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Decay rates of tunneling centers coupled to phonons: An instanton approach

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In this paper, we continue our study of defect tunneling in the presence of phonon modes. We compute the zero-temperature decay rate of the excited state of an asymmetric double well coupled to phonons. We compare the instanton decay rate with that of the traditional models of atomic tunneling (which either treat the defect as a two-level "spin" system or which work in the Condon approximation). We conclude that the traditional models are usually accurate only in a renormalized sense; any attempts to use bare tunneling matrix elements must apply the more sophisticated techniques proposed here. To illustrate this point we use instanton methods to study OH^- defect tunneling in alkali halides.

INTRODUCTION

This paper is the second by this author on the application of instantons to defect tunneling in solid-state physics. The first paper[1] dealt with the precise nature of the tunneling event. As a model system, it used a symmetric double well coupled to phonons. It computed the tunnel splitting between the symmetric ground state and the antisymmetric first excited state of the system. In this paper we turn to the interaction between tunneling events. We use an asymmetric double well coupled to phonons, and we will consider the decay rate of the first excited state.

The methods used here in treating many-body tunneling problems are phrased in terms of single-particle wave function evolving in a many-dimensional space. If one can ignore the effects of spin and indistinguishability of particles, the Schrödinger equation of a many-body system is

$$i\hbar\frac{\partial\psi}{\partial t}=\sum_j\frac{-\hbar^2}{2m_j}\frac{\partial^2}{\partial x_j^2}\psi+V(\vec{x})\psi\ .$$

If one scales each coordinate by the square root of the associated mass, the time evolution of the wave function is that of a single particle under a many-dimensional configuration-space potential $\mathscr{V}$,

$$i\hbar\frac{\partial\psi}{\partial t}=-\frac{\hbar^2}{2}\vec{\nabla}^2\psi+\mathscr{V}(\vec{Q})\psi\ .$$

Tunneling can be thought of as motion of this particle through classically inaccessible regions of configuration space. If only one coordinate is involved, tunneling can be understood asymptotically in powers of $\hbar$ using WKB techniques (Fig. 1). The methods used here are generalizations of WKB to systems with many degrees of freedom.

There are two ways in which the many-coordinate tunneling formalism presented in these two papers should be useful. First, the instanton methods provide a qualitative insight into the nature of the tunneling process. The instanton path can be thought of as the actual time-dependent collective motion during the tunneling process. Treatments which start with energy eigenstates hide this information; approximations based on these treatments will often be unphysical. For example, Hopfield[2] is developing a model of electron transport in photosynthesis, in which estimates of the decay rates (transfer rates) are used to explain the reaction mechanisms. Very little is known about these systems, and it is crucial to know what to ignore as unimportant; the direct physical nature of the path integral formalism should be useful.

In the other extreme, there are many tunneling defects in crystals which are already reasonably well understood, where the formalism can provide a first-principles, detailed microscopic picture of the phonon coupling. The coupling of these centers to electromagnetic radiation can be expanded in the number of photons involved, because the fine-structure constant $\alpha=e^2/\hbar c$ describing the coupling is small ($\sim\frac{1}{137}$). On the other hand, the coupling to elastic radiation in general is not weak, and multiple-phonon effects dominate the behavior. For there to be a well-defined excited

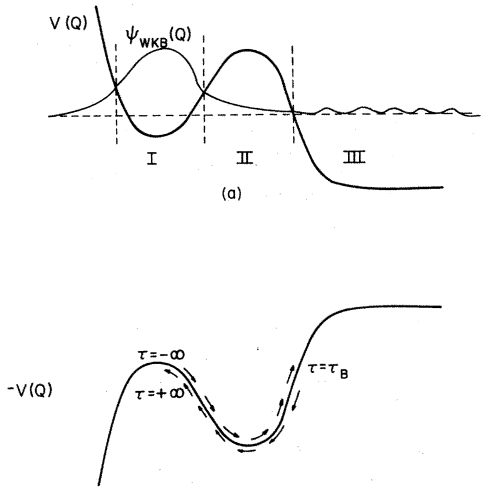

FIG. 1. (a) WKB resonance. The WKB approximation to the one-dimensional decay rate is given by matching solutions in regions I and II with a solution in region III of outgoing boundary conditions. (b) Instanton bounce in one dimension. The instanton-bounce path is a stationary point of the Euclidean action; thus it obeys a classical equation of motion in a potential $-V$. It starts at the top of the upper-well hill at $\tau=-\infty$, bounces off the slope at $\tau=\tau_B$, and slowly works its way up again by $\tau=\infty$. Note that it never explores the region where $V(Q)$ is less than the initial potential energy.

state, the decay time must be long. The stability of the excited state of these tunneling centers is maintained not by weak coupling, but by a small tunneling amplitude.

Pirc and Gosar[3] and Sander and Shore[4] were early in the study of phonon effects on these tunneling defects. They pioneered the procedure of perturbing in the tunneling matrix element Δ to study multiphonon processes. They bypass the problem of many-coordinate tunneling by simplifying the system, keeping only a few defect states (one for each local minimum in the potential). Only then do they couple to phonons. In the previous paper,[1] this truncation approximation was shown to be invalid. The decay is normally mediated by the high-energy defect states, and is best studied in configuration space, rather than energy space. Nevertheless, the theories of these authors and their successors have been quite successful in describing decay processes in these centers.

Thus the second way in which this formalism will prove useful is in studying these better-understood defects. In this paper, we will concentrate on explaining the successes and failures of the existing applications of the truncation approximation. This approximation is analogous to that of Drude and Sommerfeld's noninteracting electron gas, which reproduces many of the results of the quasiparticle description of Fermi liquids. In some cases, the high-frequency modes dress the defect, and the low-frequency decay modes see a renormalized defect which does have only two important energy states. The instanton method automatically performs both the renormalization and the truncation when these approximations are appropriate.

Despite the importance of tunneling in systems with more than one degree of freedom, the generalizations of WKB used here have developed only recently. Banks, Bender, and Wu[5,6] pointed out that tunneling in many dimensions remains essentially a one-dimensional process. Since the tunneling amplitude decreases exponentially with the barrier height, tunneling will occur in a small tube about the path of least resistance, with corrections exponentially small. Coleman[7] noted that this path satisfies the equations of motion of an analogous classical system with the sign of the potential reversed. Callan and Coleman[8] then developed a path-integral formulation of the theory. By rotating to imaginary time, the complex integrand reduces to a real positive one. Callan and Coleman observed that certain stationary points of this integrand (the instanton-bounce paths) follow the most probable escape path of Banks, Bender, and Wu. Quadratic fluctuations about the instanton bounce provide the decay rate. (Coleman and Callan draw heavily on Langer's[9] classical nucleation theory.)

So far, most of the applications of this theory have been in high-energy physics and cosmology. Coleman and Callan discuss the fate of the false vacuum. Callan, Dashen, and Gross[10] have used instantons to argue that quantum chromodynamics confines quarks. There have been attempts to treat supercurrent decay in Josephson junctions,[11] nucleation rates in liquid-helium phase transitions,[12] and soliton-pair creation[13] using these methods.

The version of the theory presented here was inspired by the configuration-space picture of tunneling centers in glasses described by Anderson, Halperin, and Varma.[14] It also draws upon the path-integral treatments of the Kondo effect due to Yuval and Anderson.[15]

The bulk of this paper is devoted to studying the links between the truncation approximation, the instanton-bounce calculation, and the true decay

rate. Section II discusses the rival schools of thought on tunneling-center—phonon interactions. Section III reviews the traditional decay-rate calculations of these schools, and discussed the unphysical consequences of the truncation approximation. Section IV motivates the instanton-bounce calculation by linking it with WKB methods. Section V uses the instanton techniques on the truncated problem—where they reduce to the method of steepest descents. Finally Sec. VI derives a renormalized truncation approximation as a limiting case of the instanton-bounce methods. This method essentially allows accurate computation of the screening of the defect by high-frequency phonons.

There are two main conclusions of this work. First, the truncation approximation has often been blindly applied in situations where there was no formal justification for believing it. The separate treatment of defect and phonon coordinates is usually artificial; the physical picture of the tunneling process painted by the truncation approximation is wrong. Second, in contrast, the workers in the field were largely correct in presuming the truncation approximation would work. Decay rates calculated in the truncation approximation will be valid outside it; approximations necessary to do calculations do not affect the validity of the answer. The Condon approximation, for example, is often made when it cannot be justified; the answers will nevertheless come out correct. *So long as discussion of bare matrix elements is avoided,* this approximation is far more useful than it first appears.

To illustrate these two points, I conclude in Sec. VII with a discussion of OH^- defects in alkali halides. Shore and Sander,[16] working within the truncation approximation, have made a very careful study of the bare tunneling matrix elements in these systems. The dynamics of these centers are well described by the truncation approximation, so they were surprised to find that the implied bare tunneling elements were unreasonably large (1.4×10^6 K for RbI:OH^-). Using a crude model, I demonstrate that this problem is rectified by using the renormalized version of the theory. By treating the defect more realistically these problems disappear, while the predicted dynamics remain unaltered.

II. THE TRUNCATION APPROXIMATION: OVERVIEW

Most calculations of tunneling rates begin by truncating the energy spectrum of the defect. Only one state is retained for each local minimum in the potential energy. For example, the Hamiltonian for a particle in a double well $V(Q)$ (Fig. 2) is modeled as a 2×2 matrix. The diagonal elements ($\pm\epsilon$) represent the asymmetry between the two wells; the off-diagonal elements ($-\Delta$) are due to tunneling through the barrier.

This vastly simplifies the problem. Δ is very small. Calculating to second order in Δ gives a complete description to all orders in the phonon coupling. The nature of the truncation approximation, however, becomes mysterious in the presence of phonons. For example, there are at least three different methods of introducing the phonons into the truncated Hamiltonian.

One school summarizes the effects of the phonons into a local strain field s. The strain field couples to the defect by changing the relative energies in the two well (diagonal coupling),

$$\mathscr{H}=\begin{bmatrix}-\epsilon & -\tilde{\Delta}\\ -\tilde{\Delta} & \epsilon\end{bmatrix}+Bs\begin{bmatrix}-1 & 0\\ 0 & 1\end{bmatrix}. \tag{2.1}$$

Computation of decay rates and phonon-scattering cross sections proceeds without ever introducing the phonon modes. Anderson, Halperin, and Varma[14] and Phillips[17] used this approach to study tunneling centers in glasses. This method essentially treats high- and low-frequency phonons separately. The response of the high-frequency phonons acts largely to renormalize the tunneling matrix element Δ; the motion of nearby atoms suppresses the tunneling. Since the local atomic structure around the tunneling center is not known

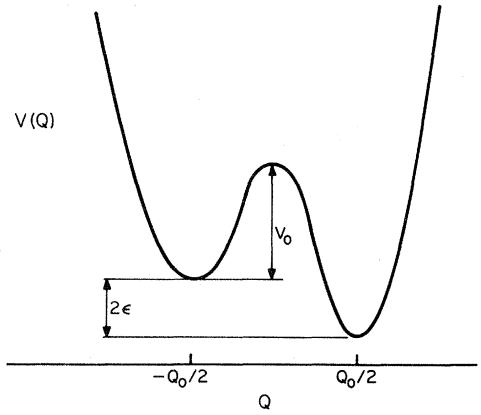

FIG. 2. Double-well defect potential. A defect in a double-well potential usually is modeled with a 2×2 Hamiltonian $\begin{pmatrix}-\epsilon & -\Delta\\ -\Delta & \epsilon\end{pmatrix}$. The bare tunneling matrix element Δ is assumed very small; it is exponentially suppressed by the barrier size $\sqrt{MV_0}Q_0$.

in glasses, the renormalized $\tilde{\Delta}$ is used from the start, and the high-frequency phonons are ignored. The low-frequency phonons mediate decays, and the strain-field coupling leads to the correct one-phonon decay rate.

The other two schools explicitly introduce phonon modes. Both end up with essentially the same Hamiltonian,

$$\mathscr{H}=\begin{bmatrix}-\epsilon & -\Delta \\ -\Delta & \epsilon\end{bmatrix}+\sum_k \frac{p_k^2}{2m}+\tfrac{1}{2}m\omega_k^2 q_k^2 + \lambda_k q_k \begin{bmatrix}-Q_0/2 & 0 \\ 0 & Q_0/2\end{bmatrix}. \tag{2.2}$$

The phonon modes are not plane waves; they are the normal modes of the lattice with the defect coordinate removed. The coupling again is diagonal. The two schools differ in the way they describe the defect. Sander and Shore[4] and Pirc and Gosar[3] model tunneling defects in crystals; they treat the two defect states as fixed local ground states, independent of the phonon positions. Theories of electron tunneling and tunneling of light atoms are usually more careful; they picture the two defect states as adiabatically changing with the phonon motion. Theories in this school include Holstein's[18] small polaron tunneling, Hopfield's[2] and Jortner's[19] electron tunneling in biophysics, Flynn and Stoneham's[20] quantum diffusion of light interstitials in metals, and Phillips's[21] electron-pair tunneling in amorphous semiconductors. Unfortunately, all of these latter theories found it necessary to make the "Condon approximation" that the tunneling matrix element Δ is independent of the phonon positions. The physical picture of this last school may be better, but the approximation is equivalent.

III. THE DECAY RATE: TRUNCATION APPROXIMATION

The total potential energy of a double well coupled to phonons does have two local minima (Fig. 3). It seems clear that such a double-well defect should be described by an effective Hamiltonian with two levels, at least if $V(Q)$ is not too asymmetric:

$$\tilde{\mathscr{H}}=\begin{bmatrix}\tilde{e}_1 & -\tilde{\Delta} \\ -\tilde{\Delta} & \tilde{e}_2\end{bmatrix}, \tag{3.1}$$

where $\tilde{\Delta}$ will represent the matrix element between the two local ground states of the many-body wave function. $\tilde{e}_2$ will have an imaginary part, reflecting the mixing of the upper-well ground state with low-frequency excitations of the lower-well ground state.

The difficulty with the truncation approximation is not that it concentrates on two states; it is the separation it makes between defect and phonon coordinates. Especially in atomic tunneling problems, this separation is artificial. The tunneling process is a collective motion through configuration space; the wave function strongly mixes defect and phonon coordinates.

In this section, we discuss the form of $\tilde{\mathscr{H}}$ found in the truncation approximation (2.2). Eventually, we will compare this calculation with the path-integral methods of the next section. For the time

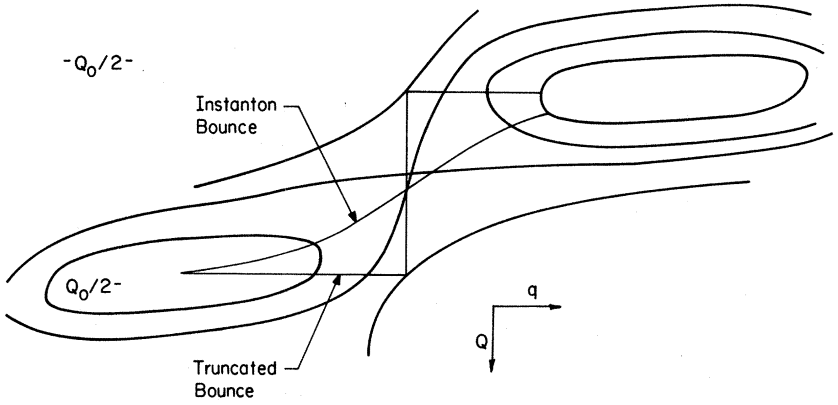

FIG. 3. Example of the truncated and untruncated instanton-bounce paths for a two-dimensional potential. The instanton-bump path moves from the upper well to a point of equal potential energy and back, retracing its path. Note that the flip of the truncated path takes place when the two defect-state energies are equal.

being, think of a path integral in the discrete defect coordinate; a representative path will flip between $\pm Q_0/2$ at irregular intervals (Fig. 4). The effect of the phonons is to provide nonlocal time-retarded interactions between flips.

We begin with the renormalized tunneling matrix element $\tilde{\Delta}$. It is given by the self-interaction of a flip. In the truncation approximation, the wave function in each well is forced to factor into a defect part and a phonon part. In turn, $\tilde{\Delta}$ factors into Δ times the overlap of the phonon ground states,

$$\tilde{\Delta}=\Delta e^{-W}=\Delta \exp\left[-\sum_k (\lambda_k^2 Q_0^2)/(4hm\omega_k^3)\right] . \tag{3.2}$$

This phonon overlap is known as the Frank-Condon factor in some groups, and as the Debye-Waller factor in others. It is dominated by high frequencies, it represents the rearrangement of the nearby atoms in response to the defect motion. The validity of this form for $\tilde{\Delta}$ is very dependent upon the Condon approximation that Δ is independent of the phonon positions. Δ will be most sensitive to the positions of nearby atoms; if the Condon approximation is at all weak, the exponent in (3.2) can be too large by 30%.[1] The problem is, the truncation approximation forces the defect to flip abruptly from one well to the other; intermediate defect positions correspond to higher energy states which are ignored. In practice the transition will often be slow enough to allow adiabatic relaxation of the high-frequency modes (i.e., the nearby atoms) during tunneling. This reduces the phonon suppression of the rate.

We now turn to $\tilde{e}_2$, the renormalized upper-well energy. It is renormalized to zeroth order by the phonon relaxation, and to second order in Δ by the time-retarded interactions between flips:

$$\tilde{e}_2=\epsilon-\sum_k \frac{\lambda_k^2 Q_0^2}{8m\omega_k^2} - \frac{i\tilde{\Delta}^2}{\hbar}\int_0^\infty ds\, e^{2i\epsilon s/\hbar}(e^{Q_0^2\mathscr{U}(s)}-1) , \tag{3.3}$$

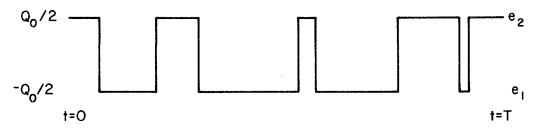

FIG. 4. Typical path in the discrete path integral. A typical path; this path would contribute to $(e^{-iHT/\hbar})_{22}$, as it begins and ends in position state 2.

$$\mathscr{U}(s)=\sum_k \frac{\lambda_k^2}{2m\omega_k^3} e^{-i\omega_k s} . \tag{3.4}$$

The zeroth-order term is the energy shift due to the relaxation of the nearby lattice. Although it involves high-frequency phonons, it does not involve tunneling and the truncation approximation is adequate.

The second-order term comes from the time-retarded interaction between flips. $\mathscr{U}(s)$ dies away with a power law for large s (Appendix A), so only nearby flips interact. Consider a path with an isolated bump of length s into the lower state (Fig. 5). It has two flips, so compared to the path which stays in the upper state it is suppressed by a factor of $[(\tilde{\Delta}dt)/\hbar]^2$. In addition, it spends a time s in the lower state, and thus picks up a relative phase $2i\epsilon s/\hbar$. Finally, the time-retarded interaction between two flips of $\pm Q_0$ a time s apart is $Q_0^2\mathscr{U}(s)$. Integrating the phonon part of the contribution of this bump path over flip lengths s gives the second-order term in (3.3).

This flip-flip interaction gives $\tilde{e}_2$ an imaginary part, which is the decay width of the first-excited state. If we expand the last exponential in the second-order term,

$$-\mathrm{Im}(\tilde{e}_2)=\frac{\tilde{\Delta}^2}{2\hbar}\int_{-\infty}^{\infty} ds\, e^{2i\epsilon s/\hbar} \times\left[\frac{Q_0^2\mathscr{U}(s)}{\hbar}+\frac{1}{2}\left[\frac{Q_0^2\mathscr{U}(s)}{\hbar}\right]^2+\cdots\right] , \tag{3.5}$$

$$=\frac{\tilde{\Delta}^2}{\hbar}\sum_k \frac{\lambda_k^2 Q_0^2\pi}{2m\omega_k^3}\delta(2\epsilon-\hbar\omega_k)+O(\lambda^4) , \tag{3.6}$$

we get the width of the upper energy level as a sum over multipole-phonon decays. The decay rate in this form clearly depends only upon phonons whose energies are less than the energy split-

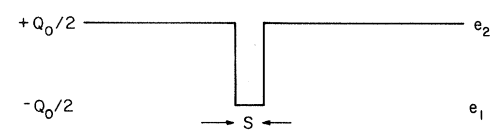

FIG. 5. An isolated bump. Phonon-mediated interactions between the two sides of the bump give the renormalized upper energy to second order in Δ. Interactions between three flips will renormalize Δ; groups of four will again renormalize the e_i, and so on.

ting. Nearby atoms are not important (except in determining $\tilde{\Delta}$) and this form is valid beyond the truncation approximation. The energy $\tilde{\epsilon}_1$ of the lower well is given by (3.3) with ϵ negative; it clearly gains no imaginary part to order Δ^2. Finally, (3.6) provides the link to the strain-field coupling methods of the glass-defect school. If one uses the Debye approximation $\omega_k = ck$ and the elastic monopole contribution $\lambda_k \propto k$ (Appendix A) the one-phonon decay rate reproduces their results.

IV. THE INSTANTON BOUNCE

The path-integral and instanton-bounce machinery may be somewhat forbidding to those unused to formalism (see Appendix B). Its success is based on a very simple idea. In the classically forbidden region $\mathscr{V}(\vec{Q}_0) - E > 0$, the wave function is exponentially damped. If configuration space $(\vec{Q})$ is one dimensional, this damping is given by the WKB exponent

$$\psi(Q_0) \propto \exp\left[-\frac{1}{\hbar}\int^{Q_0}\sqrt{2M[V(Q)-E]}\,dQ\right] . \tag{4.1}$$

In many-body systems, there are many paths leading to a given point Q_0 in the forbidden region. The exponential damping of the wave function is determined by the easiest such path.

Let $\vec{Q}(\tau)$ be a path leading from the classically allowed region to $\vec{Q}_0$, parametrized in some arbitrary way by τ. Let the components of $\vec{Q}$ be rescaled to the same mass M (see the Introduction). The damping is then given by minimizing the action in the exponent of (3.1) over all paths $\vec{Q}(\tau)$. This action,

$$\int^{Q_0}\{2M[\mathscr{V}(Q)-E]\}^{1/2}dQ ,$$

is in turn the minimum of

$$\int\left[\frac{1}{2}M\dot{Q}^2+\mathscr{V}(Q)-E\right]d\tau ,$$

under all reparametrizations of $\vec{Q}(\tau)$. Thus we are led by a simple WKB procedure to look at paths which minimize the action in the potential $-\mathscr{V}(Q)$.

Consider now a defect in a double well, coupled to phonons,

$$\mathscr{H} = \frac{P^2}{2M} + V(Q) + \sum_k \frac{p_k^2}{2m} + \tfrac{1}{2}m\omega_k^2 q_k^2 + \lambda_k q_k Q . \tag{4.2}$$

Let us consider the classical equations of motion for the phonons, with the potential energy inverted:

$$m\ddot{q}_k = m\omega_k^2 q_k + \lambda_k Q . \tag{4.3}$$

Harmonic oscillators are easy. Given $Q(\tau)$ and boundary conditions, one can solve (4.3) explicitly for $q_k(\tau)$, and for the phonon contribution to the action. The path $Q(\tau)$ must then minimize the total action:

$$S(Q) = \int_{-\infty}^{\infty} d\tau\left[\tfrac{1}{2}M\dot{Q}^2 + \tilde{V}(Q) + \tfrac{1}{2}\int_{-\infty}^{\infty} d\sigma\,\dot{Q}(\sigma)\dot{Q}(\tau)U(\sigma-\tau)\right] . \tag{4.4}$$

A derivation of (4.4) from more standard formulas is given in a previous paper.[1] The potential $\tilde{V}(Q)$ is the defect potential assuming adiabatic phonon relaxation,

$$\tilde{V}(Q) = V(Q) - \sum_k \frac{\lambda_k^2 Q^2}{2m\omega_k^2} . \tag{4.5}$$

The time-retarded velocity-velocity interaction is the flip-flip interaction (3.4) continued to imaginary time:

$$U(\rho) = \sum_k \frac{\lambda_k^2}{2m\omega_k^3} e^{-\omega_k|\rho|} . \tag{4.6}$$

It embodies the effects of the ringing of the lattice on the motion of the defect. It is not normally negligible. The WKB methods cannot be applied directly either to V or to $\tilde{V}$. In some limits, there are simple approximations for the effects of this time retarded interaction, which I have treated in detail in Ref. 1.

We want to calculate a decay rate. Decay rates are probability flows, and probability is an absolute square of a wave function. The exponent of the damping of the decay rate will be twice that of the wave function in (3.1). We are interested in the classical path which crosses the barrier *twice*.

Consider the form of the inverted potential. The upper well forms a hill, which is overshadowed on one side by the hill from the lower well. The path of interest starts at $\tau = -\infty$ at the top of the upper-well hill, and slowly rolls down (Fig. 6). At some finite time it rolls up the side of the lower-well hill, and bounces back exactly as it came. As

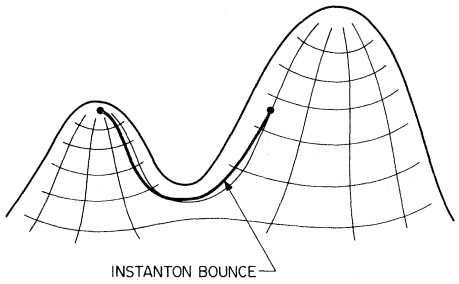

FIG. 6. Instanton bounce in inverted potential. The instanton-bounce path obeys the classical equations of motion for the system with the potential energy inverted. This path dominates the decay rate; it is the most probable escape path.

$\tau \to \infty$, it rolls back to the peak of the upper well. This is the instanton-bounce path.

The instanton-bounce path obeys the equations of motion, so the action is stationary near it. However, it is saddle point, not a minimum of the action. Paths like it which spend either more or less time in the lower well will have lower action. In some important sense, paths spending more time in the lower well correspond to successful decays, while paths spending less time are unsuccessful assaults on the barrier. The detailed theory makes use of quadratic fluctuations about the instanton path to give the WKB prefactor. For our saddle-point path the fluctuations which decrease the action contribute a negative eigenvalue, which gives the ground-state energy an imaginary part. This gives the decay rate (see Appendix B).

Although these quadratic fluctuations are formally very interesting, we shall not spend much time on them. The instanton path gives the exponential suppression of the rate; the fluctuations set the scale. Normally the scale up to a numerical factor can be guessed on physical grounds; this will suffice for our purposes.

V. STEEPEST DESCENTS AND THE TRUNCATED BOUNCE

The use of quadratic fluctuations about an instanton bounce to calculate the decay rate has been interpreted as a multidimensional generalization of the method of steepest descents.[8] It behooves us to apply the method of steepest descents to our truncated problem. In this section we show that it does indeed agree with the corresponding instanton-bounce calculation.

The decay rate in the truncation approximation is given by the imaginary part of (3.3). We may ignore the last (-1); it contributes only to the real part of the energy shift,

$$\mathrm{Im}(\tilde{e}_2)=\mathrm{Im}\left\{\frac{i\tilde{\Delta}^2}{\hbar}\int_0^\infty ds\,\exp\{[2i\epsilon s+Q_0^2\mathscr{U}(s)]/\hbar\}\right\}. \tag{5.1}$$

The remaining integral is now somewhat ill defined; however, it is now possible to apply the method of steepest descents.

We begin by deforming our integration contour (Fig. 7) to pass through the (pure imaginary) point s_I where the exponent $F(s)$ in (5.1) is stationary:

$$F'(s_I)=2i\epsilon+Q_0^2\mathscr{U}'(s_I)=0\,. \tag{5.2}$$

The first leg of our path contributes only to the real part of the energy shift. Along the second leg the magnitude of the integrand decreases very quickly if $\hbar$ is small. We therefore expand F about s_I:

$$\begin{aligned}\mathrm{Im}(e_2)&=-\frac{\tilde{\Delta}^2}{\hbar}\mathrm{Re}\left\{\int_{s_I}^\infty ds\,\exp\left[\left[F(s_I)+\frac{(s-s_I)^2}{2}F''(s_I)\right]\Big/\hbar\right]\right\}\\&=-\frac{\tilde{\Delta}^2}{\hbar}\left[\frac{-\pi\hbar}{2F''}\right]^{1/2}e^{F(s_I)/\hbar}\,.\end{aligned} \tag{5.3}$$

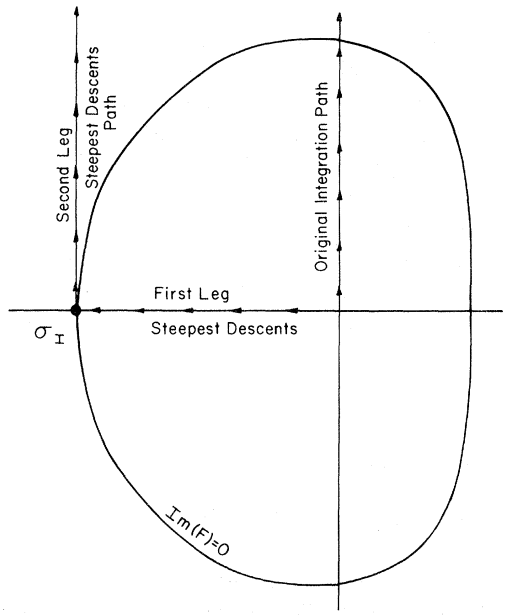

FIG. 7. Steepest descents path. Original integration path is deformed in order for the magnitude of the integrand to decrease as fast as possible. $F(s)$ on the second leg is approximated by $F(-i\sigma_I)+[(s+i\sigma_I)^2/2]F''(-i\sigma_I)$.

This is the steepest descent form of the truncated decay rate.

We now look at the corresponding instanton-bounce calculation, according to the prescription given by Callan and Coleman.[8] Once again, consider a path $[Q(\tau),\vec{q}(\tau)]$ in imaginary time, for which $Q(\tau)$ has a bump of length σ into the lower state from the upper. Such a path contributes

$$\left[\frac{\Delta}{\hbar}d\tau\right]^2 \exp\left[-\frac{1}{\hbar}\int d\tau\left[e+\sum_k \tfrac{1}{2}mq_k^2 + \tfrac{1}{2}m\omega_k^2 q_k^2+\lambda_k q_k Q\right]\right] .$$

The instanton-bounce path is a saddle point of the action in the space of all paths. It is of minimum Euclidean action with respect to variations in the phonon paths, and of maximum action (minimum contribution) with respect to variations about the instanton bounce length σ_I.

Clearly, the saddle point s_I of the steepest descent calculation ought to equal $-i\sigma_I$. As noted in the last section, the Euclidean action contributed by the phonon modes is given by the time-retarded interaction $\mathscr{U}$ continued to the imaginary axis. Thus steepest descents and instanton bounce find saddle points of the same action functional, and σ_I is indeed is_I. The quadratic expansion about the instanton bounce also agrees with the expansion of F about s_I in (5.3), so the decay rates agree. The instanton bounce is a path in phonon space as well (Fig. 3). It obeys the classical equations of motion

$$\begin{aligned} m\ddot{q}_k &= m\omega_k^2 q_k+\lambda_k Q , \\ 2\epsilon &= \sum_k \lambda_k Q_0\left[\frac{q_k(\sigma_I/2)+q_k(-\sigma_I/2)}{2}\right] . \end{aligned} \tag{5.5}$$

This path is interesting in its own right. This is the "escape path" through the classically forbidden region. One can check, for example, that the upper-state energy equals the energy at $\sigma=0$; the turning point occurs on the boundary of the classically allowed region. More interesting is the position of the flip. Since the phonons will respond symmetrically about $\sigma=0$, we find at the time $\pm\sigma_I/2$ of the flips the bare-energy splitting is exactly cancelled by the phonon coupling:

$$\begin{aligned} &\epsilon+\sum_k \lambda_k q_k(\pm\sigma_I/2)Q_0/2 \\ &\quad = -\epsilon+\sum_k \lambda_k q_k(\pm\sigma_I/2)(-Q_0/2) . \end{aligned} \tag{5.6}$$

The phonon deformation at $\tau=-\infty$ lowers the upper state below the lower state. As τ increases, the phonons deform and raise the upper-state energy. As the two energy levels cross, the transition takes place. This phenomenon, in weakly coupled electronic systems where the truncation approximation is good, is well known at higher temperatures. It was noted some time ago by Landau.[22]

This picture breaks down if the phonon coupling is not strong enough to lower the upper-state energy below the lower state. The steepest descent method still can be used on (3.3), but the instanton-bounce length is negative. Concern is definitely warranted; the flip and antiflip in this limit merge [Fig. 8(b)]. We shall discuss this in the next section.

VI. THE RENORMALIZED TRUNCATION APPROXIMATION

The truncation approximation has been very successful in describing a wide variety of low-frequency properties of tunneling systems. In many of these systems this approximation misses essential features of the tunneling process. Section III explained, qualitatively, why truncation is so successful. Essentially, low-frequency modes "see" the defect as a two-level system; only high-frequency phonons probe the details of the tunneling process. In this section we make this explanation precise, by deriving a renormalized truncation approximation as a limiting case of the instanton-bounce calculation.

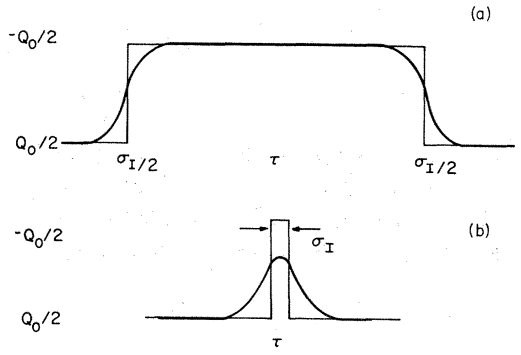

FIG. 8. (a) Truncated and untruncated instanton bounce: small asymmetry. For small asymmetry, the flip and antiflip are well separated, and the truncation approximation can be applied to a renormalized defect. (b) Truncated and untruncated instanton bounce: Large asymmetry. For larger asymmetry, the flip and antiflip will have large interactions, and the truncation picture disagrees with the instanton calculation.

Before using estimates, let us gain a qualitative idea of what this approximation does. For small asymmetries, the time spent in the lower well by the important paths is long compared to the flip time (the time spent crossing the barrier), as shown in Fig. 8(a). We want to approximate the contribution of this path with that of the truncated path shown, and with a suitably chosen truncated 2×2 Hamiltonian for the defect.

The most obvious qualitative difference between the two paths in Fig. 8(a) is the nature of each of the two transitions. The truncated transitions are abrupt giving the high-frequency phonon modes no time to relax with the defect as it tunnels. All phonon modes in the truncation approximation suppress tunneling by their Frank-Condon overlap integral. The corresponding self-interaction of a flip in the untruncated system will suppress tunneling less. The high-frequency modes in atomic tunneling will generally adiabatically relax with the defect motion, and contribute an effective mass—not a phonon wave-function overlap integral. The self-interaction of a flip has been treated with some care in the first paper.[1] Here, it can be absorbed into a redefinition of the truncated tunneling matrix element. It must be remembered that the bare matrix element in the truncation approximation has no physical meaning; in some sense it is too large by the ratio of the true phonon suppression to the phonon-overlap integral.

There remain two important differences between the two paths in Fig. 8(a), which cannot be embedded in a renormalized defect Hamiltonian. First, the nonzero flip time will affect the flip-flip interaction; this is the dominant correction as the time between flips gets large. Second, the defect approaches the bottom of the lower well only asymptotically, and there will be corrections due to $Q(0)+Q_0/2\neq0$. We shall estimate the importance of these two corrections, and show that they become unimportant as the time between flips gets large.

The Euclidean action we use in this section was introduced in Sec. IV:

$$S_E(Q)=\int d\tau\,\tfrac{1}{2}M\dot{Q}^2+\tilde{V}(Q)+\tfrac{1}{2}\int d\sigma\dot{Q}(\sigma)\dot{Q}(\tau)U(\sigma-\tau)\,,$$
$$\tilde{V}(Q)=V(Q)-\sum_k\frac{\lambda_k^2Q^2}{2m\omega_k^2},\quad U(\rho)=\sum_k\frac{\lambda_k^2}{2m\omega_k^3}e^{-\omega_k|\rho|}\,. \tag{6.1}$$

Consider now a typical path probing the well at $\tau=0$. We may split the action into three parts, one for each of the two flips and one part giving the flip-flip interaction:

$$\begin{aligned}S_E(Q)=&\int_0^\infty d\tau\left[\tfrac{1}{2}M\dot{Q}^2+\tilde{V}(Q)+\tfrac{1}{2}\int_0^\infty d\sigma\,\dot{Q}(\sigma)\dot{Q}(\tau)U(\tau-\sigma)\right]\\&+\int_{-\infty}^0 d\tau\left[\tfrac{1}{2}M\dot{Q}^2+\tilde{V}(Q)+\tfrac{1}{2}\int_{-\infty}^0 d\sigma\,\dot{Q}(\sigma)\dot{Q}(\tau)U(\tau-\sigma)\right]\\&+\int_0^\infty d\tau\int_{-\infty}^0 d\sigma\,\dot{Q}(\tau)\dot{Q}(\sigma)U(\tau+\sigma)\end{aligned} \tag{6.2}$$

The first two parts in this equation describe the self-interaction of the two flips. For the instanton path they are equal to each other; they give the exponential part of $\tilde{\Delta}$. Their value is slightly distorted by the presence of the other flip, but this effect is of higher order than the two discussed below.

The third part gives the flip-flip interactions. If the flips were abrupt, this term would be the truncated flip-flip interactions $-Q_0^2U(\sigma_0)$. $\dot{Q}(\sigma)$ for this path will be reasonably well localized around the times of the flip and antiflip. We define the time between these flips as

$$\sigma_0=\frac{1}{Q_0/2-Q(0)}\int_{-\infty}^\infty d\tau\dot{Q}(\tau)\tau\,, \tag{6.3}$$

and expand $U(\tau+\sigma)$ about σ_0:

$$U(\tau+\sigma)\simeq U(\sigma_0)+(\tau+\sigma-\sigma_0)U'(\sigma_0)+(\tau+\sigma-\sigma_0)^2U''(\sigma_0)/2\,. \tag{6.4}$$

The third part of (6.2) now becomes

$$\begin{aligned}&\int_0^\infty d\tau\int_{-\infty}^0 d\sigma\,\dot{Q}(\tau)\dot{Q}(\sigma)U(\tau-\sigma)-[Q_0/2-Q(0)]^2U(\sigma_0)\\&\quad-[U''(\sigma_0)/2]\int_0^\infty d\tau\int_{-\infty}^0 d\sigma\,\dot{Q}(\tau)\dot{Q}(\sigma)(\tau+\sigma-\sigma_0)^2\,.\end{aligned} \tag{6.5}$$

The second term in (6.5) is $U''(\sigma_0)$ times the square of a characteristic fliptime σ_F. If U dies off with a power law (see Appendix B) this term will be smaller than the flip-flip interaction by a factor of $(\sigma_F/\sigma_0)^2$.

The first term of (6.5) would equal the truncated flip-flip interaction if $Q(0)=-Q_0/2$. We now need to estimate $Q(0)$ as $\sigma_0\to\infty$. We specialize to the instanton-bounce path: "Typical" paths will have a spread of values at $\tau=0$ about $Q_I(0)$. $Q_I(\tau)$ obeys the equations of motion

$$M\ddot{Q}=\tilde{V}'(Q)-\int d\sigma\,\dot{Q}(\sigma)U'(\tau-\sigma)\,,$$

$$M\ddot{Q}(0)\approx m\omega^2[Q(0)+Q_0/2]-Q_0(U'(-\sigma_I/2)-U'(\sigma_I/2))\,.$$

Now $\ddot{Q}$ dies away faster than Q by two powers of τ. If $U(\rho)\propto 1/\rho^n$ as $\rho\to\infty$,

$$Q(0)+Q_0/2\sim\frac{2Q_0U'(-\sigma_I/2)}{m\omega^2}=O(1/\sigma_I^{n+1})$$

For point defects, $n\geq 2$ (see the Appendix) so the corrections to the first term will be even smaller than those of the flip time (the second term).

Thus, if the time σ_I spent in the lower well is large compared to the time σ_F spent crossing the barrier, the system will decay as would a corresponding two-level system—with no mention of truncation or the Condon approximation. The correct two-level system, however, involves both defect coordinates and high-frequency phonon coordinates; this complication affects only the calculation of the renormalized tunneling matrix element $\tilde{\Delta}$.

In many situations even this condition is not necessary for the validity of the renormalized truncation approximation. If the intrinsic asymmetry between the two wells is larger than the phonon coupling [Fig. 8(b)] the instanton-bounce calculation will disagree with a renormalized truncation approximation. On the one hand, the arguments of Sec. III still apply, so long as the asymmetry is not so large as to involve excited states in the lower well. On the other hand, the instanton picture certainly applies to large asymmetry—it was developed for quantum nucleation problems, where the asymmetry is in some sense infinite. In truth, the appropriate picture depends upon the widths of the lower-well excited states. If their widths are large compared to their spacing, the instanton methods apply. If the widths are small, coherent backscattering from the lower well becomes important, and truncation approximations describe the physics.

VII. OH^- IN ALKALI HALIDES

I conclude this paper with a discussion of OH^- tunneling defects in several alkali halides. The OH^- ion sits on a halide lattice site; the dipole has six (100) equilibrium orientations. The major tunneling events are 90° shifts of the dipole. There is a reasonably large lattice deformation associated with each relaxed equilibrium. Thus there is a substantial phonon motion associated with tunneling, which suppresses the rate.

The OH^- defect in alkali halides has been exhaustively studied[23] both experimentally and theoretically. OH^- tunneling centers are also of current interest[24]; they play a major role in the low-temperature behavior of glasses. The truncation approximation is clearly successful in describing decay rates of these defects. It has clearly failed in predicting tunneling rates from sensible bare tunneling matrix elements.

Shore and Sander[16] made a very careful study of the phonon suppression of the decay rate, working within the truncation approximation. They studied both electromagnetic and elastic coupling of the dipole to the lattice. The electromagnetic coupling was estimated by correcting the experimental electric-dipole moment for screening effects. The elastic coupling to the various group-theoretic modes was estimated from the experimental stress-splitting factors. The phonon modes were integrated numerically over the Brillouin zone, using published shell-model fits to neutron-diffraction data. Using this information, they computed the phonon wave-function overlap integral e^{-W} between two defect orientations 90° apart.

They then use experimental decay rates measured by Kapphan.[25] Using a one-phonon decay-rate expression, they extract renormalized tunneling matrix elements for the various alkali halides. They then make the mistake of dividing these by the overlap integrals to get "bare" tunneling matrix elements. As one can see from Table I, this results in unphysically large values of Δ_0.

Shor and Sander realized, of course, that something was wrong. They correctly pointed out that the magnitudes of the overlap exponents W seem

TABLE I. OH^- defects in alkali halides.

	KCl	RbCl	KBr	RbBr	RbI
Tunneling matrix element[a,b] $\tilde{\Delta}$ (K)	0.25	7.5×10^{-3}	2.3×10^{-3}	3×10^{-4}	7×10^{-4}
Phonon overlap integral[a] W	8.44	10.69	12.0	15.45	21.45
Bare tunneling matrix element[b] Δ (K)	1160	330	374	1540	1.4×10^{6}
Typical optical frequency[c] ω (sec^{-1})	3×10^{13}	2.7×10^{13}	0.4×10^{13}	2×10^{13}	1.6×10^{13}
Dimensionless coupling Λ	2.0	1.1	0.67	1.1	2.6
Dimensionless frequency Ω	0.86	0.54	0.15	0.39	0.45
Barrier height[d] V_0 (K)	230	475	130	500	240

[a]Reference 25.
[b]Reference 16.
[c]Shell and model fits referenced in 16.
[d]Low barrier for KBr comes from low shell-model optical frequency, the physics of which is unclear to the author.

uniformly too high. This is now, of course, expected; the nearby atoms will tunnel with the defect, and suppress the tunneling less than anticipated. I will use a very crude model (discussed at length in a previous paper[1] by this author) to show that this effect is in fact important and fixes the problem. I will use Shore and Sander's calculations of $\tilde{\Delta}$ and W, although I certainly abuse their careful estimates in my rough analysis.

The model I use consists of a single-phonon mode coupled linearly to a symmetric, quartic double well. A single-phonon mode of course cannot describe decays, but it can represent the high-frequency modes. I choose the phonon frequency ω to roughly match optical frequencies in the salts. I use the hydrogen mass M for the defect. The OH^- bond length is always very close to 1 Å; the tunneling distance Q_0 is therefore $\pi/2$ Å. Finally, I choose not to compute quadratic fluctuations, since they are tedious and make small corrections. I choose to use a prefactor for $\tilde{\Delta}$ of 138 K; this is a prefactor for an uncoupled well of characteristic frequency $4\hbar/MQ_0^2$.

The model can be reduced to a relationship between three dimensionless quantities. $\Omega=\omega/\omega_{DW}$ is a phonon frequency, where the double-well frequency

$$\omega_{DW}=4(V_0/MQ_0^2)^{1/2}$$

is the curvature at the top of the barrier. $\Lambda=\lambda^2/m\omega^2M\omega_{DW}^2$ is a dimensionless coupling. Finally, the action for the instanton path divided by $\sqrt{MV_0}Q_0$ is S. The dimensionless action S is estimated with a variational technique.[26]

Using $\tilde{\Delta}$, one can find

$$S/\Omega=-4\hbar/M\omega Q_0^2\ln(\Delta/138\text{ K})\,.$$

Using W, one knows $\Lambda/\Omega^2=(4\hbar/M\omega Q_0^2)W$.

Knowing these two quantities, we solve for Λ, Ω, and finally V_0, the barrier height of the relaxed potential. The results are shown in Table I. The barrier heights should not be trusted beyond a factor of 2 or 3 due to the rough approximations and the simple model.

The barrier heights shown are physically reasonable; they fall in a fairly narrow range and have realistic values. Corresponding bare tunneling matrix elements (physically meaningless) would range from 1—10 K; Shore and Sander chose 3 K as a reasonable value. Thus, even a crude model which allows the phonon to participate in the tunneling process gives a sensible microscopic picture.

To put the OH^- systems in a broader perspective, we can plot them on the $\Lambda\Omega$ plane (Fig. 9). The characteristic frequency of the dipole, despite the small hydrogen mass, is comparable to the phonon frequencies. This was foreshadowed by our analysis of lithium substitutional defects in KCl,[1] where the lithium motion was very slow. In both cases, the barrier heights must be low to allow tunneling, which leads to low defect frequencies. The coupling of the dipole to the lattice is quite strong; as in KCl:Li^+ it is roughly comparable to the lattice spring constants. This coupling would have to be much smaller for the truncation approximation (or the Condon approximation) to be valid.

The moral of this story is simple. Tunneling defects do act as "spin" systems, but the low-energy states mix up defect and high-frequency phonon coordinates in a nontrivial way. The truncation approximation captures the spin structure; it will describe well physical behavior depending only upon low-frequency phonons and renormalized matrix elements. Within these limits, the truncation approximation is more widely useful than generally believed. Physical behavior outside these limits must study the tunneling event in more detail. Instantons and path integrals provide workable tools for this study.

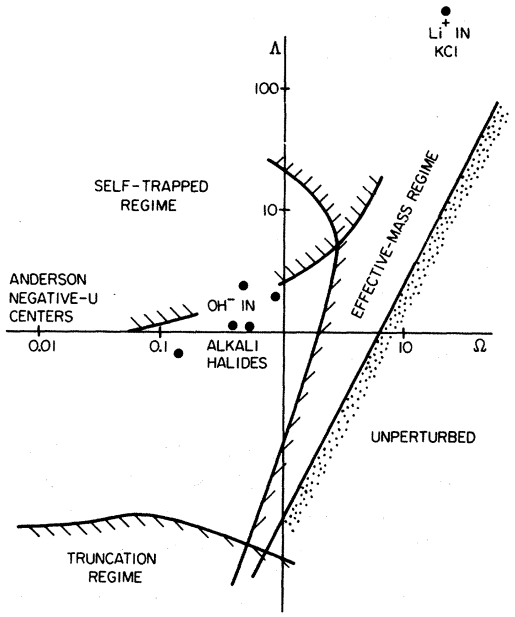

FIG. 9. Coupling and frequencies. Note the positions of various tunneling defects. (KCl:Li^+) is well within the effective-mass regime, where the phonons relax adiabatically as the defect tunnels. Anderson negative-U centers in amorphous semiconductors are self-trapped; their attractive potential is entirely due to phonon deformation. Tunneling can be viewed entirely in terms of phonon motion with adiabatic electron relaxation. OH^- defects lie in an intermediate region; they cannot, however, be described by the truncation approximation.

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APPENDIX A: DEFECTS WITH NONZERO ELASTIC MONOPOLE

In general, unless some special symmetry exists, the equilibrium states of a tunneling defect will occupy different volumes. The resulting shift in the far strain field for a local difference in volumes ΔV is

$$\vec{q}(\vec{x})=\frac{\Delta V}{4\Pi |x|^2}\frac{\vec{x}}{|x|} .$$

The remarkable fact that this volume is not shielded by compression[27] is easy to derive. It follows from the assumption that there is no local rotation ($2\omega_{ij}=\partial_i q_j-\partial_j q_i=0$). This follows, for example, from spherical symmetry. The strain field will minimize the energy

$$W=\int d^3x\,\mu[e_{ij}e_{ij}-\tfrac{1}{3}(e_{kk})^2]+\tfrac{1}{2}K(e_{kk})^2\ ,$$

where μ is the shear modulus, K is the bulk modulus, and e_{ij} is the strain tensor $\partial_i q_j$. If $\omega_{ij}=0$, then

$$\begin{aligned}e_{ij}e_{ij}-e_{kk}^2&=\partial_i q_j\partial_i q_j-\partial_i q_i\partial_j q_j\\&=\partial_i(q_j\partial_j q_i-q_i\partial_j q_j)\ ,\end{aligned}$$

is a perfect divergence, so

$$W=\int d^3x\,(\tfrac{2}{3}\mu+\tfrac{1}{2}K)(e_{kk})^2+\text{const}\ ,$$

and the strain field will minimize the compressional energy by propagating ΔV out to infinity.

We can use this far-field shift to calculate the coupling to low-frequency longitudinal modes of odd parity at the defect; these in turn will dominate the long-time asymptotic behavior of the time-retarded interaction. The displacement for a longitudinal mode in the z direction is

$$\begin{aligned}q_k(k_z)&=\frac{1}{\sqrt{N}}\sum_i \sin(kz_i)\vec{q}(\vec{x}_i)\cdot\hat{z}=\frac{1}{\sqrt{N}a^3}\int_0^R dr\int_{-r}^{r}(2\pi r)dz\sin(kz)\frac{\Delta V}{4\pi r^2}\hat{r}\cdot\hat{z}\\&=\frac{1}{k}\frac{\Delta V}{\sqrt{N}a^3}\int_0^{RK}d\rho\left[\frac{\sin\rho}{\rho^2}-\frac{\cos\rho}{\rho}\right]\to\frac{1}{k}\frac{\Delta V}{\sqrt{N}a^3}\ ,\end{aligned}$$

as $R\to\infty$ for N atoms in a sphere of radius R and interatomic spacing a. We know the equilibrium displacement $q(k)=\lambda_k Q_0/m\omega_k^2$. Since $\omega_k=ck$ as $k\to 0$ (where c is the speed of sound), the coupling constant $\lambda_k\propto k$ as $k\to 0$ is

$$\lambda_k=k\left[\frac{mc^2\Delta V}{\sqrt{N}Q_0a^3}\right]\ .$$

This in turn implies

$$\begin{aligned}U(\rho)&=\sum_k\frac{\lambda_k^2}{2m\omega_k^3}e^{-\omega_k|\rho|}\\&=\frac{(\Delta V)^2m}{4\pi^2Q_0^2a^3c}\frac{1}{\rho^2}\propto\frac{1}{\rho^2}\end{aligned}$$

as $\rho\to\infty$.

APPENDIX B: DECAY RATES AND THE INSTANTON BOUNCE

We are interested in the phonon decay time of excited states of defects. The excited state is not an energy eigenstate, of course. It is a resonance—a superposition of a continuum of true energy eigenstates which behaves as if it had a complex energy

$$\tilde{E}=E-\frac{i\gamma}{2}\ ,$$

giving it a decay rate γ/h. It is not clear, given a specific Hamiltonian, how to define a resonance. It is necessary to start with a family of Hamiltonians, analytically dependent upon a parameter. The true energy eigenvalues then can be followed into the continuum by analytic continuation. Once they mix with the continuum they leave the spectrum of the Hamiltonian, gain an imaginary part, and become resonances.

In our problem of an asymmetric double well coupled to phonons, we can define the resonance as the analytic continuation of the ground state as we change the asymmetry from negative to positive. To see how this works, consider the ground-state energy E of a two-level (truncated) system,

$$\begin{aligned}H&=\begin{bmatrix}-\epsilon & -\Delta\\ -\Delta & \epsilon\end{bmatrix},\quad \epsilon<0\\E&=-(\epsilon^2+\Delta^2)^{1/2}=\epsilon+\frac{\Delta^2}{2\epsilon}-\frac{\Delta^4}{8\epsilon^3}\cdots\\&=E^{(n)}+O(\Delta^{n+1})\ .\end{aligned}$$

If we analytically continue E to positive asymmetry ($\epsilon>0$), we stay in the ground state. However, if we first expand E as a power series in Δ, then to any finite order n the analytic continuation of $E^{(n)}$ leads us into the first excited state. Here the continuation is independent of the route around the singularity at $\epsilon=0$ and leads to another real eigenstate. When we coupled this system to phonons (Sec. III) we were able to explicitly perform this continuation. There for $\epsilon>0$ the energy $E^{(2)}$ picks up an imaginary part, and the first excited state is a resonance.

The instanton-bounce method of Coleman and Callan[7,8] does this analytic continuation (for the untruncated problem) to order Δ^2. (More precisely, it gives the term of order Δ^2 asymptotically as $\hbar\to 0$.) The terms of higher order in Δ correspond

to bounce-bounce interactions which are neglected in the dilute gas approximation. A brief discussion of the limits of this approximation seems necessary.

For very small asymmetries this expansion breaks down. If the tunneling matrix element is larger than the asymmetry, the first excited state is qualitatively an antisymmetric superposition of a Gaussian in each well. Analytically continuing from a state of large negative asymmetry where the ground state is qualitatively localized in the right-hand well is not sensible, and does not work. One can define a resonance for nearly symmetric wells by analytically continuing the first excited state from zero coupling. One can compute both the weak coupling and the large asymmetry decay times in the truncation approximation[26]; it is reassuring to note that they agree where they overlap (double wells with large asymmetry coupled weakly to phonons).

This breakdown at small asymmetry is a special case of a more general problem. Barrier penetration in one variable can be treated using the WKB method; a careful calculation of the WKB decay time agrees with that of the instanton bump (see Fig. 1). Both decay times are independent of the potential after the second turning point (region III). The WKB solution assumes at this point that the wave function in the classically forbidden region II matches onto a solution in region III with outgoing boundary conditions. For a double well (Fig. 2) there are no decays—the wave function in region III is not outgoing. The instanton-bump path never actually probes the bottom of the lower well; the calculation assumes that the decays are irreversible. Constructive or destructive interference of the wave function after it leaks into the lower well will not be adequately dealt with by the instanton approximation. Sec. VI discussed this question.

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