Effects of electronic energy-band structure on the energy distribution of field-emitted electrons

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Current three-dimensional formulations of field emission of (noninteracting) electrons are critically examined and compared. It is shown that the kinetic-theory description for the energy distribution of field-emitted electrons (FEED) can be brought into a complete formal agreement with the theory of Penn and Plummer (PP). The reinterpretations of the parameters in the PP theory enable us to demonstrate its relationship to a nearly-free-electron theory. It is shown that the claim that FEED measures the "one-dimensional local density of states" as defined by PP is an approximation which may neglect some possibly significant band-structure effects in transition metals. In FEED these manifest themselves in the contribution of states with reduced two-dimensional wave vectors differing from zero. The relationship between Penn and Plummer's theory and a recent, more exact application of Appelbaum and Brinkman's transfer-Hamiltonian formalism, by Nicolaou and Modinos is discussed. A new expression for FEED is derived from Feuchtwang's many-body theory of tunneling. The limitations of the kinetic formulation are contrasted with a complete transfer-Hamiltonian formulation such as Nicolaou and Modinos's and a more exact tunneling theory by Feuchtwang. It is shown that the kinetic theory does not allow for either inelastic tunneling or surface-band-structure effects. It is also shown that the kinetic formulation of FEED involves a "coarse average" over an appropriate "surface" plane of the local density of states in contrast to the more complete theories in which the FEED depends on the full spectral density.

I. INTRODUCTION

In the past fifteen years, a considerable amount of effort has gone into the examination of the influence of the bulk electronic energy-band structure and many-body effects on tunneling in "metal-insulator-metal" junctions,[1] and on the "field emission energy distribution" (FEED) of electrons from metals.[2-21] Some of these analyses were based on the early version of the transfer-Hamiltonian formalism, which was introduced first by Bardeen[22] and Cohen, Falicov, and Phillips,[23] and then adapted by Harrison.[3] Most, however, were based on the more elementary kinetic formulation of tunneling for noninteracting systems.[5]

It has recently been suggested that the tunneling current[1] and FEED are sensitive to, and hence can probe the "one-dimensional (local) density of states" at some appropriate reference plane.[19-21] This conclusion is based on an adaptation, by Penn et al.,[20] of the reformulation of the transfer-Hamiltonian formalism by Appelbaum and Brinkman.[14]

Proceeding from Keldysh's[24] perturbation theory for nonequilibrium processes in many-body systems, Caroli et al. reached a somewhat similar conclusion.[25] In a series of papers they show that the tunneling current[1] depends on the mixed second derivative of appropriately defined spectral densities for the uncoupled electrodes, evaluated at an appropriate reference plane.[26] It should be mentioned that Caroli et al.[25] differ with Penn et al.,[19-21] in some important details. The former

find the tunneling current depends on the derivatives of the spectral density, rather than simply on the local density of states, which (within a factor of 2π) is the spectral density with both position variables equal.

Feuchtwang[27] used Keldysh's perturbation theory in a significantly different approach and corroborated the Caroli et al. findings. He also demonstrated that the dependence of the tunneling current on the mixed second derivative of the spectral densities, found by Caroli et al., was an artifact of their particular convention in defining the spectral densities. Feuchtwang showed that, in a strictly one-dimensional theory, the tunneling current can be expressed in terms of the local densities of states at appropriate reference planes provided that a different convention for the spectral densities of the uncoupled electrodes is adopted, i.e., provided the wave functions of the uncoupled electrodes satisfy Neumann rather than Dirichlet boundary conditions at the surface. Both Caroli et al. and Feuchtwang's theories differ from those invoking the transfer-Hamiltonian formalism in that the tunneling "matrix element" is replaced by a functional of the full single-particle Green's function of the system, which in the one-dimensional theories is an explicit function of the corresponding Green's functions of the uncoupled electrodes. It is not clear under what restrictions the two theories assume their respective "transfer-Hamiltonian-like" form for realistic models of interacting systems—if such representation is at all possible! The difficulty, as pointed out by

Caroli et al.,[28] is not a limitation of the basic formulation, but rather formal, viz. the proper definition of the "uncoupled" electrodes in the presence of an interaction (such as the electron-electron and/or electron-phonon interactions) represented by a nonlocal self-energy operator.[29]

Most workers treat the tunneling problem for (i) a planar junction, subject to the assumption that the tunneling barrier is one dimensional, and (ii) a separable effective single-particle potential characterizing the "uncoupled" electrodes. Both of these assumptions are necessary if tunneling in a three-dimensional junction is to be reduced to an effective one-dimensional problem. In the kinetic formulations, the usual procedure is to invoke an effective-mass approximation[30] and to assume the normal to the junction plane coincides with a principal axis of the effective-mass tensor.[31] The transfer-Hamiltonian formulations often assume the system to be translationally invariant in the plane of the junction.[32] The same assumption was made by Caroli et al. in most of their work.[33] A general expression for FEED from an arbitrary noninteracting metal was given by Caroli et al., without detailed derivation[34]; another, presumably equally general expression for the tunneling current based on the transfer-Hamiltonian formalism, is given by Appelbaum and Brinkman.[35] Feuchtwang considered the general case of a nonplanar junction as well as the ordered planar junction.[36,37] While the explicit expressions for the tunneling current derived by these three groups differ in detail, they all predict the current to depend on a weighted average, over the interface, of the product of the spectral densities of the uncoupled electrodes.

At this point three obvious questions suggest themselves:

(a) What if any is the relation between the four formulations of tunneling? Specifically, is there any physical content in the theories based on the transfer-Hamiltonian formalism which is not accounted for by the kinetic formulation of tunneling?

(b) Is Penn et al.'s formulation completely equivalent to Appelbaum and Brinkman's?

(c) How is the latter formulation related to the theories of Caroli et al. and of Feuchtwang, and how are these two related?

The answer to the first two questions constitutes the substance of this paper. The remaining question has been dealt with in previous publications: Appelbaum and Brinkman's tunneling theory, based on their reformulation of the transfer-Hamiltonian formalism, has been shown to correspond physically to a "thick-barrier approximation" of Feuchtwang's[36,38] theory. The relation between

the theories of Caroli et al. and Feuchtwang has been discussed in Ref. 27 and further elaborated in a recent publication.[39]

In Sec. II, we shall discuss the relation between Penn et al.'s theory and the simplified kinetic theory. A new expression for FEED is derived from Feuchtwang's many-body tunneling theory and is contrasted with the other theories. In Sec. III, we compare the more complete kinetic theory of Nicolaou and Modinos[12] with the theories of Penn et al., Appelbaum and Brinkman, and Feuchtwang.

In Sec. IV, we summarize our analysis of the inter-relations of the different formulations of field emission. We also consider the relationship between current and earlier treatments of field emission from the d bands of transitions metals. Finally we discuss critically, and elaborate on, the physical significance of the "one-dimensional local density of states."

II. RELATION BETWEEN PENN'S AND THE KINETIC FORMULATION OF FIELD EMISSION

A. Derivation of the simplified kinetic formulation

1. Basic assumptions and procedures

In this section, we develop a simplified kinetic formulation of field emission, which, however, is significantly more general than the Fowler-Nordheim theory. The purpose of this discussion is to elucidate the weakest set of assumptions and consequent limitations of the traditional formulation of field emission. A more complete kinetic formulation which overcomes some of these limitations will be considered in the next section.

A strict kinetic formulation of field emission involves the factorization of the flux, or current density, into a product of a (group) velocity and a particle (or probability) density.[40] This factorization is exact only for eigenstates of the momentum.[40] It retains a limited validity, to be elaborated below, for Bloch states in a periodic potential. We therefore restrict ourselves to a semi-infinite emitter bounded by a single planar surface.

The following additional assumptions are also essential: (i) The electrons can be represented as a system of noninteracting quasiparticles, (ii) the electrons experience a static potential, and (iii) the electrons encounter an "effectively one-dimensional" tunneling barrier.

By "effectively" we mean that the barrier may exhibit a dependence on the two transverse coordinates in the plane of the surface, provided this dependence has a period which is commensurate with that of bulk lattice planes parallel to the surface.

Additional assumptions will be invoked in our derivation of the kinetic formulations. These will be numbered consecutively.

Clearly the crystal potential spoils the separability of the single-particle Hamiltonian. However, a reduction to an essentially one-dimensional problem can still be achieved by two different procedures:

(a) The first involves the effective mass method as discussed, for example, by Duke.[41] This approach is implicit in all of the early theoretical analysis of field emission,[2-5] all of which assume a strictly one-dimensional barrier.

(b) The alternative procedure takes advantage of the residual, two-dimensional periodicity of the problem, and of the consequent conservation of the reduced two-dimensional wave vector $\vec{k}_\rho$: The three-dimensional partial differential Schrödinger equation is transformed into a system of coupled one-dimensional ordinary differential equations. This procedure has both conceptual and practical advantages. In fact, it is the basis of a systematic approximation scheme to calculate the elastically back-scattered intensity of a low-energy electron beam incident at the surface from the outside.[42,43] It is also the basis of more complete kinetic analyses of field emission first formulated by Itskovitch,[6] and Politzer and Cutler,[11] and more recently by Nicolaou and Modinos.[12]

2. Definition of basis set

It is now convenient to introduce the basis set for the semi-infinite lattice to which we shall refer throughout our discussion. There exists a complete orthonormal set of single-particle "outgoing scattering states" for the semi-infinite solid extending over the half space $z \leq 0$, which satisfies the asymptotic boundary conditions

$$\lim_{z \to -\infty} \Psi^{(+)}(\vec{r}; \vec{k}_\rho, E; k_z^\mu)$$

$$= \psi_B^{(in)}(\vec{r}; \vec{k}_\rho, E; k_z^\mu)$$

$$+ \sum_\nu R_{\mu\nu}(\vec{k}_\rho, E) \psi_B^{(out)}(\vec{r}; \vec{k}_\rho, E; k_z^\nu), \quad (2.1)$$

$$\lim_{z \to \infty} \Psi^{(+)}(\vec{r}; \vec{k}_\rho, E; k_z^\mu)$$

$$= \sum_m e^{i(\vec{k}_\rho + \vec{K}_m) \cdot \vec{\rho}} T_{\vec{K}_m}(\vec{k}_\rho, E; k_z^\mu) \, \phi(z; \vec{k}_\rho, E; \vec{K}_m).$$

$$(2.2)$$

$$\vec{K}_m \equiv 2\pi(m_1 \vec{b}_1 + m_2 \vec{b}_2);$$

$$m \equiv (m_1, m_2), \quad m_1, m_2 \text{ integers}, \quad (2.3)$$

is a vector in the two-dimensional lattice reciprocal to the two-dimensional lattice defined by the

surface plane, and spanned by the primitive basis vectors $\{\vec{a}_1, \vec{a}_2\}$. That is

$$\vec{a}_i \cdot \vec{b}_j = \delta_{ij}; \quad i, j = 1, 2. \quad (2.4)$$

The functions ϕ satisfy the asymptotic condition

$$\lim_{z \to \infty} -i\left(\phi^* \frac{d}{dz}\phi - \frac{d}{dz}(\phi^*)\phi\right) \geq 0. \quad (2.5)$$

In the absence of any external field and neglecting the classical image charge potential

$$\phi(z; \vec{k}_\rho, E; \vec{K}_m) = \exp\{i \, [(2m/\hbar^2)E - (\vec{k}_\rho + \vec{K}_m)^2]^{1/2} z\}. \quad (2.6)$$

The functions ψ_B are the Bloch functions normally labeled by the reduced three-dimensional wave vector $\vec{k}$ and the band index n. Here however they are labeled by the two-dimensional reduced wave-vector $\vec{k}_\rho$, the energy E, and the index μ. This index labels the branches of the multivalued function $k_z(\vec{k}_\rho, E)$, which is the inverse of the multi-valued energy dispersion relation

$$E - \epsilon(\vec{k}_\rho, k_z) = 0, \quad (2.7)$$

whose branches are labeled by n. The superscript in (out) denotes that the z component of the group velocity in these states is positive (negative). That is, the sum over μ includes all of the real-valued roots of Eq. (2.7) such that

$$v_{g_z}(\vec{k}_\rho, k_z = k_z^\mu; E) = \frac{1}{\hbar}\frac{\partial \epsilon}{\partial k_z}(\vec{k}_\rho, k_z; E)\bigg|_{k_z = k_z^\mu} \geq 0. \quad (2.8)$$

The quantum numbers $(\vec{k}_\rho, E)$ specify a finite set of linearly independent (and hence orthogonalizeable) functions $\Psi^{(+)}$ whose elements we label by the *index k_z^μ* or μ for short. Here we emphasize that while k_z is a convenient label it does not correspond to a conserved quantity in the states $\Psi^{(+)}$, which are not eigenstates of the lattice translation operator normal to the surface plane.[44]

$\Psi^{(+)}$ may be interpreted as the complete field associated with a single incoming Bloch state $\psi_B^{(in)}$, with the (back) scattering at the surface region properly accounted for. It is well known that $\Psi^{(+)}$ can be expanded in terms of so-called generalized Bloch functions.[42,45] It is important to realize that the incoming component of $\Psi^{(+)}$ is multiplied by a position dependent amplitude $|A(z; k, E)|$ < 1 which only tends to unity as $z \to -\infty$. This amplitude accounts for intensity scattered out of the asymptotic incident wave component, $\psi_B^{(in)}$, by the long-range deviations from perfect periodicity of the crystalline potential in the region to the left of z, due to the surface at $z = 0$. We shall denote the incoming component of $\Psi^{(+)}$ by $\psi^{(in)}(\vec{r}; \vec{k}_\rho; E; k_z^\nu)$. This *partial* field is an approximate solution of the

wave equation which tends to the exact solution $\psi_B^{(in)}$ deep inside the metal as $z \to -\infty$. As z tends to the surface, the deviation of the potential from perfect periodicity gives rise to a scattered field which is not included in $\psi^{(in)}$. Furthermore, $\psi^{(in)}$ does not satisfy the boundary conditions imposed on the complete field $\Psi^{(+)}$ at $z = 0$. The (partial) current carried by $\psi^{(in)}$ has therefore a divergence, though it tends to a divergenceless limit as $z \to -\infty$. We shall write,

$$\psi^{(in)}(\vec{r};\vec{k}_\rho,E;k_z^\nu) \approx A(z;\vec{k}_\rho,E;k_z^\nu)$$
$$\times \psi_B^{(in)}(\vec{r};\vec{k}_\rho,E;k_z^\nu), \qquad (2.9)$$

where

$$|A(z;\vec{k}_\rho,E;k_z^\nu)|^2 = \left(\int_{\Omega_0(z)} |\psi^{(in)}(\vec{r};\vec{k}_\rho,E;k_z^\nu)|^2 d^3r \right)$$
$$\times \left(\int_{\Omega_0} |\psi_B^{(in)}(\vec{r};\vec{k}_\rho,E;k_z^\nu)|^2 d^3r \right)^{-1}.$$
$$(2.10)$$

Here Ω_0 is the nonprimitive unit cell defined by the vectors $\{\vec{a}_1,\vec{a}_2\}$ in the plane of the surface and the basis vector $\vec{a}_z$ normal to this plane. $\Omega_0(z)$ signifies that the integral is to be taken over a unit cell located at z.

An alternative treatment of this effect is to modify the Bloch functions to account for the z dependence of the "local" periodic potential.[46] We shall assume this position dependence—and hence also that of A—to be negligible over distances of the order of the nonprimitive basis vector $|\vec{a}_z|$.

Within the effective-mass method, and for a strictly one-dimensional barrier the sum in Eq. (2.1) is approximated by the single term for which $k_z^\mu = -k_z^\nu$.

3. Definition of transmission probability

We now define the two-dimensional space average, over a plane parallel to the surface, of the normal or z component of the partial current, $\vec{j}^{in}$, carried by the $\psi^{(in)}$ component of $\Psi^{(+)}$:

$$\frac{1}{S} \int \int_{z=const} \vec{j}^{in}(\vec{r};\vec{k}_\rho,E;k_z^\nu) \cdot d\vec{s} \equiv \langle j_z^{in}(z;\vec{k}_\rho,E;k_z^\nu) \rangle.$$
$$(2.11)$$

S is the cross-sectional area of the emitter, and is an integral multiple of the area "A" of the two-dimensional unit cell in the surface plane. In the following the angular brackets denote an average over the plane $z = const$.

We note that for a Bloch state conservation of current ensures that the quantity

$$\langle j_{z,B}(\vec{k}_\rho,E;k_z^\nu) \rangle$$

$$= \mathrm{Re}\left(\frac{1}{S} \int \int_{z=z_0} \psi_B^*(\vec{r};\vec{k}_\rho,E;k_z^\nu) \right.$$
$$\left. \times \frac{\hbar\vec{\nabla}}{mi} \psi_B(\vec{r};\vec{k}_\rho,E;k_z^\nu) \cdot d\vec{s} \right) \quad (2.12)$$

is independent of z_0.[47] Therefore,

$$S\langle j_{z,B}(\vec{k}_\rho,E;k_z^\nu)\rangle = v_{g_z}(\vec{k}_\rho,E;k_z^\nu)$$
$$\times |L^{-1/2}N(\vec{k}_\rho,E;k_z^\nu)|^2, \quad (2.13)$$

where $SL = \Omega$ is the normalization volume of the Bloch functions whose normalization constant is N. The discussion in Sec. II, of the slow variation of the "local" periodic potential implies that the z dependence of j_z^{in} can be accounted for by the amplitude factor A [of Eq. (2.10)] which exhibits a correspondingly weak z dependence. Therefore

$$S\langle j_z^{in}(z;\vec{k}_\rho,E;k_z^\nu)\rangle \approx S|A(z;\vec{k}_\rho,E;k_z^\nu)|^2\langle j_{z,B}(\vec{k}_\rho,E;k_z^\nu)\rangle$$
$$= v_{g_z}(\vec{k}_\rho,E;k_z^\nu)|L^{-1/2}A(z;\vec{k}_\rho,E;k_z^\nu)N(\vec{k}_\rho,E;k_z^\nu)|^2$$
$$\equiv v_{g_z}(\vec{k}_\rho,E;k_z^\nu)|L^{-1/2}\mathfrak{N}(\vec{k}_\rho,E;k_z^\nu;z)|^2. \quad (2.14)$$

Outside the surface plane, conservation of current ensures that the *net* average z component of the flux

$$S\langle j_z(\vec{k}_\rho,E;k_z^\nu)\rangle$$

$$= \mathrm{Re}\left(\int \int_{z=z_0>0} \Psi^{(+)*}(\vec{r};\vec{k}_\rho,E;k_z^\nu) \right.$$
$$\left. \times \frac{\hbar}{mi} \vec{\nabla}\Psi^{(+)}(\vec{r};\vec{k}_\rho,E;k_z^\nu) \cdot d\vec{s} \right)$$
$$(2.15)$$

is independent of z_0. Here Eqs. (2.2)–(2.5) guarantee that this flux is equal to the transmitted or outgoing average normal flux as $z \to +\infty$. Equations (2.13)–(2.15) represent implicitly the starting point of any kinetic theory of field emission.

We now can define the "transmission probability" across the region bounded by the planes $z = z_1, z_2$ by the ratio of the average transmitted normal flux, incident at z_2, to the average incident normal flux, incident at $z = z_1$:

$$D_{z_1 z_2}(\vec{k}_\rho,E;k_z^\nu) = \frac{\langle j_z^{in}(z=z_2;\vec{k}_\rho,E;k_z^\nu)\rangle}{\langle j_z^{in}(z=z_1;\vec{k}_\rho,E;k_z^\nu)\rangle}$$

$$\text{for } z_1, z_2 < 0 \quad (2.16)$$

and

$$D_{z_1 z_2}(\vec{k}_\rho,E;k_z^\nu) = \frac{\langle j_z(\vec{k}_\rho,E;k_z^\nu)\rangle}{\langle j_z^{in}(z=z_1;\vec{k}_\rho,E;k_z^\nu)\rangle}$$

$$\text{for } z_1 < 0 < z_2. \quad (2.17)$$

If the planes $z = z_1, z_2$ enclose the "physical" surface barrier, then the definition stated by Eq. (2.17) agrees with the usual barrier transmission coefficient calculated within the effective-mass method. However, it should be emphasized that this requires the effective-mass envelope function f and the quantity $(1/m^*)(df/dz)$ to be continuous across a plane of discontinuity of m^*, such as the surface plane.[41] If, in particular, the planes $z = z_1, z_2$ are located at the classical turning point of the one-dimensional field emission barrier, as shown in Fig. 1, then the transmission probability $D_{z_1 z_2}(\vec{k}_\rho, E; k_z^\nu)$ is reasonably approximated by the usual WKB-type exponential,[18]

$$\exp\left(-2 \int_{z_1}^{z_2} \kappa_z^\nu(z)dz\right).$$

4. Field-emitted energy distribution

The small value of the transmission probability for field-emitted electrons at the Fermi energy suggests that the steady-state tunneling current into the vacuum do not significantly disturb the thermal equilibrium of the electrons in the semi-infinite solid.[48,49] We therefore assume:

(iv) The electrons in the emitter are weakly coupled to the vacuum. The equilibrium Fermi distribution function characterizes the distribution of electrons incident at the surface.

This assumption is equivalent to the thick-barrier-approximation underlying Appelbaum and Brinkman's theory.[14] It also corresponds to the "rigid-occupancy" approximation invoked by Duke,

Kleiman, and Stakelon in their many-body theory of tunneling.[50] The total field emitted current can now be expressed with the help of Eqs. (2.14) and (2.17),[4,10,11]

$$S\langle j_z(z_2)\rangle = \frac{S}{\Omega_{BZ}} \int_{1/2BZ} \sum_n \langle j_z^{\text{in}}(z_1; \vec{k}, n)\rangle$$

$$\times D_{z_1 z_2}(\vec{k}, n; F) f(\epsilon_n(\vec{k})) d^3k,$$

$$(2.18)$$

where $f(\epsilon_n(\vec{k}))$ is the Fermi distribution $\{1 - \exp[(\epsilon - \mu)/k_B T]\}^{-1}$; Ω_{BZ} is the volume of the Brillouin zone and n is the "band index" introduced in Eq. (2.7). The integral extends only over that half of the Brillouin zone labeling states for which $v_{g_z}(\vec{k}, n) \geq 0$. The argument F of $D_{z_1 z_2}$ denotes the dependence of the transmission probability on the applied electric field. In writing Eq. (2.18), we used the multivalued energy dispersion relation of the periodic solid, Eq. (2.7), to perform a transformation of variables $E \to k_z$. Following standard procedures we define

$$D_{z_1 z_2}(\vec{k}_\rho, E; k_z^\nu; F) = D_{z_1 z_2}(\vec{k}_\rho, k_z^\nu(\vec{k}_\rho, E); F)$$

$$\equiv D_{z_1 z_2}(\vec{k}; n; F)$$

and

$$\langle j_z^{\text{in}}(z_1; \vec{k}_\rho, E; k_z^\nu)\rangle = \langle j_z^{\text{in}}(z_1; \vec{k}_\rho, k_z^\nu(\vec{k}_\rho, E))\rangle$$

$$\equiv \langle j_z^{\text{in}}(z_1; \vec{k}; n)\rangle \geq 0. \qquad (2.19)$$

There is no simple relation between the two discrete indices ν and n. The former labels the branches of the function $k_z = k_z(\vec{k}_\rho, E)$, while n labels the branches of the inverse function $E = \epsilon(\vec{k}_\rho, k_z)$. The averaged energy density of field
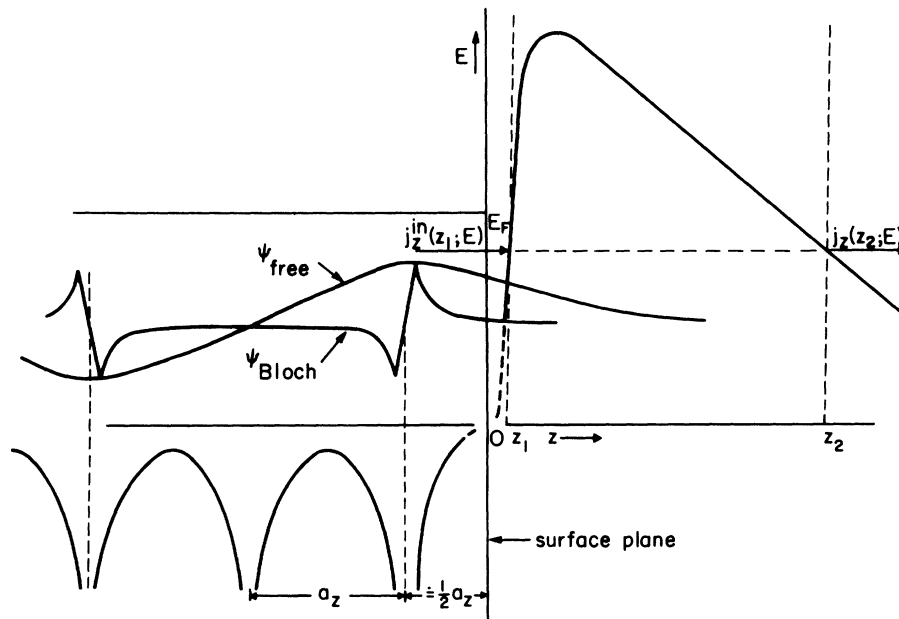

FIG. 1. Schematic illustration of field emission. The periodic potential with a unit vector $\vec{a}_z$ is indicated with the effective surface barrier. The conduction electrons occupy the states from the bottom of the band at $E = 0$ to the Fermi level $E = E_F$. The classical turning points, z_1 and z_2, for the state of energy E are indicated, as well as the "surface" plane in our convention. Finally, a typical free electron, and Bloch electron in a higher angular momentum state are sketched to illustrate the reduced local density of states for the latter at the "surface," discussed in Sec. IV.

emitted electrons is

$$\frac{d}{dE} S\langle j_z \rangle \equiv j'(E)$$

$$= \frac{S}{\Omega_{BZ}} \int_{1/2BZ} \sum_n \delta(E - \epsilon_n(\vec{k})) \langle j_z(z_1; \vec{k}; n) \rangle$$

$$\times D_{z_1 z_2}(\vec{k}; n; F) f(\epsilon_n(\vec{k})) d^3k. \qquad (2.20)$$

Substituting Eq. (2.14) into Eq. (2.20), we obtain

$$j'(E) = 2\frac{\hbar}{m} f(E) \sum_{\vec{k},n}{}' \delta(E - \epsilon_n(k))$$

$$\times \left[\frac{m}{\hbar} v_{\epsilon_z}(\vec{k}, n) \, | L^{-1/2} \mathfrak{N}(\vec{k}, n; z_1) |^2 \right] D_{z_1 z_2}(\vec{k}; n; F). \qquad (2.21)$$

In Eq. (2.21) the factor of 2 represents a sum over spins. We have also replaced the integration over half the Brillouin zone by a correspondingly restricted sum designated by a prime. To obtain the "free-electron-like" or Fowler-Northeim expression for $j'(E)$, it is necessary to use either of the following two approximations; consisting of approximations (v) and (vi) or approximation (vii), respectively.

(v) The effective mass approximation, providing that the z axis coincides with a principal axis of the effective-mass tensor. Note that the effective mass approximation did not have to be invoked in deriving Eq. (2.20).

(vi) The application of the WKB approximation for the solution of the one-dimensional effective-mass equation for the z dependence.

These two steps lead to the usual Fowler-Nordheim field emission equation.

The alternative procedure it to invoke the well-known result from the "$\vec{k} \cdot \vec{p}$" perturbation theory,[51] (vii)

$$\langle n, \vec{k} | \vec{p}_j | n, \vec{k} \rangle \approx \hbar \sum_{i=1}^{3} k_i \left(\frac{m}{m_n^*} \right)_{ij} = m v_{\epsilon_z}(\vec{k}, n),$$
$$(2.22)$$

where the index $j = 1, 2, 3$ represent x, y, z. If the z axis is a principal axis of the effective-mass tensor $\vec{m}_n^*$, we obtain

$$j'(E) = 2\frac{\hbar}{m} f(E) \sum_{\vec{k},n}{}' \delta(E - \epsilon_n(\vec{k}))$$

$$\times \left[k_z \left(\frac{m}{m_n^*} \right)_{zz} | L^{-1/2} \mathfrak{N}(\vec{k}, n; z_1) |^2 \right] D_{z_1 z_2}(\vec{k}; n; F). \qquad (2.23)$$

Although both sets of assumptions lead to formally identical expressions for $j'(E)$, the quantity k_z has different meaning in each.

Assumptions (v) and (vi) lead to the interpretation of k_z as a semiclassical wave vector,

$$k_z \equiv \kappa_z = \left(\frac{2m}{\hbar^2} [W - V(z)] \right)^{1/2}, \qquad (2.24)$$

where the normal energy W is given by

$$W = E - (\hbar k_p)^2 / 2m. \qquad (2.25)$$

Here $V(z)$ is the barrier potential in the effective-mass equation as implied in assumption (v), $\vec{k}_p$ is an ordinary (i.e., not a reduced) two-dimensional wave vector. On the other hand, the k vector introduced by Eq. (2.22) is the z component of the reduced Bloch wave vector characterizing $\psi^{(+)}$. It is furthermore customary, though not really essential, to invoke the following simplifying assumption suggested by the free-electron model.

(viii) The transmission probability depends only on the normal energy defined in Eq. (2.25),

$$D_{z_1 z_2}(\vec{k}, k_z^\nu(\vec{k}_p, E); F) \equiv D_{z_1 z_2}(W; \nu; F). \qquad (2.26)$$

Furthermore, the dependence of the transmission probability on the energy W, dominates any energy dependence of the factors in square braces in Eqs. (2.21) and (2.23), so that these can be pulled out of the sum. This assumption, although widely used, is of limited validity and several examples where it fails are discussed in the literature.[13,52,53]

B. Comparison with Penn et al.'s theory

1. Penn's formalism in terms of kinetic theory

In the preceding section, we derived a generalization of the usual expression for the averaged energy distribution of field emitted electrons in the three-dimensional independent-particle model. We listed all the assumptions necessary to obtain Eq. (2.23) to determine the dependence of the result on the validity of the WKB approximation. It is important to emphasize that Eq. (2.23) could be derived independently of the WKB approximation though this still required a weak-coupling assumption (iv).

In order to make contact with the recent formulations of field emission in terms of the local density of states (i.e., Penn et al.[20] and others[13]), we use Eq. (2.14) to eliminate $\mathfrak{N}$ from Eqs. (2.21) and (2.23),

$$\left| L^{-1/2} \mathfrak{N}(\vec{\mathbf{k}}, n; z_1) \right|^2$$

$$= \frac{1}{L}\left[\left(\int_{\Omega_0(z_1)} |\psi^{(\text{in})}(\vec{\mathbf{r}}; \vec{\mathbf{k}}_\rho, E; k_z^\nu)|^2 d^3r\right) \middle/ \left(\frac{1}{S}\int \int_{z=z_1} |\Psi(\vec{\mathbf{r}}; \vec{\mathbf{k}}_\rho, E; k_z^\nu)|^2 ds\right)\right] \frac{1}{S}\int \int_{z=z_1} |\Psi(\vec{\mathbf{r}}; \vec{\mathbf{k}}_\rho, E; k_z^\nu)|^2 ds.$$

$$(2.27a)$$

Substituting Eq. (2.27a) into Eq. (2.21) or (2.23), we obtain a reformulation of the kinetic theory which does not necessarily depend on the effective-mass method:

$$\left(\frac{2\hbar}{m} Sf(E)\right)^{-1} j'(E) = \sum_{\vec{\mathbf{k}}, n}' \left[\frac{m}{\hbar L} v_{\varepsilon_z}(\vec{\mathbf{k}}_\rho, E; k_z^\nu)\right.$$

$$\times \left(\int_{\Omega_0} |\psi^{(\text{in})}(\vec{\mathbf{r}}; \vec{\mathbf{k}}_\rho, E; k_z^\nu)|^2 d^3r\right) \middle/ \left(\int \int_{z=z_1} |\Psi(\vec{\mathbf{r}}; \vec{\mathbf{k}}_\rho, E; k_z^\nu)|^2 ds\right)\right] D_{z_1 z_2}(\vec{\mathbf{k}}, n; F)$$

$$\times \delta(E - \epsilon_n(\vec{\mathbf{k}}))|\langle \psi(z_1; \vec{\mathbf{k}}_\rho, E; k_z^\nu)\rangle|^2.$$

$$(2.27b)$$

This equation should be compared with a corresponding expression derived by Penn and Plummer,[54] and written below,

$$\left(\frac{2\hbar}{m} Sf(E)\right)^{-1} j'(E) = \lambda^{-2}(E) \sum_m D(W) |\psi_m(z_1)|^2 \delta(E - \epsilon_m).$$

$$(2.28)$$

In Penn's expression, m labels the electronic states of the metal (emitter), and $D(W)$ is the transmission probability, assumed to depend only on the normal energy W. The quantities $\lambda^{-2}(E)$ and $|\psi_m(z_1)|^2$ introduced by Penn can be identified respectively with the factor enclosed by square braces on the right of Eq. (2.27b), and an appropriate rms value of the wave function $\psi(\vec{\mathbf{r}}; \vec{\mathbf{k}}_\rho, E; k_z^\nu)$.

Using (2.9)–(2.13) and (2.27) we can obtain an equivalent and simpler definition of λ^{-2}:

$$\lambda^{-2}(E) = \lambda^{-2}(E, \vec{\mathbf{k}}_\rho; k_z^\nu) = \text{Re}\left(\int \int_{z=z_1} \psi^{(\text{in})*}(-i\vec{\nabla})\psi^{(\text{in})} \cdot d\vec{\mathbf{s}}\right) \middle/ \left(S \int \int_{z=z_1} |\psi|^2 ds\right).$$

$$(2.29)$$

It is important to note that in this formulation, the function Ψ in Eqs. (2.27a)–(2.29) can be chosen for convenience. Furthermore, ψ is an incompletely defined state, because its behavior at $z = 0$ is not, and does not have to be, specified.

Substituting Eq. (2.29) into Eq. (2.27b) we obtain

$$\frac{\hbar}{2} j'(E) = f(E) \sum_{\vec{\mathbf{k}}_\rho, k_z^\nu}' \left(\frac{\hbar^2}{m} \lambda^{-2}(E, \vec{\mathbf{k}}_\rho; k_z^\nu) D_{z_1 z_2}(W, \nu; F)\right.$$

$$\times [\delta(E - \epsilon(\vec{\mathbf{k}})) S |\langle \psi(z_1; \vec{\mathbf{k}}_\rho, E; k_z^\nu)\rangle|^2].$$

$$(2.30)$$

Equation (2.30) is formally identical with Eq. (2.28) derived by Penn and Plummer.[55] However the two expressions for $j'(E)$ require different interpretations of corresponding quantities. We shall return to this point in Sec. III.

2. Relation of Feuchtwang's formulation of field emission to the kinetic theory

a. *Derivation of new many-body formulation of field emission*. Feuchtwang's tunneling theory for a three-dimensional junction[36] is easily specialized to a field-emission configuration. Before we discuss this we shall summarize the pertinent results of the tunneling theory.[56]

The average of the tunneling current over the plane of the junction located at $z = z_1$ is expressed as an integral with respect to energy,

$$\int \int_{z=z_1} \vec{\mathbf{j}}(\vec{\mathbf{r}}) \cdot d\vec{\mathbf{s}} = S\langle j\rangle = S \int_{-\infty}^{\infty} j'(E) dE.$$

$$(2.31)$$

$\vec{\mathbf{j}}$ is to be interpreted as the ensemble average of the current density operator. In Eq. (2.32), below, we express the energy density, $j'(E)$, in terms of the "partial" spectral densities, $\rho_i(\vec{\mathbf{r}}, \vec{\mathbf{r}}'; E, \nu); i = 1, 2$, of the two uncoupled electrodes.[57] These fundamental quantities are discussed in Appendix A. Here we wish only to note that the spectral density with both spatial variables set equal defines the so-called *local density of states*:

$$\frac{\hbar}{2}j'(E)2\pi[f_1(E)-f_2(E)]^{-1}S\left(\frac{2m}{\hbar^2}\right)$$

$$=\sum_{\nu_1,\nu_2}\int_{z=z_1}\int_{z'=z_1}\int_{z''=z_1}\int_{z'''=z_1}ds\,ds'ds''ds'''\,\rho_1(\vec{r},\vec{r}';E,\nu_1)\rho_2(\vec{r}'',\vec{r}''';E,\nu_2)\;\Gamma^r(\vec{r}',\vec{r}'';E)\Gamma^a(\vec{r}''',\vec{r};E). \qquad (2.32)$$

Here (Ref. 57) $f_i(E)$; $i=1,2$ are the Fermi distributions, $\{\exp[(E-\mu_i)\beta]+1\}^{-1}$, characterizing the thermal equilibrium of the uncoupled electrodes. The transfer matrices $\Gamma^{r,a}$ are defined by the relation,

$$\frac{\hbar^2}{2m}\int_{z=z_1}\int_{z'=z_1}ds\,ds'\,\Gamma^{r,a}(\vec{r},\vec{r}';E)$$

$$\times\left(\sum_{\nu_1}g_1^{r,a}(\vec{r}',\vec{r}'';E,\nu_1)+\sum_{\nu_2}g_2^{r,a}(\vec{r}',\vec{r}'';E,\nu_2)\right)=\delta_{zz''}. \qquad (2.33)$$

An integral representation of the Green's functions, $g_{1,2}^{r,a}$, of the uncoupled electrodes is

$$g_i^{r,a}(\vec{r},\vec{r}';E)=\sum_{\nu_i}g_i(\vec{r},\vec{r}';E,\nu_i), \qquad (2.34a)$$

and

$$g_i^{r,a}(\vec{r},\vec{r}';E,\nu_i)=\lim_{\delta\to 0^+}\int_{-\infty}^{\infty}\frac{\rho_i\,(r,r';E',\nu_i)}{E'-E\pm i\delta}\frac{dE'}{2\pi}$$

$$=[g_i^{a,r}(\vec{r},\vec{r}';E,\nu_i)]^\dagger;\quad i=1,2. \qquad (2.34b)$$

For the ordered junction,[37] we can simplify Eqs. (2.32)–(2.34) with the help of a two-dimensional lattice Fourier-expansion of the spectral densities. Using the notation introduced by Eqs. (2.2)–(2.4) we obtain,

$$\rho(\vec{r}_1,\vec{r}_2;E,\nu)=\frac{1}{S}\sum_{m,n}\sum_{\vec{k}_\rho}e^{i(\vec{K}_m\cdot\vec{\rho}_1-\vec{K}_n\cdot\vec{\rho}_2)}$$

$$\times e^{i\vec{k}_\rho\cdot(\vec{\rho}_1-\vec{\rho}_2)}\rho_{mn}(z_1,z_2;\vec{k}_\rho;E,\nu),$$

where $\qquad (2.35)$

$$m\equiv(m_1,m_2),\quad n\equiv(n_1,n_2).$$

The coefficients ρ_{mn} can be interpreted as the $(m\,n)$ element of the matrix $\underline{\rho}$, and it is easily verified that Eq. (2.32) reduced to Eq. (2.36),

$$\frac{\hbar}{2}j'(E)[f_1(E)-f_2(E)]^{-1}S\frac{2m}{\hbar^2}$$

$$=\mathrm{Tr}\left[\sum_{\vec{k}_\rho,\nu}\underline{\rho}_1(z_1,z_1;\vec{k}_\rho;E,\nu)\left(\sum_\mu\underline{\Gamma}^r(z_1,z_1;\vec{k}_\rho;E)\underline{\rho}_2(z_1,z_1;\vec{k}_\rho;E,\mu)\underline{\Gamma}^a(z_1,z_1;\vec{k}_\rho;E)\right)\right]. \qquad (2.36)$$

In Eq. (2.36) we interpret the products of the quantities Γ and ρ as matrix products. Similarly, we find that Eq. (2.33) reduces to Eq. (2.37),

$$\frac{\hbar^2}{2m}\underline{\Gamma}^{r,a}(z_1,z_1;\vec{k}_\rho;E)$$

$$=[\underline{g}_1^{r,a}(z_1,z_1;\vec{k}_\rho;E)+\underline{g}_2^{r,a}(z_1,z_1;\vec{k}_\rho;E)]^{-1}. \qquad (2.37)$$

Equations (2.36) and (2.37) can now be applied to a field emission configuration. We only have to recall that the second "electrode" of the junction now is the vacuum. In the absence of any tunneling, the chemical potential of the vacuum is obviously equal to $-\infty$. Thus we shall write in the following

$$\rho_2\equiv\rho_v,\quad \mu_2\to-\infty;\quad \rho_1\equiv\rho. \qquad (2.38)$$

It is convenient to consider the factor in square brackets on the right of Eq. (2.36) as the squared magnitude of an effective matrix element, i.e.,

$$\left(\frac{\hbar}{2m}\right)^{-2}|M|^2_{mn}(z_1,z_1;\vec{k}_\rho;E,\nu;F)$$

$$=\sum_{m_1,m_2}\Gamma^r_{mm_1}(z_1,z_1;\vec{k}_\rho;E;F)$$

$$\times\rho_{v,m_1m_2}(z_1,z_1;\vec{k}_\rho;E,\mu;F)\Gamma^a_{m_2n}(z_1,z_1;\vec{k}_\rho;E,F). \qquad (2.39)$$

Here we have indicated, through the argument F, the explicit electric field dependence of the several quantities in Eq. (2.39). We note that Eq. (2.37) and (2.39) imply that $|M|^2$ does not depend explicitly on the index ν, which we shall continue to indicate as an argument of the square effective matrix.

Substituting Eqs. (2.38) and (2.39) into Eq. (2.36), we obtain the following expression for the FEED,

$$\frac{\hbar}{2} j'(E) = \frac{f(E)}{2\pi} \operatorname{Tr} \sum_{\vec{k}_\rho, \nu} S^{-1} \underline{\rho}(z_1, z_1; \vec{k}_\rho; E, \nu) |\underline{M}|^2 (z_1, z_1; \vec{k}_\rho; E, \nu; F). \tag{2.40}$$

In the coordinate representation Eq. (2.40) becomes

$$\frac{\hbar}{2} j'(E) = \frac{f(E)}{2\pi} \sum_\nu \int_{z'=z_1} \left(\int_{z''=z_1} S^{-1} \rho(\vec{r}', \vec{r}''; E, \nu) |M|^2 (\vec{r}'', \vec{r}'; E, \nu) ds'' \right) ds'. \tag{2.41}$$

Equations (2.40), (2.39), (2.37), and (2.34) constitute our formulation of field emission in terms of the spectral density function of the emitter. (See Appendix A.) This formulation depends explicitly on the convention that at $z = z_1$ the Green's function for the "uncoupled" emitter, $g(r, r'; E)$ satisfies Neumann conditions at the "surface plane" $z = z_1$. The sensitivity of Feuchtwang's tunneling theory to these boundary conditions and its significance are discussed, in detail, in I–IV.

b. Comparison with kinetic formulation. We shall now demonstrate that the kinetic formulation of field emission corresponds to a fairly obvious approximation of our more complete many-body formulation. Specifically, in the kinetic formulation one replaces the two factors in the integrand of Eq. (2.41) by their "coarse-grain" average over the plane $z = z_1$.

This may be interpreted as approximating the "product" in the integrand with respect to the primed variable, which is averaged over the plane $z' = z_1$, by the "product" of appropriate (i.e., coarse-grain) averages. The coarse-grain average, defined below, depends on the coordinates $\vec{\rho}_1$ and $\vec{\rho}_2$ only through their difference, i.e.,

$$\langle \rho(\vec{r}_1, \vec{r}_2; E, \nu) \rangle_{\text{coarse}} \equiv \bar{\rho} = \bar{\rho}(z_1, z_1; \vec{\rho}_1 - \vec{\rho}_2; E, \nu) \equiv \frac{1}{S} \sum_{\vec{k}_\rho} \operatorname{Tr} \rho(z_1, z_1; \vec{k}_\rho; E, \nu) e^{i \vec{k}_\rho \cdot (\vec{\rho}_1 - \vec{\rho}_2)}$$

$$\equiv \frac{1}{S^2} \sum_m \sum_{\vec{k}_\rho} \left[\int_{z'=z_1} \int_{z''=z_1} \rho(\vec{r}', \vec{r}''; E\nu) e^{-i(\vec{k}_\rho + \vec{k}_m) \cdot (\vec{\rho}' - \vec{\rho}'')} ds'' ds' \right] e^{i \vec{k}_\rho \cdot (\vec{\rho}_1 - \vec{\rho}_2)}. \tag{2.42}$$

Equation (2.42) is not an ordinary two-dimensional Fourier expansion, because the spectral density depends separately on the variables $\vec{\rho}_1, \vec{\rho}_2$ and not just on their difference, $\vec{\rho}_1 - \vec{\rho}_2$.

Comparing Eqs. (2.35) and (2.42), we note that if the two arguments $\vec{\rho}_1, \vec{\rho}_2$ are set equal in a coarse-grain average, the effect is to eliminate the generally rapid spatial variation of the original function of $\vec{\rho}_1 = \vec{\rho} = \vec{\rho}_2$ over the two-dimensional unit cell. Thus, using Eq. (2.42), we find for the local density of states, defined as $(2\pi)^{-1} \rho(\vec{r}, \vec{r}; E, \nu)$,

$$2\pi \langle \rho(\vec{r}_1; E, \nu) \rangle_{\text{coarse}} \equiv \langle \rho(\vec{r}_1, \vec{r}_1; E, \nu) \rangle_{\text{coarse}}$$

$$\equiv \frac{1}{S} \sum_{\vec{k}_\rho} \operatorname{Tr} \rho(z_1, z_1; \vec{k}_\rho; E, \nu). \tag{2.43}$$

It should be noted that the coarse-grain average local density of states is defined by equating the arguments in the corresponding average spectral density *after the average* [defined by Eq. (2.42)] *was performed.*

Equation (2.43) corresponds to the approximation of the $\vec{\rho}$ dependence of the Bloch function by a plane wave in $\vec{\rho}$, in which $|\psi_B|$ is represented by its rms value over the plane $z = z_1$,

$$\psi_B(\vec{r}; \vec{k}, n) = e^{i \vec{k} \cdot \vec{r}} S^{-1/2} \left(\int_{z=z_1} |u(\vec{r}; \vec{k}, n)|^2 ds \right)^{1/2}. \tag{2.44}$$

Approximating the factors in Eq. (2.41) by their coarse-grain averages, as defined by Eq. (2.42), we obtain

$$\frac{\hbar}{2} j'(E) \approx f(E) \sum_{\vec{k}_\rho, \nu} S^{-1} \frac{1}{2\pi} \operatorname{Tr} \underline{\rho}(z_1, z_1; \vec{k}_\rho; E, \nu)$$

$$\times \operatorname{Tr} |\underline{M}|^2 (z_1, z_1; \vec{k}_\rho; E, \nu; F). \tag{2.45}$$

It is shown in Appendix B that

$$\delta(E - \epsilon(\vec{k})) S |\langle \Psi(z_1; \vec{k}_\rho, E; k_z^\nu) \rangle|^2 \equiv \frac{1}{2\pi} \operatorname{Tr} \underline{\rho}(z_1, z_1; \vec{k}_\rho; E, \nu), \tag{2.46}$$

so that the right sides of Eqs. (2.30) and (2.45) are formally identical and

$$\frac{\hbar^2}{m} \lambda^{-2} D \equiv S^{-1} \operatorname{Tr} |\underline{M}|^2. \tag{2.47}$$

We conclude that in the kinetic formulation of FEED the right side of Eq. (2.40) is replaced, or rather approximated by the right side of Eq. (2.45).

3. Discussion

Our derivation of Eq. (2.30) indicated that the many-body formalism of Penn and Plummer, when applied to a noninteracting system is equivalent to the kinetic formulation of field emission. Both theories explicitly depend on assumptions (i)–(iv). However, Penn's analysis relies strongly on an explicit application of the WKB approximation, and does not distinguish between the consequences of this particular approximation and general features of the theory. For example, the factor $|\psi_m(x_m)|^2$ in Eq. (2.28) is identified as the squared magnitude of the single-particle state ψ_m, while our analysis identifies it properly as the surface average of this quantity. The difference in interpretation occurs because Penn *et al.* replace the three-dimensional metal potential by its planar average, without however interpreting the resulting wave function as an appropriate planar average. In a subsequent publication, Penn[21] considered this problem but did not completely resolve it, because his modified expression for $|\psi_m|^2$ still excluded band-structure effects associated with the periodicity in the surface or $\vec{\rho}$ plane. More recently, Penn has correctly defined this term[58] by defining

$$|\psi_m(z_1)|^2 \equiv \left| \int_{z \,=\, z_1} e^{-i \vec{k}_\rho \cdot \vec{\rho}} \psi_m(r) ds \right|^2 . \qquad (2.48)$$

According to Eqs. (2.35), (2.46), and (A.2) this implies that the Penn-Plummer (PP) expression for the field emitted energy density, $j'(E)$, [Eq. (2.28)], depends on the quantity

$$\delta(E - \epsilon(\vec{k})) S |\psi_m(z_1)|^2 = (2\pi)^{-1} \rho_{00}(z_1, z_1; \vec{k}_\rho; E, \nu). \qquad (2.49)$$

As will be shown in Sec. IV, this quantity may be interpreted as an *average (partial) local one-dimensional density of states.*

Equations (2.48) and (2.28) correspond to an approximation used by Nicolaou and Modinos[13] in their calculation of $j'(E)$ applying Appelbaum and Brinkman's transfer-Hamiltonian formalism, to be discussed in Sec. III B.

Note added in manuscript. We wish to point out that this most recent reformulation of the PP theory[58] is essentially equivalent to the direct treatment by Nicolaou and Modinos.[13] It is to be emphasized that this "equivalence" is subject to certain qualifications which were first explicitly derived in the present analysis and are referred to in the "Note Added in Proof" at the end of Penn's latest paper.[58]

It should be emphasized that the $\vec{k}_\rho \neq 0$ contribution to $j'(E)$ may be very significant. This is demonstrated by the explicit calculations of Politzer and Cutler[11] and Nicolaou and Modinos.[12,13]

The latter authors have developed a procedure to be discussed in Sec. III for dealing with a strictly one-dimensional barrier without eliminating the significant $\vec{\rho}$ dependence of the problem.

Returning to our discussion of Eqs. (2.28) and (2.30), we note that PP[20] and Penn[21,58] assert that the factor λ^{-2} depends only weakly on the energy and not at all on $\vec{k}_\rho$.[20] However on examining an explicit calculation of λ, which the authors outline, one finds a dependence on the normal energy W (*and hence on E and $\vec{k}_\rho$*). Furthermore, our calculation [see Eqs. (2.27) and (2.29)] identifies λ^{-2} as proportional to the z component of the group velocity, which exhibits a marked dependence on both $\vec{k}_\rho$ and E for any non-free-electron band. In fact the $\vec{k}_\rho$ dependence of $\lambda^{-2}D$ contradicts the assertion that the transmission probability $D(W)$ always singles out the $\vec{k}_\rho = 0$ states. The dependence of λ^{-2} on $\vec{k}_\rho$ and E has another consequence. It can make the identification of structure in FEED with the local density of states at the surface more complicated than indicated by PP. For example, while Eqs. (2.30) and (2.45) seem to emphasize the (coarse grain planar average of the) local density of states at the "surface" (i.e., at $z = z_1$), λ^{-2} clearly contains bulk band-structure information. To conclude, λ^{-2} cannot, in general, be removed from the sum over m, indicated in Eq. (2.28). However, if the PP theory is understood to be represented by Eqs. (2.27b) and (2.30), then it becomes formally equivalent to Nicolaou and Modino's formulation.

The definition of λ^{-2} and $|\langle \Psi \rangle|^2$ given by Eqs. (2.27a)–(2.29), emphasizes the arbitrariness of these quantities, which by themselves have no unique physical significance, although their product $\lambda^{-2}|\langle \Psi \rangle|^2$ has a unique physical meaning. In particular, in any kinetic formulation, the precise boundary conditions to be imposed on Ψ (at $z = 0$) do not have to be specified. Although this ambiguity is similar to that encountered in Feuchtwang's many-body theory of tunneling, he selects a "convenient" set of boundary conditions, by the requirement that the functional dependence of FEED on the "local density" of states be given by Eq. (2.41). Here a formal difference between Eqs. (2.28), (2.30), and (2.41) should be pointed out: In Eq. (2.28), PP chose z_1 to be the (energy dependent) classical turning point in the effective barrier potential. In Eq. (2.41), z_1 is the surface plane at which the wave functions satisfy Neumann conditions.[27] While neither the kinetic theory [Eq. (2.30)] nor Penn *et al.*'s analysis require z_1 to be any particular point,[58(a)] Feuchtwang's analysis singles out the interface and defines it as the plane, located beyond the last atomic plane, on which Ψ satisfies Neumann conditions.

Each of the three formulations of FEED discussed above involves a phenomenological parameter, i.e., the location of the plane on which the local density of states is evaluated. This parameter and the nature of the boundary conditions to be imposed on the single particle states of the semi-infinite solid are inherently "disposable," though they tend to be more restricted the more formal the theory, as for example in Feuchtwang's analysis.

A final point that ought to be considered is the role of surface states and (scattering) resonances. The former enter Eq. (2.41) explicitly as isolated singularities of the transfer matrix $\Gamma^r(z_1, z_1; k_\rho; E)$, which do not fall onto one of the allowed energy bands of the solid. These in turn would manifest themselves in peaks of $|M|^2$ at values of $\vec{k}_\rho$ totally unrelated to those for which the product $v_{g_z} D(W)$ peaks.[36] Similarly, surface resonances manifest themselves in peaks of $v_{g_z} D(W)$ which occur at "unexpected" values of $(\vec{k}_\rho, E)$. Thus, the assertion by Penn *et al.*, concerning the *unique, sharp peak of* $j'(E)$ *for* $\vec{k}_\rho = 0$, is valid for a nearly-free-electron-band and *in the absence of surface states and, or resonances*. The recent model calculation for field emission from tungsten by Modinos and Nicolaou[13] provides an excellent illustration of this point, which has been recently conceded by Penn (see note added in proof).[58]

III. RELATION BETWEEN THE KINETIC FORMULATION OF NICOLAOU AND MODINOS AND THE THEORIES OF PENN *ET AL*. AND FEUCHTWANG

A. Comparison of calculation of Nicolaou and Modinos and Penn *et al.*'s theory

Nicolaou and Modinos published a very complete analysis of the total energy distribution of field emitted electrons from tungsten,[12] within the framework of the kinetic formulation developed in Sec. II. Besides the basic assumptions (i)–(iv), Nicolaou and Modinos make the following three simplifying approximations in calculating the states $\Psi^{(+)}$ defined in Sec. IIA 2:

(ix) They restrict the basis set of the generalized Bloch functions used in expanding $\Psi^{(+)}$ to a set of $2n$ functions, n incoming and n outgoing waves. This approximation is closely related to approximation (x).

(x) The two-dimensional Fourier (plane wave) expansion of the $\vec{\rho}$ dependence of $\Psi^{(+)}$ (and of the generalized Bloch functions) can be truncated after n terms. Finally, Nicolaou and Modinos make an assumption in (xi).

(xi) The long-range deviations from perfect

periodicity of the crystalline potential in the region to the left of $z = 0$ can be neglected. (The surface plane, $z = 0$, is located half a lattice constant to the right of the last atomic plane.)

The assumption of perfect periodicity up to the surface plane implies that our factor $A(z; \vec{k}_\rho, E; k_z^\nu)$ is identically equal to unity, and hence, the factor $\mathfrak{N}(\vec{k}_\rho, E; k_z^\nu; z)$ in the right member of Eq. (2.14) is independent of z; thus $\mathfrak{N}$ reduces to

$$N(\vec{k}_\rho, E; k_z^\nu) = (LS)^{1/2} . \tag{3.1}$$

The rest of their analysis is exact, i.e., they evaluate the transmission probability $D_{0^-0^+}(\vec{k}_\rho, E; k_z^\mu; F)$ by matching the logarithmic derivative across the plane $z = 0$. They determine $j'(E)$ from Eq. (2.21), which now reduces to

$$j'(E) = \frac{2Sf(E)}{2\pi} \sum_\mu \sum_{\vec{k}_\rho} D_{0^-0^+}(\vec{k}_\rho, E; k_z^\mu; F) . \tag{3.2}$$

Here the sum over $\vec{k}_\rho$ ranges over the projected area of the constant energy surface into the $\vec{k}_\rho$ plane. The equivalence of Eqs. (2.21) and (3.2) follows if one notes that the delta function in Eq. (2.21) denotes the normalized single-particle density of states which, in the continuum normalization of Modinos and Nicolaou, is represented by $|\nabla_k \epsilon_n(k)|^{-1}$. Thus Eq. (2.21) corresponds to an integral over a constant energy surface, whereas in Eq. (3.2) this integral is now replaced by an integration over the projection of the constant energy surface into the $\vec{k}_\rho$ plane.[59]

It should be noted that Nicolaou and Modinos do not invoke any of the assumptions (v)–(viii). Thus, their calculation is only limited by the validity of the basic assumptions of the kinetic formulation. The avoidance of the unnecessary simplifying assumptions (v)–(viii) paid off in providing a clear counter example to the accepted "lore" that the barrier transmission probability is only peaked at $\vec{k}_\rho = 0$, so that the energy distribution of field emitted electrons is almost completely determined by the $\vec{k}_\rho = 0$ component of the (coarse averaged) local density of states. It should be noted that these results confirm those of Politzer and Cutler.[11]

In assuming that the quantity λ^{-2} in Eq. (2.28) depends only on energy, PP and Penn do not account for the $\vec{k}_\rho$ dependence of the group velocity v_{g_z}. This dependence is accounted for by Nicolaou and Modinos, who correctly omit the contributions to the integral over $\vec{k}_\rho$ from portions of the constant energy surface that have no projection onto the $\vec{k}_\rho$ plane. Nicolaou and Modinos explicitly demonstrate the existence of peaks of the transmission probability at "unexpected" values of $(\vec{k}_\rho, E)$. The identification of some of these peaks with surface resonance (or quasisurface states) was proposed

by Modinos and Nicolaou in a second paper utilizing the transfer Hamiltonian.[13] These results contrast with the conclusion of PP and Penn, that the energy distribution is primarily a measure of the local normal or one-dimensional density of states. The latter quantity, which they denote $N_m^2(E,E)\rho_m'(E)$ is,[60] in our notation,

$$N_m^2(E,E)\rho_m'(E) \equiv \frac{m}{\hbar^2 SL}\left|\mathfrak{N}(\vec{k}_\rho,E;k_z^\nu;z_1)\right|^2_{\vec{k}_\rho=0} . \quad (3.3)$$

Nicolaou and Modinos conclude that Penn et al. must have assumed the nearly free-electron model for the emitter.[13] The same conclusion can be derived as a consequence of the requirement of the Applebaum and Brinkman theory that the "left" and "right" states diagonalize the Hamiltonians for the left and right half-spaces: Penn and Plummer denote the left states of Appelbaum and Brinkman's theory by ψ_m. They chose the wave functions ψ_m to be WKB-type free-electron-like functions. This follows from the requirement that at the plane $z = z_m$, which [in the notation of Eq. (2.2)] corresponds to the turning point of $\phi(z;\vec{k}_\rho,E;\vec{K}_m=0)$ closest to the first atomic plane, ψ_m is represented by a single plane wave in $\vec{\rho}$.[61] Comparison with our $\Psi^{(+)}$ demonstrates that functions ψ_m satisfying this requirement cannot diagonalize the Hamiltonian, with the potential periodic in $\vec{\rho}$, for the left half-space. Here it should be noted that Penn[21] argues that the "normalization constant" $N_m(E)$ accounts for band-structure effects (i.e., deviations from the free-electron model) such as found by Politzer and Cutler,[11] and confirmed by Nicolaou and Modinos.[12,13] This claim is neither substantiated by Penn, nor by our analysis. Penn further argues that $N_m(E)$ could vanish along a symmetry line in the Brillouin zone.[21] Although our analysis[54] confirms this, this is unexpected behavior for a normalization constant, and it implies ψ_m is a pseudo-wave function, required to vanish whenever the normal component of the current $\int j_z ds$ carried by the corresponding state vanishes. This in turn poses difficulties in interpreting $N_m(E - E_m)$ as an (averaged) local density of states.[62] Recently Penn generalized his formalism,[21] and redefined his local (normal) density of states

$$\rho_m(E,z_1) \equiv \sum_m' \left| \int_{z=z_1} \psi_m(\vec{r})ds \right|^2 \delta(E - E_m) , \quad (3.4)$$

where the primed sum includes all "metal states with momentum normal to the metal surface."[63] Presumably it was meant to restrict the sum to include only states such that $v_{g_z} > 0$. This definition is strictly in accord with the kinetic formulation, and does unnecessarily eliminate from the analysis surface states, if these exist.[64] Furthermore, as

noted in our discussion of Eq. (2.45), the sum over m can include only the states with $\vec{k}_\rho = 0$. This is evidently inconsistent with the previously discussed claim that N_m, here identified as the surface average of $\psi_m(\vec{r})$, should account for band-structure (i.e., symmetry) effects which could manifest themselves in pronounced contributions of states with nonzero $\vec{k}_\rho$ values to the field emitted energy distribution. More recently Penn corrected this defintion of the local (normal) density of states, and replaced it by a quantity equivalent to $(2\pi)^{-1}\rho_{00}(z_1,z_1;\vec{k}_\rho;E,\nu)$.[58] However, the $\vec{k}_\rho$ dependence of λ^{-2} is still not considered. Thus, the latest version of the PP theory still does not fully account for the above mentioned band-structure effects.

B. Comparison of Nicolaou and Modinos' calculation with the theories of Appelbaum and Brinkman, and of Feuchtwang

Nicolaou and Modinos[13] noted the significant differences between their kinetic-theoretic calculation and Penn et al.'s analysis. This apparently prompted them to apply their method of calculating $\Psi^{(+)}$ to Appelbaum and Brinkman's version of the transfer Hamiltonian formalism. They obtained an expression for $j'(E)$, which in our notation reduces to

$$\frac{\hbar}{2} j'(E) = \frac{f(E)}{2\pi}\sum_{\vec{k}_\rho,\nu}\sum_{m,m'} S^{-1}\rho_{mm'}(0,0;\vec{k}_\rho,E;\nu)$$
$$\times \left|M\right|^2_{mm'}(\vec{k}_\rho,E;\nu;F) , \quad (3.5)$$

where

$$S^{-1}\rho_{mm'}(0,0;\vec{k}_\rho,E;\nu) = \left|\left(\frac{\partial\epsilon}{\partial k_z}\right)_{k_z=k_z^\nu}\right|^{-1}$$
$$\times C_m(\vec{k}_\rho,E;k_z^\nu)C_{m'}^*(\vec{k}_\rho,E;k_z^\nu) , \quad (3.6)$$

$$C_m(\vec{k}_\rho,E;k_z^\nu) = S^{-1/2}\int_{z=0=z_1}\Psi(r;\vec{k}_\rho,E;k_z^\nu)$$
$$\times e^{-i(\vec{k}_m+\vec{k}_\rho)\cdot\vec{\rho}}ds, \quad (3.7)$$

$$\left|M\right|^2_{mm'}(\vec{k}_\rho,E;\nu;F)$$
$$= 2\left(\frac{\hbar^2}{2m}\right)^{1/2}(W_m W_{m'})^{1/4}$$
$$\times \exp\left[-\frac{2}{3}\left(\frac{2m}{\hbar^2 e^2 F^2}\right)^{1/2}(W_m^{3/2} + W_{m'}^{3/2})\right]\delta_{mm'} , \quad (3.8)$$

and

$$W_m = -\epsilon(\vec{k}_\rho,k_z^\nu) + (\hbar^2/2m)(\vec{k}_\rho + \vec{K}_m)^2 . \quad (3.9)$$

In Eq. (3.5), $\vec{k}_p$ is summed over the projection of the constant energy surface into the $\vec{k}_p$ plane. The explicit form of the squared magnitude of the effective matrix element $|M|^2_{mm'}$, given by Eq. (3.8), reflects the model considered by Modinos and Nicolaou: an abruptly terminated periodic potential and an external potential corresponding to a uniform electric field $V(\vec{r}) = eFz$. On the other hand, the fact that the matrix $|\underline{M}|^2$ is diagonal in m is a general feature of the transfer Hamiltonian formalism used by Modinos and Nicolaou.[65] Thus we see that Eqs. (2.40) and (3.5) are formally identical. They differ, however, first in the formal definition of the squared magnitude of the effective matrix and, second, in the precise definition of the local density of states.

The first difference is due to the fact that Appelbaum and Brinkman's theory is equivalent to a "thick-barrier-approximation" of Feuchtwang's theory. Specifically, in Appelbaum and Brinkman's theory the right side of Eq. (2.32) assumes the form

$$\int_{z=z_1} \int_{z'=z_1} ds\, ds' \rho_1(\vec{r}, \vec{r}'; E) \rho_2(\vec{r}', \vec{r}; E)$$
$$\times |T|^2(\vec{r}', \vec{r}; E)\,, \qquad (3.10)$$

where $|T|^2$ is essentially the normalized squared magnitude of the "transition-current" of Bardeen.[22] Equation (3.10) has been shown to be the thick-barrier limit of Eq. (2.32).[36] The second difference between Eq. (2.40) and (3.5) is more subtle, and is due to the different boundary conditions imposed by the two theories on the semi-infinite solid in the absence of any tunneling current: Appelbaum and Brinkman require the states of the semi-infinite solid to vanish infinitely far, outside the solid; Feuchtwang requires them to obey Neumann conditions at the boundary surface $z = z_1$.[66]

Nicolaou and Modinos do not discuss the characteristic, formal difference between their kinetic theoretical expression and their transfer-Hamiltonian analysis: The former involves only the coarse average of the local density of states, i.e., it involves $\int_{z=0} |\psi|^2 ds \propto \mathrm{Tr}\rho$. The latter, just like the theory of Feuchtwang, involves the full matrix ρ.[67] This difference becomes unimportant in the context of the calculation of Nicolaou and Modinos because they assume that the contributions of all but the $(0,0)$ matrix element of ρ are negligible. In this approximation, the kinetic and the transfer-Hamiltonian formulations reduce to identical forms. Both, however, disagree with the PP and Penn theory which as already discussed before, is identified as a nearly-free-electron formulation; as mentioned before, this formulation does not con-

sider the strong dependence of the spectral density in transition metals (i.e., of the d states' wave functions in those metals) on $\vec{k}_p$.

Here it should be emphasized that the agreement between the kinetic and transfer-Hamiltonian calculations of Nicolaou and Modinos is accidental. Even for the strictly noninteracting system considered by Nicolaou and Modinos, the two theories differ because the kinetic formulation cannot include the effect of strict surface bands, which are orthogonal to the scattering states $\Psi^{(+)}$.[64] On the other hand, the transfer-Hamiltonian theory, just as the theory presented in Eqs. (2.34), (2.37), (2.39), and (2.41) has no such limitation. Nicolaou and Modinos' calculation did not seem to be affected by this fact. They did not search for true surface states, and thus their calculation did not include their contribution to the FEED. Their results suggest that if surface states exist on the (100) face of W, their contribution to FEED is unimportant.

IV. CONCLUSION: BAND STRUCTURE REVISITED

In the preceding section we have examined the basic approximations and consequent limitations of four current formulations of field emission.

The "naive" kinetic theory is normally derived subject to assumption (i)–(vi) and (viii), which emphasize the similarity to the nearly-free electron model of s-electron emission. We have seen that the more "exact" kinetic formulation invokes only assumptions (i)–(iv). Both are thick-barrier approximations which do not account for either inelastic field-emission or electronic surface-band-structure effects.[64, 68]

Here it is instructive to pursue the naive kinetic theory further than was done in Sec. II. Using Eqs. (2.21) and (2.23), we can describe the energy distribution of field-emitted d electrons by the expression

$$R_d(E) \equiv j'_d(E)/j'_s(E)$$

$$= \frac{v_{\varepsilon_z}(E, d)}{v_{\varepsilon_z}(E, s)} \frac{|\Re(\vec{k}_p = 0, k_z(\vec{k}_p = 0, E), d; z_1)|^2}{|\Re(\vec{k}_p = 0, k_z(\vec{k}_p = 0, E) s; z_1)|^2}$$

$$= \frac{m^*_s}{m^*_{d_{zz}}} \left| \frac{\Re(\vec{k}_p = 0, k_z(\vec{k}_p = 0, E), d; z_1)}{\Re(\vec{k}_p = 0, k_z(\vec{k}_p = 0, E), s; z_1)} \right|^2 \,,$$

$$(4.1)$$

where

$$\frac{|\Re(k, d; z_1)|^2}{L} = \int_{z=z_1} |\psi_B(\vec{r}; \vec{k}, d)|^2 ds \,, \qquad (4.2)$$

and s, d label electrons from the s, d bands.

In writing Eq. (4.1) we assumed that

$D_{z_1 z_2}(W; \nu; F)$ can be calculated by the WKB approximation and is thus the same for d and s electrons. Furthermore, the factors $v_{g_z}\mathfrak{R}$ were assumed to vary slowly with W and thus were evaluated at $\vec{k}_\rho = 0$ and taken out of the summation. $j_s'(E) = j_0'(E)$ is the standard, free-electron energy distribution. Taking a phenomenological point of view, we can interpret $R_d(E)$ as a measure of the reduced transmission probability of d electrons as compared to free or s electrons. This point of view has been adopted by Gadzuk[6] in an earlier analysis of d-electron emission.

In the sense that $R_d(E)$ is proportional to a surface average of ψ_B at z_1, it is evidently a measure of the local density of states. For s and d electrons having the same energy, the effect of the lattice potential is to localize an electron in the narrow d bands closer to the ion cores than a nearly free electron in the broader s bands. Then, assuming that the surface plane $z = z_1$ is roughly half a lattice constant from the last atomic plane, we find that $|\mathfrak{R}(d)/\mathfrak{R}(s)|^2$ is significantly smaller than unity. This effect is further enhanced by the factor $m_s^*/m_{d_{zz}}^* \sim m v_{g_z}^d/\hbar k_z$, and leads to $R_d(E) \ll 1$.[8,10,17,19] Thus Gadzuk's earlier calculation of a reduction of FEED from d bands compared to s bands is seen to be confirmed. (See Fig. 1.)

The transfer Hamiltonian formulation of Appelbaum and Brinkman does not explicitly involve assumptions (i) and (ii). That is, while it is a thick barrier approximation, like the kinetic formulation, it can describe many-body effects such as inelastic field emission. Finally, unlike the kinetic theory, the transfer-Hamiltonian formalism can account for surface-band-structure effects.

The Penn-Plummer adaptation of the transfer-Hamiltonian formalism invokes, in addition to assumptions (ii)–(iv), effectively the nearly free-electron model. This point has been amply discussed in Sec. III, and needs no further elaboration.

Feuchtwang's tunneling theory does not invoke a "weak coupling assumption," so that his formulation of field emission, given by Eqs. (2.40) and (2.41), is different from the preceding three by being independent of assumption (iv), the so-called thick barrier approximation. The theory accounts explicitly for surface band structure which manifests itself in singularities of (i) the transfer matrix Γ^r, and (ii) of the squared magnitude of the effective matrix element $|M|^2$, which do not fall into one of the bulk energy bands.[36]

Finally, a comment concerning the ubiquitous "one-dimensional, local density of states." Equation (2.41) shows that FEED depends on a weighted average of the spectral density at the surface. If we adopt the approximation, suggested by Nicolaou and Modinos, of keeping only the $(0, 0)$ element in all matrices, then Eqs. (2.40) and (2.45) show that FEED probes a weighted coarse-grain average of the full local density of states. This conclusion may also be explained as follows; we may interpret the quantity

$$(1/2\pi)\rho_{00}(z_1, z_1; \vec{k}_\rho; E, \nu) \equiv \langle \rho(z_1; \vec{k}_\rho; E, \nu) \rangle \quad (4.3)$$

on an average, partial, local one-dimensional density of states probed by FEED. This expression is only a partial local density of states because it depends not only on the energy E but also on the additional variables $\vec{k}_\rho$ and ν. A sum over $\vec{k}_\rho$ and ν has to be performed in order to obtain the corresponding full (average) local density of states which is defined as a weighted surface average of the spectral density $\sum_\nu \rho(\vec{r}', \vec{r}''; E, \nu)$,

$$\sum_{\vec{k}_\rho} \left[\frac{1}{S^2} \int_{z'=z_1} \int_{z''=z_1} \left(\frac{1}{2\pi} \sum_\nu \rho(\vec{r}', \vec{r}''; E, \nu) \, e^{-i\vec{k}_\rho \cdot (\vec{r}' - \vec{r}'')} \right) ds' \, ds'' \right] = \langle \rho(z_1; E) \rangle . \quad (4.4)$$

Here we wish to note that our analysis introduced four distinct quantities, each of which could be referred to as a (surface average of a) local density of states, and each of which has an appropriate physical significance.

First we have the coarse-grain average of the local density of states, introduced by Eq. (2.43).

$$\langle \rho(\vec{r}; E) \rangle_{\text{coarse}} = \sum_\nu \langle \rho(\vec{r}; E, \nu) \rangle_{\text{coarse}} . \quad (4.5)$$

This quantity is in fact equal to the *simple surface average* of the *local density of states*,

$$\langle \rho(\vec{r}; E) \rangle = \frac{1}{S} \int_{z=z_1} \left(\frac{1}{2\pi} \sum_\nu \rho(\vec{r}, \vec{r}; E, \nu) \right) ds$$

$$= \langle \rho(\vec{r}, E) \rangle_{\text{coarse}}$$

$$= \frac{1}{S} \sum_{\vec{k}_\rho, \nu} \frac{1}{2\pi} \text{Tr} \underline{\rho}(z_1, z_1; \vec{k}_\rho; E, \nu).$$

$$(4.6)$$

Equation (2.45) shows that in the kinetic formulation the FEED depends on the partial density corresponding to $\langle \rho(\vec{r}, E) \rangle_{\text{coarse}}$, i.e., on

$$\langle \rho(\vec{r}, \vec{k}_\rho; E, \nu)\rangle_{\text{coarse}} \equiv (2\pi s)^{-1}\, \text{Tr}\underline{\rho}(z_1, z_1; \vec{k}_\rho; E, \nu).$$

Second, we have the quantities $\langle \rho(z_1; \vec{k}_\rho; E, \nu)\rangle$ and $\langle \rho(z_1; E)\rangle$ defined respectively as weighted surface averages of the spectral density by Eqs. (4.3) and (4.4). We have seen that to a good approximation the analysis predicts that FEED can probe these quantities.

Finally we have the *simple surface average* of the *spectral density*, which using Eq. (4.3) can be written

$$\frac{1}{2\pi}\langle \rho(\vec{r}, \vec{r}'; E)\rangle$$

$$= \frac{1}{S^2}\int_{z=z_1}\int_{z'=z_1}\left(\frac{1}{2\pi}\sum_\nu \rho(\vec{r}, \vec{r}'; E, \nu)\right) ds\, ds'$$

$$= \sum_\nu \langle \rho(z_1; \vec{k}_\rho = 0; E, \nu).$$

It is the last quantity which was called by Penn and Plummer the "normal or one-dimensional density of states."[69]

It should be noted that the Penn-Plummer analysis may not be able to describe some experimental band-structure effects because it is formulated in terms of a parameter, i.e., a local density of states, which is an inappropriate surface average.

Each one of the above "local densities of states" depends only on the z (or normal) coordinate, and may be called a "one-dimensional density of states." This designation is obviously a misleading description of an appropriate surface average, since a complete analysis of FEED always involves functions of three spatial variables. In other works, the $\vec{\rho}$ dependence of the functions (i.e., of the spectral density and the local density of density of states) is eliminated by appropriate integrations over the "surface" plane at $z = z_1$, which define the corresponding weighted surface averages.

ACKNOWLEDGMENTS

APPENDIX A: THE SPECTRAL DENSITY AND LOCAL DENSITY OF STATES FUNCTIONS

In this Appendix we shall briefly summarize some facts about the spectral density of states.

The complex partial spectral density function, $\rho(\vec{r}_1, \vec{r}_2; E, \nu)$ for a noninteracting system is most conveniently represented in terms of the complete orthonormal set of single particle states $\{\psi(\vec{r}; E, \nu)\}$,

$$\rho(\vec{r}_1, \vec{r}_2; E, \nu)\, dE = 2\pi \int_E^{E+dE} \psi^*(\vec{r}_1; E', \nu)\psi(\vec{r}_2; E', \nu)dE'.$$
(A1)

An equivalent more compact notation is,

$$\rho(\vec{r}_1, \vec{r}_2; E', \nu)$$
$$= 2\pi\psi^*(\vec{r}_1; E', \nu)\psi(\vec{r}_2; E', \nu)\delta(E'(\nu) - E). \quad (A2)$$

Here, ν is a (discrete or continuous) index labeling the set of states degenerate at the energy E. The full spectral density is obtained by summing over ν. More generally we have,

$$g^r(\vec{r}_1, \vec{r}_2; E, \nu) = \lim_{\epsilon \to 0+}\int_{-\infty}^{\infty}\frac{\rho(\vec{r}_1, \vec{r}_2; E', \nu)}{E' - E + i\epsilon}\frac{dE'}{2\pi}$$

$$= P\int_{-\infty}^{\infty}\frac{\rho(\vec{r}_1, \vec{r}_2; E', \nu)}{E' - E}\frac{dE'}{2\pi}$$

$$-\frac{i}{2}\rho(\vec{r}_1, \vec{r}_2; E, \nu), \quad (A3)$$

where P denotes the Cauchy principal part of the integral.

The partial local density of states is defined by the following relations

$$\rho(\vec{r}; E, \nu) \equiv -(1/\pi)\,\text{Im}\,g^r(\vec{r}, \vec{r}; E, \nu)$$
$$= (1/2\pi)\rho(\vec{r}, \vec{r}; E, \nu) \geq 0. \quad (A4)$$

The local density of states is related to the usual density of states

$$\sum_\nu \int_{\text{all space}}\rho(\vec{r}; E, \nu)\, d^3r = \rho(E). \quad (A5)$$

APPENDIX B: THE ROLE OF COARSE-GRAIN AVERAGING IN THE KINETIC FORMULATION OF FEED: PROOF OF EQ. (2.46)

Referring to Eq. (A1), we used a set of single-particle states which is appropriate to the two-dimensional periodicity of the system, such as defined by Eqs. (2.2)–(2.6). The degeneracy label ν of Eq. (A2) is now represented by the continuous two-dimensional wave vector $\vec{k}_\rho$ and the discrete index k_z^ν. Thus,

$$\delta(E - \epsilon(k))\int_{z=z_1}|\Psi(\vec{r}; \vec{k}_\rho, E; k_z^\nu)|^2\, ds$$

$$= \frac{1}{2\pi}\int_{z=z_1}\rho(\vec{r}_1, \vec{r}_1; \vec{k}_\rho; E, \nu)\, ds. \quad (B1)$$

The periodicity of the system enables us to expand the local density of states in a two-dimensional

lattice-Fourier series

$$\rho(\vec{r}, \vec{r}; \vec{k}_\rho, E; k_z^\nu) = \frac{1}{S} \sum_{m,m'} \rho_{mm'}(z, z; \vec{k}_\rho; E, \nu)$$
$$\times e^{i(\vec{k}_m - \vec{k}_{m'}) \cdot \vec{\rho}}. \quad (B2)$$

Substituting Eq. (B2) into Eq. (B1) we obtain Eq. (2.46), i.e.,

$$\delta(E - \epsilon(k))S|\langle \Psi(z_1; \vec{k}_\rho, E; k_z^\nu)\rangle|^2$$
$$= \frac{1}{2\pi} \sum_m \rho_{mm}(z_1, z_1; \vec{k}_\rho; E, \nu). \quad (B3)$$

The identification of $(\hbar^2/m)\lambda^{-2}D$ with a trace such as shown in Eq. (2.47) follows directly from Eqs. (2.2), (2.15), (2.17), and (2.30). For,

$$\frac{\hbar^2}{m} \lambda^{-2}D = \frac{\hbar^2}{m} \text{Re}\left(\int \int_{z=\text{const}>0} \Psi^{(+)*}(-i\vec{\nabla})\Psi^{(+)} \cdot d\vec{s} \right)$$
$$\times \left(S \int \int_{z=z_1} |\Psi|^2 \, ds \right)^{-1}. \quad (B4)$$

We may interpret the denominator as a normalization constant. The numerator reduces directly to

$$\text{Re}\left[-\frac{i\hbar^2}{m} \sum_m | T_{\vec{k}_m}|^2 \phi^*(z; \vec{k}_\rho, E; \vec{K}_m) \right.$$
$$\left. \times \frac{d}{dz} \phi(z; \vec{k}_\rho, E; \vec{K}_m) \right]. \quad (B5)$$

This expression is manifestly the trace of a matrix. The explicit varification of Eq. (2.47) poses no difficulties and is omitted.

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[26]See comment following Eq. (12) of Ref. 25(e). The spectral density and local density of states are briefly discussed in Appendix A.

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[28]See Ref. 25(d), and in particular the discussion following Eq. (7).

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[30]See for instance Refs. 3 and 5.

[31]See Ref. 2, p. 26 for a more extensive discussion of this point; see also Ref. 25(e), footnote on p. 238.

[32]See, e.g., Ref. 14, Eq. (3.14) and following comment; also Ref. 15, Eq. (2.8).

[33]See, e.g., Ref. 25(c), Sec. 3; Ref. 25(d), Sec. 4.

[34]See Ref. 25(e), Sec. (2.3) and particularly Eq. (17). This equation has an error, i.e., $[G_\omega^q(x_0, \vec{p}_2|x_0, \vec{p}_3)]^*$ should have $\vec{p}_2$ and $\vec{p}_3$ interchanged.

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[51]See C. Kittel, Quantum Theory of Solids (Wiley, New York, 1963), p. 198, Eq. (140).

[52]Examples are the uniform field model of pn junctions (Ref. 2, p. 41) and tunneling in heterojunctions (Ref. 2, p. 55).

[53]Tunneling from d bands in transition metals clearly suggests that the transmission probability must depend on additional parameters such as the band index (angular momentum) and the reduced k vector, $\vec{k}_p$. See Ref. 18.

[54]Equation (2.28) is Eq. (31) of Ref. 20. Equation (30) in that reference defines λ by the relation

$$N_m \lambda = \psi_m(z_1) . \tag{30}$$

Note that the "normalization" constant N_m corresponds to our expression

$$\left[\frac{k_z}{LS} \left(\frac{m}{m^*_{n,zz}} \right) \right]^{1/2} \mathfrak{N}(\vec{k}, n; z_1)$$

$$= \left(\frac{1}{LS} \frac{m v_{g_z}}{\hbar} \right)^{1/2} \mathfrak{N}(\vec{k}, n; z_1)$$

$$= \lambda^{-1} | \langle \Psi(z_1; \vec{k}_p, E; k_z^\nu) \rangle | .$$

Furthermore, λ^{-2} has the dimensions of inverse length.

[55]See Eq. (31) in Ref. 20.

[56]Equation (2.32) corresponds to Eq. [IV (3.19)] and Eq. (2.36) to Eq. [IV (3.28)]. To obtain Eq. (2.40) let $\mu_2 \to -\infty$ in Eq. [IV (3.28)]. Furthermore, note the changed convention concerning the total current: In IV

$$\langle J \rangle = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \langle J(\omega) \rangle .$$

The field emitted current is always expressed as

$$\langle J \rangle = \int_{-\infty}^{\infty} dE \, j'(E) .$$

[57]Note that in the analysis of the ordered junction in IV we implicitly assumed and index ν to assume only one value. However, in the present case ν labels (i) The set of states $\Psi^{(+)}$ all of which have the same values of $(\vec{k}_p, E)$, and (ii) possible surface (band) states $(\vec{k}_p, E)$ having no incoming component $\psi_B^{(in)}$ and hence excluded from the set of scattering states $\Psi^{(+)}$.

[58]D. R. Penn, Phys. Rev. 14, 849 (1976). See, in particular, Eqs. (9) and (10), noting that in these equations that the right side of Eq. (2.49) is denoted $\alpha_0^{(m)}(x)$.

[58a]The arbitrary nature of z_1 in the PP theory is emphasized by the discussion in Sec. (b) of Ref. (58).

[59]Equation (3.2) is identical with Eq. (26) in Ref. 12. The restriction, of the sum over $\vec{k}_p$ to the projected area of the constant E-surface, is not stated by Nicolaou and Modinos. It is however a direct consequence of their explicit representation of the density of states $\delta(E - \epsilon(\vec{k}))$.

[60]Equation (3.3) corresponds to Eq. (32) in Ref. 20.

[61]See Eqs. (16a) and (24a) in Ref. 20.

[62]This is the interpretation of $N_m^2 \delta(E - E_m)$ required by Eq. (23) in Ref. 20.

[63]See Ref. 21, the paragraph following Eq. (6). Equation (3.4) is obtained by substituting Eq. (7) of Ref. 21 into Eq. (6) of Ref. 21.

[64]In a strictly noninteracting system, surface states cannot contribute to the steady-state field emission current, since once they are emptied, they cannot be repopulated. Our "weak-coupling" assumption corrects this deficiency, for it implies that the surface states have at all times their equilibrium occupancy, hence they could contribute a steady current. However, this contribution to the current cannot be described within a kinetic theory since in a surface state $v_{g_z} = 0$ (i.e., no current is incident from $z = -\infty$). We wish to thank J. W. Gadzuk for his comments and insight regarding these points.

[65]Equations (3.5)–(3.9) are identical to Eqs. (37), (32), and (14a) of Ref. 13.

[66]A more complete discussion of this point is found in Sec. IV of IV.

[67]This point is partly obscured by the fact that in the transfer-Hamiltonian formalism only the diagonal elements of ρ contribute to $j'(E)$, because of the diagonal structure of the effective (squared) matrix element (see Eq. (3.8)).

[68]This limitation on the equivalence of the kinetic theory and Feuchtwang's theory of tunneling for noninteracting systems has not been indicated in III.

[69]Note that this is the case even in the latest interpretation of the PP theory mentioned in Ref. 58.