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Eigenvalues of the One-Dimensional Smoluchowski Equation

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The eigenvalues and eigenfunctions of the Smoluchowski equation are investigated for the case of potentials with N deep wells. The small parameter $\delta = kT/V$, which measures the ratio of the thermal energy to a typical well depth, is used in connection with the method of matched asymptotic expansion to obtained asymptotic approximations to all the eigenvalues and eigenfunctions. It is found that the eigensolutions fall into two classes, namely (i) the top-of-the-well and (ii) the bottom-of-the-well eigensolutions. The eigenvalues for both classes of solutions are integer multiples of the squares of the frequencies at the top or bottom of the various wells. The eigenfunctions are, in general, localized to the top or bottom of the corresponding well. The very small eigenvalues require special consideration because the asymptotic analysis is incapable of distinguishing them from the zero eigenvalue with multiplicity N. Another approximation reveals that, in addition to the true zero eigenvalue, there are $N-1$ eigenvalues of order $\exp(-\delta)$. The case of other possible multiple eigenvalues is also examined.

KEY WORDS: Smoluchowski equation; deep-well potentials; eigenvalues; matched asymptotic expansions.

INTRODUCTION: THE CLASS OF POTENTIAL

It is a well-known fact that the time evolution of a system governed by a linear partial differential equation can be inferred from the knowledge of the eigensolutions of the corresponding eigenvalue problem. This is the case for the time-dependent Kramers and Smoluchowski problems. For this reason, there are numerous studies of the eigensolutions of the Kramers and Smoluchowski operators (see Risken[(1)]).

Incidentally, we are using the terms "Smoluchowski equation" and "Smoluchowski problem" to denote the high-friction limit of the full Kramers equation or Kramers problem (see, e.g., Risken[(1)] and Gardiner[(2)]).

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We want to reconsider the problem of finding the eigenvalues of the one-dimensional Smoluchowski equation. There are at least three reasons for revisiting this problem.

First, most of the previous analyses have focused on either one- or two-well potentials (see, e.g., Hänggi and Thomas[3]). We would like to study the case of a multiwell potential. Such wells might occur in models of ion transport through protein channels (see, e.g., Barcilon *et al.*[4]). Also, in studies of two-dimensional crossings with large anisotropy, it is convenient to have results of the general one-dimensional case on tap (see, e.g., Klosek *et al.*[5]).

Second, the cases which have received the greatest amount of attention are those of the small eigenvalues. We would like to compute all the eigenvalues and all the eigenfunctions, at least approximately.

Finally, many technical questions related to a systematic mathematical approach to the computation of the eigensolutions of the Kramers problem remain in spite of the efforts of numerous applied mathematicians (see, e.g., Hänggi *et al.*[6] for a very complete list of references). For example, it would be desirable to develop an approximation scheme which would enable us to obtain, without any *ad hoc* approximations, the crossover formulas (see Mel'nikov and Meshkov[7]). Also, it would be useful to revisit by analytical means the problem for a periodic potential extensively discussed by Ferrando *et al.*[8] Of course, we cannot address these questions here since we are using the Smoluchowski equation as our starting point. Nevertheless, it is our hope that the method of matched asymptotic expansion developed here can be extended to the full Fokker–Planck equation.

In this analysis, we shall focus our attention on a class of potentials $V(x)$ which have the following three properties.

(i) They have $N \geqslant 2$ quadratic minima. Furthermore, if m_i is the location of the ith minimum, then in the neighborhood of m_i we can write

$$V = v_i + \tfrac{1}{2}\omega_i^2 (x - m_i)^2 + \cdots \tag{0.1}$$

(ii) They have $N - 1$ quadratic maxima. In the neighborhood of the ith maximum located at M_i, the potential can be written as

$$V = V_i - \tfrac{1}{2}\Omega_i^2 (x - M_i)^2 + \cdots \tag{0.2}$$

(iii) The potentials become large and positive as x tends to either positive or negative large values. The growth at infinity is such that

$$\int_{-\infty} \frac{dt}{V'(t)}, \qquad \int^{\infty} \frac{dt}{V'(t)} < \infty \tag{0.3}$$

where a prime denotes a derivative with respect to x.

1. THE EIGENVALUE PROBLEM

We want to find the eigensolution $\{p_k, \sigma_k\}$ of the problem

$$\mathscr{L} p_k = \sigma_k p_k \tag{1.1}$$

where the operator $\mathscr{L}$ is the familiar Smoluchowski operator

$$\mathscr{L} = -\frac{d}{dx}\left[\delta \frac{d}{dx} + V'\right] \tag{1.2}$$

In the above equation, δ is a dimensionless number which measures the ratio of thermal energy kT to depth of a typical well. For deep wells

$$\delta \ll 1 \tag{1.3}$$

To Eq. (1.1) we add the requirement that the eigenfunctions decay at infinity, or more specifically

$$p_k \in L^2(\mathbf{R}, e^{V/\delta}\, dx) \tag{1.4}$$

The adjoint of the above eigenvalue problem is the problem for $P_k(x)$, which is related to $p_k(x)$ as

$$p_k = P_k\, e^{-V/\delta} \tag{1.5}$$

The eigenvalue problem (1.1) now reads

$$\delta \frac{d}{dx}\left[e^{-V/\delta} \frac{dP_k}{dx}\right] + \sigma_k e^{-V/\delta} P_k = 0 \tag{1.6}$$

or equivalently

$$\delta \frac{d^2 P_k}{dx^2} - V' \frac{dP_k}{dx} + \sigma_k P_k = 0 \tag{1.7}$$

We require the solutions of (1.7) to satisfy the analog of (1.4), namely

$$P_k \in L^2(\mathbf{R}, e^{-V/s}\, dx) \tag{1.8}$$

We adopt (1.7)–(1.8) as the working formulation of the eigenvalue problem for the Smoluchowski operator. We note in closing the orthogonality relation

$$\int_{-\infty}^{\infty} P_l P_k\, e^{-V/\delta}\, dx = 0 \qquad \text{if} \quad \sigma_l \neq \sigma_k \tag{1.9}$$

Of course, we can also cast the eigenvalue problem into the canonical Sturm–Liouville form

$$\delta \frac{d^2\varpi_k}{dx^2} + (q + \sigma_k)\, \varpi_k = 0 \tag{1.10}$$

where

$$\varpi_k = P_k e^{-V/2\delta} \tag{1.11}$$

and the "potential" q is

$$q = \frac{1}{2} V'' - \frac{1}{4\delta} V'^2 \tag{1.12}$$

A general treatment of eigenvalue problems such as (1.11)–(1.12) can be found in classical treatises such as those of Titchmarsh[9] and Coddington and Levinson.[10] For instance, Titchmarsh[9] (pp. 107, 127) states that the study of the spectrum falls into one of four distinct categories. One such category is that for which

$$\begin{gathered} q(x) \to -\infty \qquad \text{as} \quad x \to \pm\infty \\ \int_{-\infty}^{\infty} |q(x)|^{-1/2}\, dx < \infty \end{gathered} \tag{1.13}$$

In view of the smallness of δ, this is precisely the case of interest to us. Note that the integrability of $|q|^{-1/2}$ is related to condition (0.3). Incidentally, in this case, the spectrum is discrete. We should mention that potentials which have a linear growth at infinity are excluded from this class; in particular, piecewise linear potentials fall outside of this analysis.

2. DOMAIN DECOMPOSITION

We shall take advantage of the smallness of δ to obtain the solution as an asymptotic expansion in δ. In particular, we shall use the method of limit-process expansion (Kevorkian and Cole[11]) to obtain asymptotic expansions valid in different overlapping domains. The method will become clear in the sequel; suffice it to say at this stage that we shall consider four different types of domains. In each of these types of domains we shall solve an appropriate version of the differential equation governing the eigenvalue problem; finally we shall synthesize an eigensolution by piecing together bits of those solutions. For instance, the first such type of domains will consist of the well bottoms, say $\mathscr{B}_i$, where (see Fig. 1)

$$\mathscr{B}_i = \{x \mid |x - m_i| \sim \delta^{1/2}\}, \qquad i = 1, \dots, N \tag{2.1}$$

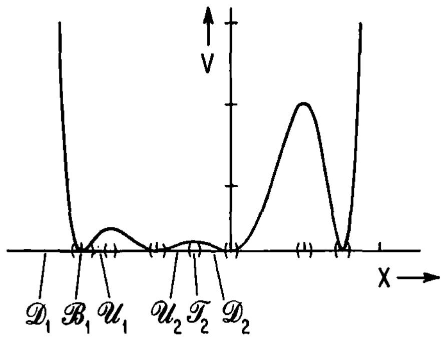

Fig. 1. Typical potential and decomposition of domain.

The second type of domains, say $\mathscr{T}_i$, will be centered around the well tops. We shall see that

$$\mathscr{T}_i = \{x \mid |x - M_i| \sim \delta^{1/2}\}, \qquad i = 1,..., N-1 \tag{2.2}$$

Not surprisingly, the third and fourth types of domains, say $\mathscr{U}_i$ and $\mathscr{D}_i$, will deal with the regions away from the well extrema where the potential goes either "up" or "down," i.e.,

$$\left. \begin{aligned} \mathscr{D}_i &= \{x \mid M_{i-1} + \delta^{1/2} < x < m_i - \delta^{1/2}\} \\ \mathscr{U}_i &= \{x \mid m_i + \delta^{1/2} < x < M_i - \delta^{1/2}\} \end{aligned} \right\}, \qquad i = 1,..., N \tag{2.3}$$

In the above definitions, we have tacitly used the fact that

$$M_0 = -\infty, \qquad M_N = \infty \tag{2.4}$$

The rationale for this domain decomposition is easy to understand. Indeed, in view of the fact that δ is small, we might feel justified in neglecting the first term in (1.7) since it is multiplied by δ. This approximation leads to the simpler equation

$$-V' \frac{dF}{dx} + \sigma F = 0 \tag{2.5}$$

This equation does indeed yield approximations to the desired eigenfunctions in intervals where V' does not vanish, i.e., in the $\mathscr{U}$ and $\mathscr{D}$ domains. However, as we approach points where V' vanishes, i.e., as we enter into the $\mathscr{B}$ and $\mathscr{T}$ domains, the first term in (1.7), which we previously neglected, is no longer small vis-à-vis the second one. Therefore, a different approximation must be obtained. All these different approximations must be matched in regions where the various domains overlap.

Incidentally, the condition (0.3) on the integrability of $1/V'$ arises naturally in the process of solving (2.5).

3. THE $\mathcal{U}$, $\mathcal{D}$ DOMAINS

In the method of limit-process expansions, the asymptotic expansions associated with the $\mathcal{U}$, $\mathcal{D}$ domains are obtained by holding $x \in \mathcal{U}$ or $\mathcal{D}$ fixed and letting $\delta \downarrow 0$.

3.1. The "Up" Domains

To fix our ideas, let us assume that $x \in \mathcal{U}_i$: then we look for a solution of the form

$$P = v_i^{(0)}(\delta)\, U_i^{(0)}(x) + v_i^{(1)}(\delta)\, U_i^{(1)}(x) + \dots \qquad \text{for} \quad x \in \mathcal{U}_i \tag{3.1}$$

Note that for the ease of reading we have suppressed temporarily the index k of the eigenfunction. The factors $v_i^{(0)}(\delta)$, $v_i^{(1)}(\delta)$,..., which form an asymptotic sequence, give the explicit magnitude of the various terms of the asymptotic series. The actual shape of the solution is provided by $U_i^{(0)}(x)$, $U_i^{(1)}(x)$,.... To simplify the analysis, we shall anticipate some results, and write form the outset (3.1) as

$$P = v_i(\delta)[\, U_i^{(0)}(x) + \delta^{1/2} U_i^{(1)}(x) + \dots] \qquad \text{for} \quad x \in \mathcal{U}_i \tag{3.2}$$

We must also write an asymptotic series for the eigenfunction

$$\sigma = \sigma^{(0)} + \delta^{1/2}\sigma^{(1)} + \dots \tag{3.3}$$

Because the asymptotic representations are in terms of power series, transcendentally small terms in either the eigenvalues of eigenfunctions and invariably lost. Although such terms are asymptotically small (i.e., as $\delta \downarrow 0$), their numerical values and relevance may not be negligible. In fact, they are of great physical significance in this problem. To evaluate such terms, we shall have to resort to some *ad hoc* means.

Substituting these expressions in (1.7), we see that to leading order

$$-V' \frac{dU_i^{(0)}}{dx} + \sigma^{(0)} U_i^{(0)} = 0 \tag{3.4}$$

The integration of this equation is straightfoward. However, in anticipation of the matching at the ends of the $\mathscr{U}_i$ domain, we write

$$\frac{1}{V'(t)}=\left[\frac{1}{V'(t)}-\frac{1}{\omega_i^2(t-m_i)}+\frac{1}{\Omega_i^2(t-M_i)}\right] + \frac{1}{\omega_i^2(t-m_i)}-\frac{1}{\Omega_i^2(t-M_i)} \tag{3.5}$$

Making use of this expression, it is easy to see that

$$U_i^{(0)}(x)=u_i\frac{(x-m_i)^{\sigma^{(0)}/\omega_i^2}}{(M_i-x)^{\sigma^{(0)}/\Omega_i^2}} \times \exp\left[\sigma^{(0)}\int_{m_i}^{x}\left(\frac{1}{V'(t)}-\frac{1}{\omega_i^2(t-m_i)}+\frac{1}{\Omega_i^2(t-M_i)}\right)dt\right] \tag{3.6}$$

where u_i is a constant of integration.

As a result,

$$U_i^{(0)}(x)\sim\begin{cases} u_i(M_i-m_i)^{\sigma^{(0)}/\omega_i^2}I_i\cdot(M_i-x)^{-\sigma^{(0)}/\Omega_i^2} & \text{as}\quad x\to M_i \\ u_i(M_i-m_i)^{-\sigma^{(0)}/\Omega_i^2}\cdot(x-m_i)^{\sigma^{(0)}/\omega_i^2} & \text{as}\quad x\to m_i \end{cases} \tag{3.7}$$

where

$$I_i=\exp\left[\sigma^{(0)}\int_{m_i}^{M_i}\left(\frac{1}{V'(t)}-\frac{1}{\omega_i^2(t-m_i)}+\frac{1}{\Omega_i^2(t-M_i)}\right)dt\right] \tag{3.8}$$

3.2. The "Down" Domains

The analysis of the generic "down" domains $\mathscr{D}_i$ follows along very similar lines. The asymptotic series representation is taken to be

$$P=\delta_i(\delta)[D_i^{(0)}(x)+\delta^{1/2}D_i^{(1)}(x)+\ldots] \qquad \text{for}\quad x\in\mathscr{D}_i \tag{3.9}$$

To leading order, the equation for $D_i^{(0)}$ is identical to (3.4). Therefore, we can immediately write

$$D_i^{(0)}(x)=d_i\frac{(m_i-x)^{\sigma^{(0)}/\omega_i^2}}{(x-M_{i-1})^{\sigma^{(0)}/\Omega_{i-1}^2}} \times \exp\left[\sigma^{(0)}\int_{M_{i-1}}^{x}\left(\frac{1}{V'(t)}-\frac{1}{\omega_i^2(t-m_i)}+\frac{1}{\Omega_{i-1}^2(t-M_{i-1})}\right)dt\right] \tag{3.10}$$

where d_i is another constant of integration.

As a result

$$D_i^{(0)}(x) \sim \begin{cases} d_i(m_i - M_{i-1})^{-\sigma^{(0)}/\Omega_{i-1}^2} J_i \cdot (m_i - x)^{\sigma^{(0)}/\Omega_i^2} & \text{as } x \to m_i \\ d_i(m_i - M_{i-1})^{\sigma^{(0)}/\omega_i^2} \cdot (x - M_{i-1})^{-\sigma^{(0)}/\Omega_{i-1}^2} & \text{as } x \to M_{i-1} \end{cases} \tag{3.11}$$

where

$$J_i = \exp\left[\sigma^{(0)} \int_{M_{i-1}}^{m_i} \left(\frac{1}{V'(t)} - \frac{1}{\omega_i^2(t - m_i)} + \frac{1}{\Omega_{i-1}^2(t - M_{i-1})}\right) dt\right] \tag{3.12}$$

Note that the approximations (3.5) and (3.10) to the eigenfunction are valid for all values of $\sigma^{(0)}$, i.e., they do not determine the eigenvalue.

3.3. First and Last Domains

The forms of the solutions in the first and last intervals are slightly different from that in the other intervals, namely,

$$D_1^{(0)}(x) = d_1(m_1 - x)^{\sigma^{(0)}/\omega_1^2} \exp\left[\sigma^{(0)} \int_{-\infty}^{x} \left(\frac{1}{V'(t)} - \frac{1}{\omega_1^2(t - m_1)}\right) dt\right] \tag{3.13}$$

and

$$U_N^{(0)}(x) = u_N(x - m_N)^{\sigma^{(0)}/\omega_N^2} \exp\left[\sigma^{(0)} \int_{m_N}^{x} \left(\frac{1}{V'(t)} - \frac{1}{\omega_N^2(t - m_N)}\right) dt\right] \tag{3.14}$$

As a result,

$$D_1^{(0)}(x) \sim d_1 J_1 \cdot (m_1 - x)^{\sigma^{(0)}/\omega_1^2} \qquad \text{as } x \to m_1 \tag{3.15}$$

where

$$J_1 = \exp\left[\sigma^{(0)} \int_{-\infty}^{m_1} \left(\frac{1}{V'(t)} - \frac{1}{\omega_1^2(t - m_1)}\right) dt\right] \tag{3.16}$$

Similarly,

$$U_N^{(0)}(x) \sim d_N \cdot (x - m_N)^{\sigma^{(0)}/\omega_N^2} \qquad \text{as } x \to m_N \tag{3.17}$$

3.4. Unavoidable Singularities

Before considering the top and bottom intervals, we should inquire as to whether it might be possible to hookup *directly* a "down" solution to an "up" solution across a domain $\mathscr{B}$. In other words, if we focus on, say, the generic minimum m_i, why can we not tie the expressions in (3.7) and (3.11) by setting

$$u_i(m_i - M_i)^{-\sigma^{(0)}/\Omega_i^2} = d_i(m_i - M_{i-1})^{-\sigma^{(0)}/\Omega_{i-1}^2} J_i \tag{3.18}$$

thus taking advantage of the fact that the behavior of $D_i^{(0)}$ is identical to that of $U_i^{(0)}$ near $x = m_i$? The reason why this procedure is not acceptable is to be found in the computation of the higher order corrections. Recalling the expansion (3.2) for the "up" solution, we know that

$$\begin{aligned} -V' \frac{dU_i^{(1)}}{dx} + \sigma^{(0)} U_i^{(1)} &= -\sigma^{(1)} U_i^{(0)} \\ -V' \frac{dU_i^{(2)}}{dx} + \sigma^{(0)} U_i^{(2)} &= -\sigma^{(1)} U_i^{(1)} - \sigma^{(2)} U_i^{(0)} - \frac{d^2 U_i^{(0)}}{dx^2} \end{aligned} \tag{3.19}$$

Now on account of (3.4)

$$\begin{aligned} \frac{d^2 U_i^{(0)}}{dx^2} &= -\frac{\sigma^{(0)} V''}{V'^2} U^{(0)} + \frac{\sigma^{(0)}}{V'} \frac{dU_i^{(0)}}{dx} \\ &= -\frac{\sigma^{(0)} V''}{V'^2} U^{(0)} + \frac{\sigma^{(0)2}}{V'^2} U_i^{(0)} \\ &= \sigma^{(0)} \frac{\sigma^{(0)} - V''}{V'^2} U^{(0)} \end{aligned} \tag{3.20}$$

As a result, in the neighborhood of the minimum m_i, the equation for the second-order corrections reads

$$\begin{aligned} \frac{dU_i^{(2)}}{dx} - \frac{\sigma^{(0)}}{V'} U_i^{(2)} &= \frac{\sigma^{(1)}}{V'} U_i^{(1)} + \frac{\sigma^{(2)}}{V'} U_i^{(0)} + \frac{1}{V'} \frac{d^2 U_i^{(0)}}{dx^2} \\ &= \frac{\sigma^{(1)}}{V'} U_i^{(1)} + \frac{\sigma^{(2)}}{V'} U_i^{(0)} + \sigma^{(0)} \frac{\sigma^{(0)} - V''}{V'^3} U_i^{(0)} \end{aligned} \tag{3.21}$$

Because of the last term on the right-hand side, the above equation is usually not integrable. The exception occurs when $\sigma^{(0)}/\omega_i^2 - 3 > -1$. However, even if this condition is satisfied, a more stringent one appears when we go to the next order. In fact, unless $\sigma^{(0)}$ is a integral multiple of ω_i^2, a case which requires special study and which we shall revisit, we must conclude that we cannot hook up directly an "up" solution to a "down" solution at a minimum.

3.5. Zero Solutions

In closing, we should not dismiss the possibility that the solutions in either an "up" or a "down" domain are identically equal to zero, i.e., that

$$U_i^{(0)} = 0 \tag{3.22}$$

or

$$D_i^{(0)} = 0 \tag{3.23}$$

We shall see that this will indeed be the case whenever these outer solutions must be matched to inner solutions which have an exponential decay.

4. THE TOP-OF-THE-HILL DOMAINS

If the outer solution in a generic domain, say $\mathscr{U}_i$, is nonzero, i.e., is given by (3.6), then as can be seen from (3.7), this outer solution blows up as we approach the maximum M_i. Clearly, we must examine the vicinity of this maximum to see how to prevent such singular behavior. To that effect, we introduce a stretched variable ζ_i such that

$$\zeta_i = \frac{\Omega_i}{(2\delta)^{1/2}} (x - M_i) \tag{4.1}$$

and look for the eigenfunction, in the domain $\mathscr{T}_i$, as an asymptotic series of the form

$$P = \theta_i(\delta)[t_i(\zeta_i) + \delta^{1/2} T_i^{(1)}(\zeta_i) + \dots] \tag{4.2}$$

The factor of $\delta^{1/2}$ in the definition of the stretched variable is dictated by our desire to reinstate the previously neglected second derivative of P in the governing equation. The other factors are simply there for the simplifications of the results to be derived.

In limit-process expansion parlance, we are looking for a solution with ζ_i fixed and $\delta \downarrow 0$. We see that to leading order, Eq. (1.7) implies that

$$\frac{d^2 T_i^{(0)}}{d\zeta_i^2} + 2\zeta_i \frac{dT_i^{(0)}}{d\zeta_i} + 2\frac{\sigma^{(0)}}{\Omega_i^2} T_i^{(0)} = 0 \tag{4.3}$$

We temporarily drop the superscript and subscript and digress from our main goal to consider the properties of the solutions of

$$\frac{d^2 T}{d\zeta^2} + 2\zeta \frac{dT}{d\zeta} + 2sT = 0 \tag{4.4}$$

We can check, say by constructing series solutions, that the most general solution of this equation is

$$T(\zeta; s) = t_1 M\left(\frac{s}{2}, \frac{1}{2}, -\zeta^2\right) + t_2 \zeta M\left(\frac{s}{2} + \frac{1}{2}, \frac{3}{2}, -\zeta^2\right) \tag{4.5}$$

where t_1 and t_2 are arbitrary constants and $M(a, b, z)$ is the confluent hypergeometric function (see Abramowitz and Stegun,[12] No. 13.1.2, p. 504).

For the purpose of matching this solution to the neighboring "up" and "down" solutions, we shall need to know its asymptotic behavior as $\zeta \to \pm\infty$. We can find it by using formula No. 13.5.1 in Abramowitz and Stegun,[12] but we must be careful to compute the argument of $-\zeta^2$ correctly.

For example, if we define

$$\zeta = |\zeta| \, e^{i\alpha} \tag{4.6}$$

and then write

$$-\zeta^2 = |\zeta|^2 \, e^{i(2\alpha + \pi)} \tag{4.7}$$

we must use different expressions for the asymptotic expansions depending upon whether $-\pi/2 < 2\alpha + \pi < 3\pi/2$ or $-3\pi/2 < 2\alpha + \pi < -\pi/2$, i.e., depending upon whether $-3\pi/4 < \alpha < \pi/4$ or $-5\pi/4 < \alpha < -3\pi/4$. In particular, negative values of ζ correspond to an argument of $-\pi$. The correct result is

$$\begin{aligned} T^{(0)} \sim & \left[t_1 \frac{\Gamma(1/2)}{\Gamma(1/2 - s/2)} + t_2 \frac{\zeta}{|\zeta|} \frac{\Gamma(3/2)}{\Gamma(1 - s/2)} \right] \\ & \times \sum_{n=0} \frac{(1 + s/n)_n \, (\frac{1}{2} + s/2)_n}{n! \, \zeta^{2n}} \cdot |\zeta|^{-s} + \left[t_1 \frac{\Gamma(1/2) \, e^{i\pi(s-1)/2}}{\Gamma(s/2)} \right. \\ & \left. + t_2 \frac{\zeta}{|\zeta|} \frac{\Gamma(3/2) \, e^{i\pi(s/2 - 1)}}{\Gamma(1/2 + s/2)} \right] e^{-\zeta^2} |\zeta|^{s-1} + \dots \qquad \text{as} \quad \zeta \to \pm\infty \end{aligned} \tag{4.8}$$

It is important to note that for certain choices of t_1 and t_2, the top-of-the-hill solution can be made to have exponential decay on either the left- or right-hand side. Finally by choosing appropriate values of s, i.e., for certain eigenvalues, the solution can decay exponentially on both sides. We discuss these cases next.

Summary

Three special top-of-the-hill solutions will play a key role in the sequel. First, if we set

$$t_1 \frac{\Gamma(1/2)}{\Gamma(1/2-s/2)} + t_2 \frac{\Gamma(3/2)}{\Gamma(1-s/2)} = 0 \tag{4.9}$$

i.e., if we define

$$t_1 = \frac{\pi r}{\Gamma(1/2)\,\Gamma(1-s/2)} \tag{4.10}$$

$$t_2 = -\frac{\pi r}{\Gamma(3/2)\,\Gamma(1/2-s/2)} \tag{4.11}$$

where r is an arbitrary constant, then the resulting solution of (4.4), which we label $R(\zeta; s)$, namely

$$R(\zeta; s) = \pi \left[\frac{M(s/2, 1/2, -\zeta^2)}{\Gamma(1/2)\,\Gamma(1-s/2)} - \zeta \frac{M(s/2+1/2, 3/2, -\zeta^2)}{\Gamma(3/2)\,\Gamma(1/2-s/2)} \right] \tag{4.12}$$

decays exponentially to the right (see Fig. 2). In fact, substituting (4.10) and (4.11) in (4.8), we see that

$$\begin{aligned} R(\zeta; s) &\sim \left[\frac{\pi e^{i\pi(s-1)/2}}{\Gamma(s/2)\,\Gamma(1-s/2)} - \frac{\pi e^{i\pi(s/2-1)}}{\Gamma(1/2+s/2)\,\Gamma(1/2-s/2)} \right] e^{-\zeta^2} |\zeta|^{s-1} + \ldots \\ &= \left[-i \sin\left(\frac{\pi s}{2}\right) + \cos\left(\frac{\pi s}{2}\right) \right] e^{i\pi s/2}\, e^{-\zeta^2} |\zeta|^{s-1} + \ldots \end{aligned} \tag{4.13}$$

i.e.,

$$R(\zeta; s) \sim e^{-\zeta^2} |\zeta|^{s-1} + \ldots \qquad \text{as} \quad \zeta \to \infty \tag{4.14a}$$

whereas

$$R(\zeta; s) \sim \frac{2\pi}{\Gamma(1-s/2)\,\Gamma(1/2-s/2)} |\zeta|^{-s} + \ldots \qquad \text{as} \quad \zeta \to -\infty \tag{4.14b}$$

Alternatively, if we set

$$t_1 \frac{\Gamma(1/2)}{\Gamma(1/2-s/2)} - t_2 \frac{\Gamma(3/2)}{\Gamma(1-s/2)} = 0 \tag{4.15}$$

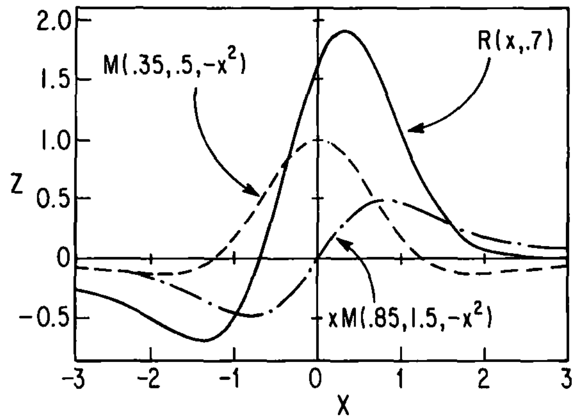

Fig. 2. Plot of $M(0.35, 0.5, -x^2)$, $xM(0.85, 1.5, -x^2)$, and $R(x, 0.7)$. Note the rapid decay of the R-function for positive values of x.

or, equivalently, define

$$t_1 = \frac{\pi l}{\Gamma(1/2)\,\Gamma(1-s/2)}$$
$$t_2 = \frac{\pi l}{\Gamma(3/2)\,\Gamma(1/2-s/2)} \tag{4.16}$$

where l is another arbitrary constant, then the corresponding solution of (4.4), which we denote by $L(\zeta; s)$, namely

$$L(\zeta; s) = \pi \left[\frac{M(s/2, 1/2, -\zeta^2)}{\Gamma(1/2)\,\Gamma(1-s/2)} + \zeta \frac{M(s/2+1/2, 3/2, -\zeta^2)}{\Gamma(3/2)\,\Gamma(1/2-s/2)} \right] \tag{4.17}$$

decays exponentially to the left. In fact

$$L(\zeta; s) \sim e^{-\zeta^2} |\zeta|^{s-1} + \ldots \qquad \text{as} \quad \zeta \to -\infty \tag{4.18a}$$

On the other hand,

$$L(\zeta; s) \sim \frac{2\pi}{\Gamma(1-s/2)\,\Gamma(1/2-s/2)} |\zeta|^{-s} + \ldots \qquad \text{as} \quad \zeta \to \infty \tag{4.18b}$$

These "right" and "left" solutions will be needed to cut off those eigenfuntions which are confined to one particular well.

The third type of solution of note is one which decays exponentially on both sides. This type of solution is obtained not only by selecting t_1 and/or t_2, but also by restricting s to particular values. We shall see that this leads to a class of eigensolutions.

We return to the asymptotic behavior (4.8): we can get rid of the algebraic decay by either setting

$$t_1 = 0$$
$$1 - \frac{s}{2} = -n, \qquad n = 0, 1,... \tag{4.19}$$

or

$$t_2 = 0$$
$$\frac{1}{2} - \frac{s}{2} = -n, \qquad n = 0, 1,... \tag{4.20}$$

Of course, if (4.9) holds, then the solution (4.5) reduces to

$$\begin{aligned} T(\zeta; s) &= t_2 \zeta M(n + \tfrac{1}{2}, \tfrac{3}{2}, -\zeta^2) \\ &= t_2 e^{-\zeta^2} \cdot \zeta M(-n, \tfrac{3}{2}, \zeta^2) \\ &= t_2 e^{-\zeta^2} \cdot 2^{-2n-1} H_{2n+1}(\zeta) \end{aligned} \tag{4.21}$$

where $H_{2n+1}(\zeta)$ is the Hermite polynomial of order $2n+1$. In arriving at this last result, we have used the Kummer transformation (see Abramowitz and Stegun,[12] No. 13.1.27) as well as the definition of the Hermite polynomial in terms of the confluent hypergeometric function (see Abramowitz and Stegun,[12] No. 13.6.38).

Similarly, if (4.20) is chosen, then

$$\begin{aligned} T(\zeta; s) &= t_1 M\left(n + \frac{1}{2}, \frac{1}{2}, -\zeta^2\right) \\ &= t_1 e^{-\zeta^2} \cdot M\left(-n, \frac{1}{2}, \zeta^2\right) \\ &= t_1 e^{-\zeta^2} \cdot \frac{n!}{2n!} \left(-\frac{1}{2}\right)^{-n} He_{2n}(\sqrt{2}\,\zeta) \end{aligned} \tag{4.22}$$

Translating these results in terms of Eq. (4.3), this means that

$$\begin{aligned} \sigma_{in}^T &= (n+1)\,\Omega_i^2 \\ P_{in}^T &= H_n\left(\Omega_i \frac{x - M_i}{(2\delta)^{1/2}}\right) \exp\left(-\Omega_i^2 \frac{(x - M_i)^2}{2\delta}\right) \\ & i = 1,..., N-1; \qquad n = 0, 1,... \end{aligned} \tag{4.23}$$

are eigensolutions. Indeed, these expressions satisfy the Smoluchowski equation in the neighborhood of the ith top and can be smoothly extended over the entire infinite range of x by means of zero solutions. These eigensolutions are the obvious generalization of the "inverted parabolic potential" eigensolutions discussed by Risken[1] (p. 109). In (4.23), the superscript indicating the order of magnitude has been dropped for ease of reading. Instead, a new superscript T is used to reminds us that we are dealing with a top-of-the-hill eigensolution. Two additional subscripts are used to label the eigensolutions: the first subscript, i, labels the particular maximum to which the eigenfuntion is confined; the second, n, refers to the nodes. We shall see next that the bottoms of the wells determine the other class of eigensolutions.

5. THE BOTTOM-OF-THE-WELL DOMAINS

To examine the solutions in the intervals $\mathscr{B}_i$, we introduce another set of stretched variables ξ_i defined as

$$\xi_i = \frac{\omega_i}{(2\delta)^{1/2}}(x - m_i) \tag{5.1}$$

We look for the eigenfunction in the ith well as an asymptotic series of the form

$$P = \beta_i(\delta)[B_i^{(0)}(\xi_i) + \delta^{1/2} B_i^{(1)}(\xi_i) + \ldots] \tag{5.2}$$

Substituting in (1.7), we see that the leading-order equation is

$$\frac{d^2 B_i^{(0)}}{d\xi_i^2} - 2\xi_i \frac{dB_i^{(0)}}{d\xi_i} + 2\frac{\sigma^{(0)}}{\omega_i^2} B_i^{(0)} = 0 \tag{5.3}$$

Following the same approach as for the intervals $\mathscr{T}_i$, we first examine the properties of the solutions of the equation

$$\frac{d^2 B}{d\xi^2} - 2\xi \frac{dB}{d\xi} + 2sB = 0 \tag{5.4}$$

We can check that the most general solution of this equation is

$$B(\xi; s) = b_1 M\left(-\frac{s}{2}, \frac{1}{2}, \xi^2\right) + b_2 \xi M\left(-\frac{s}{2} + \frac{1}{2}, \frac{3}{2}, \xi^2\right) \tag{5.5}$$

where, once again, b_1 and b_2 are constants and $M(a, b, z)$ is the confluent hypergeometric function.

We record the asymptotic behavior of this general solution for future matching purposes. Using formula No. 13.5.1 in Abramowitz and Stegun,[12] we deduce that

$$B \sim \left[b_1 \frac{\Gamma(1/2)\, e^{-i\pi s/2}}{\Gamma(1/2+s/2)} + b_2 \frac{\Gamma(3/2)\, e^{i\pi(-s+1)/2}}{\Gamma(1+s/2)} \right] \cdot |\xi|^s + \dots$$
$$+ \left[b_1 \frac{\Gamma(1/2)}{\Gamma(-s/2)} + b_2 \frac{\Gamma(3/2)}{\Gamma(1/2-s/2)} \right]$$
$$\times \sum_{n=0} \frac{(1/2+s/2)_n (1+s/2)_n}{n!\, \xi^{2n}} \cdot e^{\xi^2}\, |\xi|^{-s-1} \qquad \text{as} \quad \xi \to \pm\infty \qquad (5.6)$$

5.1. Second Class of Eigenvalues

Clearly, the general solution grows *exponentially* as ξ tends to either plus or minus infinity. This behavior precludes any possibility of matching this bottom-of-the-well solution to the outer solutions, which have, at best, an algebraic groth away from a minimum. The only exception from this behavior occurs if we choose either

$$b_1^{(0)} = 0$$
$$\frac{1}{2} - \frac{s}{2} = -n, \qquad n = 0, 1, \dots \qquad (5.7)$$

or

$$b_2^{(0)} = 0$$
$$-\frac{s}{2} = -n, \qquad n = 0, 1, \dots \qquad (5.8)$$

Combining these two results, we see that we must set

$$s = n, \qquad n = 0, 1, \dots \qquad (5.9)$$

We might as well abandon the generality of (5.5) and adopt instead the following normalization of the bottom-of-the-well solution corresponding to those integral values of s, namely

$$B^{(0)}(\xi; n) = H_n(\xi) \qquad (5.10)$$

By expressing (5.9) in terms of the original variables of the problem, we get the eigenvalues

$$\sigma^{(0)} = n\omega_i^2, \qquad n = 0, 1, \dots \qquad (5.11)$$

or, to parallel the notation introduced earlier,

$$\sigma_{in}^{B} = n\omega_i^2, \qquad i = 1,..., N, \quad n = 1, 2,... \tag{5.12}$$

We have deleted from the above expression the value $n = 0$, since it requires special consideration: we shall deal with it later. Whenever possible, we shall dispense with the full complement of subscripts and superscripts.

The above eigenvalues have been discussed previously by Hänggi and Thomas[3]; however, these authors did not bother to construct the corresponding eigenfunctions, which is what we want to do next. Indeed, as they stand, the bottom-of-the-well solutions (5.10) are not acceptable eigenfunctions. We must connect them to outer "up" and "down" solutions and examine whether, in turn, these "up" and "down" dolutions can be terminated by appropriate R and L functions in the neighborhood of the hills.

5.2. The Generic Case

We shall construct the eigenfunctions only for the generic case. We digress to explain what constitutes the generic case.

We have seen that the spectrum consists of two classes of eigenvalues, the T class and the B class, associated with the top-of-the-hill and bottom-of-the-well frequencies respectively, i.e.,

$$\begin{aligned} \text{spectrum} &= \sigma^T \cup \sigma^B \\ &= \left(\bigcup_{i=1}^{N-1} \{n\Omega_i^2\}_{n=0}^{\infty} \right) \cup \left(\bigcup_{i=1}^{N} \{n\omega_i^2\}_{n=0}^{\infty} \right) \end{aligned} \tag{5.13}$$

We shall define the generic case to be that in which none of the eigenvalues are repeated, with the exception of the zero eigenvalue, which is always a multiple eigenvalue. In other words, all bottom frequencies ω_i and top frequencies Ω_i are incommensurable with each other, or more accurately, there are no integers p and q such that either

$$p\omega_i^2 = q\omega_j^2 \qquad \text{or} \quad p\omega_i^2 = q\Omega_j^2 \tag{5.14}$$

When this is not the case, some eigenvalues are multiple and the results differ from those of the generic case. These special cases will be examined later.

5.3. Synthesis of the B-Eigenfunction

We consider the generic case and return to the B eigenvalue associated with the ith well. Since the squares of the frequencies in all the other wells differ from integral multiples of ω_i^2, it follows that the eigenfunction must be set equal to zero in all the other wells. In fact, though not as localized as the T-eigenfunctions, the B-eigenfunction which we are looking for will be different from zero in only five adjacent domains, namely in $\mathscr{B}_i$ and the two domains on either sides.

Therefore, we postulate that the eigensolution has the form

$$P_{in}^B(x) = \begin{cases} \theta_{i-1}(\delta)\, l_{i-1}\, L(\zeta_{i-1}, n\omega_i^2/\Omega_{i-1}^2) & \text{for} \quad x \in \mathscr{T}_{i-1} \\ \delta_i(\delta)\, D_i(x) & \text{for} \quad x \in \mathscr{D}_i \\ H_n(\xi_i) & \text{for} \quad x \in \mathscr{B}_i \\ v_i(\delta)\, U_i(x) & \text{for} \quad x \in \mathscr{U}_i \\ \theta_i(\delta)\, r_i R(\zeta_i, n\omega_i^2/\Omega_i^2) & \text{for} \quad x \in \mathscr{T}_i \end{cases} \tag{5.15}$$

We now embark on the task of connecting these various pieces of the solution. Note that we have arbitrarily taken the magnitude of the eigenfunction to be $O(1)$ in $\mathscr{B}_i$.

If the different pieces of solutions obtained thus far match on overlapping domains, then we do have a valid approximation of the eigenfunctions. To check this, we follow the procedure for matching in limit-process expansions.[11] In particular, in order to match the solution in the ith well to the neighboring "up" solution on the right, we must write both the inner variable ξ_i and the outer variable x in terms of an intermediate variable, say η_i, such that, for example,

$$\begin{aligned} x &= m_i + \frac{\sqrt{2}}{\omega_i}\delta^\lambda \eta_i \\ \xi_i &= \delta^{-1/2+\lambda}\eta_i \end{aligned} \tag{5.16}$$

with λ such that

$$0 < \lambda < 1/2 \tag{5.17}$$

but otherwise arbitrary. Next, η_i is kept fixed while $\delta \downarrow 0$. In that limit, the "up" solution and the bottom-of-the-well solution must agree (to within the order of approximation to which we are working). In other words

$$\lim_{\delta \downarrow 0} \{ H_n(\delta^{-1/2+\lambda}\eta_i) + \dots \} = \lim_{\delta \downarrow 0} \left\{ v_i(\delta)\, U_i^{(0)}\left(m_i + \frac{\sqrt{2}}{\omega_i}\delta^\lambda \eta_i \right) + \dots \right\} \tag{5.18}$$

Crudely speaking, the behavior of the bottom-of-the-well solution for large values of its argument must be the same as the "up" solution as it approaches the end point m_i. Making use of the property of the Hermite polynomials (Abramowitz and Stegun,[12] p. 775, No. 22.3.10), as well as of (3.7), we see that

$$2^n \delta^{-n/2+n\lambda} \eta_i^n + \dots = v_i(\delta)\, u_i(M_i - m_i)^{-n\omega_i^2/\Omega_i} 2^{n/2} \omega_i^{-n} \delta^{n\lambda} \eta_i^n + \dots \tag{5.19}$$

Therefore, the matching is indeed possible provided that

$$\begin{aligned} v_i(\delta) &= \delta^{-n/2} \\ u_i &= 2^{n/2} \omega_i^n (M_i - m_i)^{n\omega_i^2/\Omega_i^2} \end{aligned} \tag{5.20}$$

Similarly, we can also match the bottom-of-the-well solution to the "down" solution in $\mathscr{D}_i$ provided that

$$\begin{aligned} \delta_i(\delta) &= \delta^{-n/2} \\ d_i &= 2^{n/2} \omega_i^n (m_i - M_{i-1})^{n\omega_i^2/\Omega_{i-1}^2} J_{in}^{-1} \end{aligned} \tag{5.21}$$

where

$$J_{in} = \exp\left[n\omega_i^2 \int_{M_{i-1}}^{m_i} \left(\frac{1}{V'(t)} - \frac{1}{\omega_i^2 (t - m_i)} + \frac{1}{\Omega_{i-1}^2 (t - M_{i-1})} \right) dt \right] \tag{5.22}$$

The final step consists in terminating the outer solutions by means of an R-solution in $\mathscr{T}_i$ and an L-solution in $\mathscr{T}_{i-1}$. We turn next our attention first to the solution in $\mathscr{T}_i$. The solution there is

$$\begin{aligned} P_{in}^B &= \theta_i(\delta)\, r_i R(\zeta_i; n\omega_i^2/\Omega_i^2) \\ &= \theta_i(\delta)\, r_i R(\Omega_i(x - M_i)/(2\delta)^{1/2}; n\omega_i^2/\Omega_i^2) \end{aligned} \tag{5.23}$$

We have written the solution in $\mathscr{T}_i$ in terms of the outer variable x to shortcut the matching procedure and dispense with the intermediate variable. Holding x fixed and letting $\delta \downarrow 0$, we see from (4.14b) that

$$\begin{aligned} P_{in}^B &\sim \theta_i(\delta) \frac{2r_i \pi}{\Gamma(1 - n\omega_i^2/2\Omega_i^2)\, \Gamma(1/2 - n\omega_i^2/2\Omega_i^2)} \left(\frac{\Omega_i}{(2\delta)^{1/2}} (M_i - x) \right)^{-n\omega_i^2/\Omega_i^2} \\ &\sim \theta_i(\delta)\, \delta^{n\omega_i^2/2\Omega_i^2} \frac{2r_i \pi}{\Gamma(1 - n\omega_i^2/2\Omega_i^2)\, \Gamma(1/2 - n\omega_i^2/2\Omega_i^2)} \\ &\quad \times \left(\frac{2}{\Omega_i^2} \right)^{n\omega_i^2/2\Omega_i^2} (M_i - x)^{-n\omega_i^2/\Omega_i^2} \end{aligned} \tag{5.24}$$

For this expression to match with U_i as given in (3.6), we must set

$$\begin{aligned} \theta_i(\delta) &= \delta^{-n\omega_i^2/2\Omega_i^2} v_i(\delta) \\ r_i &= \frac{1}{2\pi} \Gamma\left(1 - \frac{n\omega_i^2}{2\Omega_i^2}\right) \Gamma\left(\frac{1}{2} - \frac{n\omega_i^2}{2\Omega_i^2}\right) \left(\frac{\Omega_i^2}{2}\right)^{n\omega_i^2/2\Omega_i^2} (M_i - m_i)^n I_{in} u_i \end{aligned} \tag{5.25}$$

where

$$I_{in}=\exp\left[n\omega_i^2\int_{m_i}^{M_i}\left(\frac{1}{V'(t)}-\frac{1}{\omega_i^2(t-m_i)}+\frac{1}{\Omega_i^2(t-M_i)}\right)dt\right] \tag{5.26}$$

The analysis of the matching of $L(\zeta_{i-1};\, n\omega_i^2/\Omega_i^2)$ to D_i is very similar to the previous one and yields

$$\begin{aligned}\theta_{i-1}(\delta)&=\delta^{-n\omega_i^2/2\Omega_{i-1}^2}\,\delta_i(\delta)\\ l_{i-1}&=\frac{1}{2\pi}\Gamma\left(1-\frac{n\omega_i^2}{2\Omega_{i-1}^2}\right)\Gamma\left(\frac{1}{2}-\frac{n\omega_i^2}{2\Omega_{i-1}^2}\right)\\ &\quad\times\left(\frac{\Omega_{i-1}^2}{2}\right)^{n\omega_i^2/2\Omega_{i-1}^2}(m_i-M_{i-1})^n d_i\end{aligned} \tag{5.27}$$

This concludes the matching procedure: we have now determined all the constants and orders of magnitude entering in the expression (5.15) for the eigenfunction. Indeed, combining (5.20), (5.21), (5.25), and (5.27), we now know that

$$\begin{aligned}\theta_{i-1}(\delta)&=\delta^{-n(\omega_i^2/2\Omega_{i-1}^2+1/2)}\\ \delta_i(\delta)&=\delta^{-n/2}\\ v_i(\delta)&=\delta^{-n/2}\\ \theta_i(\delta)&=\delta^{-n(\omega_i^2/2\Omega_i^2+1/2)}\end{aligned} \tag{5.28}$$

and

$$\begin{aligned}l_{i-1}&=\frac{1}{2\pi}\Gamma\left(1-\frac{n\omega_i^2}{2\Omega_{i-1}^2}\right)\Gamma\left(\frac{1}{2}-\frac{n\omega_i^2}{2\Omega_{i-1}^2}\right)\\ &\quad\times\left(\frac{\Omega_{i-1}^2}{2}\right)^{n\omega_i^2/2\Omega_{i-1}^2}(m_i-M_{i-1})^n d_i\\ d_i&=2^{n/2}\omega_i^n(m_i-M_{i-1})^{n\omega_i^2/\Omega_{i-1}^2}J_{in}^{-1}\\ u_i&=2^{n/2}\omega_i^n(M_i-m_i)^{n\omega_i^2/2\Omega_i^2}\\ r_i&=\frac{1}{2\pi}\Gamma\left(1-\frac{n\omega_i^2}{2\Omega_i^2}\right)\Gamma\left(\frac{1}{2}-\frac{n\omega_i^2}{2\Omega_i^2}\right)\left(\frac{\Omega_i^2}{2}\right)^{n\omega_i^2/2\Omega_i^2}(M_i-m_i)^n I_{in}u_i\end{aligned} \tag{5.29}$$

In summary, the analysis of the bottom-of-the-well domains (see Fig. 3) implies that the B-eigenvalues are

$$\sigma_{in}^B=n\omega_i^2 \tag{5.30}$$

and the corresonding eigensolutions

$$
P_{in}^{B}(x)=\begin{cases}
\dfrac{1}{2\pi}\left(\dfrac{2\omega_i^2}{\delta}\right)^{n/2}\left(\dfrac{\Omega_{i-1}^2}{2\delta}\right)^{n\omega_i^2/2\Omega_{i-1}^2}(m_i-M_{i-1})^{n+n\omega_i^2/\Omega_{i-1}^2}J_{in}^{-1} \\
\qquad\times\Gamma\left(1-\dfrac{n\omega_i^2}{2\Omega_{i-1}^2}\right)\Gamma\left(\dfrac{1}{2}-\dfrac{n\omega_i^2}{2\Omega_{i-1}^2}\right) \\
\qquad L\left(\dfrac{\Omega_{i-1}}{(2\delta)^{1/2}}(x-M_{i-1}),\dfrac{n\omega_i^2}{2\Omega_{i-1}^2}\right) & \text{for} \quad x\in\mathscr{T}_{i-1} \\
\left(\dfrac{2\omega_i^2}{\delta}\right)^{n/2}\left(\dfrac{m_i-M_{i-1}}{x-M_{i-1}}\right)^{n\omega_i^2/\Omega_{i-1}^2}(m_i-x)^n \\
\qquad\times\exp\left[n\omega_i^2\displaystyle\int_{m_i}^{x}\left(\dfrac{1}{V'(t)}-\dfrac{1}{\omega_i^2(t-m_i)}\right.\right. \\
\qquad\left.\left.+\dfrac{1}{\Omega_{i-1}^2(t-M_{i-1})}\right)dt\right] & \text{for} \quad x\in\mathscr{D}_i \\
H_n\left(\omega_i\dfrac{x-m_i}{(2\delta)^{1/2}}\right) & \text{for} \quad x\in\mathscr{B}_i \\
\left(\dfrac{2\omega_i^2}{\delta}\right)^{n/2}\left(\dfrac{M_i-m_i}{M_i-x}\right)^{n\omega_i^2/\Omega_i^2}(x-m_i)^n \\
\qquad\times\exp\left[n\omega_i^2\displaystyle\int_{m_i}^{x}\left(\dfrac{1}{V'(t)}-\dfrac{1}{\omega_i^2(t-m_i)}\right.\right. \\
\qquad\left.\left.+\dfrac{1}{\Omega_i^2(t-M_i)}\right)dt\right] & \text{for} \quad x\in\mathscr{U}_i \\
\dfrac{1}{2\pi}\left(\dfrac{2\omega_i^2}{\delta}\right)^{n/2}\left(\dfrac{\Omega_i^2}{2\delta}\right)^{n\omega_i^2/2\Omega_i^2}(M_i-m_i)^{n+n\omega_i^2/\Omega_i^2}I_{in} \\
\qquad\times\Gamma\left(1-\dfrac{n\omega_i^2}{2\Omega_i^2}\right)\Gamma\left(\dfrac{1}{2}-\dfrac{n\omega_i^2}{2\Omega_i^2}\right) \\
\qquad\times R\left(\dfrac{\Omega}{(2\delta)^{1/2}}(x-M_i),\dfrac{n\omega_i^2}{2\Omega_i^2}\right) & \text{for} \quad x\in\mathscr{T}_i
\end{cases}
\tag{5.31}
$$

The above form of the eigenfunctions is valid for the "inside" wells, i.e., for $i=2,\ldots,N-1$, provided of course that $N\geqslant 3$. The eigenfunctions for the first and last wells are slightly different.

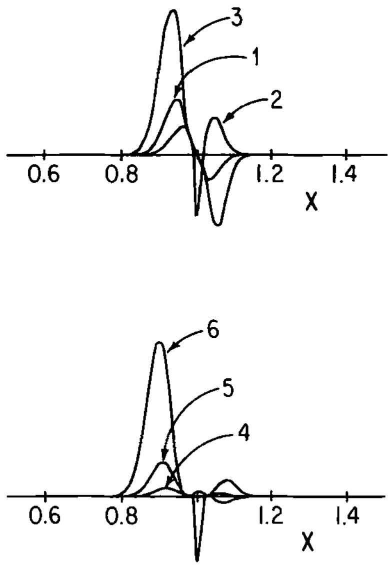

Fig. 3. Plot of bottom-of-the-well eigenfunctions for $n = 1,..., 6$ and $\delta = 0.01$. In view of our normalization, the functions become larger as n increases. Obviously, they are concentrated near the well bottom, but show a tendency for climbing the potential walls as n increases.

6. THE ZERO EIGENVALUES

We have already remarked that the zero eigenvalue, being a common eigenvalue for every well, is always an eigenvalue with multiplicity N to $O(1)$ in δ. We shall see that this multiplicity is resolved to the next order, which is a transcendentally small correction. Needless to say, this transcendentally small correction is of paramount importance in various theories, such as the theory of activated chemical reactions. For this reason, these eigensolutions have received a great deal of attention in the literature. Most of the previous work dealt with a two-well potential. For a detailed discussion of the small eigenvalues for an N-well potential, we refer the reader to Schuss[13] (p. 224). Our discussion is simply a generalization of his approach. It is interesting, though, to see how the analysis of the small eigenvalues relates to that of the higher ones.

The first step in the analysis necessary for splitting the zero eigenvalues is the construction of the related eigenfunctions. For reasons which will become clearer in a moment, we denote these eigenfunctions by P_0^B and P_{i0}^B, where the index i takes only the values $i = 1, 2,..., N-1$.

We dispose of the eigenfunction labeled P_0^B simply by noting that

$$\begin{aligned} \sigma_0^B &= 0 \\ P_0^B &= 1 \end{aligned} \tag{6.1}$$

is an exact eigensolution, correct to all orders of δ. This eigensolution is associated with the fact that

$$\bar{p}(x) = C \exp\left(-\frac{V(x)}{\delta}\right) \tag{6.2}$$

is the exact steady-state solution.

To obtain the eigenfunctions P_{i0}^B, we return to the approach of Section 3. Since the eigenvalues are now assumed to have the form

$$\sigma = \delta^{1/2}\sigma^{(1)} + \ldots \tag{6.3}$$

it follows that Eq. (3.4) for the "up" and "down" outer solutions satisfies, respectively,

$$\begin{aligned} -V' \frac{dU_i^{(0)}}{dx} &= 0 \\ -V' \frac{dD_i^{(0)}}{dx} &= 0 \end{aligned} \tag{6.4}$$

Clearly

$$\begin{aligned} U_i^{(0)} &= u_i \\ D_i^{(0)} &= d_i \end{aligned} \tag{6.5}$$

which are, of course, special cases of (3.6) and (3.10). In other words, the outer solutions are piecewise constant. The difficulties discussed in Section 3 about joining solutions across a bottom region $\mathscr{B}_i$ do not exist for such piecewise constant solutions: we simply set

$$d_i = u_i \tag{6.6}$$

Another way of justifying what might appear as an arbitrary matching is to remember that in $\mathscr{B}_i$ the solution is a Hermite polynomial and the order of this polynomial is proportional to the zeroth-order eigenvalue. In order words, the solution in $\mathscr{B}_i$ is

$$\begin{aligned} B_i^{(0)} &= b_i H_0(\xi_i) \\ &= b_i \end{aligned} \tag{6.7}$$

For all these reasons, we settle for a solution of the form

$$P^{(0)} = c_i \qquad \text{for} \quad x \in \mathscr{D}_i \cup \mathscr{B}_i \cup \mathscr{U}_i \tag{6.8}$$

The next step is to join these constant pieces across the top-of-the-hill domains $\mathscr{T}_i$. To this effect, we return to Section 4, and more particularly to (4.3), which now reads

$$\frac{d^2 T_i^{(0)}}{d\zeta_i^2} + 2\zeta_i \frac{dT_i^{(0)}}{d\zeta_i} = 0 \tag{6.9}$$

The most general solution of this equation is

$$T_i^{(0)}(\zeta_i) = a_i + t_i \operatorname{erf}(\zeta_i) \tag{6.10}$$

The matching of this inner solution to the outer solutions is trivial and yields

$$\left.\begin{aligned} a_i + t_i &= c_{i+1} \\ a_i - t_i &= c_i \end{aligned}\right\} \qquad \text{for} \quad i = 1, 2, \ldots, N-1 \tag{6.11}$$

As a result, the eigenfunctions are

$$P_{i0}^B = \begin{cases} c_i & \text{for} \quad x \in \mathscr{D}_i \cup \mathscr{B}_i \cup \mathscr{U}_i \\ \dfrac{1}{2}(c_{i+1} + c_i) + \dfrac{1}{2}(c_{i+1} - c_i) \operatorname{erf}\left(\dfrac{\Omega_i}{(2\delta)^{1/2}}(x - M_i)\right) & \text{for} \quad x \in \mathscr{T}_i \\ c_{i+1} & \text{for} \quad x \in \mathscr{D}_{i+1} \cup \mathscr{B}_{i+1} \cup \mathscr{U}_{i+1} \end{cases} \tag{6.12}$$

Note that the constants c_i are arbitrary: so, without loss of generality, we set all but one of them equal to zero and adopt the following definition of the eigenfunctions:

$$P_{i0}^B = \begin{cases} 0 & \text{for} \quad x \in \mathscr{D}_{i-1} \cup \mathscr{B}_{i-1} \cup \mathscr{U}_{i-1} \\ \operatorname{erfc}\left(\dfrac{\Omega_{i-1}}{(2\delta)^{1/2}}(x - M_{i-1})\right) & \text{for} \quad x \in \mathscr{T}_{i-1} \\ 1 & \text{for} \quad x \in \mathscr{D}_i \cup \mathscr{B}_i \cup \mathscr{U}_i \\ 1 - \operatorname{erfc}\left(\dfrac{\Omega_i}{(2\delta)^{1/2}}(x - M_i)\right) & \text{for} \quad x \in \mathscr{T}_i \\ 0 & \text{for} \quad x \in \mathscr{D}_{i+1} \cup \mathscr{B}_{i+1} \cup \mathscr{U}_{i+1} \end{cases} \tag{6.13}$$

In other words, the eigenfunction P_{i0}^B is localized to the domains $D_i \cup \mathscr{B}_i \cup \mathscr{U}_i$, and falls off exponentially to zero outside.

If we tried to pursue the asymptotic series to higher orders, we would not be able to get any corrections to the eigenvalues or eigenfunctions. For this reason, we adopt the above expressions, which are correct to within transcendentally small terms, and rely on a Rayleigh–Ritz approach to improve the eigenvalues. More specifically, making use of (1.6), we define the small eigenvalues by

$$\sigma = \frac{\delta \int_{-\infty}^{-\infty} (dP/dx)^2 \, e^{-V/\delta} \, dx}{\int_{-\infty}^{-\infty} P^2 e^{-V/\delta} \, dx} \tag{6.14}$$

where P and σ stand for P_{i0}^B and σ_{i0}^B. If we substitute in this formula the expression for P obtained in (6.13), we deduce that

$$\sigma_{i0}^B = \frac{\Omega_{i-1}}{\omega_i} \exp\left(- \frac{V_{i-1} - v_i}{\delta} \right) + \frac{\Omega_i}{\omega_i} \exp\left(- \frac{V_i - v_i}{\delta} \right) \tag{6.15}$$

As usual, this expression is valid for the inner wells, i.e., for $i = 2, \ldots, N-1$. For the first and last well, the formulas are slightly different, namely

$$\begin{aligned} \sigma_{10}^B &= \frac{\Omega_1}{\omega_1} \exp\left(- \frac{V_1 - v_1}{\delta} \right) \\ \sigma_{N-1,0}^B &= \frac{\Omega_{N-1}}{\omega_N} \exp\left(- \frac{V_{N-1} - v_N}{\delta} \right) \end{aligned} \tag{6.16}$$

These are the only expressions which involve the specific depths of the various wells!

7. COMMENSURATE SQUARE FREQUENCIES

The generic case examined previously excludes the possibility that certain eigenvalues are equal, i.e., that there exist integers p and q such that

$$p\omega_i^2 = q\omega_j^2 \tag{7.1}$$

We have also excluded the possibility that bottom and top frequencies are commensurate, namely that

$$p\omega_i^2 = q\Omega_j^2 \tag{7.2}$$

Let examine this last case first.

7.1. Commensurate Top and Bottom Frequencies

Actually, we only need to consider the cases in which the square of the frequency of a well is commensurate with the square of the frequencies of one of the two neighboring tops. Therefore, for the sake of discussion, let us assume that the ith well and ith hill are such that

$$p\omega_i^2 = q\Omega_i^2 \tag{7.3}$$

Retracing the steps we took to construct P^T_{in}, we can easily see that nothing pathological occurs. However, the situation is different for P^B_{in} and $P^B_{i+1,n}$. Indeed, these eigenfunctions require the existence of certain R and L solutions, more specifically of $R(\zeta_i; n\omega_i^2/\Omega_i^2)$. In particular, for $n=p$, we have

$$R(\zeta_i; n\omega_i^2/\Omega_i^2) = R(\zeta_i; p\omega_i^2/\Omega_i^2) \\ = R(\zeta_i; q) \tag{7.4}$$

But $R(\zeta_i, q)$, is just a "top" eigenfunction, i.e., decays exponentially on both sides! Therefore, it cannot be used to cut off the "bottom" eigenfunction. Consequently, we must reject this eigenvalue. This conclusion is not valid if the frequency of the *next* well is commensurate with the two frequencies under consideration.

7.2. Commensurate Well Frequencies

Once again, the only cases which need to be considered are those for which neighboring wells have commensurate frequencies. Therefore, let us assume that there exist two integers p and q such that

$$p\omega_i^2 = q\omega_{i+1}^2 \tag{7.5}$$

Reviewing our derivations of the various eigenfunctions, we see that nothing needs alteration in this case. However, we may want to couple the two adjacent wells and adopt different expression for the eigenfunctions P^B_{ip} and $P^B_{i+1,q}$. More specifically, rather than using

$$R\left(\frac{\Omega_i}{(2\delta)^{1/2}}(x-M_i);\, p\frac{\omega_i^2}{\Omega_i^2}\right), \qquad L\left(\frac{\Omega_i}{(2\delta)^{1/2}}(x-M_i);\, q\frac{\omega_{i+1}^2}{\Omega_i^2}\right) \tag{7.6}$$

to terminate the eigenfunctions in the vicinity of the hill at $x=M_i$, we could use even and odd solutions of (4.3) with algebraic decay.

8. A SIMPLE EXAMPLE: THE QUADRATIC POTENTIAL

In this section, we illustrate the results previously obtained by considering a very simple and well-known example, namely a quadratic a quadratic potential and more specifically the symmetric quadratic potential

$$V=(x^2-1)^2 \tag{8.1}$$

It is obvious that this potential satisfies the requirements of the Introduction. Also, we can easily see that the minima are at

$$m_1 = -1$$
$$m_2 = 1 \tag{8.2}$$

The single hill is located at the origin, i.e.,

$$M_1 = 0 \tag{8.3}$$

Also

$$v_1 = v_2 = 0$$
$$V_1 = 1 \tag{8.4}$$

Finally, the bottom frequencies are

$$\omega_1 = 2\sqrt{2}$$
$$\omega_2 = 2\sqrt{2} \tag{8.5}$$

whereas the top frequency is

$$\Omega_1 = 2 \tag{8.6}$$

Clearly, since the bottom frequencies are identical, they are commensurate. Note also that

$$\omega_1^2 = 2\Omega_1^2 = \omega_2^2 \tag{8.7}$$

Therefore, we have a case of a top square frequency being commensurate with the square frequency of a nearby well.

Spectrum

In view of the symmetry of the potential, we expect all eigenfunctions to be either even or odd functions of x.

As usual, we have the eigensolution (6.1)

$$\sigma_0^B = 0$$
$$P_0^B = 1 \tag{8.8}$$

There is one other small eigenvalue. It has the form (6.16) since there are no "interior" wells for this potential

$$\sigma_{10}^{B} = \frac{1}{\sqrt{2}} \exp\left(-\frac{1}{\delta}\right)$$
$$P_{10}^{B} = \operatorname{erf}\left(\frac{\sqrt{2}}{\sqrt{\delta}} x\right) \tag{8.9}$$

The remaining eigenvalues are

$$\sigma = (\{8n\}_1^\infty) \cup (\{4n\}_1^\infty) \cup (\{8n\}_1^\infty) \tag{8.10}$$

Consider first the simple eigenvalues of class T. The corresponding eigensolutions are as given in (4.23), namely

$$\sigma_{1,2n+1}^{T} = 4(2n+1)$$
$$P_{1,2n+1}^{T} = H_{2n+1}\left(\frac{\sqrt{2}}{\sqrt{\delta}} x\right) \exp\left(-\frac{2}{\delta} x^2\right) \tag{8.11}$$

The remaining eigenvalues have, in principle, multiplicity 3 since they are common to the hill and to the two wells. Therefore, we ought to look for three sets of eigenfunctions associated with these eigenvalues. One set of eigensolution is simply the remaining T-class eigensolution, namely

$$\sigma_{1,2n}^{T} = 4(2n)$$
$$P_{1,2n}^{T} = H_{2n}\left(\frac{\sqrt{2}}{\sqrt{\delta}} x\right) \exp\left(-\frac{2}{\delta} x^2\right) \tag{8.12}$$

The other eigenfunctions are

$$P_{\varepsilon n}^{B} = \begin{cases} \left(\dfrac{16}{\delta}\right)^{n/2} \left(\dfrac{1-x}{2x^2}\right)^n (1+x)^n & \text{for} \quad x \in \mathscr{D}_1 \\ H_n\left(\dfrac{2}{\sqrt{\delta}}(1+x)\right) & \text{for} \quad x \in \mathscr{B}_1 \\ \left(\dfrac{16}{\delta}\right)^{n/2} \left(\dfrac{1-x}{2x^2}\right)^n (1+x)^n & \text{for} \quad x \in \mathscr{U}_1 \\ (-1)^n \left(\dfrac{4}{\delta}\right)^{n/2} \left(\dfrac{2}{\delta}\right)^n \dfrac{\Gamma(1/2)}{\Gamma(n+1/2)} M\left(n, \dfrac{1}{2}, -\dfrac{2x^2}{\delta}\right) & \text{for} \quad x \in \mathscr{T}_1 \\ \left(\dfrac{16}{\delta}\right)^{n/2} \left(\dfrac{1+x}{2x^2}\right)^n (1-x)^n & \text{for} \quad x \in \mathscr{D}_2 \\ H_n\left(\dfrac{2}{\sqrt{\delta}}(1-x)\right) & \text{for} \quad x \in \mathscr{B}_2 \\ \left(\dfrac{16}{\delta}\right)^{n/2} \left(\dfrac{1+x}{2x^2}\right)^n (1-x)^n & \text{for} \quad x \in \mathscr{D}_2 \end{cases} \tag{8.13}$$

It is tempting to write the odd analogue of the above set. However, as we saw in (4.21), $xM(n+3/2, 1/2, -2x^2/\delta)$ has exponential decay and cannot be hooked to the outer solutions. Thus, as in the discussion of the previous section, the commensurability of the square frequencies of neighboring hill and well reduces the multiplicity of certain eigensolutions.

9. CONCLUSIONS

We have considered the eigenvalue problem for the one dimensional Smoluchowski equation for poentials with N wells. The wells are assumed deep: the large depth of these wells provided us with the small parameter δ which we used for our asymptotic analysis. We found that the eigensolutions fall within two classes: (i) the top-te-hill and (ii) the bottom of the well.

The eigensolutions of the first class are the union of the eigensolutions for each hill of the potential treated as a *single* inverted parabolic hill. Consequently, the eigenvalues are integer multiples of the squares of the top-of-the-hill frequencies. The corresponding eigenfunctions are Hermite polynomials modulations of Gaussian functions centered around the various hill tops.

A similar picture holds for the second class of eigensolutions. Namely, these eigensolutions are the union of the eigensolutions for the various well bottoms treated as single parabolic wells. As a result, the eigenvalues are integral multiples of the squares of the bottom frequencies. The eigenfunctions are more complicated than those of the previous class, but they share many of the same features. In particular, they are confined to the various well bottoms, and have the aspect of a Hermite polynomial modulated by a Gaussian function.

This picture is altered if either the square of the frequencies of two nearby bottoms or a bottom and a top are commensurate. In this case, the eigenfunctions can span the two wells.

For most applications, the important eigensolutions are those associated with the small eigenvalues. We found that in addition to the zero eigenvalue corresponding to the steady state, there are $N-1$ small eigenvalues. These eigenvalues are of order $\exp(-1/\delta)$ and hence transcendentally small insofar as the asymptotic sequence $\{\delta^{n/2}\}_0^\infty$ is concerned. Hence, they cannot be captured by the same asymptotic expansions as that for the large eigenvalues.

Of course, the results presented here are not uniformly valid in that eigensolutions of very large order may require special consideration. In particular, it is not clear whether these results hold for $n \sim \delta^{-1/2}$. However, this point is academic at this stage.

In closing, we note that even though higher order eigenvalues carry information about the potential, this information is not easily extracted! In fact to leading order of in the asymptotic expansion we have been using, the "kinetics" eigensolutions associated with the N smallest eigenvalues contain as much information about the potential as the higher order eigenvalues! This suggests that the inverse problem for potential with deep wells is not worth contemplating.

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