Hamilton–Jacobi formulation and quantum theory of thermal wave propagation in the solid state

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A mathematical formalism has been developed for the description of the propagation of thermal waves in solids. The theory is based on the analogy between thermal waves and mechanics as manifested upon expressing the heat conduction equation in the Hamilton–Jacobi formalism. The transition of the classical formulation to quantum mechanics is accomplished by defining thermal wave operators for the generalized coordinates and the canonically conjugated momenta. The resulting theory shows that propagating, albeit heavily damped, thermal waves can be formally described by a quantum mechanical thermal harmonic oscillator (THO). The expectation values of observables, derived from Ehrenfest's theorems, are found to be of practical importance for the description of the thermal wave field in solids with inhomogeneous thermal and thermodynamic properties.

I. INTRODUCTION

In recent years photoacoustic spectroscopy has been used for the creation and detection of thermal waves in solids in general,[1–8] and in crystalline semiconductors in particular.[9–12] The ability of thermal waves to perform nondestructive depth-profiling studies in materials has been exploited mainly qualitatively due to the lack of appropriate theoretical models in the literature. It has been recognized for some time that the depth profiling of dopant concentrations in semiconductors may be the single most important application of thermal wave physics.[10,11,13] An important theoretical obstacle, however, to the realization of the full potential of thermal wave depth profilometry appears to be the complexity of the mathematical description of thermal wave propagation in continuous solids, especially those which exhibit large local variations of their relevant thermal and thermodynamic properties, i.e., the thermal conductivity, the density, and the specific heat. As a result of the mathematical difficulties, only two theoretical treatments have appeared in the literature, which assume discrete, multilayered solid structures with constant thermal and thermodynamic properties within each thin layer.[13,14] Furthermore, Afromowitz *et al.*[15] have applied discrete Laplace transformations to the heat conduction equation to treat the production of the photoacoustic signal in a solid with continuously variable optical absorption coefficient as a function of depth, however, the thermal parameters of the solid were assumed constant. Thomas *et al.*[3] calculated the Green's function for the three-dimensional heat conduction equation describing thermal wave propagation in a thermally uniform solid with a subsurface discontinuity ("flaw"). In most experimental situations of interest one has to deal with thermal wave propagation in fields where drastic variations of thermal properties occur within a thermal wavelength[16] from the source of oscillation. In this limit the thermal wave behavior can be described formally by using the analogy between classical mechanical plane wave propagation and thermal wave motion. The crucial difference between these two types of waves is that the former kind is a result of the time harmonic solutions to the Helmholtz equation, which is a hyperbolic partial differential equation of second order in the derivative of the wave-function field, whereas the latter kind is a result of time harmonic solutions to the Fourier equation of heat conduction, which is a parabolic partial differential equation of first order in the time derivative of the thermal field wave function. The above difference has a profound effect in the nature of the two kinds of waves: the hyperbolic type is able to propagate freely within matter and suffers attenuation only when the wave vector in the medium has an imaginary component, while the parabolic type always exhibits heavy attenuation as a function of propagation distance in the medium.

In this paper the formal analogy between classical and quantum wave fields and a thermal wave field will be investigated. It will be shown that the thermal wave field Hamiltonian is nondissipative irrespective of the spatial dependence of the relevant thermal/thermodynamic properties of the system. This property, in turn, allows the definition of an eikonal equation and Fermat's principle for thermal wave propagation, as well as the definition of a fundamental spatial eigenfrequency of the thermal oscillations.

The classical mechanical Hamiltonian of the thermal wave field will be further shown to be that of a harmonic oscillator in the temperature potential field. This observation allows the quantization of the thermal wave field, which sets the foundations of the microscopic description of wave phenomena occurring within propagation distances on the order of a thermal wavelength, such as thermal diffraction. The macroscopic thermal wave equations can indeed be recovered in a quantum mechanical expectation function form after introducing expansions of the thermal wave field observables in terms of integrals over complete sets of eigenfunctions of the thermal Schrödinger equations. The formalism allows the explicit evaluation of the macroscopic tempera-

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ture field in continuous solids with nonhomogeneous thermal/thermodynamic properties as a result of the propagation of thermal wave fronts in the potential field defined by the temperature-dependent generalized coordinate. A similar approach was used successfully[17,18] in the quantization of light rays propagating in solids, where both Schrödinger-type[17] and Dirac-type[18] theories were advanced for the description of the optical wave field observables.

II. HAMILTON–JACOBI FORMULATION OF THERMAL WAVE PHYSICS

The generation of thermal waves in a medium is the result of the presence of a harmonic heat source at the origin, modulated at some angular frequency ω_0. The most commonly used heat sources are modulated laser beams,[1,3–5,8,12] electron beams,[2,9,11] or ac current sources.[19] The temperature field $\theta(\mathbf{r},t)$ in the medium excited by the heat source is given by the macroscopic Fourier heat conduction equation, which is a statement of energy balance in the medium:

$$\nabla\cdot[k(\mathbf{r})\nabla\theta(\mathbf{r},t)] - \rho(\mathbf{r})c(\mathbf{r})\frac{\partial}{\partial t}\theta(\mathbf{r},t) = 0, \tag{2.1}$$

where $k(\mathbf{r})$, $\rho(\mathbf{r})$, and $c(\mathbf{r})$ are the (generally spatially variant) thermal conductivity (W/m °K), density (kg/m^3), and specific heat (J/kg °K), respectively, of the medium. For most experimental thermal wave solid state geometries $c(\mathbf{r})$ implies the specific heat at constant volume, however, constant pressure specific heats must be used when the experimental conditions require it. In this work the one-dimensional counterpart of (2.1) will be used in order to simplify the formalism, with the three-dimensional case constituting a straightforward extension of the fundamental concepts developed herein.

A harmonic time dependence of the one-dimensional temperature field of the form

$$\theta(x,t) = T(x)\exp(i\omega_0 t) \tag{2.2}$$

yields the Fourier–Helmholtz equation

$$\frac{d}{dx}\left[k(x)\frac{d}{dx}T(x)\right] - i\omega_0\rho(x)\,c(x)\,T(x) = 0. \tag{2.3}$$

In passing we note that (2.3) is in the form of the Liouville equation with the single eigenvalue $\lambda = i\omega_0$. The Lagrangian function, which corresponds to (2.3), is[20]

$$\mathscr{L} = \frac{1}{2}k(x)\left[\frac{dT(x)}{dx}\right]^2 + i\omega_0\int_0^T y\,dy \tag{2.4}$$

and satisfies the Euler equation

$$\frac{\partial\mathscr{L}}{\partial T} - \frac{d}{dx}\frac{\partial\mathscr{L}}{\partial(dT/dx)} = 0. \tag{2.5}$$

In thermal wave configurations the following boundary conditions are usually assumed[13,14]:

$$T(x=0) = T_0, \tag{2.6a}$$

$$-k(x)\frac{dT(x)}{dx}\bigg|_{x=0} = Q_0, \tag{2.6b}$$

where the domain of the temperature field encompasses the one-dimensional volume (x). The surface (s) which encloses (x) is defined by the origin $(x=0)$ and some suitable point $L < +\infty$. The Hamiltonian is given by

$$H(x,T,p_T) = p_T\left[\frac{dT(x)}{dx}\right] - \mathscr{L}$$
$$= p_T^2/2k(x) - (i/2)\,\omega_0\rho(x)c(x)T^2, \tag{2.7}$$

with p_T the generalized momentum defined by

$$p_T = \frac{\partial\mathscr{L}}{\partial(dT/dx)} = k(x)\frac{dT(x)}{dx}. \tag{2.8}$$

Equations (2.7) and (2.8) show that for the thermal wave problem the generalized coordinate and momentum are the field temperature and heat flux, respectively. The Hamiltonian form (2.7) is not appropriate, however, for use in the consideration of thermal wave dynamics, because it is an explicit function of the spatial coordinate (x). A canonical transformation is required, such that both coordinate and momentum will be constants of the motion. Consider the following parametric transformations:

$$\zeta \equiv \frac{1}{J}\int_0^x\left[\frac{\rho(y)c(y)}{k(y)}\right]^{1/2}dy, \tag{2.9}$$

$$\tau \equiv [k(x)\rho(x)c(x)]^{1/4}T(x), \tag{2.10}$$

and

$$J \equiv \frac{1}{L}\int_0^L\left[\frac{\rho(y)c(y)}{k(y)}\right]^{1/2}dy. \tag{2.11}$$

The generating function, which produces the desired canonical transformation, is Hamilton's principal function[21] S, in which the time coordinate has been replaced by the spatial coordinate (x). The Hamilton–Jacobi equation

$$\frac{\partial S}{\partial x} = -H\left(x,T,\frac{\partial S}{\partial T}\right)$$
$$= -\frac{1}{2k(x)}\left(\frac{\partial S}{\partial T}\right)^2 + \frac{i}{2}\omega_0\rho(x)c(x)\,T^2 \tag{2.12}$$

transforms to the following equations, after introduction of the new variables ζ and τ:

$$\frac{\partial S}{\partial\zeta} = -\frac{J}{2}\left[\left(\frac{\partial S}{\partial\tau}\right)^2 - i\omega_0\tau^2\right]. \tag{2.13}$$

Using separation of variables in the form

$$S(\tau,\zeta,\alpha) = W(\tau,\alpha) - \alpha\zeta \tag{2.14}$$

yields an equation for Hamilton's characteristic function $W(\tau,\alpha)$:

$$\frac{J}{2}\left[\left(\frac{\partial W}{\partial\tau}\right)^2 - i\omega_0\tau^2\right] = \alpha = \text{const.} \tag{2.15}$$

Equation (2.15) is the canonical transformation in which the new coordinate ζ is cyclic and the transformed Hamiltonian is a constant of the motion and assumes the meaning of the total generalized energy of the thermal wave field:

$$H\left(\tau,\frac{\partial W}{\partial\tau}\right) = \alpha \equiv E. \tag{2.16}$$

In the Hamilton–Jacobi theory of thermal waves the generalized coordinate is $\tau(\zeta)$ and the generalized momentum is $p_\tau = \partial W/\partial\tau$. The functional form of the canonical Hamiltonian

$$H(\tau,p_\tau) = \tfrac{1}{2}Jp_\tau^2 + \tfrac{1}{2}K\tau^2 \tag{2.17}$$

shows that thermal wave field behavior is equivalent to that of a thermal harmonic oscillator (THO), with the effective mass $m = J^{-1}$ and spring constant K, which is subject to a restoring, conservative force $F = -K\tau$ generated by the effective harmonic potential field $V(\tau) = \frac{1}{2}K\tau^2$. The frequency of the oscillation in the canonical coordinates can be found via the use of the action-angle variable

$$I_\tau = \oint p_\tau d\tau = \oint \left[\frac{\partial W(\tau,\alpha)}{\partial \tau}\right] d\tau. \tag{2.18}$$

Defining the spring constant

$$K \equiv -i\omega_0 J, \tag{2.19}$$

the integral of (2.18) can be evaluated between 0 and 2π to yield the frequency of the motion[21] of the THO,

$$\nu_\tau = \frac{\partial H}{\partial I_\tau} = \frac{1}{2\pi}(KJ)^{1/2}, \tag{2.20}$$

so that an angular frequency can be written as

$$\Omega_\tau \equiv 2\pi\nu_\tau = (KJ)^{1/2} \; [m^{-1}]$$

or

$$\Omega_\tau(\omega_0) = \pm\frac{(1-i)}{L}\int_0^L \left[\frac{\omega_0 \rho(y) c(y)}{2k(y)}\right]^{1/2} dy$$

$$\equiv \pm\frac{(1-i)}{L}\int_0^L a_s(\omega_0, y)\, dy, \tag{2.21}$$

where $a_s(\omega_0, y)$ is the local thermal diffusion coefficient of the Rosencwaig–Gersho theory[22] at depth y in the medium. Here, Ω_τ is the spatial angular frequency of oscillation of the THO and is defined in terms of the spatial extent of the medium or, in the case of semi-infinite media, in terms of

$$\lim_{L\to\infty}\left(\frac{1}{L}\int_0^L \alpha_s(\omega_0, y)\, dy\right).$$

The Hamilton–Jacobi formulation of the thermal wave problem leads to an eikonal equation of thermal wave physics, upon combination of (2.15) and (2.16):

$$(\nabla_\tau W)^2 = p_\tau^2. \tag{2.22}$$

Equation (2.22) is the rule for the construction of the surfaces of constant phase, via the equation

$$W(\tau, \alpha) = \text{const.} \tag{2.23}$$

The thermal gradient of W determines the normal to such surfaces. Any surface (s) that satisfies the condition (2.23) is a surface of constant thermal phase and thus defines a thermal wave front. The thermal ray trajectories are determined everywhere in space by (2.22) and are perpendicular to the wave fronts, whose phase velocities are given by

$$(v_\tau)_p = \frac{E}{|\partial W/\partial \tau|} = \left(\frac{J}{2}\right)^{1/2}\frac{E}{\sqrt{E - V(\tau)}}. \tag{2.24}$$

At this stage, a variational Fermat's principle can be formulated for the description of geometrical thermal ray trajectories, analogous to those of classical mechanics and geometrical optics. This principle can be expressed as follows:

$$\delta\int\frac{ds}{(v_\tau)_p} = \delta\int p_\tau\, ds = 0, \tag{2.25}$$

where ds is the incremental length in the configuration space spanned by the generalized coordinate τ and the conjugate momentum p_τ.

Finally, it is interesting to note that there exist three Poisson brackets for the canonical variables of the one-dimensional thermal wave problem,

$$\{\tau, p_\tau\} = 1, \tag{2.26a}$$

$$\{\tau, H\} = Jp_\tau, \tag{2.26b}$$

$$\{p_\tau, H\} = i\omega_0\tau J, \tag{2.26c}$$

along with the relation

$$\frac{dH}{d\xi} = \frac{\partial H}{\partial \xi}, \tag{2.27}$$

which is a consequence of the fact that the total generalized energy of the medium is conserved over one cycle of spatial oscillation of the THO.

III. QUANTUM THEORY OF THERMAL WAVE PHYSICS

The classical theory of thermal wave fields in one dimension, which was presented in Sec. II above, is capable of describing only macroscopic thermal wave phenomena, such as the trajectories of thermal rays and the eikonal equation (2.22). In this limit of geometrical thermal wave physics the Fermat's principle (2.25) can be used successfully; however, it cannot rederive the Fourier–Helmholtz equation (2.3) through purely algebraic manipulations. Furthermore, the Fourier–Helmholtz equation is itself a reduced form of the canonical Hamilton–Jacobi equation (2.16) and thus it suffers from the mathematical disadvantages of noncanonical differential equations with regard to the degree of difficulty in obtaining the most general solution. In this section it will be shown that the thermal wave equation can be recovered and the most general solution can be obtained relatively easily from geometrical thermal ray physics via quantization, as by-products of thermal wave Ehrenfest's theorems. A complete analogy to the traditional quantum theory can be drawn upon replacing all classical variables of the Hamilton–Jacobi theory with thermal wave quantum mechanical operators:

$$\tau \to \hat{\tau} = \tau, \tag{3.1}$$

$$p_\tau \to \hat{p}_\tau = -i\hbar\frac{\partial}{\partial \tau}, \tag{3.2}$$

$$H \to \hat{H} = i\hbar\frac{\partial}{\partial \xi}. \tag{3.3}$$

The constant $\hbar$ appearing in (3.1)–(3.3) is the thermal wave equivalent of Planck's constant. The Hamiltonian operator $\hat{H}$ is in units of the generalized energy of the THO:

$$[\hat{H}] = [E] = \mathrm{W\,{}^\circ K/m^3}$$

so that

$$[\hbar] = \mathrm{W\,{}^\circ K/m^2}.$$

Equation (3.3) is now assumed to admit eigenfunction solutions

$$\hat{H}\psi = i\hbar\frac{\partial\psi}{\partial\xi}. \tag{3.4}$$

Use of the definitions (3.1) and (3.2) in (2.17) and insertion in (3.4) yields the canonical coordinate-dependent "Schrödinger equation" of thermal wave quantum mechanics:

$$-\not{b}^2\left(\frac{J}{2}\right)\frac{\partial^2}{\partial\tau^2}\psi(\tau,\zeta)+V(\tau)\psi(\tau,\zeta)=i\not{b}\frac{\partial}{\partial\zeta}\psi(\tau,\zeta), \quad (3.5)$$

where

$$V(\tau)=\tfrac{1}{2}K\tau^2. \quad (3.6)$$

Separation of variables in the form

$$\psi(\tau,\zeta)=\phi(\tau)\exp(-iE\zeta/\not{b}) \quad (3.7)$$

gives the coordinate-independent "Schrödinger equation"

$$\frac{d^2}{d\tau^2}\phi(\tau)+\frac{2}{\not{b}^2J}[E-V(\tau)]\,\phi(\tau)=0. \quad (3.8)$$

The solutions to (3.8) are, in principle, the eigenfunctions of the quantum mechanical harmonic oscillator; however, at this point it must be recognized that the constant $\not{b}$ is consistent with real values of the generalized energies only if it is a complex quantity of the form

$$\not{b}=(1+i)|\not{b}|. \quad (3.9)$$

If (3.9) is satisfied, the anticipated harmonic oscillator eigenvalues[23] $E_n=(n+\frac{1}{2})\not{b}\Omega_\tau$ will be real, as can be verified from (2.21). Using (3.9) and (2.19) in (3.8) results in the following equation:

$$|\not{b}|^2J\frac{d^2}{d\tau^2}\phi(\tau)+(\omega_0J)\tau^2\phi(\tau)=2iE\phi(\tau). \quad (3.10)$$

Defining a new variable

$$z_1\equiv(4\omega_0/|\not{b}|^2)^{1/4}\tau, \quad (3.11)$$

Eq. (3.10) becomes

$$\frac{d^2}{dz_1^2}\phi(z_1)+\left[\frac{z_1^2}{4}-i\left(\frac{E}{\omega_0|\not{b}|J}\right)\right]\phi(z_1)=0. \quad (3.12)$$

Equation (3.12) has well-defined solutions if and only if

$$E/\omega_0^{\frac{1}{2}}|\not{b}|J=p+\tfrac{1}{2} \quad (3.13a)$$

and

$$z_1=ze^{i\pi/4}, \quad (3.13b)$$

so that (3.12) may be transformed to

$$\frac{d^2}{dz^2}\phi_p(z)+\left(p+\frac{1}{2}-\frac{z^2}{4}\right)\phi_p(z)=0. \quad (3.14)$$

Equation (3.14) is a parabolic wave equation or Weber–Hermite equation[24] with eigenvalues

$$E_p=\omega_0^{\frac{1}{2}}|\not{b}|J(p+\tfrac{1}{2}). \quad (3.15)$$

For general values of p the solutions to (3.14) are the Weber functions,[25] $\phi_p(z)=D_p(z)$, where

$$D_p(z)=2^{(p/2)}e^{-z^2/4}\left\{\frac{\sqrt{\pi}}{\Gamma[(1-p)/2]}\,{}_1F_1\left(-\frac{p}{2};\frac{1}{2};\frac{z^2}{2}\right)-\frac{z\sqrt{2\pi}}{\Gamma(-p/2)}\,{}_1F_1\left(\frac{1-p}{2};\frac{3}{2};\frac{z^2}{2}\right)\right\}, \quad (3.16)$$

where ${}_1F_1(a;c;z)$ is a degenerate hypergeometric function given by[26]

$${}_1F_1(a;c;z)=\frac{e^{ia\pi}z^{-a}}{\Gamma(a)}\int_0^\infty e^{-u}u^{a-1}\left(1+\frac{u}{z}\right)^{c-a-1}du, \quad (3.17)$$

with $z=|z|e^{i\theta}$, $-\pi<\theta<\pi$. For integral values of p, i.e., for $p=n$, where n is a positive integer, the Weber functions can be expressed by means of Hermite polynomials[25]:

$$D_n(z)=2^{-(n/2)}e^{-z^2/4}H(z/\sqrt{2}) \quad (3.18a)$$

$$=(-1)^ne^{z^2/4}\frac{d^n}{dz^n}e^{-z^2/2}. \quad (3.18b)$$

In the particular case where $p=n$ the eigenvalues of the Weber–Hermite equation are

$$E_n=(n+\tfrac{1}{2})\,\omega_0^{1/2}\,|\not{b}|J. \quad (3.19)$$

Equations (2.11), (2.20), and (2.21) give

$$|\Omega_\tau|=\omega_0^{1/2}J, \quad (3.20)$$

so that (3.19) can be written

$$E_n=(n+\tfrac{1}{2})|\not{b}|\,|\Omega_\tau| \quad (3.21a)$$

$$=(n+\tfrac{1}{2})\not{b}\Omega_\tau. \quad (3.21b)$$

Now Eq. (3.21) can be used to interpret $\not{b}$ of the thermal wave quantum theory in terms of the generalized energy of thermal wave packets (thermions!), as the constant ratio of the energy to the angular frequency of such wave packets:

$$E=\not{b}\Omega_\tau=b\nu_\tau. \quad (3.22)$$

Equation (3.22) in conjunction with (2.22) and (2.24) yields a thermal wave equivalent of the de Broglie relation,

$$\lambda_{\rm th}=\frac{b}{p_\tau}=\frac{1}{2\pi}\left[\frac{\omega_0\rho(\zeta)c(\zeta)}{k(\zeta)}\right]^{1/2}. \quad (3.23)$$

Farther insight into the nature of the constant $\not{b}$ is obtained upon writing (3.22) in the form

$$\not{b}=\frac{E}{(1-i)\,[(1/L)\int_0^L a_s(\omega_0,y)\,dy]}=\frac{E}{\langle k_{\rm th}\rangle}, \quad (3.24)$$

where $k_{\rm th}$ is the one-dimensional component of the complex thermal wave vector[16]

$$\mathbf{k}_{\rm th}=k_{\rm th}\hat{\zeta}, \quad (3.25a)$$

and

$$|k_{\rm th}|=2\pi/\lambda_{\rm th}. \quad (3.25b)$$

The presence of an imaginary component in the thermal wave vector is responsible for the exponential attenuation of thermal waves propagating in a continuous medium. From another point of view, a medium whose thermal wave vector is given by (3.25) can be described as thermally lossy, in analogy to optically lossy media arising in the propagation of electromagnetic radiation.[27] Equations (3.24) and (3.25b) show that $\not{b}$ is proportional to the wavelength $\langle\lambda_{\rm th}\rangle$ of the thermal wave packet, averaged over the entire extent of the propagation medium. The proportionality of $\not{b}$ to $\langle\lambda_{\rm th}\rangle$ is analogous to that observed between the Planck's constant of the quantum theory of light rays and the wavelength of the optical radiation.[17] It is also consistent with the correspondence principle of quantum mechanics: The thermal wave Schrödinger equation (3.5) can be transformed using the substitution

$$\psi(\tau,\zeta)=A\exp[iW(\tau,\zeta)/\not{b}] \quad (3.26)$$

to an equation for W:

$$\frac{\partial}{\partial \zeta} W(\tau,\zeta) + \left(\frac{J}{2}\right)\left[\frac{\partial W(\tau,\zeta)}{\partial \tau}\right]^2 + V(\tau)$$
$$- i\hbar\left(\frac{J}{2}\right)\left[\frac{\partial^2 W(\tau,\zeta)}{\partial \tau^2}\right] = 0. \quad (3.27)$$

Letting $\hbar \to 0$ in accordance with the requirement of the correspondence principle, Eq. (3.27) becomes identical to (2.15) of the classical mechanical Hamilton–Jacobi theory:

$$H(\tau,p_\tau) + \frac{\partial}{\partial \zeta} W(\tau,\zeta) = 0, \quad (3.28)$$

with $W(\tau,\zeta)$ being Hamilton's characteristic function, for which the eikonal equation (2.22) is valid.

In the thermal wave quantum mechanical theory, the eigenvalue equation

$$\hat{H}\psi_n(\tau,\zeta) = E_n \psi_n(\tau,\zeta) \quad (3.29)$$

has the set of eigenfunctions

$$\psi_n(z,\zeta) = N_n D_n(z) \exp(-iE_n\zeta/\hbar), \quad (3.30)$$

where

$$z = (4\omega_0/|\hbar|^2)^{1/4} e^{-i\pi/4}\tau, \quad (3.31)$$

the E_n are given by (3.21), and the N_n are normalization constants, which can be determined using the orthogonality property of the Weber functions[24]:

$$\int_{-\infty}^{\infty} D_m^*(z) D_n(z) dz = (2\pi)^{1/2} n! \delta_{mn}. \quad (3.32)$$

The normalization condition for ψ_n is

$$\int_{-\infty}^{\infty} \psi_n^*(z,\zeta)\psi_n(z,\zeta) dz = 1. \quad (3.33)$$

Equations (3.30), (3.32), and (3.33) determine the normalizing constants

$$N_n = [1/(2\pi)^{1/2} n!]^{1/2}. \quad (3.34)$$

IV. EXPECTATION FUNCTIONS AND EHRENFEST'S THEOREMS

The most important application of thermal wave quantum mechanics is its ability to calculate expectation functions for various macroscopic observables, especially those which are difficult or impossible to derive explicitly from the macroscopic Fourier–Helmholtz equation, such as the temperature and the heat flux fields in the medium of thermal wave propagation. In this section we shall derive the expectation values for the potential energy of the THO, expectation functions for the temperature and the heat flux, and a macroscopic heat diffusion equation of the thermal wave center of gravity in the sense and form of Ehrenfest's theorems.

A. Potential energy of THO

We have

$$\langle V(z)\rangle_n = \int_{-\infty}^{\infty} \psi_n^*(z,\zeta) z^2 \psi_n(z,\zeta) dz \quad (4.1)$$

$$= N_n^2 |G_n(\zeta)|^2 \int_{-\infty}^{\infty} z^2 D_n^2(z) dz, \quad (4.2)$$

where

$$G_n(\zeta) = \exp(-iE_n\zeta/\hbar). \quad (4.3)$$

Using (3.18a) in (4.2), and the Hermite polynomial identity[28]

$$\int_{-\infty}^{\infty} x^2 e^{-x^2} H_n^2(x) dx = \sqrt{x}(2n+1)2^{n-1} n! \quad (4.4)$$

it can be shown that

$$\langle z^2\rangle_n = \langle V(z)\rangle_n = 2n+1 \quad (4.5)$$

and, substituting (3.31) in (4.5),

$$\langle V(\tau)\rangle_n = \tfrac{1}{2}(2n+1)(k|\hbar|/2\omega_0^{1/2} e^{-i\pi/2},$$
$$= \tfrac{1}{2}(n+\tfrac{1}{2})\omega_0^{1/2} J|\hbar|$$
$$= \tfrac{1}{2}E_n. \quad (4.6)$$

Equation (4.6) indicates that, for any value of n, the average potential energy is half of the total generalized energy per cycle of oscillation, a result similar to that obtained in the case of the classical mechanical harmonic oscillator.

B. Temperature field

It should be noticed that expectation values are calculated as integrals over the variable z, which is related to the generalized temperature τ via (3.31) and, ultimately, to the temperature T via (2.10). In the present quantum formalism, however, z is considered a dummy variable when under the integral sign, spanning the range of values $(-\infty, +\infty)$. The expectation function for $T(x)$ can be found from

$$\langle z\rangle_{n,m} = \int_{-\infty}^{\infty} \psi_n^*(z,\zeta) z \psi_m(z,\zeta) dz \quad (4.7)$$

$$= (N_n N_m / 2^{1/2(n+m)-1}) G_n^*(\zeta) G_m(\zeta) \times \begin{cases} [\sqrt{\pi}2^n(n+1)]_{m=n+1}, \\ [\sqrt{\pi}2^{n-1}n!,]_{m=n-1}, \\ 0, \quad m\neq n\pm 1. \end{cases} \quad (4.8)$$

Therefore,

$$\langle z\rangle_{n,m} = \begin{cases} \left(\frac{n+1}{2}\right)^{1/2} G_n^*(\zeta) G_{n+1}(\zeta), & m = n+1, \\ (n/2)^{1/2} G_n^*(\zeta) G_{n-1}(\zeta), & m = n-1, \\ 0, \quad m\neq n\pm 1. \end{cases} \quad (4.9)$$

For the purpose of obtaining an expression for the temperature field that is consistent with direct solutions[16] to the macroscopic Fourier-Helmholtz equation (2.3) in the limit of constant k, ρ, and c, we choose the particular eigenmodes $n = 0$, $m = 1$ in (4.9), and we get

$$\langle z\rangle_{0,1} = (1/\sqrt{2}) G_0^*(\zeta) G_1(\zeta) \quad (4.10)$$

$$= (1/\sqrt{2}) \exp[-e^{i\pi/4}|\Omega_\tau|\zeta], \quad (4.11)$$

and using (3.31), (2.9), and (2.10) in (4.11), the expectation (macroscopic) function for the temperature can be written as

$$T(x) \equiv \langle T(x)\rangle_{0,1} = \frac{|\hbar|^{1/2} e^{-i\pi/4}}{2[\omega_0 k(x)\rho(x)c(x)]^{1/4}} \times \exp\left[-\int_0^x \sigma_s(\omega_0,x')dx'\right], \quad (4.12)$$

where

$$\sigma_s(\omega_0,x') \equiv (1+i)a_s(\omega_0,x') \quad (4.13)$$

is the complex local thermal diffusion coefficient of the extended Rosencwaig–Gersho theory.[22] Equation (4.12) is valid for semi-infinite solids, for which the positive root for $\Omega_\tau(\omega_0)$ was rejected in (2.21). This situation reflects the use of thermal wave physics for quantitative analysis leading to depth-profiling at high source modulation frequencies ω_0, so that

$$1/|\sigma_s(\omega_0,L)| \ll L, \tag{4.14}$$

where L is the thickness of the propagation medium. If (4.14) is not satisfied, then the term $\exp[-\int_0^x \sigma_s(\omega_0,x')dx']$ in (4.12) must be replaced by $2\cosh[\int_0^x \sigma_s(\omega_0,x')dx']$, which is the result of the retention of the positive root for $\Omega_\tau(\omega_0)$ in (2.21). Using

$$E_0 = \tfrac{1}{2}|\hbar|\,|\Omega_\tau| = (1/J)|\Omega_\tau|^2 \tau_0^2 = Jp_T^2(0) \tag{4.15}$$

for the average total macroscopic generalized energy of the THO in (4.12), with $\tau_0 = \tau(\zeta = 0)$, the expectation function for the temperature becomes, after some algebraic manipulation and use of (2.6) and (2.8)–(2.11),

$$T(x) = \frac{Q(x)}{k(x)\sigma_s(\omega_0,x)} \exp\left[-\int_0^x \sigma_s(\omega_0,x')dx'\right], \tag{4.16}$$

where

$$Q(x) \equiv Q_0 \left[\frac{k(x)\rho(x)c(x)}{k(0)\rho(0)c(0)}\right]^{1/4} \times\left\{1 + \left(\frac{e - i\pi/4}{4\omega_0^{1/2}}\right)\left[\frac{k(0)}{\rho(0)c(0)}\right]^{1/2} \times\left[\frac{d}{dx}\ln(k\rho c)\right]_x = 0\right\}^{-1}. \tag{4.17}$$

Equation (4.16) reduces immediately to

$$T(x) = [Q_0/(1+i)k(\omega_0\rho c/2k)^{1/2}] \times\exp[-(1+i)(\omega_0\rho c/2k)^{1/2}x], \tag{4.18}$$

in the limit of constant k, ρ, and c. Equation (4.18) has been previously derived by a number of authors.[13,16,29,30]

C. Ehrenfest's theorems

These theorems can be easily formulated upon introducing quantum mechanical commutation relations to replace the Poisson brackets (2.26). For the conjugate variables τ and p_τ the following operator relations can be easily proven:

$$[\hat{\tau},\hat{p}_\tau] = i\hbar, \tag{4.19a}$$

$$[\hat{\tau},\hat{H}] = \hbar J\frac{\partial}{\partial\zeta}, \tag{4.19b}$$

$$[\hat{p}_\tau,\hat{H}] = -\hbar\omega_0 J\tau. \tag{4.19c}$$

Ehrenfest's theorem for the generalized thermal momentum can be derived from consideration of the expectation value

$$\frac{d}{d\zeta}\langle z\rangle_{n,m} = \frac{d}{\delta\zeta}\int_{-\infty}^{\infty} \psi_n^*(z,\zeta)z\psi_m(z,\zeta)dz \tag{4.20}$$

$$= \frac{i}{\hbar}\left[\int_{-\infty}^{\infty} \psi_n^*(\hat{H}z - z\hat{H})\psi_m dz\right]$$

$$= (i/\hbar)\langle[\hat{H},z]\rangle_{n,m}. \tag{4.21}$$

Equation (4.21) was obtained under the assumptions[31] that $\hat{H}$ is Hermitian and that z is not an explicit function of ζ. Equations (3.11), (3.13b), (4.19b), and (4.21) give

$$\frac{d}{d\zeta}\langle z\rangle_{n,m} = \left(\frac{4\omega_0}{|\hbar|^2}\right)e^{-i\pi/4}\left\langle\frac{d}{d\zeta}\tau(\zeta)\right\rangle_{n,m}. \tag{4.22}$$

Using the defining equations (2.9)–(2.11) the term in the brackets can be calculated:

$$\left\langle\frac{d}{d\zeta}\tau(\zeta)\right\rangle_{n,m} = \frac{1}{F^{1/4}(\zeta)}\left[\frac{d}{d\zeta}F^{1/4}(\zeta)\right]\langle\tau(\zeta)\rangle_{n,m} + [J/F^{1/4}(\zeta)]\,\langle p_\tau(\zeta)\rangle_{n,m} \tag{4.23}$$

$$= \frac{d}{d\zeta}\langle\tau(\zeta)\rangle_{n,m},$$

where

$$F(\zeta) \equiv k(\zeta)\rho(\zeta)c(\zeta). \tag{4.24}$$

The equality of expectation values,

$$\left\langle\frac{d}{d\zeta}\tau(\zeta)\right\rangle_{n,m} = \frac{d}{d\zeta}\langle\tau(\zeta)\rangle_{n,m}, \tag{4.25}$$

originates in the fact that the potential field (3.6) for the THO is harmonic and does not involve terms higher than second order.[32] Equations (4.22) and (4.23) yield the following thermal wave Ehrenfest equation, which relates the expectation values of the generalized thermal velocity $(d/d\zeta)\langle\tau\rangle$ and the generalized thermal momentum $\langle p_\tau\rangle$:

$$\frac{d}{d\zeta}\langle\tau(\zeta)\rangle_{n,m} = \frac{1}{F^{1/4}(\zeta)}\left[J\langle p_\tau(\zeta)\rangle_{n,m} + \left(\frac{d}{d\zeta}F^{1/4}(\zeta)\right)\langle\tau(\zeta)\rangle_{n,m}\right]. \tag{4.26}$$

For $F = \text{const}$, (4.26) reduces to

$$\langle p_T\rangle_{n,m} = k\frac{d}{dx}\langle T\rangle_{n,m}, \tag{4.27}$$

in agreement with (2.8).

Furthermore, an equation for the motion of the observable thermal ray center of gravity can be derived in the form of an Ehrenfest relation

$$\left\langle\frac{d^2}{d\zeta^2}\tau(\zeta)\right\rangle_{n,m} = \frac{d^2}{d\zeta^2}\langle\tau(\zeta)\rangle_{n,m} = J\frac{d}{d\zeta}\langle\Pi_\tau(\zeta)\rangle_{n,m}, \tag{4.28}$$

where $\Pi_\tau(\zeta)$ is the effective generalized thermal momentum in a medium with variable thermal/thermodynamic parameters $k(x)$, $\rho(x)$, and $c(x)$:

$$\Pi_\tau(\zeta) \equiv \frac{1}{F^{1/4}(\zeta)}\left[p_\tau(\zeta) + \frac{1}{J}\left(\frac{d}{d\zeta}F^{1/4}(\zeta)\right)\tau(\zeta)\right]. \tag{4.29}$$

Ehrenfest's theorem (4.26) can now be written in a suggestive form as

$$\frac{d}{d\zeta}\langle\tau\rangle_{n,m} = \frac{1}{J^{-1}}\langle\Pi_\tau\rangle_{n,m}, \tag{4.30}$$

where J^{-1} plays the role of a generalized mass of the system, in agreement with (2.17). Differentiating $\Pi_\tau(\zeta)$ with respect to ζ and inserting the resulting expression in (4.28) gives

$$\frac{d^2}{d\zeta^2}\langle\tau(\zeta)\rangle_{n,m} + \left[\Omega_\tau^2 - \frac{1}{F^{1/4}(\zeta)}\frac{d^2}{d\zeta^2}F^{1/4}(\zeta)\right]\langle\tau(\zeta)\rangle_{n,m} = 0. \tag{4.31}$$

Equation (4.31) is Ehrenfest's theorem, which governs the motion of the thermal ray heat centroid in the presence of a harmonic generalized potential energy field $V(\tau)$ and for general functional forms of $F(\zeta)$. An equation similar to (4.31) in structure has been derived in connection with the eigenvalue problem of the Liouville equation by Morse and Feshbach [Ref. (26), Eq. (6.3.22)]. The analogy of the Ehrenfest approach to the classical mechanical theory became apparent with (4.30), which involves generalized thermal displacement and momentum. This analogy becomes complete once (4.28) is written in terms of an integral over eigenfunctions:

$$\frac{d^2}{d\zeta^2}\langle\tau\rangle_{n,m} = \frac{e^{i\pi/4}}{(4\omega_0/|\hbar|^2)^{1/4}}\frac{d^2}{d\zeta^2}\int_{-\infty}^{\infty}\psi_n^*(z,\zeta)\,z\psi_m\,z,\zeta)\,dz$$

$$= \frac{i}{\hbar}\left[\int_{-\infty}^{\infty}\psi_n^*\,(\hat{H}\hat{\Pi}_\tau - \hat{\Pi}_\tau\hat{H})\,\psi_m\,dz\right]$$

$$= (i/\hbar)\langle[\hat{H},\hat{\Pi}_\tau]\rangle_{n,m}. \qquad (4.32)$$

To evaluate this commutator, the commutation relation

$$\hat{\Pi}_\tau f(\tau) - f(\tau)\hat{\Pi}_\tau = -i\hbar\frac{\partial f(\tau)}{\partial\tau} \qquad (4.33)$$

can be easily verified from the definition (3.2) of the generalized thermal momentum operator $\hat{p}_\tau$. Using (4.33) in (4.32) and comparing with (4.28) yields the following form of Ehrenfest's theorem (4.31):

$$\frac{d}{d\zeta}\langle\Pi_\tau\rangle_{n,m} = \left\langle-\frac{\partial U}{\partial\tau}\right\rangle_{n,m}, \qquad (4.34)$$

where U is the effective potential energy

$$U(\tau) = \tfrac{1}{2}K_{\rm eff}\tau^2, \qquad (4.35)$$

with the generalized effective spring constant

$$K_{\rm eff}(\zeta) \equiv K - \frac{1}{JF^{1/4}(\zeta)}\frac{d^2}{d\zeta^2}F^{1/4}(\zeta). \qquad (4.36)$$

Equation (4.34) is Ehrenfest's approach equivalent to the classical relationship between a restoring force, $-\nabla_\tau U$, and the rate of change of momentum due to the action of the force. The equations of motion (4.30) and (4.34) of the heat centroid of the thermal rays demonstrate the correspondence between macroscopic heat conduction theory and the expectation values of our microscopic approach.

D. Position of heat centroid and uncertainty principle

For experimental purposes the position of the heat centroid at a given modulation frequency ω_0 is extremely important, as its determination substantiates the depth-profiling capacity of thermal wave physics. The observed (measured) wave centroid is mathematically a well-defined quantity for thermal waves, unlike unattenuated electromagnetic and other plane waves, due to the damped nature of the former:

$$\langle\zeta\rangle_{0,1} = \frac{\int_0^\infty \zeta\,G_0^*(\zeta)G_1(\zeta)d\zeta}{\int_0^\infty G_0^*(\zeta)G_1(\zeta)d\zeta} \qquad (4.37)$$

$$= (\sqrt{2}/1+i)\,(|\Omega_\tau(\omega_0)|)^{-1},$$

so that

$$|\langle\zeta\rangle_{0,1}| = \frac{L}{\omega_0^{1/2}\int_0^L dx/\alpha_s^{1/2}(x)}, \quad \alpha_s(x) = \frac{k(x)}{\rho(x)c(x)}, \qquad (4.38)$$

where $\alpha_s(x)$ is the local thermal diffusivity of the propagation medium.[22] If the medium is semi-infinite, (4.38) is understood to mean

$$\langle\zeta\rangle_{0,1} = \left(\frac{1}{\omega_0^{1/2}}\right)\lim_{L\to\infty}\left(\frac{L}{\int_0^L dx/\alpha_s^{1/2}(x)}\right). \qquad (4.38')$$

A combination of (4.38) or (4.38′) and (4.16), together with a measurement of $T(x)$ or of a quantity proportional to $T(x)$, demonstrates the potential of our quantum theory for quantitative analysis of depth-profiling studies through thermal wave physics in media of arbitrarily variable $\alpha_s(x)$. This aspect of the present theory will be examined in detail in a future publication.

For completeness of the thermal wave quantum treatment an uncertainty principle with an interesting interpretation will be established. By analogy to quantum mechanics,

$$(\Delta\tau)_{n,n+1} \equiv [\langle\tau^2\rangle_{n,n+1} - \langle\tau\rangle^2_{n,n+1}]^{1/2}, \qquad (4.39)$$

$$(\Delta p_\tau)_{n,n+1} \equiv [\langle p_\tau^2\rangle_{n,n+1} - \langle p_\tau\rangle^2_{n,n+1}]^{1/2}. \qquad (4.40)$$

The expressions involve integrals of the Weber functions with powers or derivatives of τ (or z). They can be simplified upon noticing that

$$\langle z^2\rangle_{n,n+1} \propto \int_{-\infty}^{\infty} z^2 D_n^*(z)D_{n+1}(z)\,dz = 0 \qquad (4.41)$$

and

$$\langle p_\tau^2\rangle_{n,n+1}$$

$$\propto \langle p_z^2\rangle_{n,n+1} \propto -\hbar^2\int_{-\infty}^{\infty} D_n^*(z)\left[\frac{d^2}{dz^2}D_{n+1}(z)\right]dz$$

$$= -\hbar^2\left\{(n+1)n\int_{-\infty}^{\infty} D_n^*(z)D_{n-1}(z)dz\right.$$

$$-(n+1)\int_{-\infty}^{\infty} z\,D_n^*(z)D_n(z)\,dz$$

$$-\frac{1}{2}\int_{-\infty}^{\infty} D_n^*(z)D_{n+1}(z)dz$$

$$\left.+\frac{1}{4}\int_{-\infty}^{\infty} z^2 D_n^*(z)D_{n+1}(z)dz\right\} = 0, \qquad (4.42)$$

as each and every integral inside the brackets can be shown to vanish due to the orthogonality of the Weber polynomials.[24] Taking (4.41) and (4.42) into account, (4.39) and (4.40) give

$$(\Delta\tau)_{n,n+1}(\Delta p_\tau)_{n,n+1} = (\langle\tau\rangle_{n,n+1})(\langle p_\tau\rangle_{n,n+1}), \qquad (4.43)$$

where

$$\langle\tau\rangle_{n,n+1} = \frac{e^{i\pi/4}}{(4\omega_0/|\hbar|^2)^{1/4}}\left(\frac{n+1}{2}\right)^{1/2} G_n^*(\zeta)G_{n+1}(\zeta) \qquad (4.44)$$

and

$$\langle p_\tau\rangle_{n,n+1} = [(4\omega_0/|\hbar|^2)^{1/4}/e^{i\pi/4}]\langle p_z\rangle_{n,n+1} \qquad (4.45)$$

and

$$\langle p_z\rangle_{n,n+1} = -i\hbar\int_{-\infty}^{\infty}\psi_n^*(z,\zeta)\frac{\partial}{\partial z}\psi_m(z,\zeta)dz$$

$$= -i\hbar\,N_nN_{n+1}\,G_n^*(\zeta)G_{n+1}(\zeta)$$

$$\times\int_{-\infty}^{\infty} D_n(z)\left[\frac{d}{dz}D_{n+1}(z)\right]dz.$$

It can be shown that

$$\int_{-\infty}^{\infty} D_n(z)\left[\frac{d}{dz}D_{n+1}(z)\right]dz=\left(\frac{\pi}{2}\right)^{1/2}(n+1)! \qquad (4.46)$$

so that

$$\langle p_z\rangle_{n,n+1} = -(i\hbar/2)(n+1)^{1/2}\exp\left[-e^{i\pi/4}|\Omega_\tau|\zeta\right]$$

and

$$\langle p_\tau\rangle_{n,n+1} = -\left[i\hbar(4\omega_0/|\hbar|^2)^{1/4}/2e^{i\pi/4}\right] \times(n+1)^{1/2}\exp\left[-e^{i\pi/4}|\Omega_\tau|\zeta\right]. \qquad (4.47)$$

Equations (4.43), (4.44), and (4.47) yield the uncertainty principle

$$(\Delta\tau)_{n,n+1}(\Delta p_\tau)_{n,n+1} = \frac{1}{2}(n+1)\hbar\exp\left[-2\int_0^x \sigma_s(\omega_0,x')dx'\right], \qquad (4.48)$$

which indicates that the uncertainty in either the thermal wave temperature excursion or its momentum decreases with increasing modulation frequency ω_0. The form of the uncertainty principle is unlike that of ordinary quantum mechanics[23] due to the fact that the quantal thermal wave formalism requires coupling between the nth and $(n+1)$th eigenmodes to produce temperature expectation functions with the correct limiting forms. If coupling were considered entirely within the nth eigenmode, then (i) the relations $\langle\tau\rangle_{n,n}=\langle p_\tau\rangle_{n,n}=0$ would be true, also familiar from the quantum mechanical harmonic oscillator theory ($\langle x\rangle=\langle p\rangle=0$)[23]; and (ii) a more typical uncertainty relation would be obtained:

$$(\Delta\tau)_{n,n}\,(\Delta p_\tau)_{n,n}=(n+\tfrac{1}{2})\hbar. \qquad (4.49)$$

The thermal-wave uncertainty relation (4.48) is important in that it sets a lower limit in the precision with which the temperature of the heat centroid of the thermal wave packet can be measured, when the thermal flux p_τ is known with a precision $\Delta p_\tau \equiv p_0$:

$$|\Delta T(x)| > \frac{b}{4\pi p_0 F^{1/4}(x)}\exp\left[-(2\omega_0)^{1/2}\int_0^x\frac{dx'}{\alpha_s^{1/2}(x')}\right]. \qquad (4.50)$$

This inequality is a mathematical statement for the maximum depth resolution with thermal waves in a medium in which temperature is modulated at ω_0. Equation (4.48) implies the spread of thermal waves due to diffraction, as the wave packet travels away from the surface and into the medium. The rapid decrease in the uncertainty minimum with increasing ω_0 indicates a more precise thermal imaging and information transfer from subsurface features at high frequencies due to decreased diffraction limitations. This theoretical observation has been borne out in several experiments.[1,4,9,10]

V. CONCLUSIONS

The thermal wave quantum mechanical formalism developed in this work as the extension of the thermal-wave Hamilton–Jacobi theory has been shown to be capable of providing exact analytical expressions for the temperature distribution and heat flux for general solids with continuously variable thermal/thermodynamic parameters. These macroscopic expressions are in the form of Ehrenfest-type expectation functions and are expected to be useful to depth profiling analysis in solids with rapidly varying thermal parameters locally, especially close to the surface, for instance, to microelectronic processing (e.g., impurity doping, ion implantation, radiation damage).

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[1] A. Rosencwaig and G. Busse, Appl. Phys. Lett. **36**, 725 (1980).

[2] E. Brandis and A. Rosencwaig, Appl. Phys. Lett. **37**, 98 (1980).

[3] R. L. Thomas, J. J. Pouch, Y. H. Wong, L. D. Favro, P. K. Kuo, and A. Rosencwaig, J. Appl. Phys. **51**, 1152 (1980).

[4] G. Busse and A. Rosencwaig, Appl. Phys. Lett. **36**, 815 (1980).

[5] T. Sawada, H. Shimizu, and S. Oda, Jpn. J. Appl. Phys. **20**, L25 (1981).

[6] A. Rosencwaig, J. Appl. Phys. **51**, 2210 (1980).

[7] A. Rosencwaig, Thin Solid Films **77**, L43 (1981).

[8] A. Mandelis and J. D. Lymer, Appl. Spectrosc. **39**, 473 (1985).

[9] A. Rosencwaig and R. M. White, Appl. Phys. Lett. **38**, 165 (1981).

[10] A. Rosencwaig, Solid State Technol. **25**, 91 (March 1982).

[11] A. Rosencwaig, J. Photoacoust. **1**, 371 (1983).

[12] A. Rosencwaig, J. Opsal, and D. L. Willenborg, Appl. Phys. Lett. **43**, 166 (1983).

[13] J. Opsal and A. Rosencwaig, J. Appl. Phys. **53**, 4240 (1982).

[14] S. D. Campbell, S. S. Yee, and M. A. Afromowitz, IEEE Trans. Biomed. Engn. **BME-26**, 220 (1979).

[15] M. A. Afromowitz, S. P. Yeh, and S. S. Yee, J. Appl. Phys. **48**, 209 (1977).

[16] H. S. Carslaw and J. C. Jaeger, *Conduction of Heat in Solids* (Clarendon, Oxford, 1960), 2nd ed., Sec. 2.6.

[17] D. Gloge and D. Marcuse, J. Opt. Soc. Am. **59**, 1629 (1969).

[18] G. Eichmann, J. Opt. Soc. Am. **61**, 161 (1971).

[19] J. C. Murphy and L. C. Aamodt, Appl. Phys. Lett. **31**, 728 (1977).

[20] B. A. Findlayson, *The Method of Weighted Residuals and Variational Principles* (Academic, New York, 1972), Chap. 7.

[21] H. Goldstein, *Classical Mechanics* (Addison–Wesley, Reading, MA, 1965), Chap. 9.

[22] A. Rosencwaig and A. Gersho, J. Appl. Phys. **47**, 64 (1976).

[23] L. I. Schiff, *Quantum Mechanics* (McGraw–Hill, New York, 1968), Chap. 4.

[24] E. T. Whittaker and G. N. Watson, *A Course of Modern Analysis* (Cambridge U. P., Cambridge, 1963), 4th ed., Sec. 16.5.

[25] I. Ye. Kireyeva and K. A. Karpov, *Tables of Weber Functions*, translated by P. Basu (Pergamon, New York, 1961).

[26] P. Morse and H. Feshbach, *Methods of Theoretical Physics* (McGraw–Hill, New York, 1953), Sec. 5.3.

[27] A/ Yariv, *Quantum Electronics* (Wiley, New York, 1975), 2nd ed., Sec. 6.5.

[28] *Bateman Manuscript Project, Higher Transcendental Functions*, edited by A. Erdelyi (McGraw–Hill, New York, 1953), Vol. 2, Sec. 10.13.

[29] A. J. Angstrom, Ann. Phys. Lpz. **114**, 513 (1861).

[30] H. D. Arnold and I. B. Crandall, Phys. Rev. **10**, 22 (1917).

[31] A. Messiah, *Quantum Mechanics* (North-Holland, Amsterdam, 1961) Vol. I, Chap. V.

[32] D. Marcuse, *Light Transmission Optics* (Van Nostrand, New York, 1982), Sec. 3.6.