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A set of integro-differential equations describing steady-state nonisothermal dendritic growth is developed via a time-dependent approach. The steady-state equations are studied in detail for the case of isotropic, capillarity-limited growth, and it is shown that the equations assume a form particularly suitable for solution by successive linearization about the known isothermal solution. Of major importance is that the conditions necessary for the existence of a solution to the linearized equations provide a theoretical estimate of the relationship between growth rate and supercooling.

Manuscript submitted October 25, 1973.

CONTENTS

CAPILLARITY-LIMITED STEADY-STATE DENDRITIC GROWTH PART 1—THEORETICAL DEVELOPMENT

INTRODUCTION

The growth of crystals in the form of finely branched structures known as dendrites is frequently observed during the solidification of metals. Moreover dendritic crystal morphologies have profound effects on the structure, strength, and corrosion of cast materials, because the local distribution of alloying elements and impurities is to a great extent controlled by the solidification mode. Despite its importance the kinetics of dendritic growth is not yet well understood, either phenomenologically or mathematically.

In principle the theoretical time evolution of the dendritic interface can be completely determined by finding solutions to the thermal and solute diffusion equations in the solid and liquid phases such that specified initial, boundary, and interface conditions are satisfied. In practice such an approach has yet to be undertaken, and various assumptions are usually made to simplify the calculations and center attention on a particular aspect of the growth process.

The theoretical model which has received by far the most attention in the literature is the so-called steady-state model. In this theory it is assumed that the dendrite grows in a supercooled melt at a constant axial velocity in a shape-preserving manner, that is the shape of the dendritic interface remains constant with time. Experimental observations indicate that these conditions are approximately satisfied in the neighborhood of the dendrite tip. It is therefore reasonable to expect the model to furnish an approximation of the average growth rate and an approximation of the dendrite shape in the neighborhood of the tip.

Although the steady-state model affords a certain degree of simplification, it also has its disadvantages. For instance the steady-state assumptions introduce certain mathematical uniqueness problems. In addition the treatment of such inherently time-dependent effects as side-branch growth is naturally precluded. In spite of these shortcomings the steady-state model can yield useful information and has been examined by a number of workers in the field.

Ivantsov [1] and later Horvay and Cahn [2] solved the equations describing the steady-state growth of an isolated dendrite in a pure material, assuming the dendrite surface to be *isothermal.* Ivantsov showed that for axisymmetric growth the isothermal dendrite surface is a paraboloid of revolution. Horvay and Cahn generalized Ivantsov's results and showed the existence of a multitude of steady-state solutions, corresponding to families of isothermal dendrite shapes in the form of elliptic paraboloids with aspect ratios ranging from zero (parabolic cylinder) to unity (paraboloid of revoltuion). Furthermore, for a fixed aspect ratio and supercooling, Horvay and Cahn demonstrated the presence of a second family of solutions. These solutions exist for all growth rates and are characterized by a constant Péclet number $V/2\alpha\kappa_m$, where V is the axial growth rate, α is the thermal diffusivity, and κ_m is the mean tip curvature.

Note: Manuscript submitted October 25, 1973.

The nonuniqueness problems associated with the isothermal model are a consequence of the steady-state assumptions, as mentioned previously. In fact it is conceivable that other yet undiscovered families of isothermal solutions exist. Aside from these problems the isothermal model has the additional serious deficiency that no mechanism is provided for selecting the unique growth rate for a specified supercooling; that is, the relation between growth rate and supercooling is indeterminate. Since knowledge of this relation is of prime importance for understanding the kinetics of dendritic solidification, the isothermal model provides an unsatisfactory description of dendritic growth.

Horvay and Cahn [2], Temkin [3], and Bolling and Tiller [4] suggested independently that the inclusion of capillarity and molecular attachment effects in the model would force the dendritic interface to be nonisothermal, thereby providing a possible mechanism for selecting the growth rate. A number of attempts to solve the equations describing nonisothermal steady-state growth have appeared in the literature in recent years [3-8]. The results of these analyses indicate that the effect of capillarity and molecular attachment kinetics is to impose a limit on the admissible growth rates. These findings, in conjunction with the ad hoc "maximum-growth-rate hypothesis," were used to obtain specific relations between growth rate and supercooling.

The preceding studies of the nonisothermal problem all employ "shape-constrained" solutions; that is, the shape of the dendrite is prescribed in advance. This procedure considerably simplifies matters but will usually lead to incorrect results, because the dendritic growth problem is (as are all phase-transformation problems) a free-boundary problem. Conditions imposed at the phase boundary would overspecify the problem, *unless* the shape of the phase boundary is such that a self-consistent solution can be found. The predictions of the "shape-constrained" treatments must therefore be regarded with circumspection, and at present there is no satisfactory treatment of nonisothermal, steady-state dendritic growth.

The main purpose of this report, along with the companion report cited on the inside front cover, is to develop a theory of steady-state dendritic growth with no restrictions on the shape of the dendritic interface. In Part 1 (this report) a general treatment of the free-boundary problem associated with the unconstrained growth of a crystal into a supercooled melt is presented. This analysis, which is quite general and not necessarily limited to dendritic growth, serves a twofold purpose. First, it leads to a set of integro-differential equations for the shape of the growing crystal in a form *convenient for numerical solution* on currently available third-generation computers and hence sets the stage for future time-dependent treatments of dendritic growth. Second, the theory leads to a set of equations appropriate to steady-state dendritic growth in a way which makes the mathematical role of the steady-state assumptions particularly clear.

The remainder of Part 1 consists of a detailed study of the steady-state equations for the case of isotropic, capillarity-limited growth. In particular it is shown that the steady-state equations assume a form particularly suitable for solution by successive linearization about the known isothermal solution. Moreover solvability conditions on the linearized equations provide a theoretical limit on the admissible growth rates.

In Part 2 (the companion report) numerical techniques are developed for the solution of the linearized equations. Numerical calculations are presented, and for small supercoolings a universal relation between growth rate and supercooling in the form of a power law is obtained. Finally, the results of the theory are compared to previous theoretical and experimental results.

TIME-DEPENDENT FREE-BOUNDARY PROBLEM

Formulation of the Problem

In this section we develop a theoretical treatment of the free-boundary problem associated with the unconstrained growth of a crystal into a supercooled melt. It is convenient to employ a rectangular coordinate system (x_1, x_2, x_3) moving with a known velocity **V** (Fig. 1). Initially $(t = 0)$ the crystal is assumed to be at a uniform temperature T_0, which for the time being will be taken as zero, and to occupy the region D_{i0} bounded by the surface S_0. At $t = 0^+$ a perturbation is introduced into the system, causing the crystal to grow in the melt. At any time t the crystal occupies the region $D_i(t)$ bounded by the surface $S(t)$; the melt occupies the complementary domain $D_e(t)$. The problem is to determine the time evolution of the surface $S(t)$ and the temperatures in the crystal and in the melt at any point P.

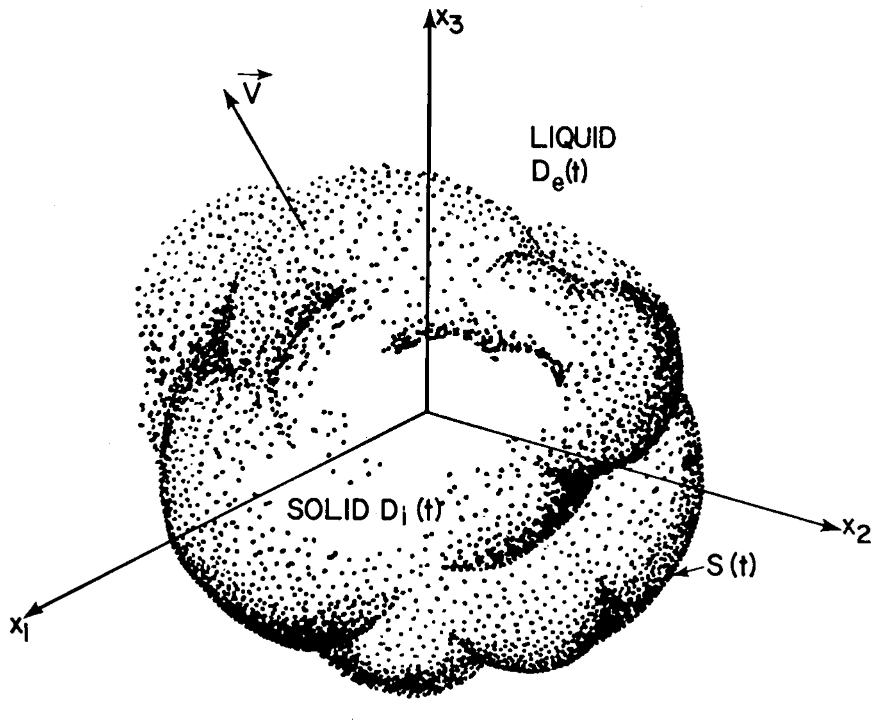

Fig. 1—Schematic representation of a crystal growing into a supercooled melt. The coordinate system is moving with velocity V. The domains D_i and D_e are internal and external to the surface S.

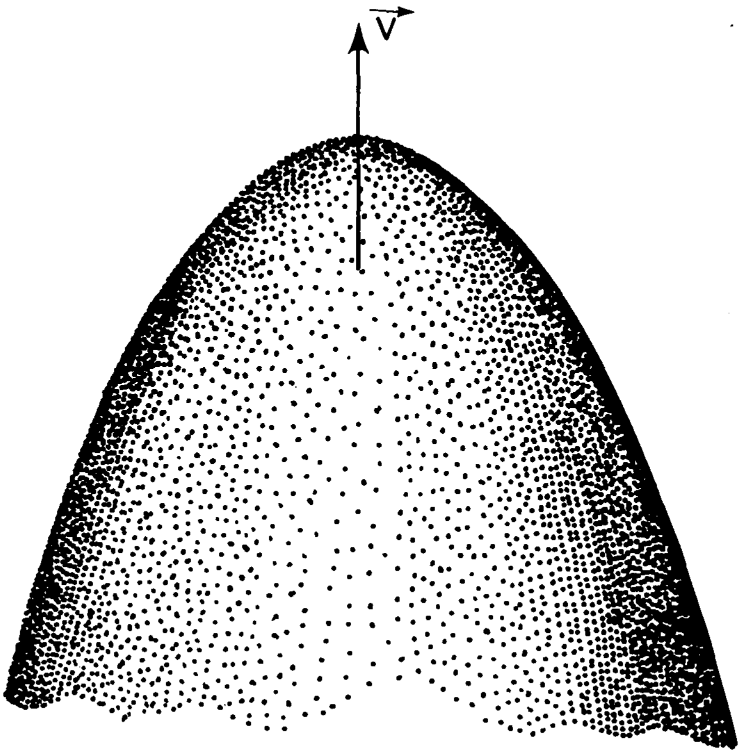

Fig. 2—A class 2 surface

For simplicity the treatment will be limited to pure materials; that is, solute diffusion is not considered. This is not a fundamental restriction, however, and the theory can readily be generalized to include the effects of coupled solute and thermal diffusion. The solid/liquid interface $S(t)$ is assumed to belong to one of two classes:

- *Class 1.* A surface is of class 1 if it is closed.

- *Class 2.* A surface is of class 2 if the surface is of infinite extent in the **V** direction and all lines parallel to **V** intersect the surface exactly once. An example of a class 2 surface is shown in Fig. 2.

Mathematically the free-boundary problem reduces to finding the temperature distributions in the crystal ($T_i(P, t), P \in D_i(t)$) and in the melt ($T_e(P, t), P \in D_e(t)$), together with the phase boundary $S(t)$, such that the following system of equations, boundary conditions, initial conditions, and interface conditions are satisfied:

$$\nabla^2 T_i + \frac{1}{\alpha_i} \mathbf{V} \cdot \nabla T_i = \frac{1}{\alpha_i} \frac{\partial T_i}{\partial t}, P \in D_i(t), \tag{1}$$

$$\nabla^2 T_e + \frac{1}{\alpha_e} \mathbf{V} \cdot \nabla T_e = \frac{1}{\alpha_e} \frac{\partial T_e}{\partial t}, P \in D_e(t), \tag{2}$$

$$T_i(P, 0) = T_e(P, 0) = T_0 = 0, \tag{3a}$$

$$S(0) = S_0, \tag{3b}$$

$$\lim_{P \to \infty} T_e(P, t) = T_0 = 0, P \in D_e(t), \tag{4}$$

$$T_i(s, t) = T_e(s, t) = \hat{T}(s, V_{n_s} + u_{n_s}), s \in S(t), \tag{5a}$$

$$k_i g_i(s, t) - k_e g_e(s, t) = \rho L(V_{n_s} + u_{n_s}), s \in S(t), \tag{5b}$$

where α_i and α_e are the thermal diffusivities of the crystal and the melt respectively, P is a general spatial point (x_1, x_2, x_3), $\mathbf{V}$ is the prescribed velocity of the coordinate system, s is a general point on the interface $S(t)$, $\hat{T}$ is the interface temperature (a specified function of the interface shape and normal velocity), $\mathbf{u}$ is the velocity of a point on the interface in the moving coordinate system; V_{n_s} and u_{n_s} are the components of $\mathbf{V}$ and $\mathbf{u}$ in the direction of the unit normal $\mathbf{n}(s)$ to $S(t)$ at s, k_i and k_e are the thermal conductivities of the crystal and the melt; g_i and g_e are the normal derivatives of the temperature fields on the solid and liquid sides of the interface ($g_i = dT_i/dn_s$ and $g_e = dT_e/dn_s$, where d/dn_s denotes the normal derivative $\mathbf{n}(s) \cdot \nabla$), ρ is the density (assumed the same in the solid and liquid), and L is the latent heat of fusion.

Equations (1) and (2) are thermal diffusion equations in the crystal and the melt respectively, written in the moving coordinate system; Eqs. (3) represent the initial conditions, Eq. (4) represents the far-field boundary condition (the condition that the temperature in the melt must approach T_0 at points far from the interface $S(t)$), Eq. (5a) represents the interface temperature condition, where the form of $\hat{T}$ is determined by the Gibbs-Thomson effect and molecular-attachment kinetics, and Eq. (5b) represents energy conservation requirements at the interface.

"Reduction" Procedure

The free-boundary problem defined by Eqs. (1) through (5) can be treated effectively by a generalization of the "reduction" technique developed by Kolodner [9] for the solution of the one-dimensional Stefan problem. In this approach a set of integro-differential equations is derived which the phase boundary $S(t)$ and the normal derivatives g_i and g_e on either side of the boundary must satisfy. In the course of the derivation integral representations for the temperature distributions $T_i(P, t)$ and $T_e(P, t)$ are also obtained in terms of $S(t)$, g_i, and g_e. Thus the problem is solved once the integro-differential equations for the phase boundary are solved. The principal advantage of this method is that the shape of the phase boundary may be calculated *without calculating the temperature distributions.* Moreover the integro-differential equations are in a form convenient for numerical solution.

The "reduction" procedure, as applied to the problem at hand, can be summarized as follows:

1. A solution $\phi_i(P, t)$ to Eq. (1) is constructed in the domain $D_i(t) \cup D_e(t)$ such that condition (3a) is satisfied and

$$[\phi_i] \equiv \lim_{\substack{P \to s \\ P \in D_e(t)}} \phi_i(P, t) - \lim_{\substack{P \to s \\ P \in D_i(t)}} \phi_i(P, t) \equiv \phi_i^+ - \phi_i^- = -\hat{T}(s, t),$$

$$\left[\frac{d\phi_i}{dn_s}\right] \equiv \lim_{\substack{P \to s \\ P \in D_e(t)}} \frac{d\phi_i}{dn_s} - \lim_{\substack{P \to s \\ P \in D_i(t)}} \frac{d\phi_i}{dn_s} \equiv \frac{d\phi_i^+}{dn_s} - \frac{d\phi_i^-}{dn_s} = -g_i(s, t).$$

2. Either ϕ_i^+ or $d\phi_i^+/dn_s$ is set equal to zero. This step insures that $\phi_i^- = \hat{T}$, $d\phi_i^-/dn_s = g_i$, and hence that $\phi_i = T_i(P \in D_i(t))$, where T_i satisfies Eqs. (1), (3), and (5a). This step also provides a relation between g_i and $S(t)$ in the form of an integro-differential equation.

3. A solution $\phi_e(P, t)$ to Eq. (2) is constructed in the domain $D_i(t) \cup D_e(t)$ such that condition (3a) is satisfied and

$$[\phi_e] \equiv \lim_{\substack{P \to s \\ P \in D_e(t)}} \phi_e(P, t) - \lim_{\substack{P \to s \\ P \in D_i(t)}} \phi_e(P, t) \equiv \phi_e^+ - \phi_e^- = \hat{T}(s, t),$$

$$\left[\frac{d\phi_e}{dn_s}\right] \equiv \lim_{\substack{P \to s \\ P \in D_e(t)}} \frac{d\phi_e}{dn_s} - \lim_{\substack{P \to s \\ P \in D_i(t)}} \frac{d\phi_e}{dn_s} \equiv \frac{d\phi_e^+}{dn_s} - \frac{d\phi_e^-}{dn_s} = g_e(s, t),$$

$$\lim_{\substack{P \to \infty \\ P \in D_e(t)}} \phi_e(P, t) = T_0 = 0.$$

4. Either ϕ_e^- or $d\phi_e^-/dn_s$ is set equal to zero. This step insures that $\phi_e^+ = \hat{T}$, $d\phi_e^+/dn_s = g_e$, and hence that $\phi_e(P, t) = T_e$ $(P \in D_e(t))$, where T_e satisfies Eqs. (2) through (5a). This step also provides a relation between g_e and $S(t)$ in the form of an integro-differential equation.

5. From the system of equations consisting of the equations obtained from steps 2 and 4 and Eq. (5b), g_i, g_e, and $S(t)$ are determined.

6. $T_i(P, t)$ and $T_e(P, t)$ are found by substituting g_i, g_e, and $S(t)$ back into the expressions for ϕ_i and ϕ_e obtained in steps 1 and 3.

Implementation of the Procedure and the Integro-differential Equations

The implementation of this procedure is facilitated by the introduction of particular solutions $U_j^{\Sigma(t)}[h](P, t)$ and $W_j^{\Sigma(t)}[f](P, t)$ to the diffusion equation

$$\nabla^2 T_j + \frac{1}{\alpha_j} \mathbf{V} \cdot \vec{\nabla} T_j = \frac{1}{\alpha_j} \frac{\partial T_j}{\partial t}, P \in D_j(t), j = i \text{ or } e,$$

that are analogous to single- and double-layer potentials (distributions of sources and dipoles). These solutions are given by

$$U_j^{\Sigma(t)}[h](P, t) = \frac{1}{8\pi^{3/2}} \int_0^t \int_{\Sigma(\tau)} \frac{h(q, \tau)}{(t - \tau)^{3/2} \alpha_j^{1/2}} F_j(\mathbf{x}(P), \mathbf{w}(q), t, \tau, \mathbf{V})\, d\Sigma_q d\tau, \tag{6}$$

$$W_j^{\Sigma(t)}[f](P, t) = \frac{1}{8\pi^{3/2}} \int_0^t \int_{\Sigma(\tau)} f(q, \tau) \left\{ \frac{[\mathbf{x}(P) - \mathbf{w}(q)] \cdot \mathbf{n}(q)}{2\alpha_j^{3/2}(t - \tau)^{5/2}} + \frac{\mathbf{V} \cdot \mathbf{n}(q)}{2\alpha_j^{3/2}(t - \tau)^{3/2}} \right\} F_j(\mathbf{x}(P), \mathbf{w}(q), t, \tau, \mathbf{V})\, d\Sigma_q d\tau, \tag{7}$$

where h and f are arbitrary functions of q and τ, $\mathbf{x}(P)$ is the position vector associated with an arbitrary point P, $\Sigma(t)$ is a class 1 or 2 surface, q is a point on $\Sigma(\tau)$ at any past time τ, $\mathbf{n}(q)$ is the outward-pointing unit normal to $\Sigma(\tau)$ at point q, $\mathbf{w}(q)$ is the position vector associated with the point q on $\Sigma(\tau)$,

$$F_j(\mathbf{x}(P), \mathbf{w}(q), t, \tau, \mathbf{V}) = \exp\left(- \left\{ \frac{[\mathbf{x}(P) - \mathbf{w}(q)] \cdot [\mathbf{x}(P) - \mathbf{w}(q)]}{4\alpha_j(t - \tau)} + \frac{\mathbf{V}}{2\alpha_j} \cdot [\mathbf{x}(P) - \mathbf{w}(q)] + \frac{\mathbf{V} \cdot \mathbf{V}}{4\alpha_j} (t - \tau) \right\} \right), \tag{8}$$

and the notation $d\Sigma_q$ emphasizes that the surface integral is to be taken over the points q.

The solutions $U_j^{\Sigma(t)}[h](P, t)$ and $W_j^{\Sigma(t)}[f](P, t)$ have the following properties†:

†Strictly speaking, $h(q, \tau)$, $f(q, \tau)$, and $\Sigma(t)$ are required to satisfy certain smoothness conditions. For a discussion of this and related topics the reader is referred to Gevrey [10], Tikhonov and Samarskii [11], Friedman [12], and Pogorzelski [13]. In this report it will be assumed that any such conditions are always satisfied.

1. They satisfy the diffusion equation

$$\nabla^2 T_j + \frac{1}{\alpha_j} \mathbf{V} \cdot \vec{\nabla} T_j = \frac{1}{\alpha_j} \frac{\partial T_j}{\partial t}$$

at all points, except perhaps on $\Sigma(t)$.

2. $$\lim_{\substack{P \to s \\ P \in \mathfrak{D}_e(t)}} U_j^{\Sigma(t)}[h](P, t) = \lim_{\substack{P \to s \\ P \in \mathfrak{D}_i(t)}} U_j^{\Sigma(t)}[h](P, t) = U_j^{\Sigma(t)*}[h](s, t),$$

where $\mathfrak{D}_i(t)$ is the domain interior to $\Sigma(t)$ and $\mathfrak{D}_e(t)$ is the domain exterior to $\Sigma(t)$,

$$U_j^{\Sigma(t)*}[h](s, t) = \frac{1}{8\pi^{3/2}} \int_0^t \int_{\Sigma(\tau)} \frac{h(q, \tau)}{(t-\tau)^{3/2} \alpha_j^{1/2}} F_j(\mathbf{w}(s), \mathbf{w}(q), t, \tau, \mathbf{V})\, d\Sigma_q\, d\tau, \tag{9}$$

and $\mathbf{w}(s)$ is the position vector associated with a point s on $\Sigma(t)$ at time t.

3. $$\lim_{\substack{P \to s \\ P \in \mathfrak{D}_e(t)}} \frac{d}{dn_s} U_j^{\Sigma(t)}[h](P, t) = -\frac{1}{2} h(s, t) + \frac{d}{dn_s} U_j^{\Sigma(t)*}[h](s, t),$$

$$\lim_{\substack{P \to s \\ P \in \mathfrak{D}_i(t)}} \frac{d}{dn_s} U_j^{\Sigma(t)}[h](P, t) = +\frac{1}{2} h(s, t) + \frac{d}{dn_s} U_j^{\Sigma(t)*}[h](s, t),$$

where

$$\frac{d}{dn_s} U_j^{\Sigma(t)*}[h](s, t) = -\frac{1}{8\pi^{3/2}} \int_0^t \int_{\Sigma(\tau)} h(q, \tau) \left\{ \frac{[\mathbf{w}(s) - \mathbf{w}(q)] \cdot \mathbf{n}(s)}{2\alpha_j^{3/2}(t-\tau)^{5/2}} \right.$$

$$\left. + \frac{\mathbf{V} \cdot \mathbf{n}(s)}{2\alpha_j^{3/2}(t-\tau)^{3/2}} \right\} F_j(\mathbf{w}(s), \mathbf{w}(q), t, \tau, \mathbf{V})\, d\Sigma_q\, d\tau. \tag{10}$$

4. $$\lim_{\substack{P \to s \\ P \in \mathfrak{D}_e(t)}} W_j^{\Sigma(t)}[f](P, t) = +\frac{1}{2} f(s, t) + W_j^{\Sigma(t)*}[f](s, t),$$

$$\lim_{\substack{P \to s \\ P \in \mathfrak{D}_i(t)}} W_j^{\Sigma(t)}[f](P, t) = -\frac{1}{2} f(s, t) + W_j^{\Sigma(t)*}[f](s, t),$$

where

$$W_j^{\Sigma(t)*}[f](s,t) = \frac{1}{8\pi^{3/2}} \int_0^t \int_{\Sigma(\tau)} f(q,\tau) \left\{ \frac{[\mathbf{w}(s) - \mathbf{w}(q)] \cdot \mathbf{n}(q)}{2\alpha_j^{3/2}(t-\tau)^{5/2}} + \frac{\mathbf{V} \cdot \mathbf{n}(q)}{2\alpha_j^{3/2}(t-\tau)^{3/2}} \right\} F_j(\mathbf{w}(s), \mathbf{w}(q), t, \tau, \mathbf{V})\, d\Sigma_q d\tau. \tag{11}$$

5. $$\frac{d}{dn_s} W_j^{\Sigma(t)}[f](P,t) = \frac{d}{dn_s} U_j^{\Sigma(t)} \left[\frac{fV_{n_q}}{\alpha_j}\right](P,t) - W_j^{\Sigma(t)} \left[\frac{fu_{n_q}(\mathbf{n}_s \cdot \mathbf{n}_q)}{\alpha_j}\right](P,t) + Y_j^{\Sigma(t)}[f](P,t),$$

where $\mathbf{n}_s$ and $\mathbf{n}_q$ denote $\mathbf{n}(s)$ and $\mathbf{n}(q)$ and where u_{n_q} and V_{n_q} denote $\mathbf{u} \cdot \mathbf{n}_q$ and $\mathbf{V} \cdot \mathbf{n}_q$. The derivation of this equation, which is not straightforward, is presented in Appendix A. $Y_j^{\Sigma(t)}[f](P,t)$ is also defined in Appendix A and is continuous across $\Sigma(t)$, that is,

$$\lim_{\substack{P \to s \\ P \in \mathfrak{D}_e(t)}} Y_j^{\Sigma(t)}[f](P,t) = \lim_{\substack{P \to s \\ P \in \mathfrak{D}_i(t)}} Y_j^{\Sigma(t)}[f](P,t) = Y_j^{\Sigma(t)*}[f](s,t).$$

It is now relatively simple to construct solutions to the free-boundary problem. Using the jump properties of the potentials $U_j^{\Sigma(t)}[h](P,t)$ and $W_j^{\Sigma(t)}[f](P,t)$, it is readily verified that

$$\phi_i(P,t) = -W_i^{S(t)}[\hat{T}](P,t) + U_i^{S(t)}\left[g_i + \frac{\hat{T}}{\alpha_i}(V_{n_q} + u_{n_q})\right](P,t), \quad P \in D_i(t) \cup D_e(t), \tag{12}$$

and

$$\phi_e(P,t) = W_e^{S(t)}[\hat{T}](P,t) - U_e^{S(t)}\left[g_e + \frac{\hat{T}}{\alpha_e}(V_{n_q} + u_{n_q})\right](P,t), \quad P \in D_i(t) \cup D_e(t), \tag{13}$$

satisfy the conditions set forth in steps 1 and 3 of the reduction procedure. It remains to insure that $\phi_i(P,t) = T_i(P,t), P \in D_i(t)$ and $\phi_e(P,t) = T_e(P,t), P \in D_e(t)$.

As indicated in steps 2 and 4 of the reduction procedure,

$$T_i(P,t) = \phi_i(P,t)$$

$$= -W_i^{S(t)}[\hat{T}](P,t) + U_i^{S(t)}\left[g_i + \frac{\hat{T}}{\alpha_i}(V_{n_q} + u_{n_q})\right](P,t), \quad P \in D_i(t), \tag{14}$$

and

$$T_e(P,t) = \phi_e(P,t)$$

$$= W_e^{S(t)}[\hat{T}](P,t) - U_e^{S(t)}\left[g_e + \frac{\hat{T}}{\alpha_e}(V_{n_q} + u_{n_q})\right](P,t), \qquad P \in D_e(t), \tag{15}$$

provided either $\phi_i^+ = \phi_e^- = 0$ or $d\phi_i^+/dn_s = d\phi_e^-/dn_s = 0$. The conditions $\phi_i^+ = \phi_e^- = 0$ can be written as

$$-\frac{1}{2}\hat{T}(s,t) - W_i^{S(t)*}[\hat{T}](s,t) + U_i^{S(t)*}\left[g_i + \frac{\hat{T}}{\alpha_i}(V_{n_q} + u_{n_q})\right](s,t) = 0, \tag{16}$$

$$-\frac{1}{2}\hat{T}(s,t) + W_e^{S(t)*}[\hat{T}](s,t) - U_e^{S(t)*}\left[g_e + \frac{\hat{T}}{\alpha_e}(V_{n_q} + u_{n_q})\right](s,t) = 0. \tag{17}$$

Similarly the conditions $d\phi_i^+/dn_s = d\phi_e^-/dn_s = 0$ can be written as

$$-\frac{1}{2}g_i(s,t) + \frac{d}{dn_s}U_i^{S(t)*}\left[g_i + \frac{\hat{T}}{\alpha_i}u_{n_q}\right](s,t)$$
$$+ W_i^{S(t)*}\left[\frac{\hat{T}u_{n_q}}{\alpha_i}(\mathbf{n}_s \cdot \mathbf{n}_q)\right](s,t) - Y_i^{S(t)*}[\hat{T}](s,t) = 0, \tag{18}$$

$$-\frac{1}{2}g_e(s,t) - \frac{d}{dn_s}U_e^{S(t)*}\left[g_e + \frac{\hat{T}}{\alpha_e}u_{n_q}\right](s,t)$$
$$- W_e^{S(t)*}\left[\frac{\hat{T}u_{n_q}}{\alpha_e}(\mathbf{n}_s \cdot \mathbf{n}_q)\right](s,t) + Y_e^{S(t)*}[\hat{T}](s,t) = 0. \tag{19}$$

Equations (16), (17), and (5b) and Eqs. (18), (19), and (5b) are systems of integro-differential equations (denoted by systems I and II respectively) involving $S(t)$, g_i, and g_e. Once either system of equations is solved, the temperature distributions can be determined from equations (14) and (15)†‡.

Both systems I and II are integro-differential equations of the Volterra type and thus may be solved numerically by "marching procedures." In particular, system II is a Volterra

†Equations (14) and (15) can also be derived using Fourier transforms. In particular, when $S(t)$ is closed (class 1), the transform method affords the more direct approach. A derivation of Eqs. (14) and (15) based on Fourier transforms is presented in Appendix B.

‡It has been implicitly assumed here that solutions to systems I and II exist, are unique, and are equivalent to solutions of the original free-boundary problem. To give the theory a firm mathematical foundation, rigorous mathematical verification of these assertions is required.

system of the second kind, since the unknowns g_i and g_e appear outside of the integral signs. Systems of this type have proved particularly amenable to numerical solution by suitably modified versions of the techniques commonly used for the numerical solution of ordinary differential equations, such as predictor-corrector methods and Runge-Kutta methods. A comprehensive survey of these techniques as applied to integral and integro-differential equations is given in Noble [14].

STEADY-STATE DENDRITIC GROWTH

The Steady-State Dendrite as an Asymptotic Solution to a Class of Time-Dependent Free-Boundary Problems

We assume the existence of a class of time-dependent free-boundary problems such that:

1. The initial domain D_{i0} is finite and bounded by the closed surface S_0.

2. At any $t < \infty$, $D(t)$ is finite and $S(t)$ remains closed.

3. At sufficiently large t there exists a region of $S(t)$, namely, $S_1(t)$, such that points on $S_1(t)$ move at a constant velocity $\mathbf{V}$; that is, $S_1(t)$ appears stationary with respect to a coordinate system moving with velocity $\mathbf{V}$.

4. $S_1(t)$ approaches a class 2 surface $\overline{S}$ as $t \to \infty$.

5. The asymptotic shape of the stationary region $\overline{S}$ depends only on the thermodynamic and transport properties of the system, and the supercooling, and is independent of initial conditions.

The time evolution of the phase boundary $S(t)$ characteristic of such problems is depicted schematically in Fig. 3. The steady-state dendrite problem, as defined in this report, is to find the asymptotic shape of the stationary region $\overline{S}$, the growth rate $\mathbf{V}$, and the limiting temperature distributions $\overline{T}_j(P)$, $P \in \overline{D}_j$ ($\overline{D}_j = \lim_{t\to\infty} D_j(t)$, $j = i$ or e), as a function of the thermodynamic and transport properties of the system, and the supercooling.

A Method for Obtaining the Asymptotic Solution

An obvious way to obtain the desired asymptotic solution is to obtain a complete time-dependent solution in a stationary coordinate system and directly ascertain the limiting behavior as $t \to \infty$. Whereas such a program is certainly possible with the aid of the methods developed for the time-dependent free-boundary problem, we will not attempt it here. Rather we will attempt to derive a set of equations which the asymptotic solution must satisfy by direct examination of the long-time behavior of the time-dependent integro-differential equations.

To derive the equations describing the asymptotic solution, we consider the free-boundary problem formulated in the preceding subsection, and suppose that the interface

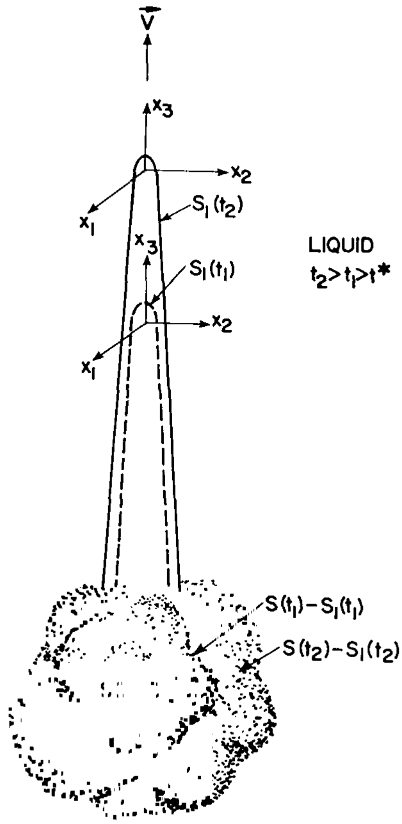

Fig. 3—Schematic representation of the development of the stationary region $\bar{S}$. The coordinate system is moving with velocity $\mathbf{V}$. As $t \to \infty$, $S_1(t) \to \bar{S}$.

shape $S(t)$, and the growth rate $\mathbf{V}$ associated with the stationary region $S_1(t)$, has been found in some time interval $0 < t < t^*$. To extend the solution to the interval $t^* < t < \infty$, suitably modified versions of the integro-differential equations developed for the time-dependent free-boundary problem can be employed. It proves to be convenient to use System I (Eqs. (5b), (16), and (17)) written in a coordinate system moving with velocity $\mathbf{V}$. Hence, with the time scale suitably shifted, $S(t)$ is determined by solving

$$-\frac{1}{2}\hat{T}(s, t) - W_i^{S(t)*}[\hat{T}](s, t) + U_i^{S(t)*}\left[g_i + \frac{\hat{T}}{\alpha_i}(V_{n_q} + u_{n_q})\right](s, t) + \psi_i(s, t) = 0, \quad (20)$$

$$-\frac{1}{2}\hat{T}(s, t) + W_e^{S(t)*}[\hat{T}](s, t) - U_e^{S(t)*}\left[g_e + \frac{\hat{T}}{\alpha_e}(V_{n_q} + u_{n_q})\right](s, t) + \psi_e(s, t) = 0, \quad (21)$$

$$k_i g_i(s, t) - k_e g_e(s, t) = \rho L(V_{n_s} + u_{n_s}), \quad (5b)$$

with initial conditions

$$T_i(P, 0) = T_i(P, t^*), \tag{22a}$$

$$T_e(P, 0) = T_e(P, t^*), \tag{22b}$$

$$S(0) = S(t^*), \tag{22c}$$

where the terms $\psi_j(P, t)$, $j = i$ or e, represent the contributions of the nonuniform initial temperatures and where $T_i(P, t^*)$, $T_e(P, t^*)$, and $S(t^*)$ are the known temperature distributions and interface shape at time t^*. We can now obtain the equations describing the asymptotic solution by examining the behavior of Eqs. (20), (21), and (5b) as $t \to \infty$.

It can be shown that

$$\lim_{t \to \infty} \psi_j(s, t) = 0. \tag{23}$$

Moreover, by rewriting the potentials as

$$W_j^{S(t)*}[\hat{T}](s, t) = W_j^{S_1(t)*}[\hat{T}](s, t) + W_j^{S(t)-S_1(t)*}[\hat{T}](s, t),$$

$$U_j^{S(t)*}\left[g_j + \frac{\hat{T}}{\alpha_j}(V_{n_q} + u_{n_q})\right](s, t) = U_j^{S_1(t)*}\left[g_j + \frac{\hat{T}}{\alpha_j}(V_{n_q} + u_{n_q})\right](s, t)$$

$$+ U_j^{S(t)-S_1(t)*}\left[g_j + \frac{\hat{T}}{\alpha_j}(V_{n_q} + u_{n_q})\right](s, t),$$

and taking t^* large enough to insure

$$W_j^{S(t)-S_1(t)*}[\hat{T}](s, t) = U_j^{S(t)-S_1(t)*}\left[g_j + \frac{\hat{T}}{\alpha_j}(V_{n_q} + u_{n_q})\right](s, t) \approx 0, s \in S_1(t),$$

$$\lim_{\substack{t \to \infty \\ s \in S_1(t)}} W_j^{S_1(t)*}[\hat{T}](s, t) = \lim_{\substack{t \to \infty \\ s \in \overline{S}}} W_j^{\overline{S}*}[\hat{T}](s, t) \equiv \overline{W}_j^{\overline{S}*}[\hat{\overline{T}}](s),$$

$$\lim_{\substack{t \to \infty \\ s \in S_1(t)}} U_j^{S_1(t)*}\left[g_j + \frac{\hat{T}}{\alpha_j}(V_{n_q} + u_{n_q})\right](s, t) = \lim_{\substack{t \to \infty \\ s \in \overline{S}}} U_j^{\overline{S}*}\left[g_j + \frac{\hat{T}}{\alpha_j} V_{n_q}\right](s, t)$$

$$\equiv \overline{U}_j^{\overline{S}*}\left[\overline{g}_j + \frac{\hat{\overline{T}}}{\alpha_j} V_{n_q}\right](s)$$

where $\hat{\bar{T}} = \lim_{t\to\infty} \hat{T}$ and $\bar{g}_j = \lim_{t\to\infty} g_j$, it is readily seen that

$$\lim_{\substack{t\to\infty \\ s\in S_1(t)}} W_j^{S(t)*}[\hat{T}](s, t) = \overline{W}_j^{\bar{S}*}[\hat{\bar{T}}](s), \tag{24a}$$

$$\lim_{\substack{t\to\infty \\ s\in S_1(t)}} U_j^{S(t)*}\left[g_j + \frac{\hat{T}}{\alpha_j}(V_{n_q} + u_{n_q})\right](s, t) = \overline{U}_j^{\bar{S}*}\left[\bar{g}_j + \frac{\hat{\bar{T}}}{\alpha_j} V_{n_q}\right](s). \tag{24b}$$

Using these results the integro-differential equations, Eqs. (20), (21), and (5b), assume the following form as $t \to \infty$:

$$-\frac{1}{2}\hat{\bar{T}}(s) - \overline{W}_i^{\bar{S}*}[\hat{\bar{T}}](s) + \overline{U}_i^{\bar{S}*}\left[\bar{g}_i + \frac{\hat{\bar{T}}}{\alpha_i} V_{n_q}\right](s) = 0, \tag{25}$$

$$-\frac{1}{2}\hat{\bar{T}}(s) + \overline{W}_e^{\bar{S}*}[\hat{\bar{T}}](s) - \overline{U}_e^{\bar{S}*}\left[\bar{g}_e + \frac{\hat{\bar{T}}}{\alpha_e} V_{n_q}\right](s) = 0, \tag{26}$$

$$k_i\bar{g}_i(s) - k_e\bar{g}_e(s) = \rho L V_{n_s}, \tag{27}$$

where $\overline{U}_j^{\bar{S}*}[h](s)$ and $\overline{W}_j^{\bar{S}*}[f](s)$ (h and f being arbitrary source and dipole distributions) are given by

$$\overline{U}_j^{\bar{S}*}[h](s) = \frac{1}{4\pi}\int_{\bar{S}} \frac{h(q)}{|\mathbf{w}(s) - \mathbf{w}(q)|} e^{-(\mathbf{V}/2\alpha_j)\cdot(\mathbf{w}(s)-\mathbf{w}(q))-(|\mathbf{V}|/2\alpha_j)|\mathbf{w}(s)-\mathbf{w}(q)|}\, d\bar{S}_q, \tag{28}$$

$$\begin{aligned} \overline{W}_j^{\bar{S}*}[f](s) = \frac{1}{4\pi}\int_{\bar{S}} f(q) \Bigg\{ & \frac{[\mathbf{w}(s) - \mathbf{w}(q)]\cdot \mathbf{n}(q)}{|\mathbf{w}(s) - \mathbf{w}(q)|^3} + \frac{|\mathbf{V}|\,[\mathbf{w}(s) - \mathbf{w}(q)]\cdot \mathbf{n}(q)}{\alpha_j |\mathbf{w}(s) - \mathbf{w}(q)|^2} \\ & + \frac{\mathbf{V}\cdot \mathbf{n}(q)}{2\alpha_j |\mathbf{w}(s) - \mathbf{w}(q)|} \Bigg\} e^{-(\mathbf{V}/2\alpha_j)\cdot(\mathbf{w}(s)-\mathbf{w}(q))-(|\mathbf{V}|/2\alpha_j)|\mathbf{w}(s)-\mathbf{w}(q)|}\, d\bar{S}_q. \end{aligned} \tag{29}$$

Equations (25), (26), and (27) are a set of integro-differential equations relating the steady-state shape S and the growth rate $\mathbf{V}$. These equations will henceforth be referred to as the "steady-state" equations.

Using a similar limiting process, integral representations for the steady-state temperatures $\bar{T}_i(P)$ and $\bar{T}_e(P)$ may be constructed. $\bar{T}_i(P)$ and $\bar{T}_e(P)$ are given by

$$\bar{T}_i(P) = -\bar{W}_i^{\bar{S}}[\hat{\bar{T}}](P) + \bar{U}_i^{\bar{S}}\left[\bar{g}_i + \frac{\hat{\bar{T}}}{\alpha_i} V_{n_q}\right](P), \qquad P \in \bar{D}_i, \tag{30}$$

$$T_e(P) = +\bar{W}_e^{\bar{S}}[\hat{\bar{T}}](P) - \bar{U}_e^{\bar{S}}\left[\bar{g}_e + \frac{\hat{\bar{T}}}{\alpha_e} V_{n_q}\right](P); \qquad P \in \bar{D}_e, \tag{31}$$

where

$$\bar{U}_j^{\bar{S}}[h](P) = \frac{1}{4\pi}\int_{\bar{S}} \frac{h(q)}{|\mathbf{x}(P) - \mathbf{w}(q)|} e^{-(\mathbf{V}/2\alpha_j)\cdot[\mathbf{x}(P)-\mathbf{w}(q)] - (|\mathbf{V}|/2\alpha_j)|\mathbf{x}(P)-\mathbf{w}(q)|}\, d\bar{S}_q, \tag{32}$$

$$\bar{W}_j^{\bar{S}}[f](P) = \frac{1}{4\pi}\int_{\bar{S}} f(q)\left\{\frac{[\mathbf{x}(P) - \mathbf{w}(q)]\cdot\mathbf{n}(q)}{|\mathbf{x}(P) - \mathbf{w}(q)|^3} + \frac{|\mathbf{V}|[\mathbf{x}(P) - \mathbf{w}(q)]\cdot\mathbf{n}(q)}{\alpha_j|\mathbf{x}(P) - \mathbf{w}(q)|^2}\right.$$

$$\left. + \frac{\mathbf{V}\cdot\mathbf{n}(q)}{2\alpha_j|\mathbf{x}(P) - \mathbf{w}(q)|}\right\} e^{-(\mathbf{V}/2\alpha_j)\cdot[\mathbf{x}(P)-\mathbf{w}(q)] - (|\mathbf{V}|/2\alpha_j)|\mathbf{x}(P)-\mathbf{w}(q)|}\, d\bar{S}_q. \tag{33}$$

Nonuniqueness of the Steady-State Equations

The most prominent feature of the steady-state equations is that there are more unknowns than equations: three equations and four unknowns ($\bar{S}$, $\mathbf{V}$, g_i, g_e). This implies that the steady-state equations cannot furnish a unique asymptotic solution but can only give compatible $\bar{S}$—$\mathbf{V}$ pairs (sets of interface shapes compatible with a specified growth rate). This behavior, which was observed in previous steady-state treatments and was discussed in the Introduction, is solely a consequence of the limit-taking procedures used in obtaining the steady-state equations. In other words the steady-state equations provide only a partial asymptotic solution. A complete time-dependent treatment would doubtless yield a unique interface shape and growth rate.

Physical Relevance of the Steady-State Problem

Solutions to the time-dependent free-boundary problem having the properties enumerated at the beginning of this section on steady-state dendritic growth should, under certain conditions, exist in a mathematical sense. On the other hand, dendritic growth without side branching is never observed in physical systems; thus the question of the physical relevance of the steady-state solutions arises. The point of view adopted in this report is that solutions to the steady-state equations will furnish reasonable approximations of the average growth rate, and of the shape of the dendrite in the neighborhood of the tip, provided that the thermal interaction between the tip and the side branches is sufficiently small. This assertion will be justified to some extent in subsequent sections of this report.

The Steady-State Equations for Equal Thermal Properties in the Solid and Liquid

When the thermal properties are the same in the solid and liquid, it is possible to reduce the three steady-state equations to a single equation for the interface shape. Thus, defining

$\alpha \equiv \alpha_e = \alpha_i,$

$k \equiv k_e = k_i,$

$c \equiv c_i = c_e$ (c_j, where $j = i$ or e, are the specific heats),

$\overline{U}^{\overline{S}*}[h](s) \equiv \overline{U}_e^{\overline{S}*}[h](s) = \overline{U}_i^{\overline{S}*}[h](s),$

$\overline{W}^{\overline{S}*}[f](s) \equiv \overline{W}_e^{\overline{S}*}[f](s) = \overline{W}_i^{\overline{S}*}[f](s),$

adding Eqs. (25) and (26), and substituting Eq. (27), gives

$$-\hat{\overline{T}} + \frac{L}{c}\,\overline{U}^{\overline{S}*}\left[\frac{V_{n_q}}{\alpha}\right](s) = 0. \tag{34}$$

A simplified expression for the steady-state temperature in both phases $\overline{T}(P)$, $P \in \bar{D}_i \cup \bar{D}_e$, can be obtained in a similar way. Defining

$$\overline{U}^{\overline{S}}[h](P) \equiv \overline{U}_e^{\overline{S}}[h](P) = \overline{U}_i^{\overline{S}}[h](P),$$

$$\overline{W}^{\overline{S}}[f](P) \equiv \overline{W}_e^{\overline{S}}[f](P) = \overline{W}_i^{\overline{S}}[f](P),$$

adding Eqs. (30) and (31), noting that

$\overline{T}_i(P) = 0, P \in \overline{D}_e,$

$T_e(P) = 0, P \in \overline{D}_i,$

and substituting Eq. (27), gives

$$\overline{T}(P) = \frac{L}{c}\,\overline{U}^{\overline{S}}\left[\frac{V_{n_q}}{\alpha}\right](P) = 0, P \in \bar{D}_i \cup \bar{D}_e. \tag{35}$$

Equations (34) and (35) are precisely the equations obtained with the "method of sources" [15].

THE EQUATIONS DESCRIBING ISOTROPIC, CAPILLARITY-LIMITED, STEADY-STATE GROWTH AND THEIR FORMAL SOLUTION

The Axisymmetric Problem

The remaining portions of this report will be concerned exclusively with steady-state, isotropic, capillarity-limited dendritic growth. We employ a cylindrical coordinate system (R, Z, ψ) moving with velocity $\mathbf{V}$, where $\mathbf{V}$ is assumed to be directed in the $+Z$ direction along the Z axis†. The dendritic interface $\overline{S}$ is assumed to be a surface of revolution, described by rotating the curve $\Omega(R)$ about the Z axis. This assumption is consistent with the postulated isotropic behavior. The problem is to find compatible Ω-V pairs ($V = |\mathbf{V}|$) and the range of velocities over which steady-state solutions exist for a specified supercooling. For simplicity, only the case of equal thermal properties in the solid and liquid will be considered.

The Axisymmetric Steady-State Potentials

In the theoretical development to follow, extensive use will be made of the axisymmetric counterparts to the steady-state potentials $\overline{U^S}[h](P)$ and $\overline{W^S}[h](P)$. Expressions for these potentials (in nondimensional form) are readily derived from Eqs. (32) and (33). Hence

$$\overline{U}^{\omega}[h](r, z) = \frac{1}{2\pi}\int_0^{\infty} \frac{xh(x)}{\cos\theta(x)}\, e^{-[z-\omega(x)]} G(r, z, w, \omega(x))\, dx, \tag{36}$$

$$\overline{W}^{\omega}[f](r, z) = \frac{1}{2\pi}\int_0^{\infty} \frac{xf(x)}{\cos\theta(x)}\, \frac{d}{dn_x}\left\{e^{-[z-\omega(x)]} G(r, z, x, \omega(x))\right\} dx, \tag{37}$$

where r, z, and ω are nondimensional variables related to the dimensional variables R, Z, and Ω by

$$r = \frac{VR}{2\alpha}, \quad z = \frac{VZ}{2\alpha}, \quad \omega = \frac{V\Omega}{2\alpha}, \tag{38}$$

$h(x)$ and $f(x)$ are nondimensional source and dipole distributions, $\overline{U}^{\omega}[h](r, z)$ and $\overline{W}^{\omega}[h](r, z)$ are the nondimensional single- and double-layer potentials,

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†Strictly speaking, dendritic growth is never isotropic, and the direction of $\mathbf{V}$ is selected by the anisotropic character of the interfacial free energy and/or the molecular attachment kinetics. A complete anisotropic, steady-state analysis should then predict compatible $\overline{S}$-$\mathbf{V}$ pairs. In the present treatment (which should properly be called a "quasi-isotropic" treatment) the anisotropy is assumed to be sufficiently weak to insure that the shapes and limiting growth rates can be reasonably approximated by an analysis which ignores the orientation dependence of the interfacial free energy. Such an analysis cannot predict the direction of $\mathbf{V}$; rather it is assumed to be preselected by the anisotropy, and the coordinate system is then rotated so that $\mathbf{V}$ is parallel to the Z axis.

$$G(r, z, x, \omega(x)) = \int_{-1}^{+1} \frac{e^{-\{r^2+x^2+(z-\omega(x))^2+2rxt\}^{1/2}}}{[r^2 + x^2 + (z - \omega(x))^2 + 2rxt]^{1/2} (1 - t^2)^{1/2}} \, dt, \tag{39}$$

$$\frac{d}{dn_x} = \sin\theta(x) \frac{\partial}{\partial x} + \cos\theta(x) \frac{\partial}{\partial \omega(x)}, \tag{40}$$

θ is the angle shown in Fig. 4, and $\sin\theta(x)$ and $\cos\theta(x)$ are given by

$$\sin\theta(x) = \frac{-\omega'(x)}{[1 + \omega'^2(x)]^{1/2}} \quad \text{(primes denote differentation),} \tag{41a}$$

$$\cos\theta(x) = \frac{1}{[1 + \omega'^2(x)]^{1/2}} . \tag{41b}$$

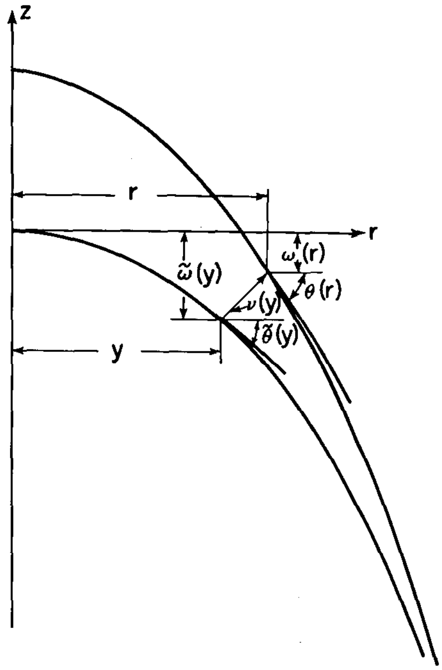

Fig. 4—Generation of the nonisothermal solution by a normal shift of points $(y, \omega(y))$ on a known class 2 surface of revolution formed by rotating the curve $\omega(y)$ about the z axis

The jump relations associated with the axisymmetric potentials can be derived directly from the expressions given in the list of properties on p. 8. Several of these relations will be used in the subsequent analysis and hence are written out explicitly below:

$$1. \quad \lim_{\substack{(r,z)\to(y,\,\omega(y))\\(r,z)\in\overline{D}_e}} \overline{U}^{\omega}[h](r,z) = \lim_{\substack{(r,z)\to(y,\,\omega(y))\\(r,z)\in\overline{D}_i}} \overline{U}^{\omega}[h](r,z) = \overline{U}^{\omega *}[h](y), \tag{42a}$$

where the point $(y, \omega(y))$ lies on the interface and

$$\overline{U}^{\omega *}[h](y) = \frac{1}{2\pi}\int_0^\infty \frac{xh(x)}{\cos\theta(x)}\, e^{-[\omega(y)-\omega(x)]} G(y, \omega(y), x, \omega(x))\, dx. \tag{42b}$$

$$2. \quad \lim_{\substack{(r,z)\to(y,\,\omega(y))\\(r,z)\in\overline{D}_e}} \frac{d}{dn_y}\overline{U}^{\omega}[h](r,z) = -\frac{1}{2}h(y) + \frac{d}{dn_y}\overline{U}^{\omega *}[h](y) \tag{43a}$$

and

$$\lim_{\substack{(r,z)\to(y,\,\omega(y))\\(r,z)\in\overline{D}_i}} \frac{d}{dn_y}\overline{U}^{\omega}[h](r,z) = +\frac{1}{2}h(y) + \frac{d}{dn_y}\overline{U}^{\omega *}[h](y), \tag{43b}$$

where

$$\frac{d}{dn_y} = \sin\theta(y)\frac{\partial}{\partial r} + \cos\theta(y)\frac{\partial}{\partial z}, \tag{43c}$$

$$\frac{d}{dn_y}\overline{U}^{\omega *}[h](y) = \frac{1}{2\pi}\int_0^\infty \frac{xh(x)}{\cos\theta(x)}\frac{d}{dn_y}\left\{e^{-[z-\omega(x)]}G(r,z,x,\omega(x))\right\}_{\substack{z=\omega(y)\\r=y}} dx, \tag{43d}$$

and

$$\sin\theta(y) = \frac{-\omega'(y)}{[1+\omega'^2(y)]^{1/2}}, \quad \cos\theta(y) = \frac{1}{[1+\omega'^2(y)]^{1/2}}. \tag{43e}$$

$$3. \quad \lim_{\substack{(r,z)\to(y,\,\omega(y))\\(r,z)\in\overline{D}_e}} \overline{W}^{\omega}[f](r,z) = +\frac{1}{2}f(y) + \overline{W}^{\omega *}[f](y) \tag{44a}$$

and

$$\lim_{\substack{(r,z)\to(y,\,\omega(y))\\(r,z)\in\overline{D}_i}} \overline{W}^{\omega}[f](r,z) = -\frac{1}{2}f(y) + \overline{W}^{\omega *}[f](y), \tag{44b}$$

where

$$\overline{W}^{\omega *}[f](y) = \frac{1}{2\pi}\int_0^\infty \frac{xh(x)}{\cos\theta(x)}\frac{d}{dn_x}\left\{e^{-[z-\omega(x)]}G(y, z, x, \omega(x))\right\}_{z=\omega(y)} dx. \tag{45}$$

The Steady-State Equation for the Dendrite Shape

For capillarity-limited growth the interface temperature $\hat{\overline{T}}$ is determined from the Gibbs-Thomson equation

$$\hat{\overline{T}}(R) = \Delta T + \frac{\gamma_{s\ell}}{\Delta S_f}\kappa(R), \tag{46}$$

where ΔT is the supercooling (regarded as specified), $\gamma_{s\ell}$ is the solid/liquid interfacial free energy (a constant), ΔS_f is the entropy of fusion per unit volume, and $\kappa(R)$ is the total interface curvature (the sum of the principal curvatures):

$$\kappa(R) = \left\{\frac{\Omega''(R)}{[1+\Omega'^2(R)]^{3/2}}\right\} + \left\{\frac{\frac{1}{R}\Omega'(R)}{[1+\Omega'^2(R)]^{1/2}}\right\} = 2\kappa_{\mathrm{mean}}(R). \tag{47}$$

By introducing the nondimensional temperature $\Theta = Tc/L$ and using Eqs. (36), (38), and (46), the nondimensional, axisymmetric counterpart of Eq. (34) (the steady-state equation) is readily derived. Hence

$$\Delta\Theta + \lambda\kappa(r) = \overline{U}^{\omega *}\left[\frac{2V_{n_x}}{V}\right](r) = \overline{U}^{\omega *}[2\cos\theta](r)$$

$$= \frac{1}{\pi}\int_0^\infty xe^{-[\omega(r)-\omega(x)]}G(r, \omega(r), x, \omega(x))\, dx, \tag{48}$$

where

$$\Delta\Theta = \frac{c}{L}\Delta T, \tag{49a}$$

$$\kappa(r) = \frac{\omega''(r)}{[1+\omega'^2(r)]^{3/2}} + \frac{\frac{\omega'(r)}{r}}{[1+\omega'^2(r)]^{1/2}}, \tag{49b}$$

and

$$\lambda = \frac{V\gamma_{s\ell}c}{2\alpha\Delta S_f L}. \tag{49c}$$

The term $\overline{U}^{\omega *}[2 \cos \theta](r)$ in Eq. (48) can be regarded physically as the temperature field due to a distribution of latent heat sources acting at the moving interface $\overline{S}$. Hence Eq. (48) states that at each point on the moving interface the temperature due to latent heat sources must equal the local equilibrium freezing temperature. This equation, together with properly specified boundary conditions, may be used to obtain $\omega(r)$ in terms of λ (equivalent to finding compatible Ω-V pairs).

If $\Delta\Theta$ is restricted to values less than unity (hypercooling [16] is thus excluded), the appropriate boundary conditions are

$$\omega'(0) = 0 \tag{50a}$$

(from symmetry) and

$$\lim_{r \to \infty} \omega(r) = \text{solution of Eq. (48) with } \lambda = 0 \tag{50b}$$

(from an enthalpy balance).

The Normal-Shift Formulation

For the special case $\lambda = 0$, Eq. (48) reduces to an integral equation whose solution is given by $\omega_0(y) = -y^2/2a_0$ where a_0 is found from the solution of the transcendental equation

$$\Delta\Theta = a_0 e^{a_0} E_1(a_0), \qquad E_1(a_0) = \int_{a_0}^{\infty} \frac{e^{-\xi}}{\xi}\, d\xi. \tag{51}$$

This result is equivalent to that of Ivantsov [1] and Horvay and Cahn [2] for the isothermal dendrite problem.

In the more general case $\lambda \neq 0$, it proves convenient to reformulate the problem slightly by regarding the solution $\omega(r)$ to Eq. (48) to be generated by shifting points $(y, \tilde{\omega}(y))$ on a known class 2 surface of revolution $\tilde{S}$ (formed by rotating the curve $\tilde{\omega}(y)$ about the z axis) an unknown distance $\nu(y)$ along the normal at $(y, \tilde{\omega}(y))$, as illustrated in Fig. 4.† The problem then reduces to finding ν-λ pairs which satisfy Eq. (48).

An explicit form for Eq. (48) in terms of the normal shift can be found from geometrical considerations. Thus, using the relations

$$r = y + \nu(y) \sin \tilde{\theta}(y) \tag{52a}$$

$$\omega(r) = \tilde{\omega}(y) + \nu(y) \cos \tilde{\theta}(y), \tag{52b}$$

†Though it is possible to treat Eq. (48) directly, the resulting equations prove to be numerically ill behaved. On the other hand the normal-shift formulation, though more complicated in a superficial sense, leads to equations which are suitable for numerical solution.

it can be shown that

$$\kappa(r) = F_1^{\tilde{\omega}}(y, \nu(y), \nu'(y), \nu''(y)), \tag{53}$$

where an explicit form for $F_1^{\tilde{\omega}}$ is derived in Appendix C. Also, with

$$x = q + \nu(q) \sin \tilde{\theta}(q), \tag{54a}$$

$$\omega(x) = \tilde{\omega}(q) + \nu(q) \cos \tilde{\theta}(q), \tag{54b}$$

$$\frac{dx}{dq} = 1 + \nu(q)\,(\sin \tilde{\theta}(q))' + \nu'(q) \sin \tilde{\theta}(q), \tag{54c}$$

the integral part of Eq. (48), expressed in terms of the normal shift, is

$$\begin{aligned}
\overline{U}^{\omega\,*}[2\cos\theta](r) = \frac{1}{\pi}\int_0^\infty & [q + \nu(q)\sin\tilde{\theta}(q)]\left\{1 + \nu(q)\,[\sin\tilde{\theta}(q)]' + \nu'(q)\sin\tilde{\theta}(q)\right\} \\
& \times \exp\left\{-\,[\tilde{\omega}(y) + \nu(y)\cos\tilde{\theta}(y) - \tilde{\omega}(q) - \nu(q)\cos\tilde{\theta}(q)]\right\} \\
& \times G[y + \nu(y)\sin\tilde{\theta}(y), \tilde{\omega}(y) + \nu(y)\cos\tilde{\theta}(y), \\
& \qquad q + \nu(q)\sin\tilde{\theta}(q), \tilde{\omega}(q) + \nu(q)\cos\tilde{\theta}(q)]\; dq \\
\equiv \int_0^\infty & F_2^{\tilde{\omega}}(q, y, \nu(y), \nu(q), \nu'(q))\; dq,
\end{aligned} \tag{55}$$

and upon substitution of Eqs. (53) and (55), Eq. (48) becomes

$$\Delta\Theta + \lambda F_1^{\tilde{\omega}}(y, \nu(y), \nu'(y), \nu''(y)) = \int_0^\infty F_2^{\tilde{\omega}}(q, y, \nu(y), \nu(q), \nu'(q))\; dq. \tag{56}$$

If $\tilde{\omega}(y)$ is taken such that $\lim_{y\to\infty} \tilde{\omega}(y) = \omega_0(\infty)$, where ω_0 denotes the isothermal solution ($\lambda = 0$), then the boundary conditions on ν, corresponding to Eqs. (50), become

$$\nu'(0) = 0 \text{ (from symmetry)}, \tag{57a}$$

$$\nu(\infty) = 0. \tag{57b}$$

The Operator Formulation

Equation (56), which is a nonlinear integro-differential equation in $\nu(y)$, can also be regarded as a nonlinear operator equation in a suitable Banach space†. Thus, defining

$$M_1^{\tilde{\omega}}\langle\nu\rangle \equiv F_1^{\tilde{\omega}}(y, \nu(y), \nu'(y), \nu''(y)), \tag{58a}$$

$$M_2^{\tilde{\omega}}\langle\nu\rangle \equiv \Delta\Theta - \int_0^\infty F_2^{\tilde{\omega}}(q, y, \nu(y), \nu(q), \nu'(q))\, dq, \tag{58b}$$

where $\nu \in E^{\tilde{\omega}}$ and where $M_1^{\tilde{\omega}}$ and $M_2^{\tilde{\omega}}$ are nonlinear operators with domain $E^{\tilde{\omega}} \subset C^2[0, \infty]$‡, Eq. (56) can be written as

$$\lambda M_1^{\tilde{\omega}}\langle\nu\rangle + M_2^{\tilde{\omega}}\langle\nu\rangle \equiv \mathfrak{M}_\lambda^{\tilde{\omega}}\langle\nu\rangle = 0, \qquad \nu \in E^{\tilde{\omega}}. \tag{59}$$

The main advantage of this formulation, aside from the convenient shorthand notation, is that the methods of functional analysis may be employed to ascertain the character of the solutions as a function of λ.

The Newton-Kantorovich method [17a] and the implicit-function theorem, as formulated for nonlinear operators in a Banach space, provide particularly effective means for obtaining the required solutions and ascertaining the range of λ values over which steady-state solutions exist. Hence we digress a moment and discuss these techniques in some detail.

The Newton-Kantorovich Method

The Newton-Kantorovich method [17a] is one of the few methods available for obtaining solutions to nonlinear integral, and integro-differential, equations. Suppose P is a nonlinear operator in a Banach space X, and further suppose that it is required to find an element x^*, $x^* \in X$, such that

$$P\langle x^*\rangle = 0; \tag{60}$$

†The appropriate space for the operators considered here is $C^2[0, \infty]$, that is, the collection of functions which have continuous second derivatives and are bounded at infinity. Suitable norms for this space are

$$\|\nu\| = \max_{[0,\infty]} |\nu(y)| + \max_{[0,\infty]} |\nu'(y)| + \max_{[0,\infty]} |\nu''(y)|,$$

$$\|\nu\| = \max\left\{\max_{[0,\infty]} |\nu(y)|,\ \max_{[0,\infty]} |\nu'(y)|,\ \max_{[0,\infty]} |\nu''(y)|\right\}.$$

‡$E^{\tilde{\omega}}$ is the set in $C^2[0, \infty]$ whose elements both satisfy the boundary conditions, Eqs. (57), and make $\omega(r)$ a single-valued function, thus insuring that the dendritic interface $\overline{S}$ is a class 2 surface.

that is, a solution x^* to the nonlinear operator equation, Eq. (60), is required. One approach to solving Eq. (60) might be to find a linear equation whose solution is in some sense close to the solution of the nonlinear equation. Since the theory and techniques for solving linear equations are highly developed, such an approach has considerable potential and indeed is the idea behind the Newton-Kantorovich method.

Suppose there exists a bounded, linear operator $P'(x_0)$, such that

$$\lim_{\substack{\|\Delta x\|\to 0 \\ (\Delta x, x_0 \in X)}} \frac{\|P\langle x_0 + \Delta x\rangle - P\langle x_0\rangle - P'(x_0)\langle \Delta x\rangle\|}{\|\Delta x\|} = 0, \tag{61}$$

where $\|y\|$, $y \in X$, denotes the norm of y. Then Eq. (61) implies that

$$P\langle x\rangle = P\langle x_0\rangle + P'(x_0)\langle x - x_0\rangle + \eta\langle x - x_0\rangle, \qquad x, x_0 \in X, \tag{62}$$

where η is a nonlinear operator such that

$$\lim_{\|x - x_0\|\to 0} \frac{\|\eta\langle x - x_0\rangle\|}{\|x - x_0\|} = 0,$$

that is, $\|\eta\langle x - x_0\rangle\| = o\|x - x_0\|$. Equation (62) provides a linear approximation to the operator P in the neighborhood of the point x_0, analogous to a one-term Taylor expansion for scalar functions. Indeed $P'(x_0)$ is generally called the first derivative of P at x_0, or the Fréchet derivative of P [17b].

If in Eq. (62) x is replaced by x^*, then, since $P\langle x^*\rangle = 0$, Eq. (62) becomes

$$P\langle x_0\rangle + P'(x_0)\langle x^* - x_0\rangle + \eta\langle x^* - x_0\rangle = 0. \tag{63}$$

Moreover, if x_0 is chosen sufficiently close to x^*, then the term $\eta\langle x^* - x_0\rangle$ may be neglected and Eq. (63) may be written as

$$P\langle x_0\rangle + P'(x_0)\langle x - x_0\rangle = 0. \tag{64}$$

Equation (64) is the desired linear equation; if x_0 is chosen sufficiently close to x^*, then the solution x_1 to Eq. (64) will be close to the sought-after solution x^*.

To improve the approximate solution x_1, the following iteration procedure is often used:

i. A solution x_0 is assumed and substituted into Eq. (64), which is then inverted to obtain a new approximate solution x_1.

ii. The approximate solution x_1 is substituted for x_0 in Eq. (64), which is then inverted to obtain a new approximate solution x_2.

iii. This process is repeated until satisfactory convergence is obtained.

This procedure is the Newton-Kantorovich method, and the sequence $\{x_n\}$ generated by the recursive process

$$P'(x_{n-1})\langle\Delta x_n\rangle = -P\langle x_{n-1}\rangle \qquad (n = 1, 2, ...), \qquad x_n = \Delta x_n + x_{n-1}, \tag{65}$$

is known as the Newton sequence. If $P'(x_{n-1})$ is well-enough behaved, and if x_0 is chosen sufficiently close to x^*, then by Kantorovich's theorm [18] the Newton sequence $\{x_n\}$ converges to the exact solution x^*.

In practice the evaluation of $P'(x_{n-1})$ at each step is time consuming, and an alternate approach is often used. In this approach, which is called the modified Newton-Kantorovich method, $P'(x_{n-1})$ in Eq. (65) is replaced by $P'(x_0)$. Thus the modified Newton sequence $\{x_n\}$ is generated by

$$P'(x_0)\langle\Delta x_n\rangle = -P\langle x_{n-1}\rangle \qquad (n = 1, 2, ...), \qquad x_n = \Delta x_n + x_{n-1}. \tag{66}$$

Kantorovich [19] has proved that the modified Newton sequence $\{x_n\}$ will converge to the exact solution x^* but at a slower rate than the unmodified Newton sequence. In subsequent work with Eq. (59) the modified Newton-Kantorovich procedure will be employed.

The Implicit-Function Theorem

As will be seen shortly, the problem of accessing the range of permissible λ values in Eq. (59) is equivalent to asking the following question: If P and Q are nonlinear operators in a Banach space X such that the equation

$$P\langle x\rangle + \mu Q\langle x\rangle = 0, \tag{67}$$

where μ is a scalar parameter, $x \in X$, has the solution $\widetilde{x}$ for $\mu = \widetilde{\mu}$, under what conditions will Eq. (67) fail to have a solution for $\mu = \widetilde{\mu} + \Delta\mu$ ($\Delta\mu$ small)? The answer is provided by the implicit-function theorem for operators in a Banach space, first given by Hildebrandt and Graves [19]. As applied to Eq. (67) the theorem gives the following result: for $\Delta\mu$ sufficiently small a unique solution in the neighborhood of the known solution $\widetilde{x}$ exists if and only if the operator $L = P'(\widetilde{x}) + \widetilde{\mu}Q'(\widetilde{x})$ has a bounded inverse. Thus Eq. (67) fails to have a solution in the neighborhood of $\widetilde{x}$ only if L^{-1} does not exist or is unbounded. This result is of utmost importance and will be used in subsequent work to calculate the maximum admissible steady-state growth rate consistent with a specified supercooling.

Solution of the Normal-Shift Equations by the Boot-strap Algorithm

Because Eq. (59) contains a parameter, and because a solution for a particular value of the parameter is known ($\lambda = 0$), Eq. (59) is eminently suited to solution by a bootstrap procedure. Thus, if solutions exist in the neighborhood of the known solution at $\lambda = 0$, they may be found by the Newton-Kantorovich method, taking as the initial guess the solution at $\lambda = 0$. Provided solutions to Eq. (59) exhibit a continuous dependence on λ, and provided λ is chosen sufficiently small, the convergence of the Newton sequence is assured. By increasing λ and repeating this process with the last known solution serving as the initial guess, solutions to Eq. (59) may be found for a range of λ values. An upper bound on the range of permissible λ values will be reached when solutions in the neighborhood of the last known solution cease to exist, with the nonexistence condition given by the implicit-function theorem.

An explicit formulation of the bootstrap algorithm follows:

1. Set $y = r$ and $\tilde{\omega}(y) = \omega_0(r, \lambda^0)$ (ω is now regarded as a function of both r and λ), where $\lambda^0 = 0$ and $\omega_0(r, \lambda^0)$ denotes the isothermal solution.

2. Set $\lambda^j = \lambda^{j-1} + \Delta\lambda^j$ ($j = 1$) and obtain a modified Newton sequence $\left\{\nu_k^j(y)\right\}$ ($k = 0, 1, 2, \ldots$ and $\nu_0^j(y) = 0$) by solving the linear equations

$$\lambda^j M_1'^{\tilde{\omega}}(0)\langle\delta\nu_k^j\rangle + M_2'^{\tilde{\omega}}(0)\langle\delta\nu_k^j\rangle + \lambda^j M_1^{\tilde{\omega}}\langle\nu_{k-1}^j\rangle + M_2^{\tilde{\omega}}\langle\nu_{k-1}^j\rangle = 0, \qquad k = 1, 2, \ldots, \tag{68}$$

for $\delta\nu_k^j(y)$ and setting $\nu_k^j(y) = \nu_{k-1}^j(y) + \delta\nu_k^j(y)$. Here $M_i'^{\tilde{\omega}}(0)$ ($i = 1$ or 2) are the Fréchet derivatives of $M_i^{\tilde{\omega}}$ (explicit expressions for $M_i'^{\tilde{\omega}}(0)$ are derived in Appendix C), and $\Delta\lambda^j$ is to be chosen sufficiently small to insure the convergence of the sequence $\left\{\nu_k^j\right\}$.

3. With $\nu^j(y) = \lim\limits_{k\to\infty} \left\{\nu_k^j(y)\right\}$, calculate $\omega(r, \lambda^j)$ using the parametric relations

$$r = y + \nu^j(y)\sin\tilde{\theta}(y), \tag{69a}$$

$$\omega = \tilde{\omega}(y) + \nu^j(y)\cos\tilde{\theta}(y). \tag{69b}$$

4. Set $y = r$ and $\tilde{\omega}(y) = \omega(r, \lambda^j)$.

5. Examine the operator $M_2'^{\tilde{\omega}}(0) + \lambda^j M_1'^{\tilde{\omega}}(0) = \mathfrak{M}'^{\tilde{\omega}}_{\lambda^j}(0)$. If $\left\{\mathfrak{M}'^{\tilde{\omega}}_{\lambda^j}(0)\right\}^{-1}$ does not exist or is unbounded, then λ^j is an upper bound on the range of permissible λ values by the implicit-function theorem; therefore $\lambda^j = \lambda_{max}$ and the problem is solved.

6. If $\left\{\mathfrak{M}'^{\tilde{\omega}}_{\lambda^j}(0)\right\}^{-1}$ is bounded, set $j = j + 1$ and repeat steps 2 through 5.

APPROXIMATIONS FOR SMALL VALUES OF λ

Normal-Shift Estimate

The bootstrap algorithm developed in the preceding subsection constitutes a formal exact solution to the problem and in principle can be used to calculate ω-λ pairs and λ_{max} regardless of the magnitude of λ. However, if λ is small in the sense that the maximum temperature change at the dendrite tip is small compared to the nominal supercooling $\Delta\Theta$, then it is possible to obtain accurate estimates of both the normal shifts and λ_{max} without employing the entire bootstrap procedure.

To obtain an estimate of the normal shift, it is useful to regard Eq. (59) as an operator equation of the form

$$\mathfrak{M}^{\tilde{\omega}}\langle \lambda, \nu \rangle = 0, \tag{70}$$

where the operator $\mathfrak{M}^{\tilde{\omega}}$ acts on both λ and ν. Setting $\tilde{\omega} = \omega_0(y, \lambda^0)$ $(\lambda^0 = 0)$, $\mathfrak{M}^{\omega\,0}$ can be expanded about the point (ν_0, λ^0) $(\nu_0 = 0)$ using arguments similar to those employed in the section on the Newton-Kantorovich method. Hence, upon noting that $M_2^{\omega\,0}\langle 0 \rangle = 0$ for the isothermal solution, Eq. (70) can be written as

$$\begin{aligned}\mathfrak{M}^{\omega\,0}\langle \lambda, \nu \rangle &= M_2^{\omega\,0}\langle \nu_0 \rangle + \lambda^0 M_1^{\omega\,0}\langle \nu_0 \rangle + \lambda^0 M_1'^{\omega\,0}(\nu_0)\langle \nu - \nu_0 \rangle + M_2'^{\omega\,0}(\nu_0)\langle \nu - \nu_0 \rangle \\ &\quad + (\lambda - \lambda^0) M_1^{\omega\,0}\langle \nu_0 \rangle + o(\|\nu - \nu_0\|) + o(\lambda - \lambda^0) \\ &= M_2'^{\omega\,0}(0)\langle \nu \rangle + \lambda M_1^{\omega\,0}\langle 0 \rangle + o(\|\nu\|) + o(\lambda)\end{aligned} \tag{71}$$

for (ν, λ) close to (ν_0, λ^0). Neglecting the terms $o(\|\nu\|)$, $o(\lambda)$ in Eq. (71) then gives the linear equation†

$$M_2'^{\omega\,0}(0)\langle \delta\nu \rangle = -\lambda M_1^{\omega\,0}\langle 0 \rangle. \tag{72}$$

Provided λ is sufficiently small, the solutions $\delta\nu$ to Eq. (72) should serve as reliable estimates of the true normal shift ν.

Physically the term $M_2'^{\omega\,0}(0)\langle \delta\nu \rangle$ in Eq. (72) represents a linear approximation to the temperature change caused by shifting points on the isothermal interface $\omega_0(y)$ a distance $\delta\nu(y)$ along the normal to $\omega_0(y)$ at the point $(y, \omega_0(y))$. Moreover the term $M_1^{\omega\,0}\langle 0 \rangle$ is simply the total curvature of the isothermal interface. Thus Eq. (72) states that to first order in ν and λ the normal shift $\delta\nu(y)$ must be such that the change in temperature at a point $(r, \omega(r))$ on the nonisothermal interface equals $-\lambda$ times the curvature of the isothermal interface at the corresponding point $(y, \omega_0(y))$.

Equation (72), which is a linear integro-differential equation in $\delta\nu(y)$, can be written out explicitly as follows. By Eq. (58a) and the expression for $F_1^{\tilde{\omega}}(y, \nu(y), \nu'(y), \nu''(y))$ in Appendix C

$$M_1^{\omega\,0}\langle 0 \rangle = F_1^{\omega\,0}(y, 0, 0, 0) = \kappa_0(y) = -\frac{1 + \xi(y)}{a_0 \xi^{3/2}(y)}, \tag{73}$$

where $\kappa_0(y)$ is the total curvature of the isothermal interface and $\xi(y) = 1 + (y/a_0)^2$. Moreover, from the expressions for the Fréchet derivatives derived in Appendix C,

$$\begin{aligned}M_2'^{\omega\,0}(0)\langle \delta\nu \rangle = \frac{\delta\nu(y)}{\xi^{1/2}(y)} - \frac{1}{\pi}\int_0^\infty e^{-[\omega_0(y) - \omega_0(q)]} \Bigg\{ &\frac{d}{dn_q}\, G(y, z, q, \omega_0(q)) \Bigg|_{z=\omega_0(y)} \\ &+ \frac{1}{2a_0 \xi^{1/2}(y)}\, G(y, \omega_0(y), q, \omega_0(q)) \Bigg\} q\,\delta\nu(q)\, dq\end{aligned} \tag{74}$$

Continued

†Equation (72) may also be obtained from Eq. (68) with $j = k = 1$ by assuming $\nu = O(\lambda)$ and neglecting terms of $O(\lambda^2)$.

$$
- \frac{1}{\pi} \int_0^\infty e^{-[\omega_0(y) - \omega_0(q)]} G(y, \omega_0(y), q, \omega_0(q)) \left\{ \left[\frac{1}{\xi^{1/2}(q)} \left(1 + \frac{1}{2a_0}\right) \right.\right.
$$

$$
\left.\left. + \frac{1}{a_0 \xi^{3/2}(q)} \right] \delta\nu(q) + \frac{q}{a_0 \xi^{1/2}(q)} [\delta\nu(q)]' \right\} q\, dq, \tag{74}
$$

where $G(y, z, q, \omega_0(q))$ and the operation d/dn_q are defined in Eqs. (39) and (40). Thus Eq. (72) becomes

$$
\frac{\delta\nu(y)}{\xi^{1/2}(y)} - \int_0^\infty C_1(y, q) \delta\nu(q)\, dq - \int_0^\infty C_2(y, q) \left\{ \left[\frac{1}{\xi^{1/2}(q)} \left(1 + \frac{1}{2a_0}\right) \right.\right.
$$

$$
\left.\left. + \frac{1}{a_0 \xi^{3/2}(q)} \right] \delta\nu(q) + \frac{q}{a_0 \xi^{1/2}(q)} [\delta\nu(q)]' \right\} q\, dq = \lambda \left[\frac{1 + \xi(y)}{a_0 \xi^{3/2}(y)} \right], \tag{75}
$$

where

$$
C_1(y, q) = \frac{q}{\pi} e^{-[\omega_0(y) - \omega_0(q)]} \left\{ \frac{d}{dn_q} G(y, z, q, \omega_0(q)) \Big|_{z = \omega_0(y)} \right.
$$

$$
\left. + \frac{1}{2a_0 \xi^{1/2}(y)} G(y, \omega_0(y), q, \omega_0(q)) \right\} \tag{76a}
$$

$$
C_2(y, q) = \frac{q}{\pi} e^{-[\omega_0(y) - \omega_0(q)]} G(y, \omega_0(y), q, \omega_0(q)). \tag{76b}
$$

If λ is sufficiently less than λ_{max}, the solution to Eq. (75) should provide reliable estimates of the true normal shift. Moreover, since $\delta\nu$ is proportional to λ and Eq. (75) is linear in $\delta\nu$, Eq. (75) need be solved only once for a specified value of $\Delta\Theta$; for example, if the solution for $\lambda = 1$ is denoted by ν^*, then $\delta\nu = \lambda\nu^*$. Numerical techniques for obtaining solutions to Eq. (75) are presented in Part 2 (the companion report cited inside the front cover), along with selected results.

λ_{max} Estimate

Though the linearization procedure presented in the preceding subsection provides an effective means of obtaining $\delta\nu$, it cannot by itself provide any information regarding λ_{max}. The reason for this is that λ_{max} is essentially determined by the information contained in the higher order terms, namely, the terms which were discarded in the linearization process. Therefore, to estimate λ_{max}, it is necessary to reconsider the nonlinear formulation.

In this subsection we return to the original nonlinear formulation, Eq. (48), and use certain known properties of the solutions to obtain an interpretation of λ_{max} in terms of conditions at the dendrite tip. Such an interpretation leads naturally to an upper bound on λ_{max} which can be evaluated explicitly by the linearization procedure discussed in the preceding subsection. Of major importance is that the upper bound provides a good approximation to λ_{max} if the temperature change at the dendrite tip is small compared to the nominal supercooling $\Delta\Theta$.

Thus consider Eq. (48). Upon noting that the quantity $\Delta\Theta - \bar{U}^{\omega *}[2 \cos \theta](r)$ is actually the interfacial supercooling $\Delta\vartheta(r)$ at a point $(r, \omega(r))$ on the interface $\omega(r)$, Eq. (48) may be written as

$$-\lambda\kappa(r) = \Delta\vartheta(r). \tag{48'}$$

Now suppose that a family of solutions $\omega(r, \lambda)$ is known for $0 \leqslant \lambda \leqslant \lambda_{max}$. Then $\Delta\vartheta(r)$ and $\kappa(r)$ can be readily calculated for any $\lambda \leqslant \lambda_{max}$; moreover, for fixed values of r, a set of curves of $\Delta\vartheta$ as a function of $-\kappa$ can be plotted with λ acting as a parameter. The resulting curves, henceforth referred to as r curves, are known to have the following properties for sufficiently small r:

1. $\Delta\vartheta$ = for $\kappa = \kappa_0$ (r fixed).

2. $\lim\limits_{-\kappa\to\infty} \Delta\vartheta = \Delta\Theta$ (r fixed).

3. $\dfrac{d\Delta\vartheta}{d(-\kappa)} > 0$ and monotonically decreases to zero as $-\kappa \to \infty$ (r fixed).

4. $\dfrac{d\Delta\vartheta(0)}{d[-\kappa(0)]} < \dfrac{d\Delta\vartheta(r)}{d[-\kappa(r)]}$ ($r \neq 0$ and κ fixed).

A family of r curves is schematically shown in Fig. 5a. Each r curve can be regarded as a representation of the right-hand side of Eq. (48), as a function of $-\kappa$, for a fixed value of r. In contrast the left-hand side of Eq. (48), when plotted as a function of $-\kappa$ for various values of $\lambda \leqslant \lambda_{max}$, is represented by a single family of straight lines with slope λ for all values of r. These lines will henceforth be referred to as λ lines. If now the r curves and λ lines are plotted on the same graph, then satisfaction of Eq. (48) is equivalent to the requirement that each λ line, for $\lambda \leqslant \lambda_{max}$, intersect all r curves. But from inspection of Fib. 5b it is apparent that this requirement cannot be met if $\lambda > \{d\Delta\vartheta(0)/d[-\kappa(0)]\}_{min}$, where $\{d\Delta\vartheta(0)/d[-\kappa(0)]\}_{min}$ is the slope of the r curve for $r = 0$ (the dendrite tip) at the point of tangency with a λ line (see Fig. 5b). Thus

$$\lambda_{max} = \left\{\frac{d\Delta\vartheta(0)}{d[-\kappa(0)]}\right\}_{min}$$

This interpretation of λ_{max}, though perhaps more appealing and less formal than the previous interpretation of λ_{max} in a physical sense, is no easier to apply computationally because $\{d\Delta\vartheta(0)/d[-\kappa(0)]\}_{min}$ cannot be calculated without knowing the interface shape at λ_{max}, namely, $\omega(r, \lambda_{max})$. However the current interpretation of λ_{max} does have the

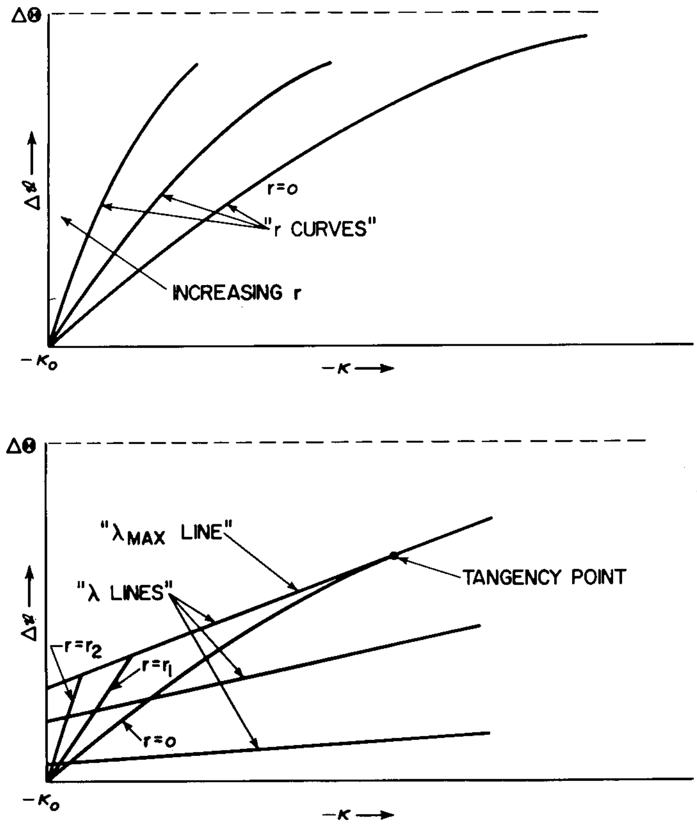

Fig. 5—(5a) Schematic representation of a family of r curves (5b) Schematic representation of families of r curves and λ lines. The slope of the r curve for $r = 0$, namely, $\{d\Delta[\vartheta(0)/d[-\kappa(0)]\}_{min}$, at the tangency point determines λ_{max}.

advantage that a rigorous upper bound on λ_{max} can be calculated using information already available.

Since $d\Delta\vartheta(0)/d[-\kappa(0)]$ is positive and decreases monotonically with $-\kappa(0)$, it is apparent that an upper bound λ^* on λ_{max} is given by

$$\lambda^* = \left.\frac{d\Delta\vartheta(0)}{d[-\kappa(0)]}\right|_{-\kappa(0)=-\kappa_0(0)}, \tag{77}$$

where $\kappa_0(0)$ is the tip curvature of the isothermal interface.

The initial slope of the r curve $d\Delta\vartheta(0)/d[-\kappa(0)]|_{-\kappa(0)=-\kappa_0(0)}$, and therefore λ^*, is readily determined from Eq. (75). Hence, if Eq. (75) is solved for $\lambda = 1$ and the solution is denoted by ν^*, as indicated in the preceding subsection, then for $\lambda = \delta\lambda$ ($\delta\lambda$ small) the corresponding normal shift $\delta\nu$ is given by

$$\delta\nu = \delta\lambda\nu^*. \tag{78}$$

The curvature change $\delta\kappa(0) = \kappa(0) - \kappa_0(0)$ associated with $\delta\nu$ is by definition $\delta\kappa(0) = \delta\lambda M'^{\omega_0}(0) < \nu^* >|_{y=0}$ or, from the results in Appendix C,

$$\delta\kappa(0) = \delta\lambda\left\{\nu^{*''}(0) + \frac{2}{a_0^2}\,\nu^*(0) + \lim_{y\to 0}\left[\frac{1}{y}\nu^{*'}(y)\right]\right\}. \tag{79}$$

Finally, since the associated change in the tip supercooling $\delta\Delta\vartheta(0)$ is, from Eq. (48′),

$$\delta\Delta\vartheta(0) = -\,\delta\lambda\kappa_0(0) = \frac{2\delta\lambda}{a_0}\,, \tag{80}$$

and, by definition,

$$= \frac{d\Delta\vartheta(0)}{d[-\kappa(0)]}\bigg|_{-\kappa(0)=-\kappa_0(0)} = -\lim_{\delta\lambda\to 0}\frac{\delta\Delta\vartheta(0)}{\delta\kappa(0)}\,,$$

Eq. (77) can be written as

$$\lambda^* = \frac{-2}{a_0\left\{\nu^{*''}(0) + \frac{2}{a_0^2}\,\nu^*(0) + \lim_{y\to 0}\left[\frac{1}{y}\nu^{*'}(y)\right]\right\}}. \tag{81}$$

Equation (81) expresses λ^* in terms of the known parameter a_0 and a solution $\nu^*(y)$ to Eq. (75) which may be found by the methods described in Part 2 (the companion report). Moreover, as illustrated in Fig. 6, λ^* will be close to λ_{max} provided the $\Delta\vartheta(0)$ versus $-\kappa(0)$ curve is approximately linear in the neighborhood of the tangency point; this will be the case if $\Delta\vartheta(0)$ at $\lambda = \lambda_{max}$ is small compared to $\Delta\Theta$. Thus λ^* provides a good approximation to λ_{max} if $\Delta\vartheta(0)|_{\lambda=\lambda_{max}}/\Delta\Theta << 1$.

Numerical values of λ^* as a function of $\Delta\Theta$ are presented in Part 2.

A Second λ_{max} Estimate

An acceptable approximation to the normal shift may also be obtained by implementing the first step in the Newton-Kantorovich solution to Eq. (59). This approach, which amounts to linearizing Eq. (59) with respect to ν about the isothermal solution, differs from the approach developed in the first subsection of this section in that terms which are nonlinear in λ are retained. While these terms do not greatly affect the calculated normal shifts, it will be demonstrated shortly that they do retain sufficient information from the nonlinear formulation to permit λ_{max} to be estimated directly from the linearized equations. As discussed in the first subsection of this section, this is not possible when the linearization is performed with respect to λ as well as ν.

For small values of λ an approximation $\delta\nu$ to the true normal shift ν can be found by setting $\tilde{\omega} = \omega_0$ and $j = k = 1$ in Eq. (68). Thus, upon noting that $M_2^{\omega_0}\langle 0\rangle = 0$, the following equation for $\delta\nu$ is obtained:

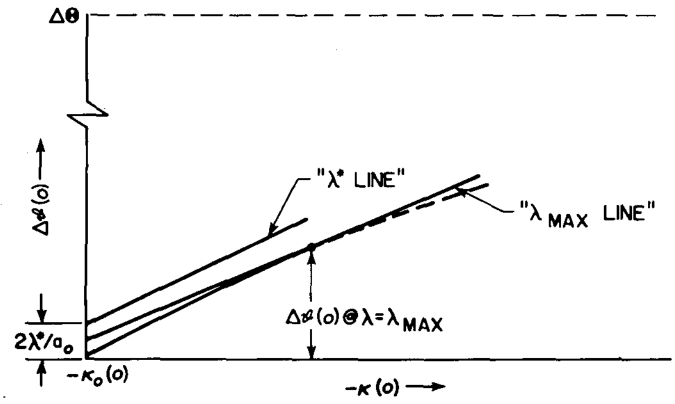

Fig. 6—The case $\Delta\vartheta(0)$ at $\lambda = \lambda_{max} << \Delta\Theta$

$$\lambda M_1'^{\omega 0}(0)\langle\delta\nu\rangle + M_2'^{\omega 0}(0)\langle\delta\nu\rangle = \mathfrak{M}_\lambda'^{\omega 0}(0)\langle\delta\nu\rangle = -\lambda M_1^{\omega 0}\langle 0\rangle. \tag{82}$$

Equation (82) is a linear integro-differential equation in $\delta\nu(y)$ and can be written out explicitly with the aid of equations (73), (74), (76), and the following expression for $M_1'^{\omega 0}(0)\langle\delta\nu\rangle$ (derived in Appendix C):

$$M_1'^{\omega 0}(0)\langle\delta\nu\rangle = \frac{1}{\xi(y)}\left\{[\delta\nu(y)]'' + \frac{1}{y\xi(y)}[\delta\nu(y)]' + \frac{1}{a_0^2}\left[1 + \frac{1}{\xi^2(y)}\right]\delta\nu(y)\right\}, \tag{83}$$

where $\xi(y) = 1 + (y/a_0)^2$. Hence an alternate form for Eq. (82) is

$$\frac{\lambda}{\xi(y)}\left\{[\delta\nu(y)]'' + \frac{1}{y\xi(y)}[\delta\nu(y)]' + \frac{1}{a_0^2}\left[1 + \frac{1}{\xi^2(y)}\right]\delta\nu(y)\right\} + \frac{\delta\nu(y)}{\xi^{1/2}(y)}$$

$$- \int_0^\infty C_1(y, q)\delta\nu(q)\,dq - \int_0^\infty C_2(y, q)\left\{\left[\frac{1}{\xi^{1/2}(q)}\left(1 + \frac{1}{2a_0}\right) + \frac{1}{a_0\xi^{3/2}(q)}\right]\delta\nu(q)\right.$$

$$\left. + \frac{q}{a_0\xi^{1/2}(q)}[\delta\nu(y)]'\right\} dq = \lambda\left(\frac{1 + \xi(y)}{a_0\xi^{3/2}(y)}\right). \tag{84}$$

Equation (84), when solved with the boundary conditions $[\delta\nu(0)]' = \delta\nu(\infty) = 0$, yields $\delta\nu$ as a function of λ.

Equation (82) differs from Eq. (72) by the term $\lambda M_1'^{\omega 0}(0)\langle\delta\nu\rangle$ which is $O(\lambda^2)$. Since for small values of λ this term has only a minor effect on $\delta\nu$, it is still preferable to use Eq. (72) to calculate $\delta\nu$, because of its simpler structure. On the other hand it is precisely this term which retains the information required to estimate λ_{max}.

It is well known from the theory of linear operator equations that Eq. (82) fails to possess a solution only if for some value of λ, say λ^{**}, the operator $[\mathfrak{M}'^{\omega 0}_{\lambda}(0)]^{-1}$ either does not exist or is unbounded. But in the formulation of the bootstrap algorithm it was shown that $\lambda = \lambda_{max}$ when $[\mathfrak{M}'^{\tilde{\omega}}_{\lambda_{max}}(0)]^{-1}$ either does not exist or is unbounded. Hence, if λ_{max} is small, so that $\mathfrak{M}'^{\omega 0}_{\lambda}(0) \approx \mathfrak{M}'^{\omega}_{\lambda}(0)$, then λ^{**} should be a good estimate of λ_{max}.

To evaluate λ^{**} numerically, a finite-difference approximation to Eq. (84) can be formulated which results in a matrix equation for $\delta\nu$ at the set of points corresponding to the nodes of the difference scheme. If the resulting matrix is regarded as an approximation to the operator $\mathfrak{M}'^{\omega 0}_{\lambda}(0)$, then the condition that $[\mathfrak{M}'^{\omega 0}_{\lambda}(0)]^{-1}$ exists and is bounded corresponds to the matrix having a nonzero determinent. Hence λ^{**} can be obtained by finding the smallest value of λ for which the determinent of the matrix is identically zero. Numerical techniques for carrying out this program are developed in Part 2 (the companion report), where numerical values for λ^{**} as function of $\Delta\Theta$ are presented.

SUMMARY OF PART 1

A general treatment of the time-dependent free-boundary problem associated with the unconstrained growth of a crystal into a supercooled melt was presented. Of major importance is that the analysis led to a set of integro-differential equations convenient for solution on currently available third-generation computers.

The time-dependent treatment was used to derive the equations which describe steady-state dendritic growth by regarding the steady-state dendrite as an asymptotic solution to a class of time-dependent free-boundary problems. This approach is particularly illuminating because it makes clear the reason for the existence of a multitude of solutions to the steady-state equations.

The equations describing isotropic, capillarity-limited, steady-state dendritic growth in pure materials were presented in a nondimensional form involving only two parameters, namely, a parameter λ (directly proportional to the growth rate V) and the nondimensional supercooling $\Delta\Theta$. Posing the problem in this way affords considerable simplification over the previous dimensional treatments, which generally involve four parameters (Péclet number, growth rate, supercooling, and a capillarity parameter). This formulation led directly to a universal relation between λ_{max} and $\Delta\Theta$. This relation, together with the expressions $\lambda_{max} = (V_{max}\gamma_{s\ell}c/2\alpha L\Delta S_f)$ and $\Delta\Theta = c\Delta T/L$, serves to determine the appropriate relation between V_{max} and ΔT for *any* pure material.

An algorithm based on the Newton-Kantorovich method and the implicit-function theorm was developed which permits both rigorous calculation of the steady-state dendrite shapes as a function of λ and rigorous determination of λ_{max} as a function of $\Delta\Theta$.

An approximate method was presented which permits accurate estimation of the shape changes induced by the nonisothermality when the supercooling at the dendrite tip is small compared to the nominal supercooling $\Delta\Theta$.

An interpretation of λ_{max} in terms of conditions at the dendrite tip was developed. This interpretation of λ_{max} leads directly to an upper-bound estimate on λ_{max}, which may be evaluated explicitly with the approximate solution discussed in the preceding paragraph.

Of major importance is that the upper bound provides an accurate approximation to λ_{max} if the supercooling at the dendrite tip is small compared to $\Delta\Theta$.

A second method for determining an independent estimate on λ_{max} was presented. In this method, which is based on a linearization of the steady-state equations about the isothermal solution, solvability conditions on the linearized equation provide the required estimate. As in the preceding paragraph the estimate obtained by this procedure provides an accurate approximation to λ_{max} if the supercooling at the dendrite tip is small compared to $\Delta\Theta$.

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Appendix A
THE NORMAL DERIVATIVE OF THE DOUBLE-LAYER POTENTIAL $W_j^{\Sigma(t)}[f](P, t)$

In principle the normal derivative of $W_j^{\Sigma(t)}[f](P, t)$, namely,

$$\frac{d}{dn_s} W_j^{\Sigma(t)}[f](P, t) = \mathbf{n}(s) \cdot \vec{\nabla} W_j^{\Sigma(t)}[f](P, t), \qquad s \in \Sigma(t),$$

for any point P not on $\Sigma(t)$, can be obtained by a straightforward differentiation of the expression

$$W_j^{\Sigma(t)}[f](P, t) = \frac{1}{8\pi^{3/2}} \int_0^t \int_{\Sigma(\tau)} f(q, \tau) \left\{ \frac{[\mathbf{x}(P) - \mathbf{w}(q)] \cdot \mathbf{n}(q)}{2\alpha_j^{3/2}(t-\tau)^{5/2}} + \frac{\mathbf{V} \cdot \mathbf{n}(q)}{2\alpha_j^{3/2}(t-\tau)^{3/2}} \right\} \cdot F_j(\mathbf{x}(P), \mathbf{w}(q), t, \tau, \mathbf{V})\, d\Sigma_q d\tau, \tag{A1}$$

where

$$F_j(\mathbf{x}(P), \mathbf{w}(q), t, \tau, \mathbf{V}) = \exp\left(- \left\{ \frac{[\mathbf{x}(P) - \mathbf{w}(q)] \cdot [\mathbf{x}(P) - \mathbf{w}(q)]}{4\alpha_j(t-\tau)} + \frac{\mathbf{V}}{2\alpha_j} \cdot [\mathbf{x}(P) - \mathbf{w}(q)] + \frac{\mathbf{V} \cdot \mathbf{V}}{4\alpha_j} (t-\tau) \right\} \right) \tag{A2}$$

Thus $\frac{d}{dn_s} W_j^{\Sigma(t)}[f](P, t)$ can always be written as

$$\frac{d}{dn_s} W_j^{\Sigma(t)}[f](P, t) = \frac{1}{8\pi^{3/2}} \int_0^t \int_{\Sigma(\tau)} f(q, \tau) \mathbf{n}(s) \cdot \vec{\nabla} \left(\left\{ \frac{[\mathbf{x}(P) - \mathbf{w}(q)] \cdot \mathbf{n}(q)}{2\alpha_j^{3/2}(t-\tau)^{5/2}} + \frac{\mathbf{V} \cdot \mathbf{n}(q)}{2\alpha_j^{3/2}(t-\tau)^{3/2}} \right\} F_j(\mathbf{x}(P), \mathbf{w}(q), t, \tau, \mathbf{V}) \right) d\Sigma_q d\tau$$

$$= \frac{1}{8\pi^{3/2}} \int_0^t \int_{\Sigma(\tau)} f(q, \tau) \left(\frac{\mathbf{n}(s) \cdot \mathbf{n}(q)}{2\alpha_j^{3/2}(t-\tau)^{5/2}} \right. \tag{A3}$$

Continued

$$- \frac{\{[\mathbf{x}(P) - \mathbf{w}(q)] \cdot \mathbf{n}(q)\}\{[\mathbf{x}(P) - \mathbf{w}(q)] \cdot \mathbf{n}(s)\}}{4\alpha_j^{5/2}(t-\tau)^{7/2}}$$

$$\left. - \frac{\{[\mathbf{x}(P) - \mathbf{w}(q)] \cdot \mathbf{n}(q)\}[\mathbf{V} \cdot \mathbf{n}(s)]}{4\alpha_j^{5/2}(t-\tau)^{5/2}} \right) F_j(\mathbf{x}(P), \mathbf{w}(q), t, \tau, \mathbf{V})\, d\Sigma_q d\tau$$

$$+ \frac{d}{dn_s} U_j^{\Sigma(t)} \left[\frac{f\mathbf{V} \cdot \mathbf{n}(q)}{2\alpha_j} \right] (P, t), \tag{A3}$$

where $\frac{d}{dn_s} U_j^{\Sigma(t)}[h](P, t) = \mathbf{n}(s) \cdot \vec{\nabla} U_j^{\Sigma(t)}[h](P, t)$ and where $U_j^{\Sigma(t)}[h](P, t)$ is given in Eq. (6).

Equation (A3), though certainly valid for any point P not on $\Sigma(t)$, is not in a form suitable for use in the reduction method, because the limiting behavior of the first integral as $P \to s$ is difficult to ascertain directly. One way to circumvent this difficulty is to obtain an alternate expression for $d/dn_s\, W_j^{\Sigma(t)}[f](P, t)$ involving only integrals whose limiting behavior is either known or easily determined. This approach, which has been used with great success for one-dimensional problems,† is the approach we adopt here.

Without loss of generality $\mathbf{w}(q)$ may be written as

$$\mathbf{w}(q) = \mathbf{w}(q)|_{t=0} + \int_0^t \mathbf{u}(q) \cdot \mathbf{n}(q)\, d\tau, \tag{A4}$$

where $\mathbf{u}(q)$ is the relative velocity of a point q on $\Sigma(\tau)$ ($u(q)$ and $\mathbf{n}(q)$ are implicit functions of τ). Moreover, using Eq. (A4), it is readily verified that

$$\frac{1}{\alpha_j} \frac{\partial}{\partial \tau} \left\{ \frac{F_j(\mathbf{x}(P), \mathbf{w}(q), t, \tau, \mathbf{V})}{\alpha_j^{1/2}(t-\tau)^{3/2}} \right\} \mathbf{n}(q) \cdot \mathbf{n}(s)$$

$$= \left\{ \frac{3\mathbf{n}(s) \cdot \mathbf{n}(q)}{2\alpha_j^{3/2}(t-\tau)^{5/2}} - \frac{\{[\mathbf{x}(P) - \mathbf{w}(q)] \cdot [\mathbf{x}(P) - \mathbf{w}(q)]\}[\mathbf{n}(s) \cdot \mathbf{n}(q)]}{4\alpha_j^{5/2}(t-\tau)^{7/2}} \right.$$

$$+ \frac{\{[\mathbf{x}(P) - \mathbf{w}(q)] \cdot \mathbf{n}(q)\}[\mathbf{u}(q) \cdot \mathbf{n}(q)][\mathbf{n}(s) \cdot \mathbf{n}(q)]}{2\alpha_j^{5/2}(t-\tau)^{5/2}} + \frac{(\mathbf{V} \cdot \mathbf{V})[\mathbf{n}(s) \cdot \mathbf{n}(q)]}{4\alpha_j^{5/2}(t-\tau)^{3/2}}$$

$$\left. + \frac{[\mathbf{V} \cdot \mathbf{n}(q)][\mathbf{u}(q) \cdot \mathbf{n}(q)](\mathbf{n}(s) \cdot \mathbf{n}(q))}{2\alpha_j^{5/2}(t-\tau)^{3/2}} \right\} F_j(\mathbf{x}(P), \mathbf{w}(q), t, \tau, \mathbf{V}). \tag{A5}$$

†I.I. Kolodner, Comm. Pure and Applied Math 9 (1956).

Multiplying Eq. (A5) by $1/8\pi^{3/2}\, f(q, \tau)$, integrating over $\Sigma(\tau)$ and τ, adding and subtracting the resulting term to and from Eq. (A3), and employing the definitions of $d/dn_s\, U_j^{\Sigma(t)}[f\mathbf{V}\cdot\mathbf{n}(q)/2\alpha_j]$ and $W_j^{\Sigma(t)}[f\mathbf{u}\cdot\mathbf{n}(q)\{\mathbf{n}(s)\cdot\mathbf{n}(q)\}/\alpha_j]$ then gives the following expression for $d/dn_s\, W_j^{\Sigma(t)}[f](P, t)$:

$$\frac{d}{dn_s}\, W_j^{\Sigma(t)}[f](P, t) = \frac{d}{dn_s}\, U_j^{\Sigma(t)}\left[\frac{f\mathbf{V}\cdot\mathbf{n}(q)}{\alpha_j}\right](P, t) - W_j^{\Sigma(t)}\left[\frac{f\mathbf{u}\cdot\mathbf{n}(q)\{\mathbf{n}(s)\cdot\mathbf{n}(q)\}}{\alpha_j}\right](P, t) + Y_j^{\Sigma(t)}[f](P, t), \tag{A6}$$

where

$$Y_j^{\Sigma(t)}[f](P, t) = \frac{1}{8\pi^{3/2}}\int_0^t\int_{\Sigma(\tau)} \frac{\partial}{\partial\tau}\left\{\frac{F_j(\mathbf{x}(P), \mathbf{w}(q), t, \tau, \mathbf{V})}{\alpha_j^{1/2}(t-\tau)^{3/2}}\right\}\frac{f(q, \tau)}{\alpha_j}\,[\mathbf{n}(s)\cdot\mathbf{n}(q)]\;d\Sigma_q d\tau + I_j^{\Sigma(t)}[f](P, t) \tag{A7}$$

and

$$\begin{aligned} I_j^{\Sigma(t)}[f](P, t) = \frac{1}{8\pi^{3/2}}\int_0^t\int_{\Sigma(\tau)} f(q, \tau)\Bigg[&-\frac{\mathbf{n}(s)\cdot\mathbf{n}(q)}{\alpha_j^{3/2}(t-\tau)^{5/2}} \\ &+\frac{1}{4\alpha_j^{5/2}(t-\tau)^{7/2}}\Bigg(\Big\{[\mathbf{x}(P)-\mathbf{w}(q)]\cdot[\mathbf{x}(P)-\mathbf{w}(q)]\Big\}[\mathbf{n}(s)\cdot\mathbf{n}(q)] \\ &-\{[\mathbf{x}(P)-\mathbf{w}(q)]\cdot\mathbf{n}(q)\}\{[\mathbf{x}(P)-\mathbf{w}(q)]\cdot\mathbf{n}(s)\} \\ &+\{[\mathbf{x}(P)-\mathbf{w}(q)]\cdot\mathbf{n}(s)\}[\mathbf{V}\cdot\mathbf{n}(q)](t-\tau) \\ &-\{[\mathbf{x}(P)-\mathbf{w}(q)]\cdot\mathbf{n}(q)\}[\mathbf{V}\cdot\mathbf{n}(s)](t-\tau) \\ &+[\mathbf{V}\cdot\mathbf{n}(s)](\mathbf{V}\cdot\mathbf{n}(q))(t-\tau)^2 \\ &-(\mathbf{V}\cdot\mathbf{V})[\mathbf{n}(s)\cdot\mathbf{n}(q)](t-\tau)^2\Bigg)\Bigg]\; F(\mathbf{x}(P), \mathbf{w}(q), t, \tau, \mathbf{V})\;d\Sigma_q d\tau. \end{aligned} \tag{A8}$$

The limiting behavior of the first two terms in Eq. (A6) is already known (properties 3 and 4 listed on p. 8 in the main text), and it therefore remains only to consider the term $Y_j^{\Sigma(t)}[f](P, t)$. The first term appearing in $Y_j^{\Sigma(t)}[f](P, t)$, namely,

$$\frac{1}{8\pi^{3/2}} \int_0^t \int_{\Sigma(\tau)} \frac{\partial}{\partial \tau} \left\{ \frac{F_j(\mathbf{x}(P), \mathbf{w}(q), t, \tau, \mathbf{V})}{\alpha_j^{1/2}(t-\tau)^{3/2}} \right\} \frac{f(q, \tau)}{\alpha_j} \, [\mathbf{n}(s) \cdot \mathbf{n}(q)] \, d\Sigma_q d\tau,$$

can be rewritten in a somewhat more convenient form by using the result

$$\frac{\partial}{\partial \tau} \int_{\Sigma(\tau)} A(q, \tau) \, d\Sigma_q = \int_{\Sigma(\tau)} \frac{\partial}{\partial \tau} A(q, \tau) \, d\Sigma_q + \int_{\Sigma(\tau)} A(q, \tau) \mathbf{u}(q) \cdot \mathbf{n}(q) \kappa(q) \, d\Sigma_q, \tag{A9}$$

where A is an arbitrary function of q and τ, defined on $\Sigma(\tau)$, and $\kappa(q)$ is the total curvature of the surface $\Sigma(\tau)$ at the point q. Thus applying Eq. (A9) and integrating by parts gives

$$\int_0^t \int_{\Sigma(\tau)} \frac{\partial}{\partial \tau} \left\{ \frac{F_j(\mathbf{x}(P), \mathbf{w}(q), t, \tau, \mathbf{V})}{\alpha_j^{1/2}(t-\tau)^{3/2}} \right\} \frac{f(q, \tau)}{\alpha_j} \, [\mathbf{n}(s) \cdot \mathbf{n}(q)] \, d\Sigma_q d\tau$$

$$= - \frac{1}{8\pi^{3/2}} \int_{\Sigma(0)} \left\{ \frac{F_j(\mathbf{x}(P), \mathbf{w}(q), t, \tau, \mathbf{V})}{\alpha_j^{3/2}(t-\tau)^{3/2}} \, f(q, \tau) [\mathbf{n}(s) \cdot \mathbf{n}(q)] \right\} \Bigg|_{\tau=0} d\Sigma_q \Bigg|_{\tau=0}$$

$$- U_j^{\Sigma(t)} \left[\frac{f \mathbf{u} \cdot \mathbf{n}(q) \kappa(q) \{\mathbf{n}(s) \cdot \mathbf{n}(q)\}}{\alpha_j} + \frac{\partial}{\partial \tau} \left\{ \frac{f \{\mathbf{n}(q) \cdot \mathbf{n}(s)\}}{\alpha_j} \right\} \right] (P, t). \tag{A10}$$

But the term $U_j^{\Sigma(t)}[h](P, t)$ is known to be continuous across $\Sigma(t)$ (property 2 in the main text), and moreover it can be shown that the integral

$$\frac{1}{8\pi^{3/2}} \int_{\Sigma(0)} \left\{ \frac{F_j(\mathbf{x}(P), \mathbf{w}(q), t, \tau, \mathbf{V})}{\alpha_j^{3/2}(t-\tau)^{3/2}} \, f(q, \tau) [\mathbf{n}(s) \cdot \mathbf{n}(q)] \right\} \Bigg|_{\tau=0} d\Sigma_q \Bigg|_{\tau=0}$$

is also continuous across $\Sigma(t)$. Hence it follows that the first term in $Y_j^{\Sigma(t)}[f](P, t)$ is continuous across $\Sigma(t)$.

The second term appearing in $Y_j^{\Sigma(t)}[f](P, t)$, namely, $I_j^{\Sigma(t)}[f](P, t)$, can also be shown to be continuous across $\Sigma(t)$. In fact, by transforming the surface integral in equation (A8) into a volume integral with the aid of the divergence theorem, it can be shown that $I_j^{\Sigma(t)}[f](P, t) = 0$, provided f is independent of q. It therefore follows that $Y_j^{\Sigma(t)}[f](P, t)$ is continuous across $\Sigma(t)$; hence Eq. (A6) provides the required form for $d/dn_s \, W_j^{\Sigma(t)}[f](P, t)$.

Appendix B
AN ALTERNATE DERIVATION OF EQS. (14) AND (15) VIA FOURIER TRANSFORMS

Let $f(P, t)$, $P = (x_1, x_2, x_3)$, be a function of the spatial point P and time t which satisfies the Dirichlet conditions† with respect to P. Then, if the integral

$$\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} f(P, t)\, dx_1 dx_2 dx_3$$

is absolutely convergent, the triple Fourier transform $\overline{f}(P_\xi, t) \equiv \mathfrak{F}[f(P, t)]$ given by

$$\overline{f}(P_\xi, t) = \left(\frac{1}{2\pi}\right)^{3/2} \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} f(P, t) e^{i[\mathbf{x}(P)\cdot\vec{\xi}(P_\xi)]}\, dx_1 dx_2 dx_3 \tag{B1}$$

exists; moreover the inverse transform

$$f(P, t) = \mathfrak{F}^{-1}[\overline{f}(P_\xi, t)] = \left(\frac{1}{2\pi}\right)^{3/2} \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} \overline{f}(P_\xi, t) e^{-i[\mathbf{x}(P)\cdot\vec{\xi}(P_\xi)]}\, d\xi_1 d\xi_2 d\xi_3 \tag{B2}$$

may be used to recover $f(P, t)$. Here $P_\xi = (\xi_1, \xi_2, \xi_3)$, where ξ_1, ξ_2, and ξ_3 are the transform parameters and $\vec{\xi}$ denotes the position vector associated with P_ξ in the transform space.

In this appendix the Fourier transform and its inverse are used to obtain integral representations for the interior and exterior temperature distributions $T_i(P, t)$ and $T_e(P, t)$ directly from the diffusion equations. Though this method proves to be somewhat more direct than the "reduction" procedure, it is also slightly less general, because $S(t)$ must be closed to guarantee the convergence of the integrals appearing in Eqs. (B1) and (B2).

THE INTERIOR PROBLEM

We consider first the interior diffusion equation

$$\nabla^2 T_i + \frac{1}{\alpha_i} \mathbf{V}\cdot\vec{\nabla} T_i = \frac{1}{\alpha_i}\frac{\partial T_i}{\partial t}\ , \tag{B3}$$

†I.N. Sneddon, *Fourier Transforms,* New York, McGraw Hill, 1951, Chapter 1.

and we seek a particular solution $\phi_i(P, t)$, $P \in D_i(t) \cup D_e(t)$, to Eq. (B3) which satisfies the initial condition $\phi_i(P, 0) = 0$ and has the following properties:

1. $\phi_i(P, t) = 0, P \in D_e(t)$.

2. $\displaystyle\lim_{\substack{P \to s \\ P \in D_i(t) \\ s \in S(t)}} \phi_i(P, t) = \hat{T}(s, t)$.

3. $\displaystyle\lim_{\substack{P \to s \\ P \in D_i(t) \\ s \in S(t)}} \frac{d\phi_i}{dn_s}(P, t) = g_i(s, t)$.

Since properties 2 and 3 imply that $\phi_i(P, t) = T_i(P, t)$, $P \in D_i(t)$, then finding $\phi_i(P, t)$ is completely equivalent to solving Eq. (B3) for the interior temperature distribution $T_i(P, t)$.

Let $\phi_i(P, t) = \psi_i(P, t)e^{-(\mathbf{V}/2\alpha_i)\cdot \mathbf{x}(P))}$. Then Eq. (B3) becomes

$$\nabla^2 \psi_i - \frac{\psi_i}{(2\alpha_i)^2} \mathbf{V}\cdot\mathbf{V} = \frac{1}{\alpha_i} \frac{\partial \psi_i}{\partial t}. \tag{B4}$$

Taking the Fourier transform of the left-hand side of Eq. (B4), and noting that $\psi_i(P, t) = 0$ for $P \in D_e(t)$ gives

$$\begin{aligned}
\mathcal{F}\left[\nabla^2 \psi_i - \frac{\psi_i}{(2\alpha_i)^2} \mathbf{V}\cdot\mathbf{V}\right] &= \mathcal{F}(\nabla^2 \psi_i) - \frac{\mathbf{V}\cdot\mathbf{V}}{(2\alpha_i)^2} \overline{\psi}_i(P_\xi, t) \\
&= \left(\frac{1}{2\pi}\right)^{3/2} \int_{D_i(t)} \nabla^2 T_i(P, t) e^{i[\mathbf{x}(P)\cdot\vec{\xi}(P_\xi)]}\, dV - \frac{\mathbf{V}\cdot\mathbf{V}}{(2\alpha_i)^2} \overline{\psi}_i(P_\xi, t) \\
&= \left(\frac{1}{2\pi}\right)^{3/2} \int_{D_i(t)} \psi_i(P, t) \nabla^2 e^{i[\mathbf{x}(P)\cdot\vec{\xi}(P_\xi)]}\, dV - \frac{\mathbf{V}\cdot\mathbf{V}}{(2\alpha_i)} \overline{\psi}_i(P_\xi, t) \\
&\quad + \left(\frac{1}{2\pi}\right)^{3/2} \int_{S(t)} \Big\{ e^{i[\mathbf{w}(q)\cdot\vec{\xi}(P_\xi)]}\, \vec{\nabla}\psi_i(q, t)\cdot\mathbf{n}(q) \\
&\quad - \psi_i(q, t) \vec{\nabla} e^{i[\mathbf{x}(P)\cdot\vec{\xi}(P_\xi)]}\Big|_{\mathbf{x}(P)=\mathbf{w}(q)} \cdot\mathbf{n}(q)\Big\}\, dS_q
\end{aligned} \tag{B5}$$

Continued

(by Green's theorem)

$$= -\left[|\xi|^2 + \frac{\dot{\mathbf{V}}\cdot\mathbf{V}}{(2\alpha_i)^2}\right]\overline{\psi}_i(P_\xi, t) + \left(\frac{1}{2\pi}\right)^{3/2}\int_{S(t)}\left\{\vec{\nabla}\psi_i(q, t)\cdot\mathbf{n}(q)\right.$$

$$\left. - i[\vec{\xi}(P_\xi)\cdot\mathbf{n}(q)]\,\psi_i(q, t)\right\}e^{i[\mathbf{w}(q)\cdot\vec{\xi}(P_\xi)]}\,dS_q, \tag{B5}$$

where $\overline{\psi}_i(P_\xi, t)$ is the transform of $\psi_i(P, t)$, q is a point on the interface $S(t)$, and $\mathbf{w}(q)$ is the position vector associated with q. The Fourier transform of the right-hand side of Eq. (B4) can be evaluated with the aid of Eq. (B1) and of the result

$$\frac{\partial}{\partial t}\int_{\mathfrak{D}(t)} A(P, t)\,dV = \int_{\mathfrak{D}(t)}\frac{\partial}{\partial t}A(P, t)\,dV + \int_{\Sigma(t)}\mathbf{A}(q, t)\mathbf{u}(q)\cdot\mathbf{n}(q)\,d\Sigma_q, \tag{B6}$$

where $\mathfrak{D}(t)$ is a time-dependent domain bounded by the surface $\Sigma(t)$, $A(P, t)$ is an arbitrary function of P and t, defined both in $\mathfrak{D}(t)$ and on $\Sigma(t)$, and $\mathbf{u}(q)$ is the relative velocity of a point q on $\Sigma(\tau)$. Thus

$$\mathcal{F}\,\frac{1}{\alpha_i}\frac{\partial\psi_i}{\partial t} = \left(\frac{1}{2\pi}\right)^{3/2}\int_{D_i(t)}\frac{1}{\alpha_i}\frac{\partial\psi_i}{\partial t}(P, t)e^{i[\mathbf{x}(P)\cdot\vec{\xi}(P_\xi)]}\,dV$$

$$= \frac{1}{\alpha_i}\frac{\partial}{\partial t}\left\{\left(\frac{1}{2\pi}\right)^{3/2}\int_{D_i(t)}\psi_i(P, t)e^{i[\mathbf{x}(P)\cdot\vec{\xi}(P_\xi)]}\,dV\right\}$$

$$- \left(\frac{1}{2\pi}\right)^{3/2}\int_{S(t)}\frac{1}{\alpha_i}\psi_i(q, t)\mathbf{u}(q)\cdot\mathbf{n}(q)e^{i[\mathbf{w}(q)\cdot\vec{\xi}(P_\xi)]}\,dS_q$$

$$= \frac{1}{\alpha_i}\frac{\partial}{\partial t}\overline{\psi}_i(P_\xi, t) - \left(\frac{1}{2\pi}\right)^{3/2}\int_{S(t)}\frac{1}{\alpha_i}\psi_i(q, t)\mathbf{u}(q)\cdot\mathbf{n}(q)e^{i[\mathbf{w}(q)\cdot\vec{\xi}(P_\xi)]}\,dS_q. \tag{B7}$$

Equating expressions (B5) and (B7) gives now the following equation for $\overline{\psi}_i(P_\xi, t)$:

$$\frac{1}{\alpha_i}\frac{\partial}{\partial t}\overline{\psi}_i(P_\xi, t) + \left[|\xi|^2 + \frac{\mathbf{V}\cdot\mathbf{V}}{(2\alpha_i)^2}\right]\overline{\psi}_i(P_\xi, t)$$

$$= \frac{1}{2\pi}^{3/2}\int_{S(t)}\left\{\vec{\nabla}\psi_i(q, t)\cdot\mathbf{n}(q) - i[\vec{\xi}(P_\xi)\cdot\mathbf{n}(q)]\,\psi_i(q, t)\right.$$

$$\left. + \frac{1}{\alpha_i}\psi_i(q, t)\mathbf{u}(q)\cdot\mathbf{n}(q)\right\}e^{i[\mathbf{w}(q)\cdot\vec{\xi}(P_\xi)]}\,dS_q. \tag{B8}$$

Equation (B8), which is simply a first-order ordinary differential equation in $\overline{\psi}_i(P_\xi, t)$ (with P_ξ as a parameter), can be integrated by standard techniques. Hence, recalling that

$$\overline{\psi}_i(P_\xi, t) = \left(\frac{1}{2\pi}\right)^{3/2} \int_{D_i(t)} \phi_i(P, t) e^{(\mathbf{V}/2\alpha_i)\cdot \mathbf{x}(P) + i[\mathbf{x}(P)\cdot \vec{\xi}(P_\xi)]} \, dV,$$

which in turn implies

$$\overline{\psi}_i(P_\xi, 0) = \left(\frac{1}{2\pi}\right)^{3/2} \int_{D_i(t)} \phi_i(P, 0) e^{(\mathbf{V}/2\alpha_i)\cdot \mathbf{x}(P) + i[\mathbf{x}(P)\cdot \vec{\xi}(P_\xi)]} \, dV = 0$$

(since $\phi_i(P, 0) = 0$ by Eq. (3a) in the main text, we can integrate Eq. (B8) to get

$$\overline{\psi}_i(P_\xi, t) = \left(\frac{1}{2\pi}\right)^{3/2} \int_0^t \int_{S(\tau)} \Big\{ \alpha_i \vec{\nabla}\psi_i(q, \tau)\cdot \mathbf{n}(q) - i\alpha_i [\vec{\xi}(P_\xi)\cdot \mathbf{n}(q)]\, \psi_i(q, \tau)$$
$$+ \psi_i(q, \tau)\mathbf{u}(q)\cdot \mathbf{n}(q) \Big\} e^{-[\alpha_i|\xi|^2 + (\mathbf{V}\cdot\mathbf{V}/4\alpha_i)](t-\tau) + i[\mathbf{w}(q)\cdot \vec{\xi}(P_\xi)]} \, dS_q d\tau. \qquad \text{(B9)}$$

With $\overline{\psi}_i(P_\xi, t)$ now determined, $\psi_i(P, t)$, and hence $\phi_i(P, t)$, can be found by applying the inversion formula, Eq. (B2). Thus

$$\psi_i(P, t) = \left(\frac{1}{2\pi}\right)^3 \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_0^t \int_{S(\tau)} \Big\{ \alpha_i \vec{\nabla}\psi_i(q, \tau)\cdot \mathbf{n}(q) - i\alpha_i [\vec{\xi}(P_\xi)\cdot \mathbf{n}(q)]\, \psi_i(q, \tau)$$
$$+ \psi_i(q, \tau)\mathbf{u}(q)\cdot \mathbf{n}(q) \Big\} e^{-[\alpha_i|\xi|^2 + (\mathbf{V}\cdot\mathbf{V}/4\alpha_i)](t-\tau)}$$
$$\times e^{i[\mathbf{x}(P) - \mathbf{w}(q)]\cdot \vec{\xi}(P_\xi)} \, dS_q d\tau d\xi_1 d\xi_2 e\xi_3$$
$$= \frac{1}{8\pi^{3/2}} \int_0^t \int_{S(\tau)} \Bigg\{ \frac{1}{\alpha_i^{1/2}(t-\tau)^{3/2}} \left[\vec{\nabla}\psi_i(q, \tau)\cdot \mathbf{n}(q) + \frac{1}{\alpha_i}\, \psi_i(q, \tau)\mathbf{u}(q)\cdot \mathbf{n}(q) \right]$$
$$- \frac{\psi_i(q, \tau)}{2\alpha_i^{3/2}(t-\tau)^{5/2}} \, [\mathbf{x}(P) - \mathbf{w}(q)]\cdot \mathbf{n}(q) \Bigg\} e^{-[\mathbf{x}(P) - \mathbf{w}(q)]\cdot[\mathbf{x}(P) - \mathbf{w}(q)]/4\alpha_i(t-\tau)}$$
$$\times e^{-(\mathbf{V}\cdot\mathbf{V}/4\alpha_i)(t-\tau)} \, dS_q d\tau, \qquad \text{(B10)}$$

and since

$$\psi_i(P, t) = \phi_i(P, t) e^{(\mathbf{V}/2\alpha_i)\cdot \mathbf{x}(P)} \qquad \text{(B11a)}$$

and, by properties 2 and 3,

$$\psi_i(q, \tau) = \hat{T} e^{(\mathbf{V}/2\alpha_i)\cdot \mathbf{w}(q)}, \tag{B11b}$$

and

$$\vec{\nabla}\psi_i(q, \tau)\cdot \mathbf{n}(q) = \left[g_i + \frac{\hat{T}}{2\alpha_i}\, \mathbf{V}\cdot\mathbf{n}(q)\right] e^{(\mathbf{V}/2\alpha_i)\cdot \mathbf{w}(q)}, \tag{B11c}$$

then

$$\begin{aligned}\phi_i(P, t) = \frac{1}{8\pi^{3/2}} \int_0^t \int_{S(\tau)} \Bigg\{ & \frac{1}{\alpha_i^{1/2}(t-\tau)^{3/2}} \left[g_i + \frac{\hat{T}}{2\alpha_i}\, \mathbf{V}\cdot\mathbf{n}(q) + \frac{\hat{T}}{\alpha_i}\, \mathbf{u}\cdot\mathbf{n}(q)\right] \\ & - \frac{\hat{T}}{2\alpha_i^{3/2}(t-\tau)^{5/2}} \left[\mathbf{x}(P) - \mathbf{w}(q)\right]\cdot\mathbf{n}(q)\Bigg\} F_i(\mathbf{x}(P), \mathbf{w}(q), t, \tau, \mathbf{V})\, dS_q\, d\tau \\ = - W_i^{S(t)}[\hat{T}](P, t) + U_i^{S(t)} & \left[g_i + \frac{\hat{T}}{\alpha_i}(\mathbf{V}\cdot\mathbf{n}(q) + \mathbf{u}\cdot\mathbf{n}(q))\right](P, t),\end{aligned} \tag{B12}$$

where $F_i(\mathbf{x}(P), \mathbf{w}(q), t, \tau, \mathbf{V})$, $W_i^{S(t)}[f](P, t)$, and $U_i^{S(t)}[h](P, t)$ are given by Eqs. (8), and (7), and (6), respectively in the main text. But $\phi_i(P, t) = T_i(P, t)$, $P \in D_i(t)$; therefore Eq. (B12) is precisely the same as Eq. (14) in the main text.

THE EXTERIOR PROBLEM

The treatment of the exterior problem is similar to the preceding treatment and therefore will only be outlined. Thus a solution $\phi_e(P, t)$ $P \in D_i(t) \cup D_e(t)$, to the exterior diffusion equation

$$\nabla^2 T_e + \frac{1}{\alpha_e}\, \mathbf{V}\cdot\vec{\nabla} T_e = \frac{1}{\alpha_e}\frac{\partial T_e}{\partial t} \tag{B13}$$

is constructed by transform methods such that the initial condition $\phi_e(P, 0) = 0$ is satisfied and

1. $\phi_e(P, t) = 0, P \in D_i(t)$.

2. $\displaystyle\lim_{\substack{P\to\infty \\ P\in D_e(t)}} \phi_e(P, t) = 0.$

3. $\displaystyle\lim_{\substack{P\to s \\ P\in D_e(t) \\ s\in S(t)}} \phi_e(P, t) = \hat{T}.$

4. $\lim\limits_{\substack{P \to s \\ P \in D_e(t) \\ s \in S(t)}} \dfrac{d\phi_e}{dn_s}(P, t) = g_e.$

The result is

$$\phi_e = +W_e^{S(t)}[\hat{T}](P, t) - U_e^{S(t)} \left\{ g_e + \frac{\hat{T}}{\alpha_e} [\mathbf{V} \cdot \mathbf{n}(q) + \mathbf{u} \cdot \mathbf{n}(q)] \right\} (P, t). \tag{B14}$$

But properties 3 and 4 imply that $\phi_e(P, t) = T_e(P, t)$, $P \in D_e(t)$; therefore Eq. (B14) is precisely the same as Eq. (15) in the main text.

Appendix C
DETERMINATION OF EXPLICIT EXPRESSIONS FOR $F_1^{\tilde{\omega}}(y, \nu(y), \nu'(y), \nu''(y))$, $M_1'^{\tilde{\omega}}(0)\langle\delta\nu\rangle$, AND $M_2'^{\tilde{\omega}}(0)\langle\delta\nu\rangle$

AN EXPRESSION FOR $F_1^{\tilde{\omega}}(y, \nu(y), \nu'(y), \nu''(y))$,

Since $F_1^{\tilde{\omega}}$ is defined as

$$F_1^{\tilde{\omega}}(y, \nu(y), \nu'(y), \nu''(y)) = \frac{\omega''(r)}{[1 + \omega'^2(r)]^{3/2}} + \frac{\frac{1}{r}\,\omega'(r)}{[1 + \omega'^2(r)]^{1/2}} \,, \tag{C1}$$

determining $F_1^{\tilde{\omega}}$ is tantamount to finding $\omega'(r)$ and $\omega''(r)$ in terms of $\nu(y)$, $\nu'(y)$, $\nu''(y)$, which in turn is essentially a problem in geometry and elementary calculus. Thus, since

$$r = y + \nu(y) \sin\tilde{\theta}(y) \tag{C2a}$$

and

$$\omega(r) = \tilde{\omega}(y) + \nu(y) \cos\tilde{\theta}(y)\,, \tag{C2b}$$

$$\omega'(r) = \frac{d\omega}{dr} = \frac{d\omega}{dy}\left(\frac{dr}{dy}\right)^{-1} = f_{a'}^{\tilde{\omega}}(y, \nu(y), \nu'(y))$$

$$= \frac{\tilde{\omega}(y) + \nu(y)\,\frac{d}{dy}\cos\tilde{\theta}(y) + \nu'(y)\cos\tilde{\theta}(y)}{1 + \nu(y)\,\frac{d}{dy}\sin\tilde{\theta}(y) + \nu'(y)\sin\tilde{\theta}(y)} \,, \tag{C3}$$

where

$$\sin\tilde{\theta}(y) = -\frac{\tilde{\omega}'(y)}{[1 + \tilde{\omega}'^2(y)]^{1/2}} \tag{C4a}$$

and

$$\cos\tilde{\theta}(y) = \frac{1}{[1 + \tilde{\omega}'^2(y)]^{1/2}}. \tag{C4b}$$

Moreover

$$\omega''(r) = \frac{d}{dr} f_a^{\tilde{\omega}} = \frac{d}{dy} (f_a^{\omega}) \left(\frac{dr}{dy}\right)^{-1} = f_b^{\tilde{\omega}} (y, \nu(y), \nu'(y), \nu''(y))$$

$$= \left\{ \left[1 + \nu(y) \frac{d}{dy} \sin \tilde{\theta}(y) + \nu'(y) \sin \tilde{\theta}(y)\right] \left[\tilde{\omega}''(y) + 2\nu'(y) \frac{d}{dy} \cos \tilde{\theta}(y) \right.\right.$$

$$\left. + \nu(y) \frac{d^2}{dy^2} \cos \tilde{\theta}(y) + \nu''(y) \cos \tilde{\theta}(y)\right] - \left[\tilde{\omega}'(y) + \nu(y) \frac{d}{dy} \cos \tilde{\theta}(y)\right.$$

$$\left. + \nu'(y) \cos \tilde{\theta}(y)\right] \left[2\nu'(y) \frac{d}{dy} \sin \tilde{\theta}(y) + \nu(y) \frac{d^2}{dy^2} \sin \tilde{\theta}(y) \right.$$

$$\left.\left. + \nu''(y) \sin \tilde{\theta}(y)\right]\right\} \left[1 + \nu(y) \frac{d}{dy} \sin \tilde{\theta}(y) + \nu'(y) \sin \tilde{\theta}(y)\right]^{-3}. \tag{C5}$$

Therefore

$$F_1^{\tilde{\omega}} (y, \nu(y), \nu'(y), \nu''(y)) = \frac{f_b^{\tilde{\omega}}}{[1 + (f_a^{\tilde{\omega}})^2]^{3/2}} + \frac{f_a^{\tilde{\omega}}}{[y + \nu(y) \sin \tilde{\theta}(y)]\,[1 + (f_a^{\tilde{\omega}})^2]^{1/2}} \tag{C6}$$

AN EXPRESSION FOR $M_1'^{\tilde{\omega}}(0)\langle\delta\nu\rangle$

The operator $M_1'^{\tilde{\omega}}(0)$ must by definition satisfy the relation

$$\lim_{\substack{\|\delta\nu\| \to 0 \\ \nu_0,\, \delta\nu\, \epsilon\, C^2[0,\, \infty]}} \frac{\|M_1^{\tilde{\omega}}\langle\nu\rangle - M_1^{\tilde{\omega}}\langle\nu_0\rangle - M_1'^{\tilde{\omega}}(\nu_0)\langle\delta\nu\rangle\|}{\|\delta\nu\|} = 0, \tag{C7}$$

where $\nu = \nu_0 + \delta\nu$ and $\nu_0 = 0$. In particular it can be shown that if $M_1^{\tilde{\omega}}\langle\nu\rangle$ is of the form $F_1^{\tilde{\omega}}(y, \nu(y), \nu'(y), \nu''(y))$, then Eq. (C7) can be satisfied only by taking $M_1'^{\tilde{\omega}}(0)\langle\delta\nu\rangle$ as

$$M_1'^{\tilde{\omega}}(0)\langle\delta\nu\rangle = \left.\frac{\partial F_1^{\tilde{\omega}}}{\partial \nu}\right|_{\nu=\nu'=\nu''=0} \delta\nu(y) + \left.\frac{\partial F_1^{\tilde{\omega}}}{\partial \nu'}\right|_{\nu=\nu'=\nu''=0} [\delta\nu(y)]' + \left.\frac{\partial F_1^{\tilde{\omega}}}{\partial \nu''}\right|_{\nu=\nu'=\nu''=0} [\delta\nu(y)]''. \tag{C8}$$

Equation (C8) therefore provides a practical means of determining $M_1'^{\tilde{\omega}}(0)$.

With the aid of Eqs. (C3), (C5), and (C6), it can be readily verified that Eq. (C8) takes the form

$$M_1'^{\tilde{\omega}}(0)\langle\delta\nu\rangle = \left\{\frac{\dfrac{d^2}{dy^2}\cos\tilde{\theta}(y) - \tilde{\omega}'(y)\dfrac{d^2}{dy^2}\sin\tilde{\theta}(y) + \tilde{\omega}''(y)\dfrac{d}{dy}\sin\tilde{\theta}(y)}{[1+\tilde{\omega}'^2(y)]^{3/2}}\right.$$

$$- \frac{3\tilde{\omega}''(y)\left[\dfrac{d}{dy}\sin\tilde{\theta}(y) + \tilde{\omega}'(y)\dfrac{d}{dy}\cos\tilde{\theta}(y)\right]}{[1+\tilde{\omega}'^2(y)]^{5/2}} - \frac{\cos\tilde{\theta}(y)}{y^2}\tilde{\omega}'(y)\sin\tilde{\theta}(y)$$

$$\left. + \frac{\cos\tilde{\theta}(y)}{y}\frac{d}{dy}\cos\tilde{\theta}(y) - \frac{\tilde{\omega}'(y)\left[\dfrac{d}{dy}\sin\tilde{\theta}(y) + \tilde{\omega}'(y)\dfrac{d}{dy}\cos\tilde{\theta}(y)\right]}{y[1+\tilde{\omega}'^2(y)]^{3/2}}\right\}\delta\nu(y)$$

$$+\left\{\frac{2\dfrac{d}{dy}\cos\tilde{\theta}(y) - 2\tilde{\omega}'(y)\dfrac{d}{dy}\sin\tilde{\theta}(y) + \tilde{\omega}''(y)\sin\tilde{\theta}(y)}{[1+\tilde{\omega}'^2(y)]^{3/2}} + \frac{\cos^2\tilde{\theta}(y)}{y}\right\}[\delta\nu(y)]'$$

$$+\left\{\frac{\cos\tilde{\theta}(y) - \tilde{\omega}'(y)\sin\tilde{\theta}(y)}{[1+\tilde{\omega}'^2(y)]^{3/2}}\right\}[\delta\nu(y)]'', \tag{C9}$$

which upon application of Eq. (C4) reduces to

$$M_1'^{\tilde{\omega}}(0)\langle\delta\nu\rangle = \left\{\frac{[\tilde{\omega}''(y)]^2}{[1+\tilde{\omega}'^2(y)]^3} + \frac{[\tilde{\omega}'(y)]^2}{y^2[1+\tilde{\omega}'^2(y)]}\right\}\delta\nu(y) + \left\{\frac{1}{y[1+\tilde{\omega}'^2(y)]}\right.$$

$$\left. - \frac{\tilde{\omega}''(y)\tilde{\omega}'(y)}{[1+\tilde{\omega}'^2(y)]^2}\right\}[\delta\nu(y)]' + \frac{1}{[1+\tilde{\omega}'^2(y)]}[\delta\nu(y)]'' \tag{C10}$$

For the particular case $\tilde{\omega}(y) = \omega_0(y) = -y^2/2a_0$, Eq. (C10) can be further reduced. Thus

$$M_1'^{\omega_0}(0)\langle\delta\nu\rangle = \frac{1}{\xi(y)}\left\{[\delta\nu(y)]'' + \frac{1}{y\xi(y)}[\delta\nu(y)]' + \frac{1}{a_0^2}\left[1 + \frac{1}{\xi^2(y)}\right]\delta\nu(y)\right\}, \tag{C11}$$

where

$$\xi(y) = 1 + \left(\frac{y}{a_0}\right)^2$$

AN EXPRESSION FOR $M_2'^{\widetilde{\omega}}(0)\langle\delta\nu\rangle$

To evaluate $M_2'^{\widetilde{\omega}}(0)\langle\delta\nu\rangle$, it is first necessary to introduce the one-sided Fréchet derivatives $M_2'^{\widetilde{\omega}+}(0)$ and $M_2'^{\widetilde{\omega}-}(0)$ which are defined by the relations

$$\lim_{\substack{\|\delta\nu\| \to 0 \\ \nu_0,\, \delta\nu \in C^2[0,\infty] \\ \delta\nu > 0}} \frac{\|M_2^{\widetilde{\omega}}\langle\nu\rangle - M_2^{\widetilde{\omega}}\langle\nu_0\rangle - M_2'^{\widetilde{\omega}+}(\nu_0)\langle\delta\nu\rangle\|}{\|\delta\nu\|} \tag{C12a}$$

and

$$\lim_{\substack{\|\delta\nu\| \to 0 \\ \nu_0,\, \delta\nu \in C^2[0,\infty] \\ \delta\nu < 0}} \frac{\|M_2^{\widetilde{\omega}}\langle\nu\rangle - M_2^{\widetilde{\omega}}\langle\nu_0\rangle - M_2'^{\widetilde{\omega}-}(\nu_0)\langle\delta\nu\rangle\|}{\|\delta\nu\|} \tag{C12b}$$

where $\nu = \nu_0 + \delta\nu$ and $\nu_0 = 0$. Then, if $M_2'^{\widetilde{\omega}+}(0) = M_2'^{\widetilde{\omega}-}(0)$, the Fréchet derivative $M_2'^{\widetilde{\omega}}(0)$ is defined as

$$M_2'^{\widetilde{\omega}}(0) = M_2'^{\widetilde{\omega}+}(0) = M_2'^{\widetilde{\omega}-}(0).$$

For operators of the form

$$\Delta\Theta - \int_0^\infty F_2^{\widetilde{\omega}}(q, y, \nu(y), \nu(q), \nu'(q))\, dq,$$

it can be shown that Eqs. (C12) are satisfied by taking $M_2'^{\widetilde{\omega}+}(0)\langle\delta\nu\rangle$ and $M_2'^{\widetilde{\omega}-}(0)\langle\delta\nu\rangle$ as

$$\begin{aligned} M_2'^{\widetilde{\omega}+}(0)\langle\delta\nu\rangle = &- \delta\nu(y) \lim_{\substack{\|\delta\nu\|\to 0 \\ \delta\nu > 0}} \frac{\partial}{\partial\nu(y)} \int_0^\infty F_2^{\widetilde{\omega}}\, dq \\ &- \lim_{\substack{\|\delta\nu\|\to 0 \\ \delta\nu > 0}} \int_0^\infty \left\{ \frac{\partial F_2^{\widetilde{\omega}}}{\partial\nu(q)}\, \delta\nu(q) + \frac{\partial F_2^{\widetilde{\omega}}}{\partial\nu'(q)}\, [\delta\nu(q)]' \right\} dq, \end{aligned} \tag{C13a}$$

$$\begin{aligned} M_2'^{\widetilde{\omega}-}(0)\langle\delta\nu\rangle = &- \delta\nu(y) \lim_{\substack{\|\delta\nu\|\to 0 \\ \delta\nu < 0}} \frac{\partial}{\partial\nu(y)} \int_0^\infty F_2^{\widetilde{\omega}}\, dq \\ &- \lim_{\substack{\|\delta\nu\|\to 0 \\ \delta\nu < 0}} \int_0^\infty \left\{ \frac{\partial F_2^{\widetilde{\omega}}}{\partial\nu(q)}\, \delta\nu(q) + \frac{\partial F_2^{\widetilde{\omega}}}{\partial\nu'(q)}\, [\delta\nu(q)]' \right\} dq, \end{aligned} \tag{C13b}$$

which by virtue of Eqs. (36), (37), (40), (55), and the definition of d/dn_y (Eq. (43c)) can also be written as (for $r = y + \delta\nu(y) \sin \tilde{\theta}(y)$, $z = \omega(y) + \delta\nu(y) \cos \tilde{\theta}(y)$, $\delta\nu > 0$)

$$M_2'^{\tilde{\omega}+}(0)\langle\delta\nu\rangle = -\,\delta\nu(y) \lim_{\substack{(r,z)\to(y,\tilde{\omega}(y))\\(r,z)\in\bar{D}_e}} \left\{\frac{d}{dn_y}\, \bar{U}^{\tilde{\omega}}[2\cos\tilde{\theta}](r,z)\right\}$$

$$\lim_{\substack{(r,z)\to(y,\tilde{\omega}(y))\\(r,z)\in\bar{D}_e}} \left\{\bar{W}^{\tilde{\omega}}[2\delta\nu\cos\tilde{\theta}](r,z)\right.$$

$$\left. + \bar{U}^{\tilde{\omega}} \left[\left\{\left((\sin\tilde{\theta})' + \frac{1}{q}\sin\tilde{\theta}\right)\delta\nu + \sin\tilde{\theta}(\delta\nu)'\right\} 2\cos\tilde{\theta}\right](r,z)\right\},$$

$$= +\,\delta\nu(y)\cos\tilde{C}(y) - \delta\nu(y)\,\frac{d}{dn_y}\,\bar{U}^{\tilde{\omega}*}[2\cos\tilde{\theta}](y) - \delta\nu(y)\cos\tilde{\theta}(y)$$

$$-\,\bar{W}^{\tilde{\omega}*}[2\delta\nu\cos\tilde{\theta}](y) - U^{\tilde{\omega}*}\left[\left\{\left((\sin\tilde{\theta})' + \frac{1}{q}\sin\tilde{\theta}\right)\delta\nu + \sin\tilde{\theta}(\delta\nu)'\right\}2\cos\tilde{\theta}\right](y) \tag{C14a}$$

by properties 1 through 3 (p. 19) and

$$M_2'^{\tilde{\omega}-}(0)\langle\delta\nu\rangle = -\,\delta\nu(q) \lim_{\substack{(r,z)\to(y,\tilde{\omega}(y))\\(r,z)\in\bar{D}_i}} \frac{d}{dn_y}\,\bar{u}^{\tilde{\omega}}[2\cos\tilde{\theta}](r,z)$$

$$-\lim_{\substack{(r,z)\to(y,\tilde{\omega}(y))\\(r,z)\in\bar{D}_i}} \left\{\bar{W}^{\tilde{\omega}}[2\delta\nu\cos\tilde{\theta}[(r,z)\right.$$

$$\left. + u^{\tilde{\omega}}\left[\left\{\left((\sin\tilde{\theta}) + \frac{1}{q}\sin\tilde{\theta}\right)\delta\nu + \sin\tilde{\theta}(\delta\nu)'\right\}2\cos\tilde{\theta}\right](r,z)\right\}$$

$$= -\,\delta\nu(y)\cos\tilde{\theta}(y) - \delta\nu(y)\,\frac{d}{dn_y}\,\bar{U}^{\tilde{\omega}*}[2\cos\tilde{\theta}](y) + \delta\nu(y)\cos\tilde{\theta}(y)$$

$$-\,\bar{W}^{\tilde{\omega}*}[2\delta\nu\cos\tilde{\theta}](y) - \bar{U}^{\tilde{\omega}*}\left[\left\{\left((\sin\tilde{\theta})' + \frac{1}{q}\sin\tilde{\theta}\right)\delta\nu + \sin\tilde{\theta}(\delta\nu)'\right\}2\cos\tilde{\theta}\right](y) \tag{C14b}$$

by properties 1 through 3. Therefore

$$M_2'^{\tilde{\omega}+}(0)\langle\delta\nu\rangle = M_2'^{\tilde{\omega}-}(0)\langle\delta\nu\rangle = M_2'^{\tilde{\omega}}(0)\langle\delta\nu\rangle$$

$$= -\,\delta\nu(y)\,\frac{d}{dn_y}\,\overline{u}^{\tilde{\omega}*}[2\cos\tilde{\theta}](y) - \overline{W}^{\tilde{\omega}*}[2\delta\nu\cos\tilde{\theta}](y)$$

$$-\,\overline{U}^{\tilde{\omega}*}\left[\left\{\left((\sin\tilde{\theta})' + \frac{1}{q}\sin\tilde{\theta}\right)\delta\nu + \sin\tilde{\theta}(\delta\nu)'\right\}2\cos\tilde{\theta}\right](y). \quad \text{(C15)}$$

A certain degree of simplification results if $\tilde{\omega}(y)$ is chosen as $\omega_0(y) = -\,y^2/2a_0$. Thus it is known† that the interior normal derivative of the isothermal temperature distribution, namely,

$$\lim_{\substack{(r,z)\to(y,\,\tilde{\omega}(y))\\(r,z)\in\overline{D}_i}} \frac{d}{dn_y}\,\overline{U}^{\omega_0}[2\cos\theta_0](r,z),$$

is identically zero.

Hence, by Eqs. (43a) and (43b),

$$\frac{d}{dn_y}\,\overline{U}^{\omega_0^*}[2\cos\theta_0](y) = -\cos\theta_0(y). \quad \text{(C16)}$$

Substituting Eq. (C16) into Eq. (C15) then gives with the aid of Eqs. (40), (41), and (42b), and (45) the following expression for $M_2'^{\omega_0}(0)\langle\delta\nu\rangle$:

$$M_2'^{\omega_0}(0)\langle\delta\nu\rangle = \frac{\delta\nu(y)}{\xi^{1/2}(y)} - \frac{1}{\pi}\int_0^\infty e^{-[\omega_0(y)-\omega_0(q)]}\left\{\frac{d}{dn_q}\,G(y,z,q,\omega_0(q))\Big|_{z=\omega_0(y)}\right.$$

$$\left. + \frac{1}{2a_0\xi^{1/2}(y)}\,G(y,\omega_0(y),q,\omega_0(q))\right\}q\delta\nu(q)dq$$

$$-\frac{1}{\pi}\int_0^\infty e^{-[\omega_0(y)-\omega_0(q)]}\,G(y,\omega_0(y),q,\omega_0(q))\left\{\left[\frac{1}{\xi^{1/2}(q)}\left(1+\frac{1}{2a_0}\right)\right.\right.$$

$$\left.\left. + \frac{1}{a_0\xi^{3/2}(q)}\right]\delta\nu(q) + \frac{q}{a_0\xi^{1/2}(q)}\,[\delta\nu(q)]'\right\}qdq, \quad \text{(C17)}$$

where

$$\xi(y) = 1 + \left(\frac{y}{a_0}\right)^2$$

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†C. P. Ivantsov, Dokl. Akad. Nauk SSSR 58 (1947) 567; G. Horvay and J. W. Cahn, Acta Met. 9 (1961) 695.