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Transitions between metastable states in a solid double well

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The evolution of a spinlike variable in a double potential well that depends upon both angular coordinates is investigated as the system is subjected to both deterministic damping and stochastic noise linked by the fluctuation-dissipation relationship. A variational procedure appropriate for large barrier-to-noise ratio is adopted, and it can be seen that the resulting Euler-Lagrange equation introduces an angle-dependent field conjugate to the leading Fokker-Planck eigenfunction. In this way the spectral problem of the Fokker-Planck operator is approximated by two coupled first-order partial-differential equations, whose solutions allow the determination of the relaxing probability distribution and the equilibration current in almost all phase-space regions. A detailed application to the Lipkin model of many-body theory is presented.

I. INTRODUCTION

Physical descriptions of the decay of a metastable state or the thermally activated escape out of a single well, traditionally formulated in terms of transition-state theory [1], have undergone spectacular development since the statement of Kramers's problem [2] and the solutions encountered by Kramers himself for the underdamped and the overdamped regimes of one-dimensional Brownian motion. More recently, Matkowsky, Schuss, and Tier [3] presented an appropriate generalization of Kramers's transition rate, valid for any friction strength. Decaying metastable states appear in a variety of physical and physicochemical phenomena, such as molecular autoionization and dissociation, diffusion in solids, nuclear fission, and Josephson tunneling. Furthermore, the spectrum in cases where the damped system may remain bound in neighboring potential wells incorporates as well problems of optical bistability, aspects of chemical kinetics, response of logical cells, and dynamics through porous systems. In addition to well-known textbooks [4,5] and review papers [6,7] useful references and applications of Kramers's transition theory for bistable and multistable potentials can be found in Refs. [8–11]. In particular, the investigation of diffusion over a barrier in one-dimensional bistable potentials has become an active field, and a number of special applications that allow exact or quasiexact solutions are available [12–14] (see also Ref. [10] and references therein).

Somewhat less, although still significant attention has been paid to the generalization of Kramers's theory to n-dimensional multistable potential wells [15–23]. In two earlier works, Brown [24,25] elaborated Kramers's ideas for a system with a two-dimensional configuration space related to a spin orientation, and developed a framework appropriate to describe magnetic relaxation of single-domain particles (see also Ref. [26]). However, illustration of this approach has been restricted to a situation where the anisotropy energy and the initial spin distribution do not depend on the polar angle. This case reduces then to thermally activated diffusion over a one-dimensional barrier between two minima and can be inscribed within rate-equation theory [23,27]; a variational procedure allows one to reencounter Kramers's formula for the transition rate in the low-noise–high-barrier limit. The validity of the variational approach has been recently discussed by Dekker [11] and holds in the Smoluchowski, i.e., high friction, regime. Based on a similar reasoning, Landauer and Swanson [15] formulated escape theory in an n-dimensional double well by looking for an escape near the saddle in the energy surface [23], which should be a sensible approach insofar as the noise is additive [20]. In addition, a recent calculation of the mean transition time between metastable states in a one-dimensional well by Ryter and Meyer [28–30] which closely parallels Brown's estimate of the first eigenfunction of the Fokker-Planck (FP) operator above the equilibrium state in the low-noise regime, provides a characterization of the stochastic separatrix in phase space.

On the other hand, it has been recently shown that coherent-state mappings of quantum systems with spectrum-generating algebras provide a generous supply of multistable energy landscapes for several degrees of freedom [31]. In particular, quasispin and pseudospin systems corresponding to physical objects with SU(2) and SU(1,1) dynamical groups, and with quadratic Hamiltonians, are shown to exhibit structural instabilities and undergo nonthermodynamic phase transitions to a double-minimum-plus-double-maximum configuration [32–36] in a two-dimensional phase space. The SU(2) models, which are exceedingly popular in many-body theory, become especially interesting from the topological viewpoint, since their phase space is a compact manifold—the sphere, present as well in the description of spin relaxation [24,25]—and the potential landscape presents as well two saddle points. We then intend to formulate the dynamical problem of a quasispin variable J immersed in a thermal reservoir which yields both deterministic friction and stochastic noise, within the Langevin Fokker-Planck framework, and estimate the transition rate in the double well. The treatment employed here follows earlier approaches [15,24,25] however, the appearance of the leading FP eigenfunction in the large-barrier limit is given for every region of phase space where the relaxation current remains stationary. The role of the two saddle points is discussed, and the consequences of having the variety of Morse i saddles available in higher-dimensional systems [34,37] are also mentioned.

For this purpose, in Sec. II we set the framework for the description of the stochastic evolution of the quasispin variable on its phase space, and in Sec. III the variational approach [24,25] is adopted to establish a formula for the transition rate. The characteristics and estimate of the leading FP eigenfunction are discussed in Sec. IV and the illustration for the celebrated Lipkin-Meshkov-Glick model [38] is presented in Sec. V. The summary and conclusions are the subject of Sec. VI.

II. BROWNIAN MOTION OF THE QUASISPIN VARIABLE

As shown in Refs. [31–36], given a quadratic Hamiltonian in quasispin space $\mathbf{J}$,

$$\mathcal{H}(\mathbf{J})=\mathbf{\Omega}_0\cdot\mathbf{J}+\tfrac{1}{2}\alpha_{ij}J_iJ_j \ , \tag{2.1}$$

where $\mathbf{J}$ is the expectation value of the SU(2) algebra basis vector $\hat{\mathbf{J}}$ with respect to an SU(2) coherent state, the deterministic motion on the SU(2)/U(1) sphere is ruled by a nonlinear Euler-like or Bloch equation

$$\dot{\mathbf{J}}=\mathbf{\Omega}\times\mathbf{J} \ , \tag{2.2}$$

where

$$\mathbf{\Omega}\equiv\mathbf{\Omega}(\mathbf{J})=\nabla_{\mathbf{J}}\mathcal{H} \ . \tag{2.3}$$

It is well known [31–34] that the family of Hamiltonians (2.1) can be at most bistable in phase space. If the quasispin system is now immersed in a fluctuating heat bath, a phenomenological approach to the subsequent stochastic evolution is given by the pseudovectorial Langevin equation [24],

$$\dot{\mathbf{J}}=\mathbf{\Omega}'\times\mathbf{J} \ , \tag{2.4}$$

where the effective frequency $\mathbf{\Omega}'$ now contains a conservative, a dissipative, and a random contribution. We assume, as in Ref. [24],

$$\mathbf{\Omega}'=\mathbf{\Omega}-\gamma\mathbf{\Omega}\times\mathbf{J}+\boldsymbol{\omega}(t) \tag{2.5}$$

where γ is a dissipation parameter and $\boldsymbol{\omega}(t)$ a Gaussian fluctuating frequency with a white spectrum, i.e.,

$$\langle\boldsymbol{\omega}(t)\rangle=0 \ , \tag{2.6a}$$

$$\langle\omega_i(t)\omega_j(t')\rangle=2D_{ij}(t-t') \ . \tag{2.6b}$$

Furthermore, we will assume $D_{xx}=D_{yy}=D_\perp$, $D_{zz}=D_\parallel$, and $D_{ij}=0$ if $i\neq j$.

The FP equation for the distribution $P(\mathbf{J},t)$ can then be expressed in terms of the (anti-Hermitian) angular-momentum operator in quasispin space,

$$\mathbf{L}=\mathbf{J}\times\nabla_{\mathbf{J}} \ , \tag{2.7}$$

and acquires for the form [24,25]

$$\begin{aligned}\dot{P}(\mathbf{J},t)&=\mathbf{L}\cdot[\mathbf{\Omega}(\mathbf{J})P(\mathbf{J},t)]-\gamma\mathbf{J}\times\mathbf{L}\cdot[\mathbf{\Omega}(\mathbf{J})P(\mathbf{J},t)]\\&\quad+D_{ij}L_iL_jP(\mathbf{J},t)\\&\equiv\hat{D}(\mathbf{L})P(\mathbf{J},t) \ .\end{aligned} \tag{2.8}$$

Since the stochastic motion described by Eqs. (2.4) and (2.5) takes place on the sphere $\mathbf{J}\cdot\mathbf{J}=J^2=$const, the distribution function $P(\mathbf{J},t)$ in fact refers to the angular location (ϑ,φ) of the random quasispin vector. In what follows, we take the radius J equal to unity; it is straightforward to obtain Eq. (2.8) in terms of the angular variables. It reads

$$\begin{aligned}\dot{P}(\mathbf{J},t)&=\{P,\mathcal{H}\}+\frac{1}{\sin\vartheta}\frac{\partial}{\partial\vartheta}[\sin\vartheta(\gamma\mathcal{H}_\vartheta P+D_\perp P_\vartheta)]\\&\quad+\frac{1}{\sin^2\vartheta}\frac{\partial}{\partial\varphi}[\gamma\mathcal{H}_\varphi P+(D_\perp\cot^2\vartheta+D_\parallel)P_\varphi] \ ,\end{aligned} \tag{2.9}$$

where subscripts under $\mathcal{H}$ or P indicate partial differentiation with respect to the given variable. The curly Poisson-bracket symbol here means

$$\{\ ,\ \}=\frac{1}{\sin\vartheta}\left[\frac{\partial}{\partial\varphi}\frac{\partial}{\partial\vartheta}-\frac{\partial}{\partial\vartheta}\frac{\partial}{\partial\varphi}\right]=\nabla\times\nabla \ , \tag{2.10}$$

with ∇ the angular gradient operator,

$$\nabla=\left[\frac{1}{\sin\vartheta}\frac{\partial}{\partial\varphi},\frac{\partial}{\partial\vartheta}\right] . \tag{2.11}$$

It is clear that (2.8) is a continuity equation on the sphere, in other words,

$$\dot{P}(\mathbf{J},t)=-\nabla\cdot\mathbf{j} \ , \tag{2.12}$$

where the divergence operator only contributes the angular derivatives on the current density,

$$\mathbf{j}=(j_\varphi,j_\vartheta)=\mathbf{j}_{\rm rev}+\mathbf{j}_{\rm dis}+\mathbf{j}_{\rm dif} \ ; \tag{2.13}$$

the three terms on the right are the reversible, dissipative, and diffusive contributions,

$$\mathbf{j}_{\rm rev}=\mathbf{v}P=\left[-\mathcal{H}_\vartheta,\frac{1}{\sin\vartheta}\mathcal{H}_\varphi\right]P \ , \tag{2.14a}$$

$$\mathbf{j}_{\rm dis}=-\gamma\nabla\mathcal{H}P=-\gamma\left[\frac{1}{\sin\vartheta}\mathcal{H}_\varphi,\mathcal{H}_\vartheta\right]P \ , \tag{2.14b}$$

$$\mathbf{j}_{\rm dif}=\left[D_\parallel P_\vartheta,\frac{D_\perp\cot^2\vartheta+D_\parallel}{\sin\vartheta}P_\varphi\right] . \tag{2.14c}$$

The equilibrium distribution P^0 gives then rise to a divergenceless current $\mathbf{j}^0$. It is not trivial to write down the analytical form of $P^0(\mathbf{J})$ for anisotropic diffusion; however, if the isotropy condition $D_\perp=D_\parallel\equiv D$ is fulfilled, one can find a divergenceless reversible current $\mathbf{j}^0=\mathbf{j}_{\rm rev}$, and a distribution,

$$P^0(\mathbf{J})\approx\exp\left[-\frac{\gamma}{D}\mathcal{H}(\mathbf{J})\right] \tag{2.15}$$

which corresponds to a fluctuation-dissipation relationship

$$D=\gamma T \tag{2.16}$$

for temperature T given in energy units. Hereafter, we will restrict ourselves to the isotropic diffusion problem; the FP equation consequently reads

$$\dot{P}(\varphi,\theta,t)=-\mathbf{v}_T\cdot\nabla P+\gamma P\nabla^2\mathcal{H}+\mathcal{D}\nabla^2\mathcal{P} \ , \tag{2.17}$$

with the total velocity

$$\mathbf{v}_T=\mathbf{v}-\gamma\nabla\mathcal{H} \ , \tag{2.18}$$

III. VARIATIONAL APPROACH TO THE DECAY TOWARDS EQUILIBRIUM

Several approaches have been devised to solve the FP equation [4,39]. Among the various numerical techniques [39,40], it is tempting to expand the distribution into spherical harmonics and look for the solutions of the system of coupled equations for the expansion coefficients that originates in Eq. (2.17). However, such a method has proven to be useful, in the sense that rapid convergence is achieved, when the noise source is able to rapidly randomize an initial anisotropy in the spin population [24,41]. In this work, rather than investigating the highly diffusive regime, we will be concerned with the limit of large barrier-to-noise ratio, for which it has been already shown that the most convenient approach is the eigenfunction expansion [24].

Let us now consider the spectral problem of the FP operator $\hat{D}$ defined by (2.8) and (2.9) with the current j given in Eqs. (2.12)–(2.14). The eigenfunctions $F_n(p,q)$, namely, the solutions of the partial-differential equation

$$\hat{D}F_n=-\lambda_n F_n \ , \tag{3.1}$$

satisfy the orthonormality relationship [24,25],

$$\int d\omega \exp(\mathcal{H}/T)F_nF_m=\delta_{nm} \ , \tag{3.2}$$

where $d\omega=\sin\theta d\theta d\varphi$ is the elementary angular volume. Accordingly, one may write

$$\begin{aligned}\lambda_n&=\int d\omega\, e^{\mathcal{H}/T}F_n\nabla\cdot\mathbf{j}_n\\ &=\Lambda(F_n) \ .\end{aligned} \tag{3.3}$$

The evolving distribution $P(\varphi,\vartheta,t)$ may then be expanded as

$$P(\varphi,\vartheta,t)=A_0e^{-\mathcal{H}/T}+\sum A_n e^{-\lambda_n t}F_n(\varphi,\vartheta) \ . \tag{3.4}$$

It is evident that in the long-time scale, where the evolution is dominated by the probability flow among peaks of the nonequilibrium distribution, the decay rate towards equilibrium is governed by the smallest nonvanishing eigenvalue λ_1 (hereafter, $\lambda_1=\lambda$). We will then consider

$$P(\varphi,\vartheta,t)=e^{-\mathcal{H}/T}A_0+A_1F_1(\varphi,\vartheta)e^{-\lambda t} \ . \tag{3.5}$$

As stressed by Dekker [11], in any dissipation regime, Eq. (3.3) describes the exact eigenvalue in terms of the exact eigenfunction; it has been shown [11] that in the overdamped (Smoluchowski) regime, an appropriate upper bound for λ is given by Brown's ansatz, namely, by the minimum of the functional Λ in Eq. (3.3). If we adopt the reduced eigenfunctions $\Phi_n(\omega)=e^{\mathcal{H}/T}F_n(\omega)$, the action of the FP operator can be set as

$$\hat{D}(e^{-\mathcal{H}/T}\Phi)=-\nabla\cdot(e^{-\mathcal{H}/T}\mathbf{j}_\Phi) \ , \tag{3.6}$$

with the reduced current

$$\mathbf{j}_\Phi=\mathbf{v}\Phi-D\nabla\Phi \ , \tag{3.7}$$

which makes it evident that the effect of factorizing the equilibrium distribution away in the eigenfunction is the suppression of the dissipative current. Furthermore, the set $\{\phi_n\}$ can be shown to coincide with the eigenspectrum of the adjoint FP operator $\hat{D}^\dagger$.

Equation (3.3) is then

$$\begin{aligned}\Lambda(\Phi)&=\int d\omega\, \Phi\nabla\cdot(e^{-\mathcal{H}/T}\mathbf{j}_\Phi)\\ &=\int d\omega\, e^{-\mathcal{H}/T}\nabla\Phi\cdot\mathbf{j}_\Phi \ ,\end{aligned} \tag{3.8}$$

which is an actionlike expression,

$$\Lambda(\Phi)=\int d\omega\mathcal{L}[\Phi(\varphi,\vartheta)] \ , \tag{3.9}$$

with the Lagrangian

$$\begin{aligned}\mathcal{L}(\Phi(\varphi,\vartheta))&=-e^{-\mathcal{H}/T}\nabla\Phi\cdot j_\Phi\\ &=e^{-\mathcal{H}/T}[D(\nabla\Phi)^2-\tfrac{1}{2}\{\Phi^2,\mathcal{H}\}] \ .\end{aligned} \tag{3.10}$$

In addition, the general orthonormality relation (3.2) poses two restrictions on the potential Φ, namely, (a) orthogonality with respect to the equilibrium distribution,

$$Y_1=\int d\omega\, e^{-\mathcal{H}/T}\Phi(\varphi,\vartheta)=0 \ , \tag{3.11a}$$

and (b), normalization,

$$Y_z=\int d\omega\, e^{-\mathcal{H}/T}\Phi^2(\varphi,\vartheta)=1 \ . \tag{3.11b}$$

In order to extract an approximate expression for the decay rate λ in (3.5) within the range of validity of the variational prescription, we restrict ourselves to the strong-coupling limit where some interaction parameters α_{ij} in Eq. (2.1) are much larger than a typical unperturbed frequency component Ω_i^0. This condition gives rise to high maxima and deep minima in the energy surface, $\mathcal{H}(\mathbf{J})=\mathcal{H}(\varphi,\vartheta)$ for given modulus J; this is illustrated in Figs. 1 and 2 for the Lipkin model Hamiltonian [38] (which will be further discussed in Sec. V), for interaction-strength values $\chi=1.5$ and 10, respectively, for completeness, we show as well the level curves of these surfaces in Figs. 3 and 4, where the libration and rotation zones, together with the separatrices, are clearly displayed. The equilibrium distributions (2.15) are respectively shown in Figs. 5 and 6, where we can appreciate the concentration of probability density on the libration areas around the minima. Consequently, a steepest-descent approach that generalizes the well-known one proven to be appropriate for the one-dimensional case [24] can be employed as follows [15].

We first notice that the extremum of the functional (3.9) together with (3.10) may correspond to a function

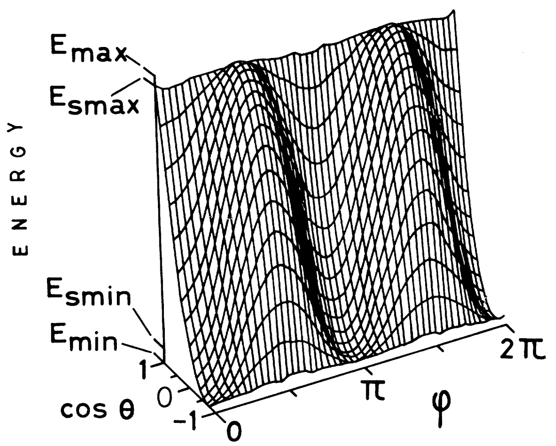

FIG. 1. The energy surface $\mathcal{H}(\varphi,\vartheta)$ associated to the Lipkin model for an interaction strength $\chi=1.5$.

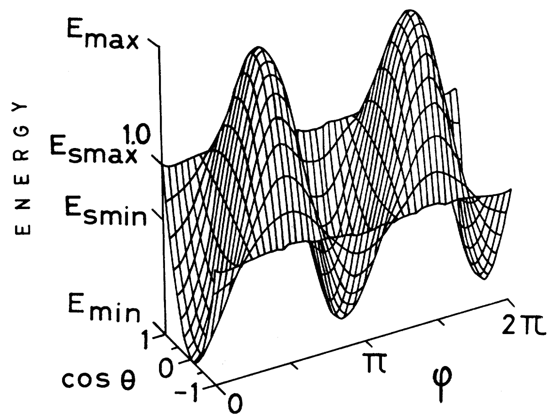

FIG. 2. Same as in Fig. 1 for an interaction strength $\varphi=10$.

$\Phi(\varphi,\vartheta)$ that remains approximately constant in those phase-space domains where the exponential is large, and that is allowed to vary only near the ridge through the double maximum and the double saddle. We then look for a field $\Phi(\varphi,\vartheta)$ such that

$$\Phi(\varphi,\vartheta q)=\begin{cases}\phi(\varphi,\vartheta) & \text{if } (\varphi,\vartheta)\notin\mu_\alpha\\ \Phi_\alpha=\text{const} & \text{if } (\varphi,\vartheta)\in\mu_\alpha\end{cases} \tag{3.12}$$

where μ_α, $\alpha=1,2,\ldots$ are conveniently chosen regions surrounding the minima. Since the integrable phase flow of the Hamiltonian (2.1) possesses well-defined separatrices between librational and rotational trajectories (cf. Figs. 1–6, or Refs. [31–35] and those cited therein) we shall consider μ_α to be some as yet unspecified inner region to the separatrix Σ_α around the energy minimum $\mathbf{J}_\alpha^{\min}$. In a similar fashion, we may define regions ν_α around the maxima $\mathbf{J}_\alpha^{\max}$.

It is clear that the most important contributions to the integrals Y_k correspond to regions μ_α. Accordingly, we set

$$Y_k\approx\sum_\alpha\Phi_\alpha^k\int_{\mu_\alpha}d\omega\, e^{-\mathcal{H}/T} \tag{3.13}$$

where the summation involves all minima. Each term in (3.13) can now be evaluated expanding the Hamiltonian up to second order and performing a two-dimensional Gaussian integration, giving

$$\begin{aligned}Y_\alpha&=\int_{\mu_\alpha}d\omega\, e^{-\mathcal{H}/T}\\ &=\frac{2\pi T}{(\Delta_\alpha)^{1/2}}e^{-\mathcal{H}_\alpha^{\min}/T},\end{aligned} \tag{3.14}$$

with Δ_α being the Hessian of $\mathcal{H}(\varphi,\cos\vartheta)$ computed at $\mathbf{J}_\alpha^{\min}$. Equations (3.11) then establish two relationships between the constants Φ_α, namely,

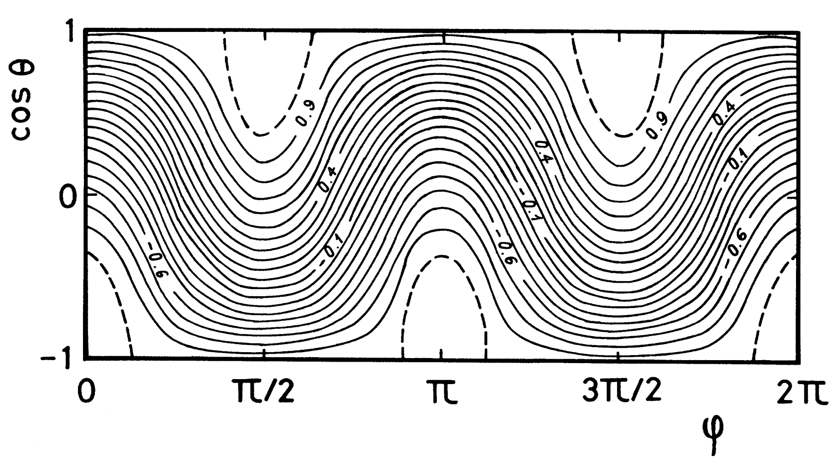

FIG. 3. The level curves of the energy surface in Fig. 1, where the dashed lines denote the separations between librational orbits surrounding extrema and rotations of the conservative flow.

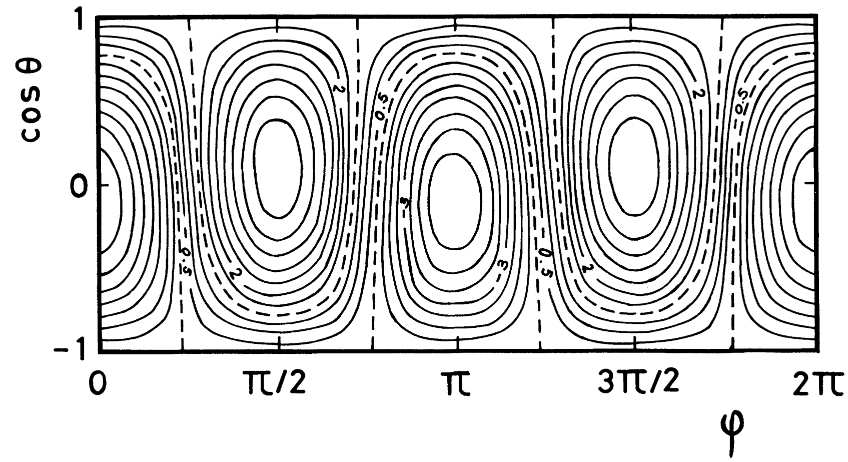

FIG. 4. Same as Fig. 3 for the energy surface in Fig. 2.

$$\sum_\alpha \Phi_\alpha \frac{e^{-\mathcal{H}_\alpha^{\min}/T}}{(\Delta_\alpha)^{1/2}}=0 \,, \tag{3.15a}$$

$$\sum_\alpha \frac{\Phi_\alpha^2 e^{-\mathcal{H}_\alpha^{\min}/T}}{(\Delta_\alpha)^{1/2}}=\frac{1}{2\pi T} \,. \tag{3.15b}$$

The system of Eqs. (3.15) can be solved, giving the constant potentials in the minima regions μ_α as

$$\Phi_1=-\left[\Delta_1\frac{e^{-(\mathcal{H}_1^{\min}-\mathcal{H}_2^{\min})/T}}{2\pi T\Delta}\right]^{1/2} , \tag{3.16a}$$

$$\Phi_2=\left[\Delta_2\frac{e^{(\mathcal{H}_1^{\min}-\mathcal{H}_2^{\max})/T}}{2\pi T\Delta}\right]^{1/2} \tag{3.16b}$$

with

$$\Delta=(\Delta_1)^{1/2}e^{-\mathcal{H}_2^{\min}/T}+(\Delta_2)^{1/2}e^{-\mathcal{H}_1^{\min}/T} \,. \tag{3.17}$$

One additionally realizes that if both minima are degenerate, Eq. (3.11a) is automatically fulfilled for $-\Phi_1=\Phi_2\equiv\Phi_0$, with

$$\Phi_0=\left[\frac{(\Delta_0)^{1/2}}{4\pi T}e^{\mathcal{H}_0^{\min}/T}\right]^{1/2} \tag{3.18}$$

being Δ_0, $\mathcal{H}_0^{\min}$ the common values of Hessian and energy at either fixed point.

The problem to be solved is now the determination of the restricted field $\phi(\varphi,\vartheta)$ defined in (3.12) in the rotational areas. We defer the discussion over this point until the next section, and here just remark that regardless of the explicit form of the eigenfunction $\phi(\varphi,\vartheta)$, the transition rate λ which corresponds to the extremum of the functional $\Lambda(\Phi)$ can be estimated by means of the follow-

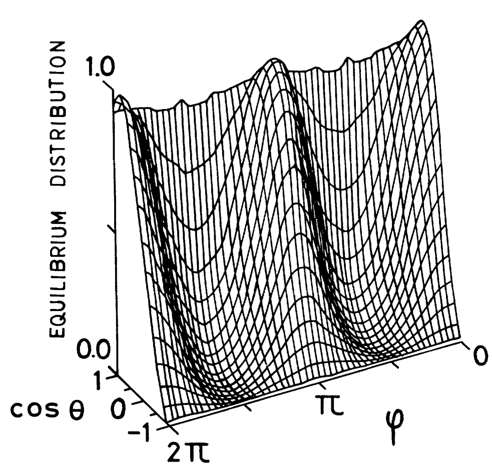

FIG. 5. The equilibrium distribution for the energy surface in Fig. 1. The temperature is set equal to unity.

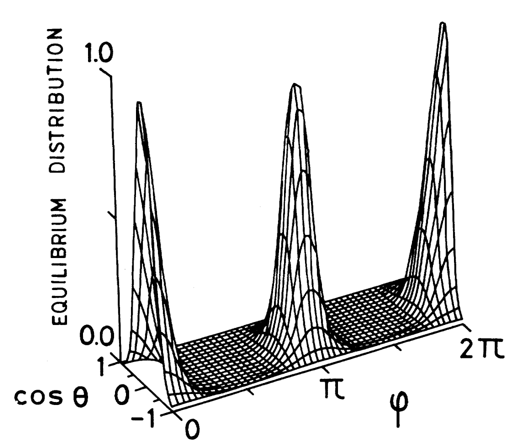

FIG. 6. The equilibrium distribution for the energy surface in Fig. 2 and $T=1$.

ing arguments [15,24]. Inspection of the conservative phase flow and the shape of the equilibrium distribution suggests that for low deviations from equilibrium, the relaxational current takes place mostly near the saddle points. One then tentatively sets

$$\lambda = \sum_{\alpha} \lambda_\alpha , \tag{3.19}$$

with the summation including every saddle, and with

$$\lambda_\alpha = \int_{\sigma_\alpha} d\omega \mathcal{L}(\nabla\phi) \tag{3.20}$$

with σ_α some region surrounding the saddle s_α.

Now let ξ and η be the eigencoordinates at s_α, i.e.,

$$\mathcal{H} \cong \mathcal{H}_\alpha^s - \tfrac{1}{2}\mathcal{H}_{\xi\xi}(\xi-\xi_\alpha)^2 + \tfrac{1}{2}\mathcal{H}_{\eta\eta}(\eta-\eta_\alpha)^2 . \tag{3.21}$$

With $\mathbf{v} = \nabla\mathcal{H} = \mathbf{0}$ at either saddle, Eq. (3.20) is actually

$$\lambda_\alpha \simeq e^{-\mathcal{H}_\alpha/T} \int_{\sigma_\alpha} d\omega \exp\left[\frac{\mathcal{H}_{\xi\xi}(\xi-\xi_\alpha)^2 - \mathcal{H}_{\eta\eta}(\eta-\eta_\alpha)^2]}{2T}\right] D(\nabla\phi)^2 . \tag{3.22}$$

We now assume that ϕ varies only in the descent direction ξ with a ξ-independent current density C [15,24]

$$C = e^{-\mathcal{H}/T} D \frac{\partial\phi}{\partial\xi} \tag{3.23}$$

and integrate ϕ over ξ across the saddle, which means switching between the minimum regions μ_α. We then get

$$C = \Delta\phi D \left[\frac{\mathcal{H}_{\xi\xi}}{2\pi T}\right]^{1/2} \exp\left[\frac{-\mathcal{H}_\alpha^s - \frac{1}{2}\mathcal{H}_{\eta\eta}(\eta-\eta_\alpha)^2}{T}\right] \tag{3.24}$$

and after replacement of $\partial\phi/\partial\xi$ in (3.22) we obtain

$$\lambda_\alpha \cong e^{(-\mathcal{H}_\alpha^s/T)} \left[\frac{\mathcal{H}_{\xi\xi}}{\mathcal{H}_{\eta\eta}}\right]^{1/2} D(\Delta\phi)^2 . \tag{3.25}$$

The expression for $\Delta\phi = \phi_2 - \phi_1$ may be recovered from Eqs. (3.16). We here quote just the result for symmetric minima, with $\Delta\phi = 2\phi_0$ as given by (3.18); in this case,

$$\lambda_\alpha \cong \frac{D}{\pi T} \left[\Delta_0 \frac{\mathcal{H}_{\xi\xi}}{\mathcal{H}_{\eta\eta}}\right]^{1/2} e^{(-\mathcal{H}_\alpha^s - \mathcal{H}_0^{\min})/T} , \tag{3.26}$$

which is equivalent to the expression obtained by Landauer and Swanson using rate equations [15]. Consequently, the lifetime of the nonequilibrium mesoscopic state is the harmonic mean of the individual lifetimes, or, for twofold symmetric minima,

$$\tau \approx \frac{1}{\sum_\alpha e^{-(\mathcal{H}_\alpha^s - \mathcal{H}_0^{\min})/T}} , \tag{3.27}$$

indicating that the saddle lying closest to the double minimum controls overall relaxation and establishes the equilibration time scale.

The relationship between this decay and the escape rate for a two-dimensional double well can be established on the same arguments as for a one-dimensional system [24–27], as indicated in Appendix A. Furthermore, in Appendix B we derive formulas equivalent to (3.25) and (3.26) for the degenerate saddle case, together with the corresponding approximate expressions for the eigenfunction ϕ in the near-saddle region.

IV. ESTIMATE OF THE REDUCED CURRENT IN THE FAR-SADDLE REGIONS

Let us now turn back to the determination of the fields $\phi(\varphi,\vartheta)$ in those angular domains that exclude the double well and the saddle or, equivalently, to the estimate of the reduced current $\mathbf{j}_\phi$ [Eq. (3.7)]. Considering the Lagrangian (3.10) and the variations $\delta\Phi_i = \partial_i(\delta\Phi)$, for $i=\varphi$ or ϑ, and $\Phi=\phi$, the functional derivative $\delta\Lambda/\delta\Phi=0$ gives rise to a divergenceless current in the above regions,

$$\nabla\cdot(e^{-\mathcal{H}/T}\mathbf{j}_\Phi) = 0 . \tag{4.1}$$

This field equation indicates that the current $e^{-\mathcal{H}/T}\mathbf{j}_\Phi$ can be derived out of a scalar potential $\Psi(\varphi,\vartheta)$, such that

$$e^{-\mathcal{H}/T}\mathbf{j}_\Phi = \nabla\times\Psi , \tag{4,2}$$

with the angular part of the rotor operator and with $\Psi = \Psi_J^J$. Equation (4.2) replaces then the assumption of a stationary current adopted in the one-dimensional case [2,24]; it permits one to write the Lagrangian (3.10) as the Lie product,

$$\mathcal{L} = \{\Psi,\Phi\} , \tag{4.3a}$$

or

$$\mathcal{L} = -\nabla\phi\cdot\nabla\times\Psi = \nabla\Psi\cdot\nabla\times\phi = \nabla\Psi\times\nabla\phi . \tag{4.3b}$$

The antisymmetric role of ϕ and Ψ suggests a plausibility argument for further characterization of either field. We will then assume that $\Psi(\varphi,\vartheta)$ is itself a solution of the variational problem for a flow with conservative generator $-\mathcal{H}(\varphi,\vartheta)$; in this context, we may regard Φ and Ψ as conjugate fields with the respective currents $e^{-\mathcal{H}/T}j_\Phi = \nabla\times\Psi$ and $e^{\mathcal{H}/T}j_\Psi = \nabla\times\Phi$. To determine either field Φ or Ψ we may then resort to a numerical procedure to solve Eq. (4.1), subject to boundary conditions on the edges of both minimum areas; several methods are available [40]. However, as the numerical processing of the approximate field equation is undertaken, one is led to the conclusion that the difficulties involved are not largely lower than those of solving the exact eigenvalue problem (3.1). Furthermore, no advantage can be taken from the fact that the FP operator $\hat{D}$ is a quadratic function of the angular-momentum operator $\mathbf{L}$; if the motion were purely diffusive, $\hat{D}_{\text{diff}}=D_{ij}L_iL_j$ would commute with L^2 and could be diagonalized within any irreducible representation of the rotation group [42]. This is not the present case, since one can verify by direct computation that neither the reversible nor the dissipative currents are rotationally invariant. It becomes evident that such a lack of symmetry is due to the presence of the coordinate-dependent frequency $\mathbf{\Omega}(\mathbf{J})=\nabla_{\mathbf{J}}\mathcal{H}$ in both currents.

In what follows, we will derive a simpler frame within which the second-order partial derivative equation (4.1) reduces to quadratures along orbits of the conservative flow. In order to do this, let us express the definition of the pair of conjugate currents and their related fields as

$$\mathbf{j}_\Phi=\mathbf{v}\phi-D\nabla\phi=e^{\mathcal{H}/T}\nabla\times\boldsymbol{\psi}\ , \tag{4.4a}$$

$$j_\Psi=-\mathbf{v}\Psi-D\nabla\Psi=e^{-\mathcal{H}/T}\nabla\times\boldsymbol{\phi}\ . \tag{4.4b}$$

These vector equations constitute a linear four-dimensional system with unknowns ϕ, Ψ, and their respective derivatives. One may then eliminate three out of the six unknowns and obtain individual first-order partial-differential equations for each field. As we eliminate ψ, ψ_φ, and ψ_ϑ we get

$$\{\mathcal{H},\phi\}=\frac{Dv^2}{D^2+1}\phi\ , \tag{4.5a}$$

with $v=|v|=|\nabla\mathcal{H}|$, and under elimination of ϕ, ϕ_φ, and ϕ_ϑ,

$$\{\psi,\mathcal{H}\}=\frac{Dv^2}{D^2+1}\psi \tag{4.5b}$$

in every region where the velocity vector is nonvanishing, i.e., Eqs. (4.5) are meaningless at the critical points, which are anyway not present in the rotation area.

Now elementary treatments of first-order partial-differential equations (PDE's) lead to the characteristic system for (4.5a),

$$\frac{d\phi}{d\varphi}=-\frac{\mathcal{H}_\varphi}{\mathcal{H}_\vartheta}\ , \tag{4.6a}$$

$$\frac{1}{\phi}\frac{d\phi}{d\vartheta}=\frac{D}{D^2+1}\frac{\sin\vartheta v^2}{\mathcal{H}_\varphi} \tag{4.6b}$$

if $\mathcal{H}_\varphi\neq0$, or

$$\frac{1}{\phi}\frac{d\phi}{d\vartheta}=-\frac{D}{D^2+1}\frac{\sin\vartheta v^2}{\mathcal{H}_\vartheta} \tag{4.6c}$$

if $\mathcal{H}_\vartheta\neq0$. The first equation here corresponds to the conservative orbits $\mathcal{H}=E$; the second one (4.6b) or (4.6c) is then the total derivative of the field with respect to an angle along each given orbit. Straightforward integration of (4.6b) then yields

$$\phi(E,\vartheta)=f(E)\exp\left[\frac{D}{D^2+1}\times\int_{\vartheta_0}^{\vartheta}d\vartheta\left[\frac{\mathcal{H}_\varphi}{\sin\vartheta}+\mathcal{H}_\vartheta^2\frac{\sin\vartheta}{\mathcal{H}_\varphi}\right]_{\vartheta,E}\right] \tag{4.7a}$$

on an orbit with energy E, with an amplitude $\phi_0(E)$ to be specified upon setting the explicit expression of $\phi(\varphi,\vartheta)$ on a given curve $\vartheta=\Gamma(\varphi)$. The solution of (4.6) is then the function $\phi(\mathcal{H}(\varphi,\vartheta),\vartheta)$; if one chooses (4.6c), one gets, instead,

$$\phi(E,\vartheta)=g(E)\exp\left[-\frac{D}{D^2+1}\int_{\varphi_0}^{\varphi}d\varphi\left[(\sin\vartheta)\mathcal{H}_\vartheta+\frac{\mathcal{H}_\varphi^2}{(\sin\vartheta)\mathcal{H}_\vartheta}\right]_{\varphi,E}\right] \tag{4.7b}$$

which is a function $\phi(\varphi,\mathcal{H}(\varphi,\vartheta))$. It should be noticed that since $\mathcal{H}_\varphi$ and $\mathcal{H}_\vartheta$ simultaneously vanish only at the critical points, Eqs. (4.7a) and (4.7b) are the appropriate expressions, respectively, for the field in the rotation areas where $\mathcal{H}_\vartheta=0$ and where $\mathcal{H}_\varphi=0$. In a similar fashion one may integrate Ψ from (4.5b).

The remaining step is to compute the field gradients appearing in the currents (4.4). One then notices that the four involved partial derivatives can indeed be written, solving the system (4.4), as a rectangular matrix equation,

$$\begin{bmatrix}\dfrac{\phi_\varphi}{\sin\theta}\\ \phi_\vartheta\\ \dfrac{\psi_\varphi}{\sin\vartheta}\\ \psi_\vartheta\end{bmatrix}=\frac{1}{D^2+1}\begin{bmatrix}-D\mathcal{H}_\vartheta & -e^{\mathcal{H}/T}\dfrac{\mathcal{H}_\varphi}{\sin\vartheta}\\ D\dfrac{\mathcal{H}_\varphi}{\sin\vartheta} & -e^{\mathcal{H}/T}\mathcal{H}_\vartheta\\ e^{-\mathcal{H}/T}\dfrac{\mathcal{H}_\varphi}{\sin\vartheta} & D\mathcal{H}_\vartheta\\ e^{-\mathcal{H}/T}\mathcal{H}_\vartheta & -D\dfrac{\mathcal{H}_\vartheta}{\sin\vartheta}\end{bmatrix}\begin{bmatrix}\phi\\ \psi\end{bmatrix}\ . \tag{4.8}$$

In view of these relationships, the extremal Lagrangian can be written in a rather symmetric fashion as

$$\mathcal{L}(\phi,\Psi)=\frac{Dv^2}{D^2+1}(e^{-\mathcal{H}/T}\phi^2+e^{\mathcal{H}/T}\psi^2)\ . \tag{4.9}$$

Furthermore, we may construct the reduced current lines which correspond to the integral curves of

$$\frac{d\vartheta}{d\varphi}=\frac{j_\vartheta}{j_\varphi}=\frac{(\mathcal{H}_\varphi/\sin\vartheta)\phi-D\phi_\vartheta}{-\mathcal{H}_\vartheta\phi-D(\phi_\varphi/\sin\vartheta)}\ , \tag{4.10}$$

i.e.,

$$\frac{d\vartheta}{d\varphi}=\frac{(\mathcal{H}_\varphi/\sin\vartheta)\phi+De^{\mathcal{H}/T}\mathcal{H}_\vartheta\psi}{-\mathcal{H}_\vartheta\phi+De^{\mathcal{H}/T}(\mathcal{H}_\varphi/\sin\vartheta)\psi}\ . \tag{4.11}$$

A similar equation can be derived for the $\mathbf{j}_\Psi$ current which corresponds to a change of sign in the velocity.

V. APPLICATION TO DOUBLY SYMMETRIC MINIMA

In order to illustrate the construction here proposed we adopt a specific phase portrait, namely, the one corresponding to the semiclassical Lipkin Hamiltonian [38],

$$\mathcal{H}(\varphi,\vartheta)=\cos\vartheta-\frac{\chi}{2}\sin^2\vartheta\cos2\varphi \;, \tag{5.1}$$

with a positive interaction strength $\chi>1$. As is well known, this energy surface on (φ,ϑ) space exhibits two symmetric minima on the southern parallel $\cos\vartheta=-1/\chi$, respectively located on the meridians $\varphi=0$ and $\varphi=\pi$, together with two maxima at $\cos\vartheta=1/\chi$ in the northern hemisphere with $\varphi=\pi/2$ and $\varphi=3\pi/2$ (cf. Figs. 1–6). In this model, the energy values at the extrema are

$$\mathcal{H}_{1,2}^{\min}=-\mathcal{H}_{1,2}^{\max}=-\tfrac{1}{2}\left[\chi+\frac{1}{\chi}\right] . \tag{5.2}$$

Let us now indicate the application of the formalism developed in the preceding section to fully determine the field $\phi(\varphi,\vartheta)$. We first examine expressions (4.7) and the velocity components,

$$-v_\varphi=\mathcal{H}_\vartheta=-\sin\vartheta(1+\chi\cos\vartheta\cos2\varphi) \;, \tag{5.3a}$$

$$v_\vartheta=\frac{\mathcal{H}_\varphi}{\sin\vartheta}=\chi\sin\vartheta\sin2\varphi \;, \tag{5.3b}$$

We immediately notice that while $\mathcal{H}_\vartheta$ vanishes only at the critical points and on the curve $\cos\theta=-1/(\chi\cos2\varphi)$, whose arcs are contained in the librational regions as indicated in Fig. 7, $\mathcal{H}_\varphi$ is zero on the meridians $\varphi=0$, $\pi/2$, and $3\pi/2$. It becomes clear that the appropriate field description corresponds to Eq. (4.7b) which is nonsingular in the rotation area. To calculate $g(E)$, we select a curve and an expression for $\phi(\varphi,\vartheta)$ on it which satisfies most requirements for the leading eigenfunction, namely, those given in Eqs. (3.12) and (B13). A possible choice among many others, which has the advantage of simplicity, is depicted in Fig. 8 and corresponds to a function $\phi(\varphi,\vartheta_0)$ on a parallel $\vartheta_0=$const near the saddle, as follows:

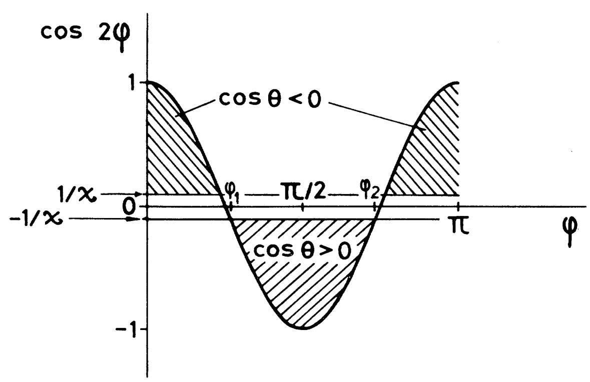

FIG. 7. The φ intervals where $\cos\vartheta=-1/(\chi\cos2\varphi)$ is a meaningful curve. If $\cos2\varphi>0$, ϑ corresponds to the southern hemisphere and the curve lies inside the librational area at the minima. If $\cos2\varphi<0$, the corresponding arc lies within the maximum region.

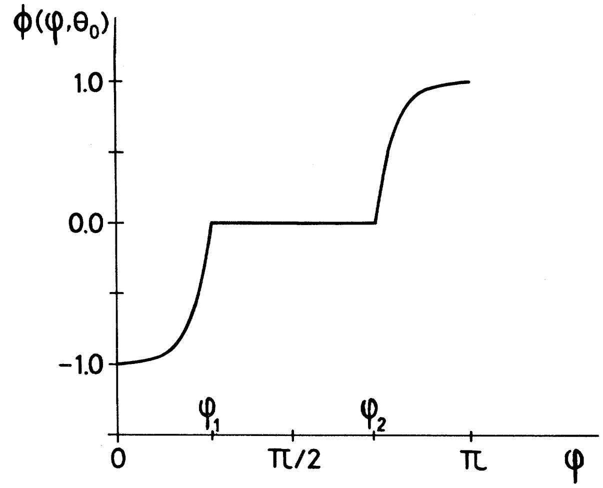

FIG. 8. The selected matching function $\phi(\varphi,\vartheta_0)$ described in Eq. (5.4) on an arbitrary parallel $\vartheta_0=$const. The parameter a has the value 2π.

$$\phi(\varphi,\vartheta)=\begin{cases}\phi_0\dfrac{1-e^{-a(\varphi-\varphi_2)}}{1-e^{-a(\pi-\varphi_2)}} & \text{if } \varphi_2\le\varphi\le\pi\\ 0 \;\text{ if } \varphi_1<\varphi<\varphi_2 & \\ -\phi_0\dfrac{1-e^{a(\varphi-\varphi_1)}}{1-e^{-a\varphi_1}} & \text{if } 0\le\varphi\le\varphi_1 \;.\end{cases} \tag{5.4}$$

Furthermore, on the given parallel we have, according to (5.1),

$$\varphi\equiv\varphi(E)=\tfrac{1}{2}\cos^{-1}\left[\frac{2}{\chi}\frac{\cos\vartheta_0-E}{\sin\vartheta_0}\right] . \tag{5.5}$$

Accordingly, one can match Eq. (5.4) to (4.7b) and extract the amplitude $g(E)$ as

$$g(E)=\phi(\varphi(E),\vartheta_0)\exp\left[-\int_0^{\varphi(E)}d\varphi' h(\varphi',E)\right] \tag{5.6}$$

where $h(\varphi',E)$ is the integrand in (4.7b).

Finally we establish the form of the transition rate λ as indicated in Sec. III and Appendix B, since this is the case where one coefficient, actually $\mathcal{H}_{\varphi\varphi}$, vanishes at the saddle. The proper integration over the angular domain thus gives, according to Eq. (B6),

$$\lambda\simeq\frac{D}{T}\left[\frac{2\pi\Delta_0\chi}{T}\right]^{1/2}e^{-(\chi-1)^2/2\chi T} \;, \tag{5.7}$$

with

$$\Delta_0=2(\chi^2-1) \;. \tag{5.8}$$

For very large barrier-to-noise ratio $r=\chi/T\gg1$, the transition rate is then

$$\lambda\cong2\pi^{1/2}Dr^{3/2}e^{-r/2} \;, \tag{5.9}$$

which exhibits the same temperature dependence as that obtained in the one-dimensional spin relaxation problem [24,25].

VI. SUMMARY AND CONCLUSIONS

The present paper has been devoted to developing an extension of Kramers's theory of transitions between states in a double well to those situations where the potential energy landscape is bivariate and exhibits double maxima and double saddle points. This is indeed the case of the quasispin models of atomic and nuclear physics [31–36], in addition to the problem of spin relaxation for single domain particles in a thermally fluctuating environment [24]. The procedure here adopted follows closely previous advances in the field [15,24], however, beyond the already established derivation of Kramers's transition probability by means of rate equations and/or variations near the saddle point, we set solvable equations for the first nonequilibrium FP eigenfunction in the rotational region of the phase portrait. The celebrated Lipkin model [39] provides an adequate framework for specializing the general ideas and working out the particular details of the present approach.

Immediate applications of the arguments and formalism here exposed concern potential shapes with asymmetric double minima [32–34], on both compact and noncompact manifolds [35,36] for which some particular realizations step on the field of collective many-body dynamics [31]. An extension of the whole theory should be developed as one intends to estimate transition rates for higher-dimensional systems like those of the SU(n) type [31]. In such a case one faces a potential landscape on an m-dimensional manifold, $m>2$, where critical points of the conservative flow are Morse i saddles [34,37]. In other words, between maxima and minima one may encounter a wide variety of partial barriers with more than one descent direction, and it is not obvious where the preferred escape should run. One may then formulate the general hypothesis that the lowest $|E_s-E_{\min}|$ barrier among every i saddle and every minimum ought to be selected by the escaping probability density; it is then of interest to examine the possible appearance of competing paths and the temperature dependence of each partial contribution to the transition rate, since any additional Gaussian integration along a descending direction incorporates a factor $T^{1/2}$. Forthcoming results along these lines will be presented elsewhere.

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APPENDIX A

In the asymptotic regime under consideration, smoothing of the probability density is governed by the flow among its time-dependent peaks, located near the minima. Quantitatively speaking, the population balance can be described in the standard manner as follows: Let

$$P_\alpha(t)=\int_{\mu_\alpha} d\omega\, P(\varphi,\vartheta,t) \tag{A1}$$

be the total probability of finding the Brownian quasispin in the librational area corresponding to minimum α. We assume expression (3.5) for $P(\varphi,\vartheta,t)$; thus using (3.14) we obtain

$$P_\alpha(t)=\frac{2\pi T}{(\Delta_\alpha)^{1/2}}(A_0+A_1\Phi_\alpha e^{-\lambda t})e^{-\mathcal{H}_\alpha^{\min}/T}\ , \tag{A2a}$$

$$\dot P_\alpha(t)=-\frac{2\pi T}{(\Delta_\alpha)^{1/2}}\lambda A_1\Phi_\alpha e^{-\mathcal{H}_\alpha^{\min}/T}e^{-\lambda t}\ . \tag{A2b}$$

According to Eqs. (3.16),

$$\dot P_1(t)=-\dot P_2(t)\ , \tag{A3}$$

i.e., $P_1+P_2=$const. Furthermore,

$$P_1+P_2=2\pi T\frac{\Delta}{(\Delta_1\Delta_2)^{1/2}}A_0\ , \tag{A4a}$$

$$P_1-P_2=2\pi T\frac{\delta}{(\Delta_1\Delta_2)^{1/2}}A_0 +2\left[\frac{2\pi T}{\Delta}e^{-(\mathcal{H}_1^{\min}+\mathcal{H}_2^{\min})/T}\right]^{1/2}A_1e^{-\lambda t} \tag{A4b}$$

with Δ given by (3.17) and

$$\delta=(\Delta_1)^{1/2}e^{-\mathcal{H}_2^{\min}/T}-(\Delta_2)^{1/2}e^{-\mathcal{H}_1^{\min}/T}\ . \tag{A5}$$

It is now straightforward, after elimination of A_0 and A_1 from (A4), to obtain the balance equation

$$\dot P_1=-\dot P_2=-\nu_1P_1+\nu_2P_2 \tag{A6}$$

with

$$\nu_\alpha=\lambda\frac{(\Delta_\beta)^{1/2}}{\Delta}e^{-\mathcal{H}_\alpha^{\min}/T}\ . \tag{A7}$$

Here β is the complementary label with respect to α. It then becomes clear that the escape rate, in other words, the nonzero eigenvalue of the system (A6) is

$$\nu_1+\nu_z=\lambda \tag{A8}$$

and that in the case of symmetric minima, one obtains

$$\nu_1=\nu_2=\frac{\lambda}{2} =\lambda_1=\lambda_2\ . \tag{A9}$$

APPENDIX B

It may happen that the quadratic form $d^2\mathcal{H}$ is degenerate at the saddle point, i.e., either $\mathcal{H}_{\xi\xi}$ or $\mathcal{H}_{\eta\eta}$ vanish together with $\mathcal{H}_{\xi\eta}$. Let us consider each of these possibilities.

If $\mathcal{H}_{\xi\xi}=0$, we have

$$\mathcal{H}\cong\mathcal{H}_\alpha^s+\tfrac{1}{2}\mathcal{H}_{\eta\eta}(\eta-\eta_\alpha)^2 \tag{B1}$$

in the neighborhood of s_α. The approximate partial eigenvalue then reads [cf. Eq. (3.22)]

$$\lambda_\alpha \cong e^{-\mathcal{H}_\alpha^s/T}\int_{\sigma_\alpha} d\omega\, e^{-\mathcal{H}_{\eta\eta}(\eta-\eta_\alpha)^2/2T} D(\nabla\phi)^2$$
$$\cong e^{-\mathcal{H}_\alpha^s/T}\Delta\xi_m \int_{\eta_\alpha}^{\eta} d\eta\, e^{-\mathcal{H}_{\eta\eta}(\eta-\eta_\alpha)^2/2T} D(\nabla\phi)^2 \qquad (B2)$$

where $\Delta\xi_m$ is the distance between minima across the descent axis. On the other hand, in order to calculate the field gradient, we proceed as in Sec. III. The current density C is computed from (3.23), considering $\partial\phi/\partial\xi = Ce^{-\mathcal{H}/T}/D$, with $\mathcal{H}$ given by (B1), and integrating across the saddle to obtain $\Delta\phi$. This gives

$$C \cong D\frac{\Delta\phi}{\Delta\xi_m} e^{-[\mathcal{H}_\alpha^s + \mathcal{H}_{\eta\eta}(\eta-\eta_\alpha)^2/2]T} \qquad (B3)$$

and consequently,

$$\frac{\partial\phi}{\partial\xi} \cong \frac{\Delta\phi}{\Delta\xi_m} . \qquad (B4)$$

Equation (B2) then yields

$$\lambda_\alpha \cong D\frac{(\Delta\phi)^2}{\Delta\xi_m}\left[\frac{2\pi T}{\mathcal{H}_{\eta\eta}}\right]^{1/2} e^{-\mathcal{H}_\alpha^s/T} \qquad (B5)$$

which, for symmetric minima, is

$$\lambda_\alpha \simeq \frac{D}{D\xi_m}\left[\frac{2\Delta_0}{\pi T\mathcal{H}_{\eta\eta}}\right]^{1/2} e^{-(\mathcal{H}_\alpha^s - \mathcal{H}_0^{\min})/T} . \qquad (B6)$$

If $\mathcal{H}_{\eta\eta}=0$, then

$$\mathcal{H} \simeq \mathcal{H}_\alpha^s - \tfrac{1}{2}\mathcal{H}_{\xi\xi}(\xi-\xi_\alpha)^2 . \qquad (B7)$$

The partial eigenvalue is now estimated as

$$\lambda_\alpha \cong e^{-\mathcal{H}_\alpha^s/T}\int_{\sigma_\alpha} d\omega\, e^{\mathcal{H}_{\xi\xi}(\xi-\xi_\alpha)^2/2T} D(\nabla\phi)^2$$
$$\cong e^{-\mathcal{H}_\alpha^s/T} LD \int_{\xi_\alpha}^{\xi} d\xi\, e^{\mathcal{H}_{\xi\xi}(\xi-\xi_\alpha)^2/2T}(\nabla\phi)^2 \qquad (B8)$$

where L is the length of coordinate η. The above procedure to calculate C now yields

$$C \cong D\Delta\phi\left[\frac{H_{\xi\xi}}{2\pi T}\right]^{1/2} e^{-\mathcal{H}_\alpha^s/T} \qquad (B9)$$

from where the field gradient can be approximate as

$$\frac{\partial\phi}{\partial\xi} \cong \Delta\phi\left[\frac{\mathcal{H}_{\xi\xi}}{2\pi T}\right]^{1/2} e^{-\mathcal{H}_{\xi\xi}(\xi-\xi_\alpha)^2/2T} . \qquad (B10)$$

Replacement in (B8) and Gaussian integration then gives

$$\lambda_\alpha \cong DL\left[\frac{\mathcal{H}_{\xi\xi}}{2\pi T}\right]^{1/2}(\Delta\phi)^2 e^{-\mathcal{H}_0^s/T} \qquad (B11)$$

and, for symmetric minima,

$$\lambda_\alpha \cong \frac{DL}{\pi T}\left[\frac{\mathcal{H}_{\xi\xi}\Delta_0}{2}\right]^{1/2} e^{-(\mathcal{H}_\alpha^s - \mathcal{H}_0^{\min})/T} . \qquad (B12)$$

Finally, we illustrate here the local appearance of the eigenfunction $\phi(\xi)$ in the near-saddle region, as arising from the integration of its gradient. Let us first consider the nondegenerate case, with nonvanishing $\mathcal{H}_{\xi\xi}$ and $\mathcal{H}_{\eta\eta}$. From (3.23) and (3.24), we obtain the same as in Eq. (B10), consequently,

$$\phi(\xi) \cong \Delta\phi\left[\frac{\mathcal{H}_{\xi\xi}}{2\pi T}\right]^{1/2}\int_{\xi_\alpha}^{\xi} d\xi\, e^{-\mathcal{H}_{\xi\xi}(\xi-\xi_\alpha)^2/2T}$$
$$= \frac{\Delta\phi}{2}\operatorname{erf}\left[\left[\frac{\mathcal{H}_{\xi\xi}}{2T}\right]^{1/2}(\xi-\xi_\alpha)\right] . \qquad (B13)$$

If (B4) holds, the field gradient is constant and given by Eq. (B4). Accordingly, one has

$$\phi(\xi) = \frac{\Delta\phi}{\Delta\xi_m}(\xi-\xi_\alpha) , \qquad (B14)$$

which is the appropriate expression for the Lipkin scenario studied in Sec. V.

[1] S. Arrhenius, Z. Phys. Chem. **4**, 226 (1889).
[2] H. A. Kramers, Physica **7**, 284 (1940).
[3] B. J. Matkowsky, Z. Schuss, and C. Tier, J. Stat. Phys. **35**, 443 (1984).
[4] H. Haken, *Synergetics* (Springer-Verlag, Berlin, 1975).
[5] N. G. van Kampen, *Stochastic Phenomena in Physics and Chemistry* (North-Holland, Amsterdam, 1986).
[6] G. H. Weiss, J. Stat. Phys. **42**, 3 (1986).
[7] P. Hanggi, J. Stat. Phys. **42**, 105 (1986).
[8] V. I. Mel'nikov and S. V. Meshkov, J. Chem. Phys. **85**, 1018 (1986).
[9] L. E. Reichl, J. Chem. Phys. **77**, 4199 (1982).
[10] H. Hron and M. Razavy, J. Stat. Phys. **38**, 655 (1985).
[11] H. Dekker, Physica A **135**, 80 (1986).
[12] M. J. Englefield, J. Stat. Phys. **52**, 383 (1988).
[13] F. Marchesoni, P. Sodano, and M. Zannetti, Phys. Rev. Lett. **61**, 1143 (1988).
[14] P. Hanggi, P. Jung, and F. Marchesoni, J. Stat. Phys. **54**, 1367 (1989).
[15] R. Landauer and J. A. Swanson, Phys. Rev. **121**, 1668 (1961).
[16] J. S. Langer, Ann. Phys. (N.Y.) **54**, 258 (1969).
[17] B. J. Matkowsky and Z. Schuss, Siam J. Appl. Math. **42**, 835 (1982).
[18] B. Caroli, C. Caroli, and B. Roulet, J. Stat. Phys. **28**, 757 (1982).
[19] C. W. Gardiner, J. Stat. Phys. **30**, 157 (1983).
[20] R. Landauer, J. Stat. Phys. **53**, 233 (1988).
[21] Ye. A. Brener, V. I. Marchenko, and S. V. Meshkov, Zh. Eksp. Teor. Fiz. **85**, 2107 (1983) [Sov. Phys.—JETP **58**, 1223 (1983)].
[22] H. A. Weidenmuller and Zhang-Jing Shang, J. Stat. Phys. **34**, 191 (1984).
[23] H. C. Brinkman, Physica **22**, 149 (1956).
[24] W. F. Brown, J. Appl. Phys. **30**, 130S (1959).
[25] W. F. Brown, Phys. Rev. **130**, 1677 (1963).
[26] D. Kumar, in *Stochastic Processes: Formalism and Applications,* edited by G. S. Agarwal and S. Dattagupta (Springer, Berlin, 1983), p. 186.

[27] L. Néel, Ann. Geophys. **5**, 99 (1949); Adv. Phys. **4**, 191 (1955).
[28] D. Ryter, Physica A **142**, 103 (1967).
[29] D. Ryter, and H. Meyer, Physica A **142**, 103 (1987).
[30] D. Ryter, J. Stat. Phys. **49**, 751 (1987).
[31] E. S. Hernandez (unpublished).
[32] D. M. Jezek, E. S. Hernandez, and H. G. Solari, Phys. Rev. C **34**, 297 (1986).
[33] D. M. Jezek and E. S. Hernandez, Phys. Rev. C **35**, 1555 (1987).
[34] C. E. Vignolo, D. M. Jezek, and E. S. Hernandez, Phys. Rev. C **38**, 506 (1988).
[35] D. M. Jezek and E. S. Hernandez, Phys. Rev. **42**, 96 (1990).
[36] Ch. C. Gerry and J. Kiefer, Phys. Rev. A **41**, 27 (1990).
[37] R. Gilmore, *Catastrophe Theory for Scientists and Engineers* (Wiley, New York, 1981).
[38] H. J. Lipkin, N. Meshkov, and A. J. Glick, Nucl. Phys. **62**, 188 (1965).
[39] H. Risken, *The Fokker-Planck Equation Methods of Solution and Applications* (Springer-Verlag, Berlin, 1984).
[40] A. R. Mitchell and D. F. Griffiths, *The Finite Difference Method* (Wiley, New York, 1980).
[41] J. F. Luciani, P. Mora, and R. Pellat, Phys. Fluids **28**, 835 (1985).
[42] M. Baldo, Physica **114A**, 88 (1982).