8) with (7.6), we obtain the additional entropy, compared to that of a uniform impurity distribution $S_{\mathrm{av}} = V_0 \ln(pe/n)$,

$$S - S_{\mathrm{av}} = \int_V d^3r \left\{ [n + z(\mathbf{r})] \ln \frac{n}{n + z(\mathbf{r})} + z(\mathbf{r}) \right\} < 0 . \tag{7.9}$$

If $z(\mathbf{r})$ decreases fast enough so that the integral (7.9) converges, the integration can be extended to infinity. The probability that some part of the volume will exhibit a fluctuation $z(\mathbf{r})$ is given by $\exp(-\Omega\{z\})$, where

$$\Omega\{z\} = -\int d^3r \left\{ [n + z(\mathbf{r})] \ln \frac{n}{n + z(\mathbf{r})} + z(\mathbf{r}) \right\} . \tag{7.10}$$

The ground-state energy $\lambda_0\{z\}$ of an electron at $\mathbf{r}$ with a potential energy $V(\mathbf{r},\{z\})$ is determined by the Schrödinger equation

$$-\frac{\hbar^2}{2m} \nabla^2 \Psi + V(\mathbf{r},\{z\}) \Psi = \lambda_0\{z\} \Psi . \tag{7.11}$$

Assuming linear screening, as in Sec. V, we obtain with Eq. (5.13)

$$V(\mathbf{r},\{z\}) = -\int \mathbf{K}(\mathbf{r} - \mathbf{r}') z(\mathbf{r}') d\mathbf{r}' . \tag{7.12}$$

The optimum fluctuation must minimize $\Omega\{z\}$, subject to the condition $\lambda_0\{z\} = -E$. Introducing the Lagrange multiplier μ, we must minimize the functional $F\{z\} = \Omega\{z\} + \mu(\lambda_0\{z\} + E)$. Varying $\Omega\{z\}$ and λ_0 [in Eq. (7.11)] we obtain, after a straightforward calculation,

$$\begin{aligned} \delta\Omega\{z\} &= \int d^3r \ln \frac{n + z(\mathbf{r})}{n} \delta z(\mathbf{r}) , \\ \delta\lambda_0\{z\} &= \int d^3r\, |\Psi|^2 \frac{\partial V(\mathbf{r},\{z\})}{\partial z} \delta z(\mathbf{r}) , \end{aligned} \tag{7.13}$$

and since $\delta F = \delta\Omega\{z\} + \mu\delta\lambda_0\{z\} = 0$, we finally obtain

$$\ln \frac{n + z(\mathbf{r})}{n} - \mu \int d^3r' |\Psi(\mathbf{r}')|^2 K(\mathbf{r} - \mathbf{r}') = 0 , \tag{7.14}$$

or, rewritten,

$$z(\mathbf{r}) = n(e^{\chi(\mathbf{r})} - 1) \tag{7.15}$$

where

$$\chi(\mathbf{r})=\frac{\mu e^2}{4\pi\epsilon}\int d^3\mathbf{r}'\frac{|\Psi(\mathbf{r}')|^2}{|\mathbf{r}-\mathbf{r}'|}e^{-\kappa|\mathbf{r}-\mathbf{r}'|} . \qquad (7.16)$$

Together with Eq. (7.11), Eq. (7.14) determines the optimal fluctuation $z^*(\mathbf{r})$. The leading term in the logarithm of the DOS then reads

$$\ln\left[\frac{\rho(E)}{\rho(0)}\right]=-\Omega\{z^*\} . \qquad (7.17)$$

C. The high-density limit: Gaussian statistics

The assumption of Gaussian statistics implies (see Appendix A) that $z(\mathbf{r})\ll n$ and $n\gg 1$. In this case, Eq. (7.10) reduces to

$$\Omega\{z\}=\frac{1}{2n}\int d^3r\, z^2(\mathbf{r}) , \qquad (7.18)$$

while (7.14) simplifies to

$$z(\mathbf{r})=\mu n\int d^3r'|\Psi(\mathbf{r}')|^2K(\mathbf{r}-\mathbf{r}') . \qquad (7.19)$$

It is interesting to note that Eq. (7.18) is more elegantly derived from a characteristic functional, as is elucidated by Feynman and Hibbs (1965). Combining Eq. (7.19) with (7.12), we find that Eq. (7.11) becomes

$$-\frac{\hbar^2}{2m}\nabla^2\Psi-\mu\Psi\int d^3r'|\Psi(\mathbf{r}')|^2W(\mathbf{r}-\mathbf{r}')=\lambda_0\{z\}\Psi , \qquad (7.20)$$

where

$$W(\mathbf{r}-\mathbf{r}')=n\int d\mathbf{r}''K(\mathbf{r}-\mathbf{r}'')K(\mathbf{r}''-\mathbf{r}') . \qquad (7.21)$$

Equation (7.20) exactly equals the fundamental equation (6.25) in the work of Halperin and Lax (1966), which also appears in the method of Zittartz and Langer (1966). In the particular case of a random system where only the ground-state energy is taken into account, Donsker and Varadhan (1975) derived an upper bound for Ψ which coincides with the lower bound. It leads to the nonlinear eigenvalue problem (7.20) [or (6.25)]. This remarkable result proves the exactness of Eq. (6.25).

D. DOS asymptotics ($E\to-\infty$)

As already mentioned above, very deep in the tail, Gaussian statistics are no longer valid. For these energies, one may intuitively argue that the situation resembles an ion-electron system. Consequently, one would expect Eq. (7.11) to possess a spherically symmetric solution, with a ground-state wave function of the form

$$\Psi(\mathbf{r})=\frac{1}{\sqrt{\pi}\,\lambda^{3/2}}e^{-r/\lambda} . \qquad (7.22)$$

In this picture, the fluctuation then represents an almost pointlike nucleus of an ion with the charge

$$Z=\int d^3r\, z(\mathbf{r}) , \qquad (7.23)$$

and the characteristic length of the exponential decay of $z(\mathbf{r})$ in Eq. (7.16) is small compared to the electron wavelength λ in the ground state. Since the ground-state energy must equal E, we have

$$E=Z^2E_0 , \qquad (7.24)$$

where

$$E_0=\frac{me^4}{2\hbar^2\varepsilon^2}\ \text{(the ground-state of the } H \text{ atom)} , \qquad (7.25)$$

$$\lambda=\frac{a}{Z}\text{the ground-state wavelength of the } H \text{ atom).} \qquad (7.26)$$

Following Efros, we now prove that this solution indeed satisfies Eqs. (7.11) and (7.15). Substituting Eq. (7.22) into (7.16) and expanding in terms of r/λ, we find the explicit form of $\chi(\mathbf{r})$ and $z(\mathbf{r})$:

$$\chi(\mathbf{r})=t-\frac{r^2}{x^2} \qquad (7.27)$$

where

$$t=\frac{\mu e^2}{4\pi\varepsilon\lambda}\quad\text{and } x^2=\frac{3\lambda^2}{2t} . \qquad (7.28)$$

The above assumption of a sharp decline of $z(\mathbf{r})$ at short distances is equivalent to $t\gg 1$. Consequently Eq. (7.15) may be written

$$z(\mathbf{r})=n[e^t\exp(-r^2/x^2)-1]\approx ne^t\exp(-r^2/x^2). \qquad (7.29)$$

Combining Eqs. (7.29), (7.24), and (7.23), we obtain a transcendental equation for t,

$$t=\ln\left[\left[\frac{2}{3\pi}\right]^{3/2}\left[\frac{E}{E_0}\right]^2\frac{t^{3/2}}{na^3}\right] , \qquad (7.30)$$

whence for sufficiently high energies we may deduce

$$t\approx\ln\left[\left[\frac{E}{E_0}\right]^2\frac{1}{na^3}\right]\gg 1 , \qquad (7.31)$$

which justifies the above approximation. Thus the described solution does, indeed, exist. To evaluate $\Omega\{z\}$, we note that $z(\mathbf{r})\gg n$ [see Eq. (7.29)] so that Eq. (7.10) simplifies to

$$\Omega\{z\}=\int z(\mathbf{r})\left[\ln\frac{z(\mathbf{r})}{n}-1\right]d^3r . \qquad (7.32)$$

Substituting Eq. (7.29), we readily obtain

$$\Omega\{z\}=Z(t-1)-\tfrac{3}{2}Z . \qquad (7.33)$$

However, this expression contains terms both of order Z

and of order Zt. A simple substitution of Eq. (7.24) would not correctly describe $\Omega\{z\}$, and corrections of Z to order t^{-1} must be included. The ground-state energy, corrected for the finite (not pointlike) nucleus size, reads (Bethe and Salpeter, 1957)

$$E=Z^2E_0\left[1-\frac{4}{3}\frac{\langle r^2\rangle}{\lambda^2}\right], \tag{7.34}$$

where

$$\langle r^2\rangle=\frac{1}{Z}\int z(\mathbf{r})r^2d^3r$$

Invoking Eq. (7.29), we obtain the corrected expression for Z,

$$Z=\sqrt{E/E_0}\left[1+\frac{3}{2t}\right]. \tag{7.35}$$

The corrections to Eq. (7.30) by using (7.34) instead of (7.24) are of order t^{-1} and can be neglected. Finally, employing (7.35) in (7.33), $\Omega\{z\}$ yields

$$\Omega\{z\}=\sqrt{E/E_0}(t-1), \tag{7.36}$$

which gives for the DOS, for very large negative energies E for which the effective-mass approach is applicable, clearly a non-Gaussian form,

$$\ln\left[\frac{\rho(E)}{\rho(0)}\right]=-\sqrt{E/E_0}\ln\left[\left[\frac{2}{3\pi}\right]^{3/2}\frac{t^{3/2}-e^{-1}}{na^3}\right], \tag{7.37}$$

where t follows from Eq. (7.30).

E. Very-deep-tail asymptotics: Lifshitz's conjecture

In this section, we present an ingenious intuitive method due to Lifshitz (1965) because it is related to the optimal-fluctuation method in some ways. Before summarizing Lifshitz's idea, we rescale the energy axis such that $\rho(E)=0$ for $E<0$. Hence the problem considered is "How does $\rho(E)$ behave as $E\to 0^+$?"

Electronic energy levels for arbitrary small energy can only come from states with wave functions localized in very large regions that are empty of impurities. Indeed, if the electronic wave function overlaps an impurity appreciably, there will be a finite potential energy of interaction, while a large region is necessary to make the kinetic energy very small. By the Poisson distribution law, the probability of a large region of volume V being free of impurities is proportional to $\exp(-nV)$. Since the volume V is very large, the low-lying levels for localized states will be insensitive to the exact conditions on the boundary ∂V of V, and we may take the wave function to be zero on ∂V. Now, clearly, the main contribution to the probability of finding a low-lying level E for the system will be proportional to the probability of finding a region V whose lowest level is E. As mentioned above, the probability of finding a region whose second level is E will be exponentially smaller because of the exponential dependence of the probability on V. Further, because of this same exponential dependence, the regions whose shape is such that V is smallest for a given lowest level will make the main contribution. Hence, by the isoperimetric theorem, this will mean spherical regions. The lowest level E in an empty spherical volume of radius R with boundary condition that the wave function vanishes on its surface is given by

$$E=\frac{\pi^2\hbar^2}{2mR^2}. \tag{7.38}$$

The probability of such a region existing is proportional to $\exp[-n(4\pi/3)R^3]$, so that the DOS of low-lying levels will be given by

$$\rho(E)\sim\exp\left[-\frac{c_0}{E^{3/2}}\right],\quad E\to 0, \tag{7.39}$$

where

$$c_0=\frac{4\pi}{3}\left[\frac{\pi^2\hbar^2}{2m}\right]^{3/2}n. \tag{7.40}$$

This conjecture (7.39) was put on a firmer mathematical basis by Friedberg and Luttinger (1975). Although their rigorous proof, departing from the general equation (5.7), is one of mathematical beauty, we give only the result,

$$\ln\frac{\rho(E)}{\rho(0)}=-(c_0E^{-3/2}+c_1E^{-1/2}+\cdots), \tag{7.41}$$

where

$$c_1=-\frac{\pi^2c}{a\lambda_0}\sqrt{\hbar^2/m} \tag{7.42}$$

and

$$a=\text{scattering length},$$

$$\lambda_0=\frac{1}{\sqrt{4\pi an}}, \tag{7.43}$$

$$c=\int_0^\infty dx[1-\sqrt{1-\exp(-x^2)}]\approx 0.628.$$

Equation (7.41) should be compared with (7.37) after rescaling the energy scales properly.

VIII. THE PATH-INTEGRAL METHOD

The famous path-integral approach to quantum mechanics was invented by R. P. Feynman and is very well described in his book (Feynman and Hibbs, 1965). For the description of disordered systems, the path-integral method was first introduced by Edwards (Abram and Edwards, 1972a, 1972b) and improved by Samathiyakanit (Samathiyakanit and Glyde, 1973; Samathiyakanit, 1974), who has extensively compared his path-integral results (Sa-yakanit, 1979; Sa-yakanit and Glyde, 1980; Sa-yakanit *et al.*, 1982) with the method of Halperin and Lax (see Sec. VI).

The central idea and basic assumptions of the following derivation were given in Feynman's polaron theory (Feynman, 1955). The action S of the random system is approximated by a trial action S_0, which contains adjustable parameters to minimize the "free energy" and which is quadratic, because for such actions the path integral can be evaluated exactly.

Once the trial action S_0 has been introduced, the average propagator can be calculated by expanding in cumulants about the corresponding trial-average propagator G_0. All this is described in Feynman and Hibbs (1965, Chap. 11). Some basics of the path-integral theory are summarized in Appendix B. Although higher cumulant corrections (Gross, 1983), are possible, we limit ourselves to the first cumulant and thus obtain G_1. In Sec. VIII.A, we formulate the problem in terms of path integrals. Section VIII.B goes into the details, and Sec. VIII.C compares Sa-yakanit's results with previously discussed methods.

A. Path-integral theory of a disordered system: statement of the problem

In the one-electron and effective-mass approximation, the doped semiconductor is described by the Hamiltonian H,

$$H=-\frac{\hbar^2}{2m}\nabla^2+\sum_{i=1}^{N}v(\mathbf{r}-\mathbf{r}_i)\ . \tag{8.1}$$

The propagator (or Green's function) $\mathcal{G}$ of such a system with a particular configuration of impurities $\{\mathbf{r}_i\}$ is expressed as a path integral,

$$\mathcal{G}(\mathbf{r}_2,\mathbf{r}_1;t;\{\mathbf{r}_i\})=\int\mathcal{D}\mathbf{r}(\tau)\exp\left[\frac{i}{\hbar}S(\{\mathbf{r}_i\})\right]\ , \tag{8.2}$$

with boundary conditions $\mathbf{r}(0)=\mathbf{r}_1$ and $\mathbf{r}(t)=\mathbf{r}_2$, where the action $S(\{\mathbf{r}_i\})$ is given by

$$S(\{\mathbf{r}_i\})=\int_0^t d\tau\left[\frac{m}{2}\dot{\mathbf{r}}^2(\tau)-\sum_{i=1}^{M}v(\mathbf{r}(\tau)-\mathbf{r}_i)\right]\ . \tag{8.3}$$

The average over all configurations reads

$$G(\mathbf{r}_2,\mathbf{r}_1;t)=\int P[\{\mathbf{r}_i\}]d[\{\mathbf{r}_i\}]\mathcal{G}(\mathbf{r}_2,\mathbf{r}_1;t;\{\mathbf{r}_i\})\ . \tag{8.4}$$

Assuming that the impurities are equally likely to be found at all points, the probability distribution is

$$P[\{\mathbf{r}_i\}]d[\{\mathbf{r}_i\}]=\prod_{N}^{\infty}\frac{d\mathbf{r}_i d\mathbf{r}_2\cdots d\mathbf{r}_N}{V_0^N}\ ,$$

$$V_0\rightarrow\infty,\quad n=\frac{N}{V_0}\ .$$

The method that results in Eq. (5.7) (Appendix A) is readily applied,[8] yielding

$$G(\mathbf{r}_2,\mathbf{r}_1;t)=\int\mathcal{D}\mathbf{r}(\tau)\exp\left\{\frac{i}{\hbar}\int_0^t d\tau\frac{m}{2}\dot{\mathbf{r}}^2(\tau)+n\int d\mathbf{R}\left[\exp\left[-\frac{i}{\hbar}\int_0^t d\tau\, v(\mathbf{r}(\tau)-\mathbf{R})\right]-1\right]\right\}\ . \tag{8.5}$$

Although Eq. (8.5) is an exact general formula, the path integral is too complicated to work with. An obvious simplification (also applied in Sec. V) is the assumption of high density ($n\rightarrow\infty$) combined with very weak scattering ($v\rightarrow 0$), so that nv^2 remains finite.

Expanding

$$\exp\left[-\frac{i}{\hbar}\int_0^t d\tau\, v(\mathbf{r}(\tau)-\mathbf{R})\right]-1$$

to second order and setting the energy origin at the mean potential of the system, we find that Eq. (8.5) becomes

$$G(\mathbf{r}_2,\mathbf{r}_1;t)=\int\mathcal{D}\mathbf{r}(\tau)\exp\left[\frac{i}{\hbar}S\right]\ , \tag{8.6}$$

where

$$S=\int_0^t d\tau\frac{m}{2}\dot{\mathbf{r}}^2(\tau)+\frac{i}{2\hbar}\eta^2\int_0^t\int_0^t d\tau\, d\sigma\, W(\mathbf{r}(\tau)-\mathbf{r}(\sigma))\ . \tag{8.7}$$

Here W denotes the correlation function (6.12), and the parameter η denotes the strength of the scattering potential. Although various correlation functions can be considered, here we confine ourselves to a Gaussian correlation function

$$W(\mathbf{r}(\tau)-\mathbf{r}(\sigma))=n(\pi L^2)^{-3/2}\exp\left[-\frac{|\mathbf{r}(\tau)-\mathbf{r}(\sigma)|^2}{L^2}\right]\ , \tag{8.8}$$

where L denotes the correlation length of the random system.

From a knowledge of the Green's function (8.6) many physical quantities can be studied. Again, we limit ourselves to the DOS, obtained by taking the trace of G and then Fourier transforming according to the standard formula,

$$\rho(E)=\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}dt\,\mathrm{Tr}G(\mathbf{r}_1,\mathbf{r}_2;t)\exp\left[\frac{i}{\hbar}Et\right]\ . \tag{8.9}$$

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[8] Analogous expressions are derived by Feynman and Hibbs (1965, Chap. 12). This expression (8.5) seems first to have appeared in Edwards and Gulyaev (1964).

Since G is obtained by averaging over all configurations of scattering potentials, it must be translationally invariant (see Sec. II.A), meaning that $G(\mathbf{r}_2,\mathbf{r}_1;t)\equiv G(\mathbf{r}_2-\mathbf{r}_1;t)$. Consequently $\mathrm{Tr}G(\mathbf{r}_2,\mathbf{r}_1;t)$ simplifies to $V_0 G(\mathbf{r}_2-\mathbf{r}_1;t)$ in Eq. (8.9).

The problem is now well described and consists in solving Eq. (8.9) together with (8.6)–(8.8).

B. A harmonic trial action: solution of the problem

Guided by Feynman's polaron theory, we consider the following trial action of a harmonic oscillator having one parameter ω:

$$S_0(\omega)=\int_0^t d\tau \frac{m}{2}\left[\dot{\mathbf{r}}^2(\tau)-\frac{\omega^2}{2t}\int_0^t d\sigma\,|\mathbf{r}(\tau)-\mathbf{r}(\sigma)|^2\right]. \tag{8.10}$$

The average propagator may be written in terms of this trial action as

$$G(\mathbf{r}_2,\mathbf{r}_1;t)=\int \mathcal{D}\mathbf{r}(\tau)\exp\left[\frac{i}{\hbar}S_0(\omega)\right]\times\exp\left[\frac{i}{\hbar}[S-S_0(\omega)]\right]$$

or, more rigorously, by explicitly expressing the path-integral normalization, with Eq. (B12)

$$G(\mathbf{r}_2,\mathbf{r}_1;t)=G_0(\mathbf{r}_2,\mathbf{r}_1;t,\omega)\langle \exp[i(S-S_0(\omega)/\hbar]\rangle_{S_0(\omega)} \tag{8.11}$$

where

$$G_0(\mathbf{r}_2,\mathbf{r}_1;t,\omega)=\int \mathcal{D}(\mathbf{r}(\tau))\exp\left[\frac{i}{\hbar}S_0(\omega)\right]. \tag{8.12}$$

When we use the exact semi-invariant or cumulant expansion (Kubo, 1962),

$$\langle e^{A}\rangle=\exp\left[\langle A\rangle+\frac{1}{2!}(\langle A^2\rangle-\langle A\rangle^2)+\frac{1}{3!}[\langle A^3\rangle-3\langle A\rangle(\langle A^2\rangle-\langle A\rangle^2)-\langle A\rangle^3]+\cdots\right] \tag{8.13}$$

to first order, Eq. (8.11) becomes

$$G_1(\mathbf{r}_2,\mathbf{r}_1;t,\omega)=G_0(\mathbf{r}_2,\mathbf{r}_1;t,\omega)\exp[i/\hbar\langle S-S_0(\omega)\rangle_{S_0(\omega)}]. \tag{8.14}$$

1. The average $\langle S-S_0(\omega)\rangle_{S_0(\omega)}$

Since the kinetic terms in the actions S and $S_0(\omega)$ are identical, only the second terms in Eqs. (8.7) and (8.10) play a role in $\langle S-S_0(\omega)\rangle_{S_0(\omega)}$, and we shall denote them $\langle S\rangle_{S_0(\omega)}$ and $\langle S_0(\omega)\rangle_{S_0(\omega)}$, respectively.

Let us first consider $\langle S\rangle_{S_0(\omega)}$, which can be exactly evaluated by expressing $W(\mathbf{r}(\tau)-\mathbf{r}(\sigma))$ as a Fourier transform. For, if $W(\mathbf{k})$ is the Fourier transform of $W(\mathbf{r})$, which equals for Eq. (8.8)

$$W(\mathbf{k})=n\exp(-L^2k^2/4), \tag{8.15}$$

then

$$\langle S\rangle_{S_0(\omega)}=\frac{i}{2\hbar}\eta^2\int_0^t\int_0^t d\tau\, d\sigma\int\frac{d^3k}{(2\pi)^3}W(\mathbf{k})\langle\exp\{-i\mathbf{k}\cdot[\mathbf{r}(\tau)-\mathbf{r}(\sigma)]\}\rangle_{S_0(\omega)}. \tag{8.16}$$

The average appearing now in Eq. (8.16) is of the type investigated in Appendix B [Eq. (B13)], because $S_0(\omega)$ is quadratic. Such path integrals can be evaluated exactly [see Eq. (B15)]. Alternatively, only the first two cumulants (8.13) are nonzero (Kubo, 1962). Consequently we get

$$\langle S\rangle_{S_0(\omega)}=\frac{i}{2\hbar}\eta^2\int_0^t\int_0^t d\tau\, d\sigma\int\frac{d^3k}{(2\pi)^3}W(\mathbf{k})\exp(a_1+a_2) \tag{8.17}$$

where

$$\begin{aligned} a_1&=i\mathbf{k}\cdot\langle[\mathbf{r}(\tau)-\mathbf{r}(\sigma)]\rangle_{S_0(\omega)},\\ a_2&=-\tfrac{1}{2}k^2[\tfrac{1}{3}\langle[\mathbf{r}(\tau)-\mathbf{r}(\sigma)]^2\rangle_{S_0(\omega)}-\langle[\mathbf{r}(\tau)-\mathbf{r}(\sigma)]\rangle^2_{S_0(\omega)}]. \end{aligned} \tag{8.18}$$

Note that the second term inside the large square brackets represents only one component of the coordinates. The k integration can be performed if $W(k)$ is given by Eq. (8.15) and yields

$$\langle S\rangle_{S_0(\omega)}=\frac{i}{2\hbar}n\eta^2\int_0^t\int_0^t d\tau\, d\sigma\left[\frac{1}{4\pi A}\right]^{3/2}\exp\left[-\frac{B^2}{4A}\right], \tag{8.19}$$

where

$$A=\frac{1}{4}L^2+\frac{1}{2}\left[\frac{1}{3}\langle[\mathbf{r}(\tau)-\mathbf{r}(\sigma)]^2\rangle_{S_0(\omega)}-\langle[\mathbf{r}(\tau)-\mathbf{r}(\sigma)]\rangle^2_{S_0(\omega)}\right] .$$
$$B=\langle\mathbf{r}(\tau)-\mathbf{r}(\sigma)\rangle_{S_0(\omega)} \tag{8.20}$$

Next we focus on $\langle S_0(\omega)\rangle_{S_0(\omega)}$, which is easily written as

$$\langle S_0(\omega)\rangle_{S_0(\omega)}=-\frac{m}{2}\frac{\omega^2}{2t}\int_0^t\int_0^t d\tau\, d\sigma\langle[\mathbf{r}(\tau)-\mathbf{r}(\sigma)]^2\rangle_{S_0(\omega)} . \tag{8.21}$$

From Eqs. (8.19) and (8.21), we see that the average $\langle S-S_0(\omega)\rangle_{S_0(\omega)}$ can be expressed solely in terms of the averages $\langle\mathbf{r}(\tau)\rangle_{S_0(\omega)}$ and $\langle[\mathbf{r}(\tau)\cdot\mathbf{r}(\sigma)]\rangle_{S_0(\omega)}$. Such averages can be obtained from Eqs. (B16) and (B17) and therefore we need the classical action S'_{cl}.

2. The classical action S'_{cl} corresponding to Eq. (8.10)

From $S'_{\text{cl}}[b,a]=S'[\xi(t)]$, the classical path ξ of Eq. (8.10) must be found, which obeys

$$\delta S'=\delta\left[S_0+\int d\tau\,\mathbf{f}(\tau)\cdot\mathbf{r}(\tau)\right]=0$$

or

$$\ddot{\xi}(\tau)+\frac{\omega^2}{t}\int_0^t d\sigma[\xi(\tau)-\xi(\sigma)]-\frac{\mathbf{f}(\tau)}{m}=0 . \tag{8.22}$$

Rewriting Eq. (8.22) as

$$\ddot{\xi}(\tau)+\omega^2\xi(\tau)=\frac{\omega^2}{t}\int_0^t d\sigma\,\xi(\sigma)-\frac{\mathbf{f}(\tau)}{m} \tag{8.23}$$

and introducing a Green's function

$$\left[\frac{d^2}{d\tau^2}+\omega^2\right]g(\tau,\sigma)=\delta(\tau-\sigma) ,$$

$$g(\tau,\sigma)=-\frac{1}{\sin\omega t}[\sin\omega(t-\tau)\sin\omega\sigma\;\theta(\tau-\sigma)+\sin\omega(t-\sigma)\sin\omega\tau\;\theta(\sigma-\tau)] ,$$

we find the general solution of Eq. (8.23) with boundary conditions $\xi(0)=\xi_1$ and $\xi(\tau)=\xi_2$,

$$\xi(\tau)=\frac{1}{\sin\omega\tau}[\xi_2\sin\omega t+\xi_1\sin\omega(t-\tau)]+\frac{1}{m}\int_0^t d\sigma\left[\omega^2\xi(\sigma)+\frac{\mathbf{f}(\tau)}{m}\right] . \tag{8.24}$$

This is an integral equation, which can be solved, yielding

$$\xi(\tau)=\frac{\xi_2\sin\omega t+\xi_1\sin\omega(t-\tau)}{\sin\omega t}$$
$$-\frac{4\sin\frac{1}{2}\omega(t-\tau)\sin\frac{1}{2}\omega\tau}{\sin\omega t}\left[(\xi_1+\xi_2)\sin\tfrac{1}{2}\omega t-\frac{2}{m\omega}\int_0^t d\sigma\;\mathbf{f}(\sigma)\sin\tfrac{1}{2}\omega(t-\sigma)\sin\tfrac{1}{2}\omega\sigma\right]+\frac{1}{m}\int_0^t\mathbf{f}(\sigma)g(\tau,\sigma) . \tag{8.25}$$

The classical action S'_{cl} is simply found by substituting $\xi(\tau)$ into

$$S'_{\text{cl}}(\xi_2-\xi_1;\omega)=\frac{m}{2}\left[\int_0^t d\tau\,\xi^2(\tau)-\frac{\omega^2}{2t}\int_0^t d\tau\int_0^t d\sigma|\xi(\tau)-\xi(\sigma)|^2\right]+\int_0^t d\tau\,\mathbf{f}(\tau)\cdot\xi(\tau) ,$$

which simplifies, after integrating the first term by parts and invoking Eq. (8.23), to

$$S'_{\text{cl}}(\xi_2-\xi_1;\omega)=\frac{m}{2}[\dot{\xi}(\tau)\xi(\tau)-\dot{\xi}(0)\xi(0)]+\tfrac{1}{2}\int_0^t d\tau\,\mathbf{f}(\tau)\cdot\xi(\tau) . \tag{8.26}$$

Explicitly, Eq. (8.26) becomes

$$S'_{\mathrm{cl}}(\xi_2-\xi_1;\omega)=\frac{m\omega}{4}|\xi_2-\xi_1|^2\cot\tfrac{1}{2}\omega t+\left[\frac{\xi_2}{\sin\omega t}\int_0^t d\tau\,\mathbf{f}(\tau)[\sin\omega\tau-2\sin\tfrac{1}{2}\omega t\,\sin\tfrac{1}{2}\omega(t-\sigma)\sin\tfrac{1}{2}\omega\tau]\right]$$
$$+\left[\frac{\xi_1}{\sin\omega t}\int_0^t d\tau\,\mathbf{f}(\tau)[\sin\omega(t-\tau)-2\sin\tfrac{1}{2}\omega t\,\sin\tfrac{1}{2}\omega(t-\sigma)\sin\tfrac{1}{2}\omega\tau]\right]$$
$$-\frac{1}{m\omega\sin\omega t}\left[\int_0^t d\tau\,\mathbf{f}(\tau)\int_0^\tau d\sigma\,\mathbf{f}(\sigma)[\sin\omega(t-\tau)\sin\omega\sigma-4\sin\tfrac{1}{2}\omega(t-\tau)\sin\tfrac{1}{2}\omega\tau\sin\tfrac{1}{2}\omega(t-\sigma)\sin\tfrac{1}{2}\omega\sigma]\right]. \tag{8.27}$$

The classical action $S_{\mathrm{cl}}(\xi_2-\xi_1;\omega)$ is then obtained by setting $\mathbf{f}\equiv 0$ in Eq. (8.27),

$$S_{\mathrm{cl}}(\xi_2-\xi_1;t,\omega)\equiv S_0(\xi_2-\xi_1;t,\omega)=\frac{m\omega}{4}|\xi_2-\xi_1|^2\cot\tfrac{1}{2}\omega t\ . \tag{8.28}$$

Invoking Eqs. (8.25), (8.26), and (8.27), we can work out Eq. (8.20). After some straightforward calculations we find for $\tau>\sigma$

$$A\equiv A(t,\tau-\sigma;\omega)=\tfrac{1}{4}L^2+\frac{i\hbar}{m\omega}\frac{\sin\tfrac{1}{2}\omega(\tau-\sigma)\sin\tfrac{1}{2}\omega[t-(\tau-\sigma)]}{\sin\tfrac{1}{2}\omega t}$$
$$B\equiv\mathbf{B}(\mathbf{r}_2-\mathbf{r}_1;t,\tau,\sigma;\omega)=\frac{\sin\tfrac{1}{2}\omega(\tau-\sigma)\cos\tfrac{1}{2}\omega[1-(\tau+\sigma)]}{\sin\tfrac{1}{2}\omega t}(\mathbf{r}_2-\mathbf{r}_1)\ , \tag{8.29}$$

and we clearly have

$$A(t,\tau-\sigma;\omega)=A(t,t-(\tau-\sigma);\omega). \tag{8.30}$$

Analogously, after performing the integration, we find that Eq. (8.21) reads

$$\langle S_0(\omega)\rangle_{S_0(\omega)}=\tfrac{3}{2}i\hbar(\tfrac{1}{2}\omega t\cot\tfrac{1}{2}\omega t-1)+\tfrac{1}{2}m[\tfrac{1}{2}\omega t\cos\tfrac{1}{2}\omega t-(\tfrac{1}{2}\omega t\csc\tfrac{1}{2}\omega t)^2]\frac{(\mathbf{r}_2-\mathbf{r}_1)^2}{2t}\ . \tag{8.31}$$

3. Evaluation of $G_0(\mathbf{r}_2,\mathbf{r}_1;t,\omega)$

Since the trial action $S_0(\omega)$ is quadratic, Eq. (8.12) can be evaluated with Eqs. (B7) and (8.28) as

$$G_0(\mathbf{r}_2,\mathbf{r}_1;t,\omega)=\exp\left[\frac{i}{\hbar}S_{\mathrm{cl}}(\mathbf{r}_2-\mathbf{r}_1;t,\omega)\right]F(t,\omega)\ . \tag{8.32}$$

The remaining problem consists in the determination of $F(t,\omega)$. Since the path integral (8.12) reduces to the propagator for a free particle as $\omega=0$, we readily obtain from Eq. (B11)

$$\lim_{\omega\to 0}F(t,\omega)=\left[\frac{m}{2\pi i\hbar t}\right]^{3/2}\ . \tag{8.33}$$

Our trial action $S_0(\omega)$ is closely related to that of a simple harmonic oscillator, as follows. The propagator $H(\mathbf{r}_2,\mathbf{r}_2;t,\mathbf{y})$ of a simple harmonic oscillator is

$$H(\mathbf{r}_2,\mathbf{r}_1;t,\mathbf{y})=\int\mathcal{D}(\mathbf{r}(\tau))\exp\left[\frac{i}{\hbar}\int_0^t d\tau\left[\frac{m}{2}\dot{\mathbf{r}}^2(\tau)-\frac{\kappa}{2}|\mathbf{r}(\tau)-\mathbf{y}|^2\right]\right]\ , \tag{8.34}$$

where $\mathbf{y}$ represents the origin of the harmonic oscillator and $\kappa=m\omega^2$ is the force constant. This path integral can be worked out exactly and can be obtained from formula (3.66) in Feynman and Hibbs (1965, p. 64) by some minor modifications. Since Eq. (8.34) is also quadratic (or Gaussian) in $\mathbf{y}$, an integration over all $\mathbf{y}$ can be accomplished, illustrating a remarkable property of Eq. (8.34):

$$\int d\mathbf{y}\,H(\mathbf{r}_2,\mathbf{r}_1;t,\mathbf{y})=\left[\frac{2\pi\hbar}{im\omega^2 t}\right]^{3/2}G_0(\mathbf{r}_2,\mathbf{r}_1;t,\omega)\ . \tag{8.35}$$

From a mathematical analogy, we may introduce a kind of "partition function Z" (Feynman and Hibbs, pp. 279), in fact an imaginary one, which would equal the "true" partition function after transforming $t \rightarrow i\hbar\beta$, where β is proportional to the inverse temperature T. Then the "partition function" corresponding to $G_0(\mathbf{r}_2,\mathbf{r}_2;t,\omega)$ is

$$Z_0=\int d\mathbf{r}\, G_0(\mathbf{r},\mathbf{r};t,\omega)=V_0 F(t,\omega)\ , \tag{8.36}$$

which also equals, with Eq. (8.35),

$$\begin{aligned}\int d\mathbf{r}\, G_0(\mathbf{r},\mathbf{r},t;\omega) &= \left[\frac{2\pi\hbar}{im\omega^2 t}\right]^{-3/2} \int d\mathbf{r} \int d\mathbf{y}\, H(\mathbf{r},\mathbf{r};t,\mathbf{y}) \\ &= \left[\frac{2\pi\hbar}{im\omega^2 t}\right]^{-3/2} (2i\sin\tfrac{1}{2}\omega t)^{-3} V_0\ .\end{aligned} \tag{8.37}$$

Hence

$$F(t,\omega)=\left[\frac{m}{2\pi i\hbar}\right]^{3/2}\left[\frac{\omega t}{2\sin\frac{1}{2}\omega t}\right]^3 , \tag{8.38}$$

and this agrees with Eq. (8.33).

4. The final expression for $\rho(E)$

Putting all the above results together to construct Eq. (8.11), we get

$$\begin{aligned} G_1(\mathbf{r}_2,\mathbf{r}_1;t,\omega) = {} & \left[\frac{m}{2\pi i\hbar t}\right]^{3/2}\left[\frac{\omega t}{2\sin\frac{1}{2}\omega t}\right]^3 \\ & \times\exp\left[\frac{3}{2}\left[\frac{\omega t}{2}\cos\frac{\omega t}{2}-1\right]+\frac{im}{4t\hbar}\left[\frac{\omega t}{2}\cot\frac{\omega t}{2}+\left[\frac{\omega t}{2}\csc\frac{\omega t}{2}\right]^2\right](\mathbf{r}_2-\mathbf{r}_1)^2\right] \\ & \times\exp\left[-\frac{n\eta^2}{2\hbar^2}\int_0^t\int_0^\tau d\tau\, d\sigma\left[\frac{1}{4\pi A(t,\tau-\sigma;\omega)}\right]^{3/2}\exp\left[-\frac{\mathbf{B}^2(\mathbf{r}_2-\mathbf{r}_1;t,\tau,\sigma,\omega)}{4A(t,\tau-\sigma,\omega)}\right]\right] . \end{aligned} \tag{8.39}$$

From Eq. (8.9), we finally achieve an expression for $\rho(E,\omega)$,

$$\rho(E,\omega)=\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dt\left[\frac{m}{2\pi i\hbar t}\right]^{3/2}\left[\frac{\omega t}{2\sin\dfrac{\omega t}{2}}\right]^3 \exp\left[\frac{iEt}{\hbar}+\frac{3}{2}\left[\frac{\omega t}{2}\cos\frac{\omega t}{2}-1\right]-\frac{n\eta^2 t}{2\hbar^2}\int_0^t dx\left[\frac{1}{4\pi A(t,x;\omega)}\right]^{3/2}\right] , \tag{8.40}$$

where $(1/V_0)\mathrm{Tr}G(\mathbf{r}_2,\mathbf{r}_1;t)=G(\mathbf{r},\mathbf{r};t)\approx G_1(0;t,\omega)$ because of translational invariance. We have used Eq. (8.28) to perform one integration in the double integral appearing in (8.39). The dependence of the variational parameter ω is explicitly expressed. An exact variational principle for the DOS exists (Sec. II.2) which completely determines the best value for for ω and hence the best $\rho(E)$, subject to the chosen trial action (8.10), the first cumulant expansion (8.14), and the assumption of a Gaussian correlation function for the potential (8.8). This optimal $\rho(E)$ can only be computed numerically.

C. Discussion and comparison with previous models

Sa-yakanit (1979; Sa-yakanit and Glyde, 1980) used the method of Sec. VIII.C to calculate the DOS assuming a screened Coulomb scattering potential (6.37), and he obtained

$$\rho(E,\omega)=\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dt\left[\frac{m}{2\pi i\hbar t}\right]^{3/2}\left[\frac{\omega t}{2\sin\dfrac{\omega t}{2}}\right]^3 \exp\left[\frac{iEt}{\hbar}+\frac{3}{2}\left[\frac{\omega t}{2}\cot\frac{\omega t}{2}-1\right]-\frac{\xi\kappa t}{2\hbar^2}\int_0^t dx\, F(x)\right] , \tag{8.41}$$

where

$$F(x)=\frac{1}{\sqrt{\pi}}\int_0^\infty dy\, y\exp(-\kappa^2 y)\left[y+\frac{i\hbar}{m\omega}\frac{\sin\frac{1}{2}\omega x\,\sin\frac{1}{2}\omega(t-x)}{\sin\frac{1}{2}\omega t}\right]^{-3/2} . \tag{8.42}$$

In the low-energy band tail, we can argue [as is generally assumed in fluctuation models (Secs. VI and VII)] that only the ground states of the potential fluctuations contribute to the DOS. Applied to path integrals, the lowest energy[9] of the system is found by considering the "partition function Z" in the limit $t \rightarrow \infty$ (Feynman and Hibbs, p. 303). This means that we should first take the limit of $G_1(\mathbf{r},\mathbf{r};t,\omega)$ [Eq. (8.39)] for $t \rightarrow \infty$, before substituting in Eq. (8.9). Employing the parabolic cylinder function formula,

$$\int_0^\infty dt(it)^p \exp(-u^2t^2-ist)=2^{-p/2}\sqrt{\pi}u^{-p-1}\exp\left[-\frac{s^2}{8u^2}\right]D_p\left[\frac{s}{u\sqrt{2}}\right] ,$$

Sa-yakanit derived the following expressions:

$$\rho(E,\omega)=\frac{1}{4}\left[\frac{\sqrt{2}}{\pi}\right]^{1/2}\omega^3\left[\frac{m}{2\pi\hbar}\right]u^{-5/2}\exp\left[-\frac{(\frac{3}{4}\hbar\omega-E)^2}{8u^2}\right]D_{3/2}\left[\frac{(\frac{3}{4}\hbar\omega-E)}{u\sqrt{2}}\right] , \tag{8.43}$$

where for a Gaussian potential

$$u^2=\frac{1}{2\hbar^2}\frac{n\eta^2}{(\pi L^2)^{3/2}}\left[1+4\frac{\hbar}{2m\omega L^2}\right]^{-3/2} \tag{8.44}$$

and for a screened Coulomb potential

$$u^2=\frac{\xi\kappa t}{2\hbar^2}\frac{1}{\sqrt{\pi}}\int_0^\infty dy\, y\exp(-\kappa^2 y)\left[y+\frac{\hbar}{2m\omega}\right]^{-3/2} . \tag{8.45}$$

From the variational principle (Sec. II.B), a supplementary equation can be derived to determine ω. For a screened Coulomb potential, we have

$$\left[\frac{2D_{-4}(z)}{D_{-3}(z)}-\frac{1}{z}\left[\frac{T}{T-T/E_\kappa}+2\right]\right]-\frac{\sqrt{\pi}(T-E/E_\kappa)^2}{4\xi\sqrt{2}\exp(z^2/4)D_{-3}(z)}\left[\frac{D_{-4}(z)}{D_{-3}(z)}-\left[\frac{2z^{-3}}{T-E/E_\kappa}\right]\right]=0 , \tag{8.46}$$

where [with Eq. (6.40)]

$$z=\frac{2E_\kappa}{\sqrt{\hbar\omega}} \tag{8.47}$$

and where T is the normalized zero-point kinetic energy of a harmonic oscillator,

$$T=\frac{1}{E_\kappa}\frac{3}{4}\hbar\omega=\frac{3}{2}z^{-2} . \tag{8.48}$$

Similarly, retaining only the high electron energy states corresponds to the $t \rightarrow 0$ limit of the "partition function Z." Performing this operation before using Eq. (8.9), we find

$$\rho(E)=\frac{\xi^{1/4}m^{3/2}}{\sqrt{2}\pi^2\hbar^3}\exp\left[-\frac{E^2}{4\xi}\right]D_{-3/2}\left[-\frac{E}{\sqrt{\xi}}\right] , \tag{8.49}$$

which exactly equals the Kane result [Eq. (5.15)]. In this limit, the resulting DOS (8.49) does not depend only ω, because only the free-particle contribution "survives," so that the semiclassical $\rho(E)$ is independent of the trial action (8.10).

The one-dimensional analog of Eq. (8.43) can be compared to the exact asymptotic formula ($\alpha=\beta=1$) [Eq. (4.53)]

$$\rho_1(E)=\alpha\frac{8E}{\pi\xi}\exp\left[-\beta\frac{16}{3\xi}\sqrt{\hbar^2/2m}\,E^{3/2}\right] ,$$

yielding $\alpha=\sqrt{2\pi/6}=0.4178$ and $\beta=\pi/3=1.0233$. Halperin and Lax found $\alpha=1/\sqrt{5}=0.4472$ and $\beta=1$. Although this result is worse than that of Halperin and Lax, Sa-yakanit shows some advantages of the path-integral method:

(1) The calculation can be improved by going beyond the first cumulant. Gross (1977) calculated $\rho_1(E)$ with the second-cumulant correction and found $\alpha=\frac{4}{3}\sqrt{\pi/6}=0.9648$ and $\beta=\sqrt{64\pi/201}=1.000\,15$. This calculation roughly agrees with the second-order correction of Halperin and Lax (1967).

(2) Analytical expressions are obtained that are much more convenient to use than results given in tables (like those of Halperin and Lax).

(3) The method can be used to obtain the DOS at high and intermediate energies.

(4) The model can be applied to the evaluation of the DOS with general statistics including correlations among the impurities, i.e., by using Eq. (8.5) and then immediately considering a cumulant expansion.

(5) The trial action $S(\omega)$ [Eq. (8.10)] can be generalized

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[9] This can be understood physically by considering the "pseudo" Heisenberg uncertainty relation for the energy and time, $Et \geq \hbar$. Making the time large corresponds to searching for low energies (and vice versa).

to a quadratic trial action with two variational parameters $S(\kappa,\Omega)$ (Sa-yakanit, 1974).

The use of a harmonic trial action is equivalent to assuming that all the fluctuating potentials have the same quadratic shape. In fact, this was the ansatz of Halperin and Lax's model, that all ground-state wave functions are assumed to have the same wave function f [Eq. (6.1)]. The harmonic-oscillator potential is equivalent to approximating Eq. (6.1) by a Gaussian. However, the use of a Gaussian for (6.1) also permits an analytical expression for Eqs. (6.20) and (6.22) in the Halperin and Lax theory.

Sa-yakanit and Glyde (1980) compare the determination of ω by the exact variational principle with two other methods. The first maximizes $\rho(E)$ to obtain ω; the second only minimizes the argument of the exponential (as in Halperin and Lax and Efros). Sa-yakanit and Glyde (1980) conclude that the results obtained by maximizing $P(E)$ (Sec. II) and $\rho(E)$ do not differ significantly, but that the result of minimizing the argument of the exponential is substantially different from the first two.

The path-integral approach, the semiclassical, and the Halperin-Lax methods are compared in Figs. 12 and 13. The normalized parameter for the energy of the potential fluctuation,

$$\xi_{\text{Sa-yakanit}}=\frac{\xi}{E_\kappa^2}\ , \tag{8.50}$$

has been calculated for various doping concentrations and temperature in n-GaAs in Fig. 11, assuming a Thomas-Fermi approximation (Sec. V). This figure gives an idea of the order of magnitude of the potential fluctuations in n-GaAs and may serve to relate Figs. 12 and 13 to doping concentration in n-GaAs. For energies deep in the tail, the results coincide with those of Halperin and Lax. At higher energies the DOS intersects the semiclassical value (5.15). At this point the result of Halperin and Lax is significantly too low. As a conclusion, Sa-yakanit *et al.* propose to use Eq. (8.43) until it crosses the semiclassical Kane $\rho(E)$ and thereafter to employ the latter.

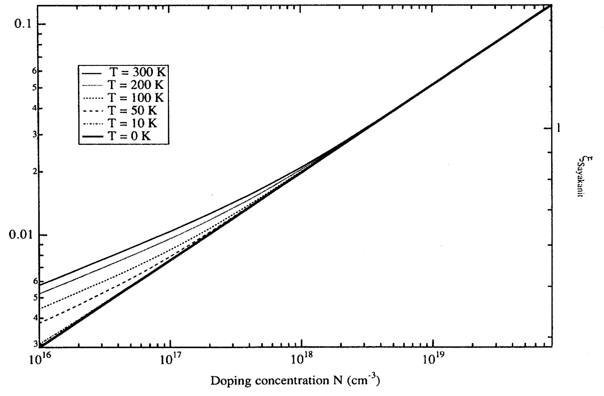

FIG. 11. The root mean square of the potential fluctuation σ_n as a function of doping concentration for n-GaAs in three dimensions. The parameter $\xi_{\text{Sa-yakanit}}$ is further used in Figs. 12 and 13.

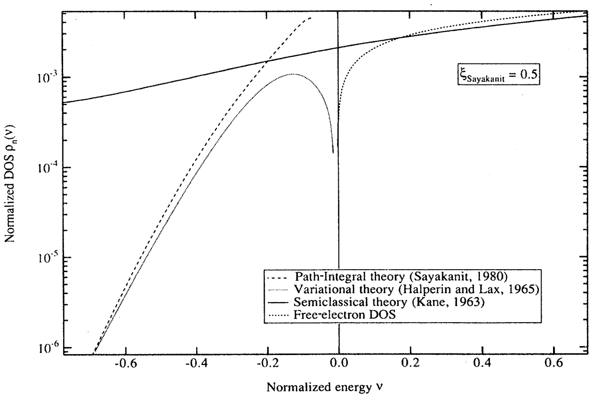

FIG. 12. Important band-tail theories for the parameter $\xi_{\text{Sa-yakanit}}=0.5$ (data extracted from Sa-yakanit and Glyde (1980) in normalized quantities: $\nu=E/E_\kappa$ [Eq. (6.41)] and

$$\rho_n(\nu)=\frac{E_\kappa\xi^2_{\text{Sa-yakanit}}}{\kappa^3}n_f(E)=a(\nu)\exp\left[\frac{b(\nu)}{2\xi_{\text{Sa-yakanit}}}\right]\ ,$$

[Eq. (6.39)].

IX. FIELD THEORY AND THE REPLICA APPROACH

The replica approach was introduced by Edwards and Anderson (1975) in their study of spin glasses. In the theory of disordered systems (mainly applied to spin glasses and amorphous materials) the replica solution has reached a high degree of sophistication. For spin glasses it is thoroughly studied in the book by Mézard, Parisi, and Virasoro (1987). Although successful in some cases, the replica approach still lacks a rigorous mathematical foundation. Cardy (1978) and Brézin and Parisi (1980) have applied techniques from statistical field theory combined with the replica "trick" to describing the electronic states in a random potential. We shall now consider the replica approach.

A. The formal description

In field theory, the Green's function is defined as the correlation of two ϕ fields (Parisi, 1988). The correlation

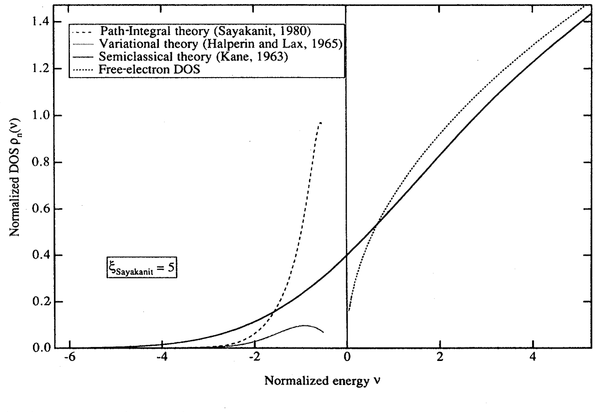

FIG. 13. Graph analogous to Fig. 12 but on a linear scale and for $\xi_{\text{Sa-yakanit}}=5$.

functions of the functional-integral approach of statistical field theory become expectation values of the time-ordered products of operators on the ground state (as in quantum field theory). Thus

$$G(\mathbf{r}_1,\mathbf{r}_2;E)\equiv\langle\phi(\mathbf{r}_1)\phi(\mathbf{r}_2)\rangle = \frac{\int\mathcal{D}\phi\, e^{-\beta H[\phi]}\phi(\mathbf{r}_1)\phi(\mathbf{r}_2)}{\int\mathcal{D}\phi\, e^{-\beta H[\phi]}} \; . \tag{9.1}$$

In order to find the DOS by Eq. (2.4), it suffices to study $G(\mathbf{r}_1,\mathbf{r}_1;E)$ because of the trace in Eq. (2.4). Substituting the Hamiltonian in d dimensions for a random potential (4.1), we find the starting expression for the Green's function (Parisi, 1988),

$$G(\mathbf{r}_1,\mathbf{r}_1;E) = \frac{\int\mathcal{D}\phi\,\phi(\mathbf{r}_1)\phi(\mathbf{r}_1)\exp\left[\frac{1}{2}\int d\mathbf{r}\,\phi(\mathbf{r})(E-H_{\text{op}})\phi(\mathbf{r})\right]}{\int\mathcal{D}\phi\exp\left[\frac{1}{2}\int d\mathbf{r}\,\phi(\mathbf{r})(E-H_{\text{op}})\phi(\mathbf{r})\right]} \; . \tag{9.2}$$

As in the path-integral approach, we are interested in the Green's function averaged over all possible potential configurations having a probability distribution function $P[V]$. Direct averaging of Eq. (9.2) is hard, but the replica approach (Appendix C) can be introduced as follows: Let

$$Z_v[g(\mathbf{r})] = \left|\int\mathcal{D}\phi\exp\left[\frac{1}{2}\int d\mathbf{r}\,\phi(\mathbf{r})[E-H_{\text{op}}+2g(\mathbf{r})]\phi(\mathbf{r})\right]\right| \; . \tag{9.3}$$

Then we find by functional derivation with respect to $g(\mathbf{r})$ that

$$G(\mathbf{r}_1,\mathbf{r}_1;E)=\frac{\delta}{\delta g(\mathbf{r})}(\ln Z_v)\bigg|_{g(\mathbf{r})\equiv 0} \; . \tag{9.4}$$

Performing the average over the potential configurations[10] gives

$$\langle G(\mathbf{r}_1,\mathbf{r}_1;E)\rangle_v \equiv \int\mathcal{D}v(\mathbf{r})P[v(\mathbf{r})]G(\mathbf{r}_1,\mathbf{r}_2;E)=\frac{\delta}{\delta g(\mathbf{r})}\left[\int\mathcal{D}v(\mathbf{r})P[v(\mathbf{r})]\ln Z_v\right]\bigg|_{g(\mathbf{r})\equiv 0} \; . \tag{9.5}$$

The expression between brackets is the continuous case of (C5). When we apply the replica trick (C10), Eq. (9.5) becomes

$$\langle G(\mathbf{r}_1,\mathbf{r}_1,E)\rangle_v=\frac{\delta}{\delta g(\mathbf{r})}\left[\lim_{M\to 0}\frac{1}{M}\ln\left|\int\mathcal{D}v(\mathbf{r})P[v(\mathbf{r})]Z_v^M\right|\right]\bigg|_{g(\mathbf{r})\equiv 0} \; . \tag{9.6}$$

Changing the limit with the functional differential operator, we obtain, after functional derivation,

$$\langle G(\mathbf{r}_1,\mathbf{r}_1;E)\rangle_v=\lim_{M\to 0}\frac{1}{M}\frac{\int\mathcal{D}v(\mathbf{r})P[v(\mathbf{r})]MZ_v^{M-1}\dfrac{\delta Z_v}{\delta g(\mathbf{r})}\bigg|_{g(\mathbf{r})\equiv 0}}{\int\mathcal{D}v(\mathbf{r})P[v(\mathbf{r})]Z_v^M} \; . \tag{9.7}$$

Substituting

$$\frac{\delta Z_v}{\delta g(\mathbf{r})}\bigg|_{g(\mathbf{r})\equiv 0}=\int\mathcal{D}\phi\,\phi(\mathbf{r}_1)\phi(\mathbf{r}_1)\exp\left[\frac{1}{2}\int d\mathbf{r}\,\phi(\mathbf{r})(E-H_{\text{op}})\phi(\mathbf{r})\right] \tag{9.8}$$

in Eq. (9.7) and using the fact that $\int\mathcal{D}v(\mathbf{r})P[v(\mathbf{r}]=1$, we find that Eq. (9.7) simplifies to

$$\begin{aligned}\langle G(\mathbf{r}_1,\mathbf{r}_1,E)\rangle_v=\lim_{M\to 0}\int\mathcal{D}v(\mathbf{r})P[v(\mathbf{r})]\\ \times\Bigg\{\int\mathcal{D}\phi\,\phi(\mathbf{r}_1)\phi(\mathbf{r}_1)\exp\left[\frac{1}{2}\int d\mathbf{r}\,\phi(\mathbf{r})(E-H_{\text{op}})\phi(\mathbf{r})\right]\\ \times\left[\int\mathcal{D}\phi\exp\left[\frac{1}{2}\int d\mathbf{r}\,\phi(\mathbf{r})(E-H_{\text{op}})\phi(\mathbf{r})\right]\right]^{M-1}\Bigg\} \; .\end{aligned}$$

Using the replica concept (C11), we arrive at

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[10] In our particular case, a somewhat more elegant approach is as follows. Instead of averaging Eq. (9.4), we can first use $\ln Z_V=\lim_{M\to 0}(Z_V^M-1)/M$. After changing the order of the limit and differential functional and executing the functional derivation, we perform the average and obtain the result (9.10) without using the more complicated replica trick [Eq. (C10)]. However, this alternative is possible due to the functional derivation with respect to $g(r)$ and is less general than the presented method.

$$G(\mathbf{r}_1,\mathbf{r}_1;E)\rangle_v=\lim_{M\to 0}\int \mathcal{D}v(\mathbf{r})P[v(\mathbf{r})]\left[\int \prod_{i=1}^{M}\mathcal{D}\phi_i\,\phi_1(\mathbf{r}_1)\phi_1(\mathbf{r}_1)\exp\left[\frac{1}{2}\int d\mathbf{r}\sum_{i=1}^{M}\phi_i(\mathbf{r})(E-H_{\mathrm{op}})\phi_i(\mathbf{r})\right]\right] . \tag{9.9}$$

We then write the explicit form of the Hamiltonian operator H_{op} [Eq. (4.1) with Eq. (4.20)], denoting by $\Phi=\{\phi_1,\phi_2,\ldots,\phi_M\}$ the M-component vector field, and reordering of the path integrals finally leads to

$$\langle G(\mathbf{r}_1,\mathbf{r}_1;E)\rangle_v=\lim_{M\to 0}\left[\int \prod_{i=1}^{M}\mathcal{D}\phi_i\phi_1(\mathbf{r}_1)\phi_1(\mathbf{r}_1)e^{S[\Phi]}\right] \tag{9.10}$$

with

$$S[\Phi]=\tfrac{1}{2}\int d\mathbf{r}\sum_{i=1}^{M}\phi_i(\mathbf{r})\left[E+\frac{\hbar^2\nabla^2}{2m}\right]\phi_i(\mathbf{r})+\ln\left[Q\left[\sum_{i=1}^{M}[\phi_i(\mathbf{r})]^2\right]\right] \tag{9.11}$$

and

$$Q\left[\sum_{i=1}^{M}[\phi_i(\mathbf{r})]^2\right]=\int \mathcal{D}v(\mathbf{r})P[v(\mathbf{r})]\exp\left[\frac{1}{2}\int d\mathbf{r}\sum_{i=1}^{M}[\phi_i(\mathbf{r})]^2 v(\mathbf{r})\right] . \tag{9.12}$$

The representation (9.10) is valid for E sufficiently large and negative with a real contour for all $\phi_i(\mathbf{r})$. To obtain a representation for Eq. (3.4) with $\eta>0$, Cardy (1978) shows that a rotation of each contour over $e^{i\pi/4}$ defines Eq. (9.10) for all nonreal E such that the contour can be distorted to enclose singularities of $G(\mathbf{r},\mathbf{r},E\pm i\eta)$. In another approach, Nitzan *et al.* (1977) inserted a convergence factor.

At this point, further elaboration requires a knowledge of the distribution function $P[v]$. The assumption of a Gaussian distribution function is obvious for several reasons. Physically, we have shown before [Eq. (A7)] that heavily doped semiconductors are satisfactorily described in that way. Mathematically, averaging over a Gaussian probability function can be performed exactly because quadratic path integrals can be analytically evaluated. The resulting expression for (9.12) is derived in Appendix D,

$$Q\left[\sum_{i=1}^{M}[\phi_i(\mathbf{r})]^2\right]=\exp\left[\frac{1}{8}\int d\mathbf{u}\int d\mathbf{r}\sum_{i=1}^{M}[\phi_i(\mathbf{r})]^2 W(\mathbf{r}-\mathbf{u})\sum_{i=1}^{M}[\phi_i(\mathbf{u})]^2\right] , \tag{9.13}$$

where the correlation function $W(\mathbf{r}-\mathbf{u})$ is defined in Eq. (6.12). Further evaluation usually consists of approximating Eq. (9.10) by the saddle-point method (Parisi, 1988) about an M-component field Φ_c satisfying

$$\left.\frac{\delta S[\Phi]}{\delta\Phi}\right|_{\Phi_c}=\sum_{i=1}^{M}\frac{\delta S[\Phi]}{\delta\phi_i(\mathbf{u})}=0 . \tag{9.14}$$

Evaluation of Eq. (9.14) for Gaussian statistics (9.13) gives

$$\left[E+\frac{\hbar^2\nabla^2}{2m}\right]\Phi_c(\mathbf{u})+\tfrac{1}{2}\Phi_c(\mathbf{u})\int d\mathbf{r}\,W(\mathbf{r}-\mathbf{u})|\Phi_c(\mathbf{r})|^2=0 . \tag{9.15}$$

The trivial solution $\Phi_c(\mathbf{u})=0$ corresponds to energies in the continuum ($E\geq 0$). After the saddle-point integration is carried out, the expression for the DOS can be written as

$$\rho(E)=A(E)\exp(S[\Phi_c]) , \tag{9.16}$$

where $A(E)$ is a (nonexponential) prefactor that is in general difficult to determine (John and Stephen, 1984). Explicitly, we can write Eq. (9.16) as

$$\rho(E)=A(E)\exp\left[\frac{1}{4}\int d\mathbf{r}\left[E[\Phi_c(\mathbf{r})]^2-\frac{\hbar^2}{2m}[\nabla\Phi_c(\mathbf{r})]^2\right]\right] \tag{9.17}$$

or equivalently

$$\rho(E)=A(E)\exp\left[-\tfrac{1}{8}\int d\mathbf{u}\int d\mathbf{r}\,\Phi_c^2(\mathbf{u})W(\mathbf{r}-\mathbf{u})\Phi_c^2(\mathbf{r})\right] . \tag{9.18}$$

The presented replica procedure exhibits a number of interesting features. First of all, we notice that Eq. (9.15) which determines the instanton in field theory is precisely the same key equation in the work of Halperin and Lax [Eq. (6.25)] and Efros [Eq. (7.20)]. Moreover, this Hartree equation appears in other theories of bandtails (Lifshitz, 1964; Zittartz and Langer, 1966). This fundamental equation returns the wave function in a potential fluctuation obeying Gaussian stochastics. Obviously, there is a close analogy between the instanton and the most probable potential: by solving the instanton equation of motion (9.15), one allows for the most general well shape possible for a Gaussian distribution. Another observation concerns Eq. (9.17), in which the argument for the exponential resembles the variational energy for the wave function Φ_c [see also the review of Thouless (1986,

p. 690)]. This again links the variational method of Halperin and Lax and the replica field approach. Perturbation theory (Cardy, 1978), is not applicable[11] to the region of localized states because a nonzero DOS and a finite localization distance are only found if perturbation theory diverges.

Considering Eq. (9.18), we deduce that the correlation function plays an important role. However, the precise form of this correlation function is hard to find and strongly depends on the kind of disorder. In their study of Urbach tails in amorphous materials, Cohen *et al.* (1988) and John *et al.* (1988) have investigated a broad class of physically interesting correlation functions. They showed that an exponential Urbach tail can be found if a short-range-order correlation function [typically of the form $W(x)=W_0\exp[-(|x|/L)^m]$ with short-range-order radius L and $m\geq 2$] is used. In contrast, in heavily doped semiconductors the potential fluctuation originates from randomly distributed ions and can be approximated (in a Thomas-Fermi approach) by random-screened Coulomb potentials. The corresponding correlation function lies closer to $m\leq 1$, for which the linear exponential regime is very narrow [in fact, rather an inflection point between the Halperin-Lax regime and the deep-tail regime (Fig. 3)].

A last remark concerns the general form of Eq. (9.12). Although the limitation to a Gaussian distribution seems a good approximation for tail states sufficiently below the unperturbed band edge ($E=0$), it remains doubtful whether energy states close to this edge (or in the intermediate region) follow Gaussian statistics.

B. White-noise Gaussian spectrum: $W(r-u)=\frac{1}{2}D\delta(r-u)$

Although the white-noise spectrum may have a limited physical significance, it enables exact results to be derived. Moreover, comparison with older methods described before may illustrate the power of the replica field approach. The white-noise correlation function (4.3) simplifies Eq. (9.13) to

$$Q\left[\sum_{i=1}^{M}[\phi_i(\mathbf{r})]^2\right]=\exp\left[\frac{D}{16}\int d\mathbf{r}\left[\sum_{i=1}^{M}[\phi_i(\mathbf{r})]^2\right]^2\right] . \quad (9.19)$$

Substitution in Eq. (9.11), bearing in mind that

$$\int d\mathbf{r}\,\phi_i(\mathbf{r})\frac{\hbar^2\nabla^2}{2m}\phi_i(\mathbf{r})=-\int d\mathbf{r}\frac{\hbar^2}{2m}[\nabla\phi_i(\mathbf{r})]^2 ,$$

gives the result of Cardy (1978) and Brézin and Parisi (1980),

$$S[\Phi]=\int d\mathbf{r}\left[\frac{1}{2}\sum_{i=1}^{M}\left[E[\phi_i(\mathbf{r})]^2-\frac{\hbar^2}{2m}[\nabla\phi_i(\mathbf{r})]^2\right]+\frac{D}{16}\left[\sum_{i=1}^{N}[\phi_i(\mathbf{r})]^2\right]^2\right] . \quad (9.20)$$

Expression (9.20) with (9.10) resembles the averaged Green's function corresponding to the M-component Landau-Ginzburg model in d dimensions (Parisi, 1988), with effective "Hamiltonian"

$$\mathcal{H}=\int d\mathbf{r}\left[\frac{1}{2}\sum_{i=1}^{M}\{\mu^2[\phi_i(\mathbf{r})]^2+[\nabla\phi_i(\mathbf{r})]^2\}+\frac{1}{4}g|\mu|^{4-d}\left[\sum_{i=1}^{M}[\phi_i(\mathbf{r})]^2\right]^2\right] . \quad (9.21)$$

Comparison between the dimensionless equation (9.21) and (9.20) reveals that

$$\begin{aligned}\mu^2&=-\frac{2mE}{\hbar^2} ,\\ g&=-\frac{D(\hbar^2/2m)^{1-d/2}}{4|E|^{2-d/2}} .\end{aligned} \quad (9.22)$$

Based on this resemblance, Brézin and Parisi (1980) derived expressions for the DOS [Eqs. (9.17) and (9.18)] in two and three dimensions for large negative energies E. In one dimension, the correct exponent and prefactor had already been obtained by Zittartz and Langer (1966). Moreover, Thouless (1986, p. 692) briefly sketches how the derivative of Eq. (4.51), the exact one-dimensional DOS first found by Frisch and Lloyd (1960), may be obtained from Eq. (9.20).

C. Conclusions

The field-theoretical method is the most general and powerful technique discussed here to handle the band-tail problem. The advantage it offers over the path-integral method (Sec. VIII) is that we are not restricted to Gaussian wave functions or to the introduction of quadratic trial actions. In addition, the use of field theory offers some technical and computational advantages (Cohen *et al.*, 1988).

X. CONCLUSION

The deviations from the free-electron DOS due to the random distribution of impurities in a heavily doped semiconductor are described by several models. The most important of these models have been discussed in detail. The exact solution of the band-tail problem in one dimension, has received much attention, as it was used to evaluate the accuracy of approximate theories. An exact solution for heavily doped semiconductors in three dimensions, however, does not exist. We have demonstrated that the semiclassical theory yields a simple asymptot-

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[11] In fact, this statement was already introduced by Wolff (1962), who showed that perturbation theory fails for localized states.

ic formula valid for all energies. This model is particularly useful for the majority carriers in degenerate semiconductors. An approximate expression for the Fermi-level shift purely due to band tailing offers the possibility of introducing band-tail effects into device simulators.

The calculation of the number of carriers in the deep energy tails requires a full quantum-mechanical treatment. The most famous model is that of Halperin and Lax, which clearly describes the fundamental underlying physics. Even today, it remains, together with Kane's semiclassical theory, the most referenced band-tail theory. Efros's optimal-fluctuation theory does not differ significantly from that of Halperin and Lax and has the advantage that non-Gaussian statistics may be treated. If we consider only noninteracting Fermi gases, then there exists an exact description of the band-tail problem in three dimensions, given in terms of a Feynman path integral, i.e., Eq. (8.5). Since this expression is exceedingly complicated, approximations of Eq. (8.5) result in the method of Sa-yakanit, yielding expressions for the whole energy region. Related to the path-integral method, we have the powerful replica method. This technique reproduces the precise solutions of older methods (e.g., the Frisch and Lloyd model in one-dimension). In addition, John *et al.* (1988) argue that for static disorder the replica method is much more efficient than even the path integral. The main advantage of the quantum-mechanical methods is that they are derived from first principles and thus may serve to check approximate models. Moreover, they can be generalized (in principle) to include other physical mechanisms (e.g., electron-phonon interactions, . . .). However, all full quantum-mechanical models lead to numerically complicated solutions, which prohibit their application in device simulators to calculate the number of minority carriers accurately. Apart from the semiclassical model, there seems to be no easy generalization for interacting Fermi liquids available.

ACKNOWLEDGMENTS

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APPENDIX A: THE DISTRIBUTION FUNCTION $P(V)$ FOR A POTENTIAL ENERGY $V(\mathbf{r},\{r_i\})=\sum_{i=1}^{N}v(r-r_i)$

Assuming that the probability of finding an impurity at a point $\mathbf{r}_i$ is constant (and thus equals V_0^{-1}), the probability for the potential energy to have the value V at position $\mathbf{r}$ is defined as

$$P(\mathbf{r},V)=\int\frac{d\mathbf{r}_1}{V_0}\int\frac{d\mathbf{r}_2}{V_0}\cdots\int\frac{d\mathbf{r}_N}{V_0}\delta(V-V(\mathbf{r}-\{\mathbf{r}_i\}))\ . \tag{A1}$$

Employing the identity

$$\delta(x-a)=\frac{1}{2\pi}\int_{-\infty}^{\infty}e^{i(x-a)t}dt\ ,$$

we can rewrite Eq. (A1) as

$$P(\mathbf{r},V)=\frac{1}{2\pi}\int_{-\infty}^{\infty}e^{iVt}f(t;\mathbf{r})dt\ , \tag{A2}$$

where

$$f(t;\mathbf{r})=\left[\int_{V_0}\frac{d\mathbf{R}}{V_0}e^{-iv(\mathbf{r}-\mathbf{R})t}\right]^N\ . \tag{A3}$$

Thermodynamically, the extensive properties of a structure do not change if the volume increases. Applying this principle, the distribution function $P(\mathbf{r},V)$ becomes

$$P(V)=\lim_{\substack{V_0\to\infty\\ N=nV_0}}\frac{1}{2\pi}\int_{-\infty}^{\infty}e^{iVt}\left[1+\frac{1}{V_0}\int_{V_0}d\mathbf{R}(e^{-iv(\mathbf{R})t}-1)\right]^N dt\ . \tag{A4}$$

Moreover, $P(V)$ turns out to be independent of position $\mathbf{r}$, because a change of variables in Eq. (A4) does not alter the integral if $V_0\to\infty$. Let

$$A=\int_{V_0}d\mathbf{R}(e^{-iv(\mathbf{R})t}-1)\ . \tag{A5}$$

If $v(\mathbf{r})$ decreases sufficiently rapidly, then A rapidly approaches a constant value, even while the volume V_0 keeps increasing. The following relationship then applies:

$$\lim_{V_0\to\infty}\left[1+\frac{A}{V_0}\right]^{nV_0}=e^{An}$$

and we finally obtain the exact result

$$P(V)=\frac{1}{2\pi}\int_{-\infty}^{\infty}\exp\left[iVt+n\int d\mathbf{R}(e^{-iv(\mathbf{R})t}-1)\right]dt\ , \tag{A6}$$

whose properties are further explored in Van Mieghem *et al.* (1991). An alternative derivation is proposed by Morgan (1965).

In the high-density limit ($n\to\infty$), $P(V)$ reduces to a Gaussian,

$$P(V)=\frac{\exp(-x^2/2)}{\sqrt{2\pi}\sigma} \tag{A7}$$

with

$$\sigma^2=b_2\ ,$$

$$x=\frac{b_1-V}{\sigma}\ ,$$

and

$$b_m=n\int d\mathbf{R}\,v^m(\mathbf{R})\ , \tag{A8}$$

which considerably simplifies both the interpretation and the calculation of $P(V)$. The shift b_1 results from the average potential of the charged impurities. Due to charge neutrality, however, this energy shift is exactly compensated by the potential energy of the electrons and will be disregarded further.

APPENDIX B: MATHEMATICAL PROPERTIES OF PATH INTEGRALS WITH QUADRATIC ACTION[12]

The simplest path integrals are those in which all of the variables appear up to second degree in an exponent. Let us consider a particle whose Lagrangian has the form

$$\begin{aligned}L(\dot{x};x;t)=a(t)\dot{x}^2+b(t)\dot{x}x+c(t)x^2\\ +d(t)\dot{x}+e(t)x+f(t)\ .\end{aligned} \tag{B1}$$

We wish to determine

$$K(b,a)=\int_a^b \exp\left[\frac{i}{\hbar}\int_{t_a}^{t_b}L(\dot{x};x,t)dt\right]\mathcal{D}x(t)\ , \tag{B2}$$

the integral over all paths that go from (x_a,t_a) to (x_b,t_b). Notice first that the form of the Lagrangian is more general than necessary for our purpose. Since we are concerned only with Eq. (B2), we could remove the factor $\dot{x}$ from those terms in which it is linear through an integration by parts.

If we denote $\xi(t)$ as the classical path between the specified end points, then $\xi(t)$ is an extremum for the action S, and we write $S_{\rm cl}[b,a]=S[\xi(t)]$. We now change the variable x in Eq. (B2) by

$$x=\xi+y\ . \tag{B3}$$

This means that, instead of defining a point on the path by its distance $x(t)$ from an arbitrary coordinate axis, we measure instead the deviation $y(t)$ from the classical path. Since the classical path $\xi(t)$ is well defined, it does not vary, and hence $\mathcal{D}x(t)=\mathcal{D}y(t)$.

The action becomes

$$\begin{aligned}S[x(t)]&=S[\xi(t)+y(t)]\\ &=\int_{t_a}^{t_b}[a(t)(\dot{\xi}^2+2\dot{\xi}\dot{y}+\dot{y}^2)+\cdots]dt\ .\end{aligned} \tag{B4}$$

If all the terms that do not involve y are collected, the resulting integral is just $S[\xi(t)]=S_{\rm cl}[b,a]$. Since ξ is so chosen that there is no change in S, to first order, for the variations of the path around ξ ($\delta S=S[\xi+y]-S[\xi]=0$), all terms that contain y as a linear factor cancel, and all that remain are the second-order terms in y. Thus Eq. (B4) equals

$$S[x(t)]=S_{\rm cl}[b,a]+\int_{t_a}^{t_b}[a(t)\dot{y}^2+b(t)\dot{y}y+c(t)y^2]dt\ , \tag{B5}$$

and the kernel (or propagator) reduces to

$$K(b,a)=\exp\left\{\frac{i}{\hbar}S_{\rm cl}[b;a]\right\}\int_0^0\exp\left[\frac{i}{\hbar}\int_{t_a}^{t_b}[a(t)\dot{y}^2+b(t)\dot{y}y+c(t)y^2]dt\right]\mathcal{D}y(t)\ . \tag{B6}$$

Since all paths $y(t)$ start and return to the point $y=0$, the integral over paths is only a function of the times at the end points, and hence

$$K(b,a)=\exp\left[\frac{i}{\hbar}S_{\rm cl}[b;a]\right]F(t_a,t_b)\ . \tag{B7}$$

The dependence upon the spatial variables x_a and x_b is completely determined. The factor $F(t_a,t_b)$ must be determined by some other property of the solution, as, for example,

$$K(b,a)=\int_{\text{all possible values of }x_c}dx_c K(b,c)K(c,a) \tag{B8}$$

or by evaluation through Fourier series expansion (Feynman and Hibbs, pp. 71–73).

An important special case of (B1) is the Lagrangian of a free particle,

$$L=\frac{1}{2}m\dot{x}^2 \tag{B9}$$

with its corresponding action

$$S[b,a]=\frac{1}{2}m\frac{(x_b-x_a)^2}{t_b-t_a} \tag{B10}$$

and kernel (where d stands for the dimension)

$$K(b,a)=\left[\frac{m}{2\pi i\hbar(t_b-t_a)}\right]^{d/2}\exp\left[\frac{im(\mathbf{x}_b-\mathbf{x}_a)^2}{2\hbar(t_b-t_a)}\right]\ . \tag{B11}$$

Let us now consider the average $\langle\cdots\rangle_S$ of a functional A through a quadratic action S, which is defined as

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[12] Most of the results are summarized from Feynman and Hibbs (1965).

$$\langle A\rangle_S=\frac{\int\mathcal{D}(\mathbf{r}(\tau))\exp\left[\frac{i}{\hbar}S\right]A}{\int\mathcal{D}(\mathbf{r}(\tau))\exp\left[\frac{i}{\hbar}S\right]} . \tag{B12}$$

If we choose for the functional A the particular form

$$A=\exp\left[\frac{i}{\hbar}\int d\tau\,\mathbf{f}(\tau)\cdot\mathbf{r}(\tau)\right] \tag{B13}$$

then the numerator exhibits an action $S'=S+\int d\tau\,\mathbf{f}(\tau)\cdot\mathbf{r}(\tau)$, which is clearly quadratic. Thus the numerator path integral can be worked out as explained above, so that

$$\int_a^b\mathcal{D}(\mathbf{r}(\tau))\exp\left[\frac{i}{\hbar}S'\right]=\exp\left[\frac{i}{\hbar}S'_{\mathrm{cl}}[b;a]\right]F'(t_a,t_b) . \tag{B14}$$

The integral over the paths $y,F'(t_a,t_b)$ does not depend on the function $\mathbf{f}(t)$, because this function appears in the action S' multiplying only a linear term in $\mathbf{r}(t)$ and, from Eq. (B6), $F'(t_a,t_b)$ contains only quadratic parts of S'. Hence $F'(t_a,t_b)=F(t_a,t_b)$, which implies that

$$\left\langle\exp\left[\frac{i}{\hbar}\int d\tau\,\mathbf{f}(\tau)\cdot\mathbf{r}(\tau)\right]\right\rangle_S=\exp\left[\frac{i}{\hbar}[S'_{\mathrm{cl}}[b;a]-S_{\mathrm{cl}}[b;a]]\right] . \tag{B15}$$

Once the classical action $S'_{\mathrm{cl}}[b;a]$ has been obtained, $S_{\mathrm{cl}}[b;a]$ can be found by simply setting $\mathbf{f}(\tau)\equiv 0$. Suppose we take the functional derivative with respect to $\mathbf{f}(\tau)$ to Eq. (B15) to obtain

$$\begin{aligned}\left\langle\mathbf{r}(\tau)\exp\left[\frac{i}{\hbar}\int d\tau\,\mathbf{f}(\tau)\cdot\mathbf{r}(\tau)\right]\right\rangle_S&=\frac{\hbar}{i}\frac{\delta}{\delta\mathbf{f}(\tau)}\left[\exp\left[\frac{i}{\hbar}(S'_{\mathrm{cl}}[b;a]-S_{\mathrm{cl}}[b;a])\right]\right]\\&=\frac{\delta S'_{\mathrm{cl}}[b;a]}{\delta\mathbf{f}(\tau)}\left[\exp\left[\frac{i}{\hbar}(S'_{\mathrm{cl}}[b;a]-S_{\mathrm{cl}}[b;a])\right]\right] .\end{aligned}$$

Evaluating both sides when $\mathbf{f}(t)\equiv 0$, we obtain

$$\langle\mathbf{r}(\tau)\rangle_S=\left.\frac{\delta S'_{\mathrm{cl}}[b;a]}{\delta\mathbf{f}(\tau)}\right|_{\mathbf{f}(\tau)\equiv 0} . \tag{B16}$$

We can continue this process to get the second derivative,

$$\langle\mathbf{r}(\tau)\cdot\mathbf{r}(\sigma)\rangle_S=\frac{\hbar}{i}\left.\left[\frac{\delta^2S'_{\mathrm{cl}}}{\delta\mathbf{f}(\tau)\delta\mathbf{f}(\sigma)}+\frac{\delta S'_{\mathrm{cl}}\delta S'_{\mathrm{cl}}}{\delta\mathbf{f}(\tau)\delta\mathbf{f}(\sigma)}\right]\right|_{\mathbf{f}\equiv 0} . \tag{B17}$$

Actually, since S' is quadratic only in $\mathbf{f}$, the average of any number of $\mathbf{r}(\tau)$, $\langle\mathbf{r}(\tau)\mathbf{r}(\lambda)\cdots\mathbf{r}(\sigma)\rangle_S$, can be directly evaluated in terms of

$$\frac{\delta^2S'_{\mathrm{cl}}}{\delta\mathbf{f}(\tau)\delta\mathbf{f}(\sigma)}\quad\text{and}\quad\frac{\delta S'_{\mathrm{cl}}}{\delta\mathbf{f}(\tau)} .$$

APPENDIX C: THE REPLICA TRICK

From the basic principle of statistical mechanics (Feynman, 1972), once the partition function Z is known, all thermodynamic properties can be found. Consider a system whose Hamiltonian H_V depends on a certain potential configuration V. This potential configuration is a stochastic variable with probability $P[V]$. For a certain choice of V we can compute the partition function

$$Z_{V(N)}=\sum_{i=1}^{N}e^{-\beta E_{V(N)}(i)} , \tag{C1}$$

where $\beta=1/k_BT$ and $E_{V(N)}(i)$ is the ith energy state belonging to H_V in a finite volume, which implies a finite number of states N. The corresponding free-energy density is

$$f_{V(N)}=-1/\beta N\ln Z_{V(N)} . \tag{C2}$$

The principle of the thermodynamic limit states that for $N\rightarrow\infty$ (infinite-volume limit) the free-energy density does not change or

$$\lim_{N\rightarrow\infty}f_{V(N)}=f_V^{\infty} . \tag{C3}$$

This principle has proven to be very useful in computations (see, for example, Appendix A).

We are interested in the average of the free-energy density of the possible potential configurations

$$\begin{aligned}\langle f_N\rangle_{V(N)}&=\sum_{V(N)}P[V(N)]f_{V(N)}\\&=-1/\beta N\sum_{V(N)}P[V(N)]\ln Z_{V(N)} .\end{aligned} \tag{C4}$$

Suppose now that direct computation of Eq. (C4) is hard but that $\sum_{V(N)}P[V(N)](Z_{V(N)})^m$ would be feasible. The replica method yields a formal solution procedure for the computation of (C4). Define

$$\langle g_N\rangle_{V(N)}=-\beta N\langle f_N\rangle_{V(N)} \tag{C5}$$

and use the relation

$$\lim_{m\rightarrow 0}\frac{1}{m}\ln|1+mA|=A , \tag{C6}$$

yielding

$$\langle g_N\rangle_{V(N)}=\lim_{m\rightarrow 0}\frac{1}{m}\ln\left|1+m\left[\sum_{V(N)}P[V(N)]\ln Z_{V(N)}\right]\right| . \tag{C7}$$

Since $\sum_{V(N)}P[V(N)]=1$, the argument of the logarithm reads

$$1+m\left[\sum_{V(N)} P[V(N)]\ln Z_{V(N)}\right] = \sum_{V(N)} P[V(N)](1+m\ln Z_{V(N)}) \; . \tag{C8}$$

Invoking the fact that

$$1+m\ln Z_{V(N)}=(Z_{V(N)})^m \quad \text{for } m\to 0 \; , \tag{C9}$$

we finally obtain the replica alternative formula for Eq. (C4),

$$\langle f_N\rangle_{V(N)}=-1/\beta N \lim_{m\to 0}\frac{1}{m}\ln\left|\sum_{V(N)} P[V(N)](Z_{V(N)})^m\right| \; . \tag{C10}$$

The name "replica" originates from the calculation of $(Z_{V(N)})^m$ by taking m duplicates of the system. Indeed,

$$\begin{aligned}(Z_{V(N)})^m &= \sum_{k_1=1}^{N} e^{-\beta N_{V(N)}(k_1)} \sum_{k_2=1}^{N} e^{-\beta E_{V(N)}(k_2)} \cdots \sum_{k_m=1}^{N} e^{-\beta E_{V(N)}(k_m)} \\ &= \sum_{k_1=1}^{N}\sum_{k_2=1}^{N}\cdots\sum_{k_m=1}^{N} \exp\left[-\sum_{j=1}^{m}\beta E_{V(N)}(k_j)\right] \; ,\end{aligned} \tag{C11}$$

meaning that the partition function of m (noninteracting) replicas of the system is the partition function of the original system to the power m.

The replica method is a formal procedure. The $m\to 0$ limit assumes a continuous variable m where one usually only disposes of integer values of m. The impossibility of analytic continuation of the free energy from its values on the integers down to its value at $m=0$ constitutes a weak point of the method. Further, the derivation demonstrates that first the limit $m\to 0$ and afterwards the $N\to\infty$ (thermodynamic limit) should be taken. However, in practice, a reversal of this order seems to be permitted, as discussed by Mézard *et al.* (1987). Finally, complications may occur in what is called "breaking of the replica symmetry," which is connected in some way with the order of the limits. For this, we refer the reader to Mézard *et al.* (1987) because it is not part of our problem.

APPENDIX D: EVALUATION OF THE AVERAGE (9.12) OVER ALL POTENTIAL CONFIGURATIONS HAVING A GAUSSIAN DISTRIBUTION FUNCTION

The problem is to calculate a path integral of the form

$$Q[f(\mathbf{r})]=\int \mathcal{D}v(\mathbf{r})P[v(\mathbf{r})]\exp\left[\tfrac{1}{2}\int d\mathbf{r}\, f(\mathbf{r})v(\mathbf{r})\right] \; , \tag{D1}$$

where the probability $P[v(\mathbf{r})]$ is assumed to be Gaussian, and characterized by the first two moments (see Sec. IV.C)

$$\begin{aligned}&\langle v(\mathbf{r})\rangle=0 \; ,\\ &\langle v(\mathbf{r})v(\mathbf{u})\rangle=A(|\mathbf{r}-\mathbf{u}|) \; .\end{aligned} \tag{D2}$$

Feynman and Hibbs (p. 333) show that the corresponding probability functional $P[v(\mathbf{r})]$ equals

$$P[v(\mathbf{r})]=\exp\left[-\tfrac{1}{2}\int d\mathbf{r}\int d\mathbf{u}\, v(\mathbf{r})B(\mathbf{r}-\mathbf{u})v(\mathbf{u})\right] \; , \tag{D3}$$

where

$$\int d\mathbf{u}\, B(\mathbf{r}-\mathbf{u})A(\mathbf{u})=\delta(\mathbf{r}) \; , \tag{D4}$$

or, the Fourier transform of the correlation function $A(\mathbf{u})$ is the inverse of the Fourier transform of the $B(\mathbf{u})$. With Eq. (D3) the path integral (D1) resembles a path integral with quadratic action, where the argument of the exponential $S[v(\mathbf{r})]$ is

$$\begin{aligned}S[v(\mathbf{r})]=&-\tfrac{1}{2}\int d\mathbf{r}\int d\mathbf{u}\, v(\mathbf{r})B(\mathbf{r}-\mathbf{u})v(\mathbf{u})\\ &+\tfrac{1}{2}\int d\mathbf{r}\, f(\mathbf{r})v(\mathbf{r}) \; .\end{aligned} \tag{D5}$$

This kind of path integral can be evaluated exactly (Appendix B). Proceeding as in Appendix B, we find the analog of the classical action by first solving

$$\frac{\delta S[v(\mathbf{r})]}{\delta v(\mathbf{u})}=0=f(\mathbf{u})-\int d\mathbf{r}\, B(\mathbf{u}-\mathbf{r})v(\mathbf{r}) \; . \tag{D6}$$

Multiplying both sides of Eq. (D6) with $A(\mathbf{x}-\mathbf{u})$, integrating over all space, and using Eq. (D4) solves (D6) with the resulting analog for the classical path

$$v_c(\mathbf{x})=\tfrac{1}{2}\int d\mathbf{u}\; A(\mathbf{x}-\mathbf{u})f(\mathbf{u}). \tag{D7}$$

Substitution of Eq. (D7) in (D5) gives the analog of the classical action,

$$S_c=\tfrac{1}{8}\int d\mathbf{u}\int d\mathbf{r}\, f(\mathbf{r})A(\mathbf{r}-\mathbf{u})f(\mathbf{u}) \; . \tag{D8}$$

According to Eq. (B7) we have for (D1)

$$Q[f(\mathbf{r})]=F\exp\left[\tfrac{1}{8}\int d\mathbf{u}\int d\mathbf{r}\, f(\mathbf{r})A(\mathbf{r}-\mathbf{u})f(\mathbf{u})\right] \; . \tag{D9}$$

The remaining constant F is found by the normalization condition for the probability, or equivalently $Q[0]=1$, yielding $F=1$.

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