Coupled Instantons In A Four-Well Potential With Application To The Tunneling Of A Composite Particle

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Coupled instantons are introduced by generalizing the double well potential to multiple mutually coupled wells. Physically this corresponds to the simultaneous tunneling of multiple degrees of freedom. A system with four equal minima is examined in detail. It has three instanton types or flavors with distinct actions. For weak coupling and subject to there being a single large (or small) parameter, the interactive system can be handled perturbatively. The zero mode problem arising from time translation symmetry is handled via the Fadeev-Popov procedure. A diagrammatic procedure allows corrections to the fluctuation determinant to be calculated systematically. Independent instanton contributions are summed over by extending the dilute gas approximation to three flavors and energy splittings of the lowest four states is calculated. All tunneling amplitudes are concisely expressed in terms of elementary functions. While the model is possibly useful for a variety of physical systems, an application is made here to the tunneling of a composite particle in one dimension.

The double well potential has long been the starting point for investigating quantum tunneling between two degenerate vacuum states. As such it provided the backdrop for the invention of instantons in the 1970's, a major development that spawned new non-perturbative methods across many areas of physics and mathematics. These have helped uncover the geometrical, topological and quantum properties of both the ground state and spectrum of Yang-Mills type gauge theories. Excellent textbooks and review papers now cover double well instantons and their extensions into various field theories [1][2][3][4][5]. The current literature abounds with applications of instantons to diverse areas such as computing chemical reaction rates [6] and neural networks [7].

Surprisingly, however, we were unable to discover any effort to extend the single double-well instanton to more general systems where two or more instantons are mutually coupled with each instanton being associated with a separate double well. For two degrees of freedom, this corresponds to both simultaneously tunneling across to their respective vacuaa. That such investigations have not been pursued may have several reasons. First, there is little incentive to investigate a mathematical problem that is apparently unconnected to some actual physical situation. Second, the task seems rather difficult because the classical level equations for instantons are non-linear and usually do not admit analytic solutions. This is true even for instantons belonging to the same potential, a fact that leaves the dilute instanton gas model as the only viable way of doing an actual calculation. Finally, at the technical level, calculating the fluctuation determinant analytically is non-trivial even in the simplest case because zero modes are an unavoidable complication in instanton theory. This is why many instanton applications

in the literature simply ignore quadratic fluctuations.

In this paper we make the case that at least one physical problem calls for studying coupled instantons, i.e. that of quantum mechanical tunneling by a composite object. Particle tunneling is commonly encountered in atomic and nuclear physics, and condensed matter physics. Perhaps the most celebrated early example is George Gamow's 1928 discovery that protons may cross each other's Coulomb barrier to fuse together, a possibility ruled out by classical mechanics [8]. Tunneling also resolved the outstanding problem of α decay from nuclei. Once considered esoteric, tunneling has everyday applications to technology such as the scanning-tunneling microscope. At the field theory end, instanton tunneling was famously used to predict how the universe may catastrophically transition from a possibly false vacuum state to a truer one [9].

All theoretical attention paid to tunneling has, however, concentrated upon structure-less point particles. For protons, α particles, and atoms, multiple length and energy scales are involved and so perturbation theory is generally of little use. In atomic and nuclear physics attempts have been made to account for compositeness using a coupled channel approach for scattering processes. This is heavily computational and seeks to directly solve the Schrödinger equation. Though straightforward in principle, little theoretical insight can be gained. Some papers are referenced in the book by Razavy [10].

The instanton approach to tunneling discussed in this paper differs radically from attempting to solve the Schrodinger through the WKB approximation or via time dependent scattering. Pioneered by Polyakov, t'Hooft, and others this approach takes the Feynman path integral as its starting point and calls for extremizing the action around solutions to the classical equations of motion in imaginary time. The instanton emerges as a solution with a finite, non-zero action. It is therefore natural to ask what the instanton method might have to say about a system where the objects that tunnel through are finite sized rather than point-like.

As a warm up we consider a one-dimensional diatomic "molecule" with two dissimilar atoms at its ends trapped in the same potential double well. Imagine that such a molecule is placed inside one well. If the atoms are totally free (or loosely bound) then, intuitively speaking, one may tunnel to the other side sooner than the other resulting in a flip of the molecule's orientation when eventually both atoms cross over. On the other hand, if the atoms are held together by a strong inter-atomic force then the tunneling probability will be quite different from that of a point particle and a flip would be unlikely to happen. As a warm up, let us first analyze the "molecule" using the semiclassical expansion under the assumption that the atoms are joined by a perfectly rigid rod of length L. The assumption of rigidity will be relaxed subsequently.

I. PRELIMINARIES

The Feynman amplitude in imaginary (or Euclidean) time t is,

$$\mathscr{A} = \left\langle a, T/2 | e^{-\frac{H}{\hbar}t} | -a, -T/2 \right\rangle = \mathscr{N} \int [dx(t)] \ e^{-\frac{S[x]}{\hbar}},$$
(1)

where S[x] is the Euclidean action. The system is in its initial state at time $\tau = -T/2$ at position y = -a and makes its way to the final state at y = a at $\tau = T/2$ by traveling on all possible paths connecting the initial to the final state. To get bound state energies and wavefunctions one eventually takes $T \to \infty$. In the semiclassical approximation, fluctuations away from these paths are allowed up to the quadratic level. In our toy model, we first consider a perfectly rigid diatomic "molecule" wherein each "atom" experiences an identical potential U(y) if it happens to be at position y

$$U(y) = \frac{m\omega^2}{16a^2}(y^2 - a^2)^2$$
(2)

For simplicity the atoms are assumed to be distinguishable but with equal masses, $m_1 = m_2 = \frac{m}{2}$. The centre of mass $y = \frac{1}{2}(y_1 + y_2)$ is equidistant from the two constituents and the relative distance $x = x_1 - x_2$ is fixed at L. The (Euclidean) Lagrangian is,

$$\mathscr{L} = \frac{m}{2}\dot{y}^2 + \bar{U},\tag{3}$$

$$\bar{U} = U\left(y + \frac{L}{2}\right) + U\left(y - \frac{L}{2}\right) \tag{4}$$

The potential \overline{U} is symmetrical under $y \to -y$, i.e. the cm may be located equally within either well. The Euler-Lagrange equation can, of course, be directly written

down but \overline{U} does not have a minimum at $y = \pm a$ for $L \neq 0$ and there is no instanton solution. However, \overline{U} can be rewritten so that it has minima at $y = \pm y_0$ with $y_0 \neq a$. Instantons may then tunnel from $-y_0$ to y_0 ,

$$\bar{U} = \frac{m\omega^2}{8a^2} \left(y^2 - y_0^2\right)^2 + \frac{1}{8}m\omega^2 L^2 \left(1 - \frac{L^2}{2a^2}\right) \quad (5)$$

$$y_0 = \pm af, \ f = \sqrt{1 - \frac{3}{4} \frac{L^2}{a^2}}.$$
 (6)

In the limit $L \to 0$, \bar{U} reduces to U. The second, yindependent, part of the potential in Eq.5 is of no consequence and can be discarded. The classical EOM becomes,

$$\ddot{y}_c = \frac{\omega^2}{2a^2} (y_c^2 - y_0^2) y_c, \tag{7}$$

with an instanton solution modified relative to the textbook form only by the factor f,

$$y_c(\tau) = \pm af \tanh \frac{\omega f}{2} (\tau - \tau') \tag{8}$$

In the above τ' is an arbitrary additive constant that owes to the invariance of Eq.7 under time translation, $\tau \to \tau + \tau'$. This solution interpolates between the shifted vacuaa that are now located at $\pm y_0$. These well localized solutions differ from the vacuum values only in the narrow range $\Delta \tau \sim 1/\omega$. From this classical solution the action contributed by a single instanton is,

$$S_{0} = \int_{-\infty}^{\infty} d\tau \left[\frac{m}{2} \dot{y}_{c}^{2} + \frac{m\omega^{2}}{8a^{2}} \left(y_{c}^{2} - y_{0}^{2} \right)^{2} \right]$$
$$= \frac{2}{3} m\omega a^{2} f^{3}$$
(9)

This coincides with the action for a point particle in the point molecule limit, $L \to 0$. Note that for $L \to 2a/\sqrt{3}$ the double minimum becomes a quartic with a single minimum at $y_0 = 0$,

$$\bar{U} \to \frac{m\omega^2}{8a^2}y^4 + \frac{1}{18}m\omega^2 a^2.$$
 (10)

There is no instanton solution in the above limit.

The above result comes from purely classical considerations. Quantum effects arise through the fluctuation factor whose calculation is identical to that of Novikov[1] et al but which, to make this discussion self contained, we shall recapitulate. Briefly, one expands y around the classical solution y_c , i.e. $y = y_c + \eta$ and then integrates over all η 's that vanish at the endpoints. This is most efficiently achieved by expanding in a complete set of eigenfunctions of the fluctuation operator,

$$\hat{O} = -m\frac{d^2}{d\tau^2} + \bar{U}''(y_c) = -m\frac{d^2}{d\tau^2} + mf^2\omega^2 \left(1 - \frac{3}{2}\mathrm{sech}^2\frac{f\omega\tau}{2}\right). \quad (11)$$

For large times this becomes the operator for the simple harmonic potential $\frac{1}{2}mf^2\omega^2(y-y_0)^2$,

$$\hat{O}_H = -m\frac{d^2}{d\tau^2} + mf^2\omega^2.$$
(12)

Doing the functional integral in Eq.1 over the fluctuations yields the single instanton contribution to the amplitude in terms of the determinant of O,

$$\mathscr{A} = \mathscr{N}\sqrt{\frac{S_0}{2\pi m\hbar}} e^{-\frac{S_0}{\hbar}} \frac{T}{\sqrt{\det'[\hat{O}]}}.$$
 (13)

In arriving at Eq.13 above, an appropriate Jacobian factor has been inserted. The determinant is the usual (infinite) product of eigenvalues but with one significant complication. Time translation invariance of the underlying EOM leads to a zero eigenvalue. This comes from the fact that the instanton's center can be displaced by any amount without costing energy. Hence $det[\hat{O}]$ vanishes unless this eigenvalue is specifically excluded. Using the discussion in ref.[1] for computing the functional determinant, and after restoring units, gives $det[\hat{O}]$ in terms of the harmonic oscillator determinant,

$$\frac{1}{\det'[\hat{O}]} = \frac{12mf^2\omega^2}{\det[\hat{O}_H]}.$$
(14)

(The prime above indicates exclusion of the zero eigenvalue.) Only the issue of the normalization constant \mathcal{N} now remains:

$$\frac{\mathcal{N}}{\sqrt{\det'[\hat{O}]}} = \frac{\mathcal{N}}{\det[\hat{O}_H]^{\frac{1}{2}}} \sqrt{12m} f \omega$$
$$= \sqrt{\frac{mf\omega}{2\pi\hbar\sinh f\omega T}} \sqrt{12} f \omega \qquad (15)$$

In the last step above, \mathcal{N} has been fixed by using the well-known result for the harmonic oscillator's propagator. Of course one also recovers the correct free particle propagator in the $\omega \to 0$ limit. Specializing to large T and inserting S_0 from Eq.9 gives,

$$\mathscr{A} = \sqrt{\frac{mf\omega}{\pi\hbar}} e^{-\frac{f\omega T}{2}} \times \sqrt{\frac{S_0}{2\pi\hbar}} e^{-\frac{S_0}{\hbar}} \sqrt{12} f\omega T$$
$$= \sqrt{\frac{mf\omega}{\pi\hbar}} e^{-\frac{f\omega T}{2}} KT$$
(16)

$$K = f\omega \sqrt{\frac{6S_0}{\pi\hbar}} e^{-\frac{S_0}{\hbar}} = f\sqrt{\frac{4m\omega^3 a^2}{\pi\hbar}} e^{-\frac{S_0}{\hbar}}$$
(17)

For large T the above single instanton amplitude is a vanishingly small contribution to the total transition amplitude. To get a finite sum we must sum over all classical paths satisfying Eq.7. Making the assumption of sufficiently large separation between instantons (i.e. dilute gas approximation) the result easily exponentiates,

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$$\mathcal{A}_{+} \equiv \mathcal{A}(-y_{0} \to y_{0})$$

$$= \sqrt{\frac{mf\omega}{\pi\hbar}} e^{-\frac{f\omega T}{2}} \sinh KT, \qquad (18)$$

$$\mathcal{A}_{-} \equiv \mathcal{A}(-y_{0} \to -y_{0})$$

$$= \sqrt{\frac{mf\omega}{\pi\hbar}} e^{-\frac{f\omega T}{2}} \cosh KT.$$
(19)

This allows the extraction from \mathscr{A}_\pm of the two lowest energies belonging, respectively, to the even and odd eigenstates,

$$E_{+} = \frac{1}{2}\hbar f\omega - \frac{2af^{5/2}}{\sqrt{\pi}}\sqrt{\hbar m\omega^{3}}e^{-\frac{S_{0}}{\hbar}}$$
(20)

$$E_{-} = \frac{1}{2}\hbar f\omega + \frac{2af^{5/2}}{\sqrt{\pi}}\sqrt{\hbar m\omega^3}e^{-\frac{S_0}{\hbar}}$$
(21)

It is well known that for point particle (f = 1) tunneling the level splittings in Eqs. 20-21 can be derived in the WKB approximation [2]. Presumably WKB can also give the present results but it is hard to see exactly how. That one can calculate the tunneling of a rigid composite object with only minimal effort encourages us to take the next step.

II. COMPOSITE TUNNELING

We will now relax the condition of perfect rigidity by adding a kinetic term for relative motion as well as an extra potential chosen to constrain x near L, now to be thought of as the length parameter determining the average length of the vibrating molecule,

$$\mathscr{L} = \frac{m}{2}\dot{y}^2 + \frac{m}{8}\dot{x}^2 + U_T.$$
 (22)

In terms of the double well potential U in Eq.2 the new potential U_T is,

$$U_T = U(y + \frac{x}{2}) + U(y - \frac{x}{2}) + \frac{m\Omega^2}{32L^2}(x^2 - L^2)^2 \quad (23)$$

One can imagine other constraints such as inserting various other powers of a/L in front of the $(x^2 - L^2)^2$ term and would constitute separate physical models. The important point is that as $\Omega \to \infty$ the molecule becomes increasingly rigid with equilibrium points close to $x = \pm L$. As with the potential in Eq.4, apriori the Euler-Lagrange equations are intractable. To proceed further, we find the minima of U_T and then re-express it with appropriately defined constants,

$$U_T = \frac{m\tilde{\Omega}^2}{32L^2}(x^2 - x_0^2)^2 + \frac{m\omega^2}{8a^2}(y^2 - y_0^2)^2 + \frac{3m\omega^2}{16a^2}(y^2 - y_0^2)(x^2 - x_0^2) + C$$
(24)

The potential minima are at $x = \pm x_0$, $y = \pm y_0$ where mensionless action is:

$$x_0, y_0$$
 and the remaining constants are:

$$x_0^2 = \frac{1 - \frac{2\omega^2}{\Omega^2}}{1 - \frac{2\omega^2 L^2}{\Omega^2 a^2}} L^2$$
(25)

$$y_0^2 = \frac{1 - \frac{3L^2}{4a^2} - \frac{\omega^2 L^2}{2a^2 \Omega^2}}{1 - \frac{2\omega^2 L^2}{a^2 \Omega^2}} a^2$$
(26)

$$\tilde{\Omega}^2 = \Omega^2 \left(1 + \frac{\omega^2 L^2}{4a^2 \Omega^2} \right) \tag{27}$$

$$C = \frac{1}{8}m\omega^2 L^2 \frac{1 - \frac{\omega^2}{\Omega^2} - \frac{L^2}{2a^2}}{1 - \frac{2L^2\omega^2}{a^2\Omega^2}}$$
(28)

The constant $C = E_{min}$ is irrelevant to the dynamics but has been listed above for completeness. Note that as $\Omega \to \infty$ the equilibrium positions shift towards the free values, $x_0 \to L, y_0 \to fa$.

Until we revert to it towards later in this paper, we shall temporarily set aside the composite particle tunneling problem and instead move to a more general formulation of coupled systems. This is important because, other than the example considered here, there are likely many other systems where it may be relevant such as a two dimensional free electron gas subjected to a perpendicular, spatially varying magnetic field. Electrons move along snake-like classical paths on either side of the line where the field crosses zero. This system of spinless electrons is described quantum mechanically by a symmetric double well potential [11]. Were one to take into account the electron's magnetic moment as well, the resulting effective action is similar to Eq.24. Suitably designed optical lattices might provide yet other opportunities. We have not investigated any of these possibilities.

III. COUPLED INSTANTONS MODEL

A single double well instanton is characterized by three parameters only two of which enter the Lagrangian. The three could, for instance, be taken as the mass, separation between the two well bottoms, and the instanton width. For our purpose a suitable expression for the generic di-

$$\frac{1}{\hbar}\int d\tau \left[\frac{1}{2}m\left(\frac{dy}{d\tau}\right)^2 + \frac{m\omega^2}{8u^2}(y^2 - y_0^2)^2\right]$$

$$\begin{array}{c} \bar{h} \int \left[2 \left(d\tau \right) & 8y_0^2 \left(3 - 50 \right) \right] \\ = \int d\tau \left(\frac{1}{2} b_1 \dot{q}^2 + \frac{1}{4} b_2 (q^2 - 1)^2 \right)$$
(29)

where $q = y/y_0$ is dimensionless and will serve as the new dynamical variable and b_1, b_2 are in Eq.32 below. The inverted potential is drawn schematically in Fig.1. Of course, to be kept in mind is that the smallness of \hbar is what makes the semi-classical formulation useful. For future use we record below the fluctuation amplitude in the present notation,

$$\langle -y_0, T/2 | e^{-\frac{H}{\hbar}t} | -y_0, -T/2 \rangle = \langle y_0, T/2 | e^{-\frac{H}{\hbar}t} | y_0, -T/2 \rangle$$
$$= \sqrt{\frac{m\omega}{\pi\hbar}} e^{-\frac{1}{2}\omega T} = \frac{\sqrt[4]{2b_1b_2}}{\sqrt{\pi}y_0} e^{-\frac{1}{2}\omega T}.$$
(30)

Note that ω_q is also expressible in terms of b_1, b_2 as $\omega_q = \sqrt{2b_2/b_1}$. Also, that $\sqrt{m\omega/\pi\hbar}$ is the square $|\psi(0)|^2$ of the SHO's ground state wavefunction at the origin.



FIG. 1. The inverted potential for two double wells. An instanton can travel from any one peak to any other peak by a variety of different paths and thus back to its starting point as well.

Consider now two instantons corresponding to two different physical variables that interact with each other and with the potential drawn schematically in Fig.1. The five independent constants a_1, a_2, b_1, b_2, c in Eq.31 are set by some underlying physical model. For composite tunneling these can be read off from Eq.24 but will be given explicitly later.

$$\frac{1}{\hbar}S[p(t),q(t)] = \int d\tau \left[\frac{1}{2}a_1\dot{p}^2 + \frac{1}{2}b_1\dot{q}^2 + \frac{1}{4}a_2\left(p^2 - 1\right)^2 + \frac{1}{4}b_2\left(q^2 - 1\right)^2 + \frac{1}{2}c\left(p^2 - 1\right)\left(q^2 - 1\right)\right].$$
(31)

$$a_1 = \frac{m_p x_0^2}{\hbar}, \ a_2 = \frac{m_p x_0^2 \omega_p^2}{2\hbar}, \ b_1 = \frac{m_q y_0^2}{\hbar}, \ b_2 = \frac{m_q y_0^2 \omega_q^2}{2\hbar}.$$
 (32)

The interaction operates only briefly at t = 0 (or, rather, t = t' for arbitrary t') and then rapidly turns itself off. For c = 0 two decoupled instantons mediate between their respective vacuum states at $p = \pm 1$ and $q = \pm 1$. As per the semi-classical prescription, the action S[p,q] in Eq.31 is expanded in a functional Taylor series around the classical path up to and including quadratic terms, $S = S_0 + S_1 + S_2$. The remainder can then be treated perturbatively.

$$S[p,q] = S[p_c,q_c] + \int dt' \left[\frac{\delta S}{\delta p} \eta + \frac{\delta S}{\delta q} \xi \right] + \frac{1}{2} \int dt' dt'' \left[\frac{\delta^2 S}{\delta p \delta p} \eta \eta + \frac{\delta^2 S}{\delta q \delta q} \xi \xi + 2 \frac{\delta^2 S}{\delta p \delta q} \eta \xi + \cdots \right]$$
(33)

To be integrated over are the arbitrary deviations from the classical path $\eta = p - p_c$ and $\xi = q - q_c$. These must obey the end point conditions,

$$\eta(-T/2) = \eta(T/2) = \xi(-T/2) = \xi(T/2) = 0.$$
(34)

Some algebra gives,

$$S_{0} = \int dt \left[\frac{1}{2} a_{1} \dot{p}_{c}^{2} + \frac{1}{2} b_{1} \dot{q}_{c}^{2} + \frac{1}{4} a_{2} \left(p_{c}^{2} - 1 \right)^{2} + \frac{1}{4} b_{2} \left(q_{c}^{2} - 1 \right)^{2} + \frac{1}{2} c \left(p_{c}^{2} - 1 \right) \left(q_{c}^{2} - 1 \right) \right], \qquad (35)$$

$$S_1 = \int dt \left[a_1 \dot{p}_c \dot{\eta} + b_1 \dot{q}_c \dot{\xi} + a_2 p_c (p_c^2 - 1)\eta + c p_c (q_c^2 - 1)\eta + b_2 q_c (q_c^2 - 1)\xi + c q_c (p_c^2 - 1)\xi \right].$$
(36)

$$S_2 = \int dt \left[\frac{a_1}{2} \dot{\eta}^2 + \frac{a_2}{2} (3p_c^2 - 1)\eta^2 + \frac{b_1}{2} \dot{\xi}^2 + \frac{b_2}{2} (3q_c^2 - 1)\xi^2 + \frac{c}{2} (q_c^2 - 1)\eta^2 + \frac{c}{2} (p_c^2 - 1)\xi^2 + 2cp_c q_c \eta \xi \right]$$
(37)

Vanishing of the first order variation, i.e. $S_1 = 0$, yields the coupled Euler-Lagrange equations for p_c and q_c ,

$$\frac{d^2 p_c}{dt^2} = \frac{a_2}{a_1} (p_c^2 - 1) p_c + \frac{c}{a_1} (q_c^2 - 1) p_c$$
$$\equiv \frac{\kappa^2}{2} (p_c^2 - 1) p_c + \mu^2 (q_c^2 - 1) p_c \qquad (38)$$

$$\frac{d^2 q_c}{dt^2} = \frac{b_2}{b_1} (q_c^2 - 1)q_c + \frac{c}{b_1} (p_c^2 - 1)q_c$$
$$\equiv \frac{\epsilon^2}{2} (q_c^2 - 1)q_c + \nu^2 (p_c^2 - 1)q_c \qquad (39)$$

The definitions used above are,

$$\kappa^2 \equiv \frac{2a_2}{a_1} = \omega_p^2, \ \epsilon^2 \equiv \frac{2b_2}{b_1} = \omega_q^2, \ \mu^2 = \frac{c}{a_1}, \ \nu^2 = \frac{c}{b_1}$$
(40)

Together with an overall scale factor, the four parameters $\kappa, \epsilon, \mu, \nu$ form a set equivalent to a_1, a_2, b_1, b_2, c . The former set is more suited for discussing approximate solutions to the EOM's above. For $\mu = \nu = 0$, the solutions are,

$$p_c^0(t) = \tanh \kappa \frac{t - t'}{2}, \ q_c^0(t) = \tanh \epsilon \frac{t - t''}{2}.$$
 (41)

Intuitively this corresponds to two independent instantons, each rolling down separate hills starting from the respective hilltop on which it was placed and reaching the other in the same time T. These hills are, of course, the hills of the inverted potential shown in Fig.1. As in Eq.8 the times t', t'' are arbitrary in the $T \to \infty$ limit. They are also independent of each other so one instanton may have nearly completed its journey to the opposite peak even as the other has barely begun to move.

For $c \neq 0$ the picture changes. Insight into the coupled system can be obtained by noting that the Euclidean energy $E \equiv -T + V$ is conserved at the classical (but not quantum) level. Writing down E,

$$E = -\frac{1}{2}a_1\dot{p}_c^2 - \frac{1}{2}b_1\dot{q}_c^2 + \frac{1}{4}a_2\left(p_c^2 - 1\right)^2 + \frac{1}{4}b_2\left(q_c^2 - 1\right)^2 + \frac{1}{2}c\left(p_c^2 - 1\right)\left(q_c^2 - 1\right), \qquad (42)$$

then taking the derivative and using the EOM's in Eqs. 38,39 yields,

$$\frac{dE}{dt} = 0. \tag{43}$$

It trivially follows that,

$$S_0 = \int_{-\infty}^{\infty} dt [a_1 \dot{p}_c^2(t) + b_1 \dot{q}_c^2(t)] = a_1 ||\dot{p}_c||^2 + b_1 ||\dot{q}_c||^2 \quad (44)$$

The fact that one may compute S_0 either from Eq.44 or from Eq.35 will turn out to be a valuable check on the correctness of approximations made in solving the EOMs as well as the subsequent integrations; the values must agree order by order. Energy conservation also means that we cannot consider the p, q instantons to move independently, i.e. $t' = t'' = t_c$ in Eq. 41 and there is only one common arbitrary time t_c . It follows that there can be only zero mode. To obtain the eigenfunction for zero eigenvalue, consider solutions of the EOM for $p_c(t, t_c), q_c(t, t_c)$ centred at $t = t_c$. This origin is arbitrary and so shifting it by any amount leaves the action unchanged. Suppose the shift is by an infinitesimal amount δt_c , i.e. $t_c \to t_c + \delta t_c$. Then,

$$S[p_{c}(t, t_{c} + \delta t_{c}), q_{c}(t, t_{c} + \delta t_{c})] = S[p_{c}(t, t_{c}), q_{c}(t, t_{c})]$$
(45)

The above condition can be expanded out using the chain rule:

$$0 = \int dt \left[\frac{\delta S}{\delta p_c(t)} \frac{\partial p_c(t)}{\partial t_c} + \frac{\delta S}{\delta q_c(t)} \frac{\partial q_c(t)}{\partial t_c} \right] \delta t_c + \int dt dt' \left[\frac{1}{2} \frac{\partial p_c(t)}{\partial t_c} \frac{\delta^2 S}{\delta p_c(t) \delta p_c(t')} \frac{\partial p_c(t')}{\partial t_c} + \frac{1}{2} \frac{\partial q_c(t)}{\partial t_c} \frac{\delta^2 S}{\delta q_c(t) \delta q_c(t')} \frac{\partial q_c(t')}{\partial t_c} + \frac{\partial p_c(t)}{\partial t_c} \frac{\delta^2 S}{\delta p_c(t) \delta q_c(t')} \frac{\partial q_c(t')}{\partial t_c} \right] \delta t_c^2 (46)$$

The first term on the RHS above is zero because we have required that the first order variations vanish, and hence the second term in Eq. 46 is also zero. After some simplification we see that the eigenvector,

$$\begin{bmatrix} \frac{dp_c}{dt} \\ \frac{dq_c}{dt} \end{bmatrix}$$
(47)

is annihilated by the matrix M,

$$\begin{bmatrix} M_{pp} & M_{pq} \\ M_{qp} & M_{qq} \end{bmatrix} \begin{bmatrix} \frac{dp_c}{dt} \\ \frac{dq_c}{dt} \end{bmatrix} = 0,$$
(48)

the entries of which are,

$$M_{pp} = -\frac{a_1}{2}\frac{d^2}{dt^2} + \frac{a_2}{2}(3p_c^2 - 1) + \frac{c}{2}(q_c^2 - 1) \quad (49)$$

$$M_{qq} = -\frac{b_1}{2}\frac{d^2}{dt^2} + \frac{b_2}{2}(3q_c^2 - 1) + \frac{c}{2}(p_c^2 - 1) \quad (50)$$

$$M_{pq} = M_{qp} = c p_c q_c \tag{51}$$

The normalized zero mode eigenfunction at leading order has components,

$$\sqrt{\frac{3\kappa}{8}}\mathrm{sech}^2\frac{\kappa t}{2}, \ \sqrt{\frac{3\epsilon}{8}}\mathrm{sech}^2\frac{\epsilon t}{2}.$$
 (52)

At next to leading order to get the zero mode eigenfunctions requires solving a pair of coupled non-linear equations. This could be done along the lines to be discussed in the next section. However such explicit solutions will not be needed here.

IV. SOLVING THE EOM'S

We shall now solve the coupled equations of motion Eqs. 38-39 to obtain the classical solutions $p_c(t), q_c(t)$. Various cases will be distinguished according to the different boundary conditions imposed upon them. As discussed in the preceding section, the same arbitrary time t_c characterizes both. For brevity this will be left implicit. The null solution $p_c^2=1,q_c^2=1$ obviously satisfies the EOM's. However it is uninteresting since this corresponds to zero action. For an arbitrary choice of parameters, the coupled non-linear system does not admit exact solutions. In general solving non-linear equations analytically, even approximately, is a daunting task. However the topological protection offered by the EOM's makes progress possible because for $t \to \pm \infty$, both p and q necessarily tend to their asymptotic values $p^2 = 1$, $q^2 = 1$. Therefore all deviations from the non-interacting case can occur only for small t.

To get analytical solutions it seems necessary to assume the existence of one large parameter κ ,

$$\kappa \gg \epsilon, \mu, \nu$$
 (53)

This means one instanton will transition much faster than

the other. For now we shall not assume any hierarchy of sizes between ϵ, μ, ν . The basic solutions of the EOM's fall into 3 types or flavors, denoted here by P, Q, R. For the P type, the p instanton gives the dominant contribution to the action. For the Q type it is the q instanton, and for the R type both contribute maximally. P, Q will sometimes be referred to respectively as fast/slow. In the context of the diatomic molecule considered earlier, P mediates a flip but no cm tunneling, Q causes cm tunneling but no flip, while R results in both cm tunneling and a flip.

As a final remark: the p, q parts of the action seem to correspond to two separate energy bumps but both start their travel and end it at the same time. Hence it is proper to speak of a single energy transporting bump (instanton) with three flavors.

A. P type

With the *P* instanton supplying the background, let us first investigate whether there can exist a stable *q* solution. More precisely, we ask whether the coupled system admits solutions satisfying $p_c(-T/2) = -1$, $p_c(T/2) = 1$ together with $q_c(\mp T/2) = -1$. This corresponds to the *p* instanton going over to its other hilltop while *q* returns to its initial position without touching the other peak. To this end insert into Eq. 39 the ansatz,

$$p_c^0(t) = \tanh \frac{\kappa t}{2}, \ q_c(t) = -1 + \alpha(t).$$
 (54)

Assuming $\alpha \ll 1$ gives the linearized equation for α ,

$$\frac{d^2\alpha}{dt^2} = \epsilon^2 \alpha - \nu^2 \operatorname{sech}^2 \frac{\kappa t}{2} (-1 + \alpha)$$
$$\approx \epsilon^2 \alpha + \nu^2 \operatorname{sech}^2 \frac{\kappa t}{2}.$$
(55)

Though apparently simple, the above equation leads to an opaque solution expressed in terms of hypergeometric functions. However the assumption $\kappa \gg \epsilon$ leads to a drastic simplification because the forcing term becomes a blip perturbation around t = 0 lasting for $O(1/\kappa)$, far shorter than the decay time scale $O(1/\epsilon)$ set by the first term. Using the homogeneous equation's propagator,

$$G_{\epsilon}(t,t') = -\frac{1}{2\epsilon} e^{-\epsilon|t-t'|}, \qquad (56)$$

and performing the required integrals gives,

$$\alpha(t) = -\frac{2\nu^2}{\kappa\epsilon} \left(\cosh\epsilon t - \sinh\epsilon t \tanh\frac{t\kappa}{2}\right).$$
 (57)

The large κ limit gives a simple form for q_c ,

$$q_c(t) = -1 - \frac{2\nu^2}{\kappa\epsilon} e^{-\epsilon|t|}$$
(58)

This confirms the stability of the q solution as well as our assumption of linearity, $\alpha \ll 1$.

With the improved q solution in hand, the back reaction on P can be calculated from Eq.38 with the ansatz,

$$p_c(t) = (1+f) \tanh \frac{\kappa t}{2} \tag{59}$$

Here it is presumed that $f(t) \ll 1$, satisfies $\dot{f}/f \sim \epsilon$ (i.e. varies slowly on the scale $O(1/\kappa)$, and vanishes at infinity, $f(\pm \infty = 0)$. Inserting into Eq.38 gives,

$$\ddot{f} - \kappa^2 f - \frac{4\mu^2 \nu^2}{\kappa^3 \epsilon} e^{-t\epsilon} = 0, \qquad (60)$$

To leading order the solution for p_c is,

$$p_c(t) = \left(1 - \frac{4\mu^2 \nu^2}{\kappa^3 \epsilon} e^{-\epsilon|t|}\right) \tanh \frac{1}{2}\kappa t \tag{61}$$



FIG. 2. **P** instanton : The dashed curve is the background instanton $p_c^0(t)$, the solid bottom curve is the motion this induces in $q_c(t)$, and the solid upper curve shows the back reaction on $p_c(t)$. The parameters used are: $\kappa = 1, \epsilon = \mu = \nu = 0.4$.

From these approximate solutions for p_c and q_c in the P case, the respective norms of \dot{p}, \dot{q} are calculated to be:

$$||\dot{p}_{c}||^{2} = \int dt \, \dot{p}_{c}^{2} = \frac{2\kappa}{3} - \frac{16\mu^{2}\nu^{2}}{3\kappa^{2}\epsilon}$$
(62)

$$|\dot{q}_c||^2 = \frac{4\nu^*}{\kappa^2\epsilon}.$$
(63)

From Eq.44 the action S_P follows,

$$S_P = a_1 ||\dot{p}_c||^2 + b_1 ||\dot{q}_c||^2 \tag{64}$$

$$= \sqrt{\frac{8a_1a_2}{9}} \left(1 - \frac{\sqrt{a_1}}{2a_2^{3/2}\sqrt{b_1b_2}}c^2 \right).$$
(65)

Unsurprisingly all five parameters a_1, a_2, b_1, b_2, c of the action are needed; the four ratios $\kappa, \epsilon, \mu, \nu$ do not include the overall energy scale.

B. Q type

The slowly varying Q instanton provides the background field for the p variable. To solve let,

$$p_c(t) = -1 + \beta(t), \ q_c^0(t) = \tanh \frac{\epsilon t}{2}.$$
 (66)

Linearization yields,

$$\ddot{\beta} - \kappa^2 \beta = \mu^2 \mathrm{sech}^2 \frac{\epsilon t}{2}.$$
(67)

For large κ this can be solved iteratively,

$$\beta = -\frac{\mu^2}{\kappa^2} \operatorname{sech}^2 \frac{\epsilon t}{2} + \cdots$$
 (68)

The back reaction on q_c requires solving,

$$\frac{d^2 q_c}{dt^2} = \frac{1}{2} \epsilon^2 (q_c^2 - 1) q_c + \frac{2\mu^2 \nu^2}{\kappa^2} q_c \operatorname{sech}^2 \frac{t\epsilon}{2}.$$
 (69)

The forcing term on the RHS above being small, and the characteristic decay time of $O(1/\epsilon)$ being long, the ansatz below becomes appropriate:

$$q_c = \tanh\frac{\epsilon t}{2} + f(t)\mathrm{sech}^2\frac{\epsilon t}{2}.$$
 (70)

Inserting this into Eq.69 and linearizing in f yields,

$$\ddot{f} - 2\epsilon\dot{f} - \frac{2\mu^2\nu^2}{\kappa^2} = 0,$$
 (71)

whose solution is,

$$f(t) = -\frac{\mu^2 \nu^2}{\epsilon \kappa^2} t. \tag{72}$$



FIG. 3. **Q** instanton : The dashed curve is the background instanton $q_c^0(t)$, the solid bottom curve is the motion this induces in $p_c(t)$, and the dashed curve shows the back reaction on $q_c(t)$. The parameters used are: $\kappa = 1, \epsilon = \mu = \nu = 0.4$.

We have thus arrived at the back-reaction corrected solutions for the Q system:

$$p_c = -1 - \frac{\mu^2}{\kappa^2} \operatorname{sech}^2 \frac{\epsilon t}{2}$$
(73)

$$c = \tanh \frac{\epsilon t}{2} - \frac{\mu^2 \nu^2}{\epsilon \kappa^2} t \operatorname{sech}^2 \frac{\epsilon t}{2}$$
 (74)

The norms of \dot{p}, \dot{q} at leading order follow:

$$||\dot{p}_{c}||^{2} = \frac{8\epsilon\mu^{4}}{15\kappa^{4}},$$
 (75)

$$||\dot{q}_{c}||^{2} = \frac{2\epsilon}{3} - \frac{4\mu^{2}\nu^{2}}{3\epsilon\kappa^{2}},$$
 (76)

as well as the action,

q

$$S_Q = \sqrt{\frac{8b_1b_2}{9}} \left(1 + \frac{\frac{2a_1}{b_1} - \frac{5a_2}{b_2}}{10a_2^2} c^2 \right)$$
(77)

C. R type

Finally, consider the system where both p, q transit to their respective opposite hills, $(-1, -1) \rightarrow (1, 1)$. The P, Q pair moves in the background,

$$p_c^0(t) = \tanh\frac{\kappa t}{2}, \ q_c^0(t) = \tanh\frac{\epsilon t}{2}.$$
 (78)

Inserting q_c from above yields, into the RHS of Eq. 38 yields,

$$\frac{d^2 p_c}{dt^2} = \frac{1}{2} \kappa^2 (p_c^2 - 1) p_c - \mu^2 \mathrm{sech}^2 \frac{\epsilon t}{2} p_c.$$
(79)

The slowly varying perturbation of the q instanton suggest the following ansatz for p_c ,

$$p_c = (1+g) \tanh\left[\frac{\kappa t}{2}(1+g)\right],\tag{80}$$

where g(t) is small and dies off slowly on the scale $O(1/\epsilon)$. A suitable candidate for g is,

$$g(t) = c \operatorname{sech}^2 \frac{t\epsilon}{2}.$$
(81)

Inserting into Eq.79 and linearizing in c gives, $c = \mu^2 / \kappa^2$. For q_c in the background of p_c^0 we must solve,

$$\frac{d^2 q_c}{dt^2} = \frac{1}{2} \epsilon^2 (q_c^2 - 1) q_c - \nu^2 \mathrm{sech}^2 \frac{\kappa t}{2} q_c.$$
(82)

together with a similar ansatz for q_c ,

$$q_c = (1+h) \tanh \frac{\epsilon t}{2}.$$
(83)

However the sudden perturbation results in a very different response,

$$h(t) = \frac{4\nu^2}{\kappa^2} \left[\frac{\kappa |t|}{2} - \log\left(2\cosh\frac{\kappa t}{2}\right) \right]$$
(84)

$$= -\frac{4\nu^2}{\kappa^2}e^{-\kappa t} + \cdots \text{ for } t \gg \kappa^{-1}.$$
 (85)

In summary, for the R system the corrected solutions are,

$$p_c = \left(1 + \frac{\mu^2}{\kappa^2} \operatorname{sech}^2 \frac{t\epsilon}{2}\right) \tanh \frac{\kappa t}{2} \tag{86}$$

$$q_c = \left(1 + \frac{4\nu^2}{\kappa^2} \left\lfloor \frac{\kappa |t|}{2} - \log\left(2\cosh\frac{\kappa t}{2}\right) \right\rfloor\right) \tanh\frac{\epsilon t}{2}(87)$$



FIG. 4. **R** instanton : The upper dashed curve is $p_c^0(t)$, the lower dotted curve is $q_c^0(t)$. They are, respectively, backgrounds for the upper/lower curves which represent $p_c(t), q_c(t)$. The parameters used are: $\kappa = 1, \epsilon = \mu = \nu = 0.4$.

The above lead to

$$||\dot{p}_{c}||^{2} = \frac{2\kappa}{3} \left(1 + \frac{4\mu^{2}}{\kappa^{2}} + \cdots \right)$$
 (88)

$$||\dot{q}_c||^2 = \frac{2\epsilon}{3} \left(1 + \frac{6\epsilon\nu^2}{\kappa^3}\right) + \cdots$$
 (89)

and the R system's action,

$$S_R = \sqrt{\frac{8a_1a_2}{9}} + \sqrt{\frac{8b_1b_2}{9}} + \frac{4}{3}\sqrt{\frac{2a_1}{a_2}}\left(1 + \frac{3a_1b_2}{2a_2b_1}\right)c \quad (90)$$

As a final comment: one can see from the expressions derived in this section for S_P , S_Q , S_R , that if one sets c =0 then the action is purely that of a single independent instanton. For P it is $8a_1a_2/9$, for Q it is $8b_1b_2/9$, aand for R it is the sum of these two actions.

V. ZERO MODE REMOVAL

Up to the present point we have engaged only with the linear term in the functional expansion for the action Eq. 33 but for calculating the Feynman amplitude \mathscr{A} one must integrate over all fluctuations around the classical path. This entails dealing with the zero mode issue. For c = 0, i.e. non-interacting instantons, the p and q dof's will have two independent zero modes since either can be arbitrarily displaced in time. However, for $c \neq 0$ there is only one. In fact we have already seen how that single zero mode eigenfunction can be calculated explicitly via Eq.48. We shall eliminate the zero mode in the present case using the Fadeev-Popov procedure. This, adapted to the single instanton case by Zinn-Justin [16], is well suited here as well for getting the correct pre-factor. The starting point is the identity,

$$\frac{1}{\sqrt{2\pi\mu}} \int_{-\infty}^{\infty} d\lambda \ e^{-\frac{\lambda^2}{2\mu}} = 1, \tag{91}$$

The arbitrary parameter μ will eventually disappear from the final result. Make the following particular choice for the integration variable λ ,

$$\lambda = \int dt \big(a_1 \dot{p}_c(t) [p(t+t^*) - p_c(t)] + b_1 \dot{q}_c(t) [q(t+t^*) - q_c(t)] \big)$$
(92)

Here t^* is chosen arbitrarily with the intent of breaking the invariance of the action under time translations. This particular form of unity in Eq.91 is then inserted into the path integral after which, following ref.[16], similar manipulations are performed. These result in the parameter t^* disappearing from the effective action and being replaced by an overall factor of T. A new form for the amplitude \mathscr{A} then emerges:

$$\mathscr{A} = \frac{T}{\sqrt{2\pi\mu}} \left(a_1 ||\dot{p}_c||^2 + b_1 ||\dot{q}_c||^2 \right) \mathscr{N} \int [d\eta] [d\xi] \ e^{-S_{\mu}}$$
(93)

As before η and ξ are deviations from the classical paths p_c, q_c . The μ dependent action S_{μ} is,

$$S_{\mu} = S_0 + S_2 + \frac{\hbar}{2\mu} \left[\int dt (a_1 \dot{p}_c \eta + b_1 \dot{q}_c \xi) \right]^2.$$
(94)

The first derivative of S_{μ} with respect to η and ξ vanishes for $\eta = \xi = 0$, i.e. there is no linear term in the expansion of S_{μ} . Thus no change needs to be made in the results of the previous section. While the first two terms in Eq.94 are time translation invariant the last one is not. Hence S_{μ} does not have a zero mode. Let $\{\phi_n(t)\}, \{\chi_n(t)\}$ be two complete basis sets of functions for expanding $\eta(t), \xi(t)$:

$$\eta = \sum_{n=0}^{\infty} a_n \phi_n, \quad \xi = \sum_{n=0}^{\infty} b_n \chi_n. \tag{95}$$

 ϕ_n and χ_n are, respectively, eigenfunctions of the operators \hat{O}_{η} and \hat{O}_{ξ} ,

$$\hat{O}_{\eta} = -\frac{d^2}{dt^2} + \frac{\kappa^2}{2}(3p_c^2 - 1)$$
(96)

$$\hat{O}_{\xi} = -\frac{d^2}{dt^2} + \frac{\epsilon^2}{2}(3q_c^2 - 1).$$
(97)

The corresponding eigenvalues are λ_n and $\tilde{\lambda}_n$, and the normalization rules are,

$$\langle f|g\rangle = \int_{-\tilde{T}/2}^{\bar{T}/2} dt \ f^*(t)g(t) \tag{98}$$

$$\langle \phi_n | \phi_m \rangle = \delta_{nm}, \ \langle \chi_n | \chi_m \rangle = \delta_{nm}$$
 (99)

Apart from a_0, b_0 , the expansion coefficients a_n, b_n are independent variables for all other n. From Eq.48 it is evident that $a_0 = b_0$ else time translational invariance will be violated. Inserting the expansion Eq.95 into Eq.93 and performing the integral over a_0 yields,

$$\mathscr{A} = \frac{T}{\sqrt{2\pi}} \frac{S_0}{a_1 ||\dot{p}_c|| + b_1 ||\dot{q}_c||} \times e^{-S_0} \mathscr{N} \int [DaDb]' e^{-S_2}$$
(100)

In arriving at the above equation the expression Eq.44 for S_0 has been used. The first factor in Eq.100 is essentially the Jacobian for the case of two dof's. In the second factor the primes on the functional measure indicate that zero mode coefficients a_0, b_0 must be excluded. Note that the arbitrary parameter μ has disappeared. For a single dof, eg. for p only, the first factor above gives back the standard result for the Jacobian:

$$\mathscr{A} = T\sqrt{\frac{S_0}{2\pi a_1}} \times e^{-S_0} \mathscr{N} \int [Da]' e^{-S_2}$$
(101)

At the next step, the integrations in Eq.100 must be performed. This requires splitting S_2 in Eq.37 into its diagonal and non-diagonal parts,

$$S_2 = S_{2D} + \delta S_2. \tag{102}$$

The diagonal part is,

$$S_{2D} = \frac{1}{2} \sum_{n}^{\prime} (\omega_n a_n^2 + \tilde{\omega}_n b_n^2)$$
(103)

$$\omega_n = a_1 \lambda_n, \quad \tilde{\omega}_n = b_1 \tilde{\lambda}_n \tag{104}$$

The non-diagonal part δS_2 is conveniently expressed in matrix form,

$$\delta S_2 = \mathbf{a} \cdot \mathbf{U} \cdot \mathbf{a} + \mathbf{b} \cdot \mathbf{V} \cdot \mathbf{b} + \mathbf{a} \cdot \mathbf{W} \cdot \mathbf{b}$$
(105)

$$U_{nm} = \frac{c}{2a_1} \langle \phi_n(q_c^2 - 1)\phi_m \rangle = \frac{\mu^2}{2} \langle \phi_n(q_c^2 - 1)\phi_m \rangle (106)$$

$$V_{nm} = \frac{c}{2b_1} \langle \chi_n(p_c^2 - 1)\chi_m \rangle = \frac{\nu^2}{2} \langle \chi_n(p_c^2 - 1)\chi_m \rangle (107)$$

$$W_{nm} = \frac{2c}{\sqrt{a_1 b_1}} \langle \phi_n p_c q_c \chi_m \rangle = 2\mu \nu \langle \phi_n p_c q_c \chi_m \rangle \qquad (108)$$

While U, V are self interactions, W owes to the interaction between fluctuations associated with the p and qdegrees of freedom. Further, U, V are determined over "distances" of order ϵ^{-1} and κ^{-1} respectively but the range of W is infinite because $p_c, q_c \to \pm 1$ as $t \to \pm \infty$. Note also that U_{nm}, V_{nm} have large off-diagonal matrix elements but W_{nm} is almost diagonal.

VI. FLUCTUATION DETERMINANT

Before proceeding to the case where there is one or more instanton, it is necessary to consider the zero instanton case. In fact this will be needed to deal with the problem mentioned in the lines above. The linear part of the action (see Eq.36) vanishes for the trivial solution of the EOM, $p_c = \pm 1$ and $q_c = \pm 1$. However the quadratic part Eq.37 does not. Moreover one sees here a feature that is absent in the single dof case, namely an interaction now exists between p and q and so pure harmonic oscillators do not exist anywhere inside the [-T/2, T/2]interval. There is, of course, no zero eigenvalue and one may expand the fluctuations η, ξ :

$$\eta = \sqrt{\frac{2}{T}} \sum_{n} a_n \sin k_n t, \ \xi = \sqrt{\frac{2}{T}} \sum_{n} b_n \sin k_n t, \ k_n = \frac{n\pi}{T}$$

This gives the zero instanton quadratic action,

$$S_{\text{zero}} = \frac{1}{2} \sum_{n} \left[a_n^2 \lambda_n + b_n^2 \tilde{\lambda}_n \pm 4c a_n b_n \right], \qquad (109)$$

$$\lambda_n = a_1 \left(k_n^2 + \kappa^2 \right), \quad \tilde{\lambda}_n = b_1 \left(k_n^2 + \epsilon^2 \right).$$
(110)

Keeping only the leading order in c, the functional integral is easily done,

$$R_{0} = \mathcal{N}' \int [da][db] \exp\left[-\frac{1}{2} \sum_{n} (\lambda_{n} a_{n}^{2} + \tilde{\lambda}_{n} b_{n}^{2} \pm 4ca_{n} b_{n})\right]$$
$$= \mathcal{N}' \prod_{n=1}^{\infty} \frac{1}{\sqrt{\lambda_{n}}} \prod_{n=1}^{\infty} \frac{1}{\sqrt{\tilde{\lambda}_{n}}} \prod_{n=1}^{\infty} \left(1 + \frac{2c^{2}}{\lambda_{n} \tilde{\lambda}_{n}} + \cdots\right) (111)$$

The first product splits further into two products,

$$\prod_{a=1}^{\infty} \frac{1}{\sqrt{\lambda_n}} = \mathcal{N}_a \times F,$$

$$\mathcal{N}_a = \prod_{n=1}^{\infty} \left(\frac{T}{a_1^{\frac{1}{2}} n \pi}\right), \quad F = \prod_{n=1}^{\infty} \frac{k_n}{\sqrt{k_n^2 + \kappa^2}}.$$
(112)

One may now take the logarithm of F, convert the product into a sum, and then convert that sum into an integral by using,

$$\sum_{n} \to \frac{T}{\pi} \int dk.$$
 (114)

Performing the integral yields,

r

$$F = \exp\left[-\frac{\kappa T}{2}\right].$$
 (115)

The same procedure is then applied to the other two factors in Eq.112. The normalization constants are then matched against those of two free particles, i.e. in the limit where $\kappa, \epsilon, c \to 0$. Using the constants μ, ν in Eq.40 yields the final form for R_0 ,

$$R_0 = \mathcal{N}' \mathcal{N}_a \mathcal{N}_b \exp\left[-(\kappa + \epsilon)\frac{T}{2} + \frac{\mu^2 \nu^2}{\kappa \epsilon (\kappa + \epsilon)}T\right] = \frac{\sqrt[4]{2a_1 a_2}}{\sqrt{\pi} x_0} \frac{\sqrt[4]{2b_1 b_2}}{\sqrt{\pi} y_0} \exp\left[-(\kappa + \epsilon)\frac{T}{2} + \frac{\mu^2 \nu^2}{\kappa \epsilon (\kappa + \epsilon)}T\right]$$
(116)

Although the energy $\mu^2 \nu^2 / [\kappa \epsilon (\kappa + \epsilon)]$ in the above exponent has emerged here from performing the functional integral, one can check that in fact it is the second order perturbation theory correction to the energy of two weakly interacting harmonic oscillators. In contrast, for a single dof one has a pure (uncoupled) oscillator.

Now consider quadratic fluctuations in the presence of a single instanton. This is different from the zero instanton case in two important ways. First, now there is a zero eigenvalue and so the functional integral below excludes integration over a_0, b_0 .

$$\mathcal{N}' \int [da]' [db]' e^{-S_2} = \mathcal{N}' \int [da]' [db]' e^{-S_D} e^{-\delta S_2}$$
$$= \mathcal{N}' \int [da]' [db]' e^{-S_D} \left(1 - \delta S_2 + \frac{1}{2} \delta S_2^2 + \cdots \right) \quad (117)$$

Second, the expanded exponential contains the interaction W. Since the $p_c^2 = q_c^2 = 1$ case was already included in calculating R_0 , this is modified to,

$$W_{nm} = 2\mu\nu\langle\phi_n(p_cq_c-1)\chi_m\rangle.$$
 (118)

(The above modification is relevant only for the R instanton; by parity the matrix element vanishes for P, Q.)

Performing the Gaussian integrations over a_n, b_n yields,

$$\mathcal{N}' \int \left[\frac{da}{\sqrt{2\pi}}\right]' \left[\frac{db}{\sqrt{2\pi}}\right]' e^{-S_2} = \frac{\mathcal{N}'}{\sqrt{\det'\hat{\omega}_\eta} \sqrt{\det'\hat{\omega}_\xi}} F_c.$$
(119)

The operators $\hat{\omega}_{\eta}, \hat{\omega}_{\xi}$ and their indicated determinants are,

$$\hat{\omega}_{\eta} = a_1 \hat{O}_{\eta}, \quad \hat{\omega}_{\xi} = b_1 \hat{O}_{\xi}, \quad (120)$$

$$\det' \hat{\omega}_{\eta} = \prod_{n=1}^{\infty} \omega_n, \ \det' \hat{\omega}_{\xi} = \prod_{n=1}^{\infty} \tilde{\omega}_n.$$
(121)

The single instanton amplitude for each flavor decomposes into three readily identifiable factors:

$$\mathscr{A}_i = R_0 K_i T$$
 where $i = P, Q, R.$ (122)

 K_i is the Jacobian factor weighted by $e^{-S_{0i}}$,

$$K_{i} = \frac{12}{\sqrt{2\pi}} \frac{\kappa \epsilon \sqrt{a_{1}b_{1}} S_{0i} e^{-S_{0i}}}{a_{1} ||\dot{p}_{ci}|| + b_{1} ||\dot{q}_{ci}||} F_{ci}$$
(123)

This result is key. R_0 is flavor independent and comes from the interacting SHO's with frequencies κ, ϵ . It is determined by the wavefunction at the center of a well (see remark below Eq.30). Flavor dependence resides entirely in K_i with each flavor having its own action S_0 and values for $||\dot{p}_c||, ||\dot{q}_c||$. These were computed in Section IV by solving the coupled EOM's. Finally, the *T* factor reminds us that each instanton can be placed anywhere in the interval (-T/2, T/2) because of time translation invariance and so its contribution will be proportional to the "volume" in which it can exist. In the limit $T \to \infty$ the contribution of a single instanton vanishes because $se^{-s} \to 0$ as $s \to 0$.

With the understanding that all sums exclude n = 0, the product of determinants is corrected by the factor F_c . Doing the integrals over a_n, b_n after expanding the exponential yields, up to second order,

$$F_{c} = 1 - \sum_{n} \frac{U_{nn}}{\lambda_{n}} + \frac{1}{2} \left(\sum_{n} \frac{U_{nn}}{\lambda_{n}} \right)^{2} + \sum_{nm} \frac{U_{nm}^{2}}{\lambda_{m}\lambda_{n}} - \sum_{m} \frac{V_{nn}}{\tilde{\lambda}_{n}} + \frac{1}{2} \left(\sum_{n} \frac{V_{nn}}{\tilde{\lambda}_{n}} \right)^{2} + \sum_{nm} \frac{V_{nm}^{2}}{\tilde{\lambda}_{m}\tilde{\lambda}_{n}} + \frac{1}{2} \sum_{nm} \frac{W_{nm}^{2}}{\lambda_{n}\tilde{\lambda}_{m}} + \cdots$$
(124)

Calculating the single and double sums in F_c requires knowledge of the two-point propagator G_{κ} (and similarly G_{ϵ}) connecting two time-separated points:

$$G_{\kappa}(t,t') = \sum_{n \neq 0} \frac{\phi_n(t)\phi_n(t')}{\lambda_n}.$$
 (125)

The presence of a zero mode means computing $G_{\kappa}(t,t')$

for the Poschl-Teller potential takes effort. After this paper was completed we became aware that other authors had obtained the propagator as well. The first attempt was by Aleinikov and Shuryak[20]. That this contained errors was pointed out by Olejnik[21]. Our result matches Olejnik's exactly in the limit $T \to \infty$ which, indeed, what the instanton procedure requires at the end of the calcu-

lation. However, strictly speaking there is no zero mode for any finite T and so in principle the solutions of the differential equation for G should vanish at finite T. Because our result was derived somewhat differently from Olejnik's and because we shall need a form more suited for calculating F_c in Eq.124, it is appropriate to briefly discuss the propagator here.

We begin by specifying the differential operator $\hat{\mathscr{L}}$ of which ϕ_n are the eigenfunctions,

$$\hat{\mathscr{L}}\phi_n = \lambda_n \phi_n, \quad \phi_n(\pm T/2) = 0$$
 (126)

$$\hat{\mathscr{L}} = -\frac{d^2}{dt^2} + \kappa^2 \left(1 - \frac{3}{2} \mathrm{sech}^2 \frac{\kappa t}{2}\right). \quad (127)$$

Being a Sturm-Liouville system, eigenfunctions belonging to two non-equal eigenvalues are automatically orthogonal but the zero mode is non-zero everywhere and so must be treated differently. Define below the functions f(t), F(t, t'),

$$f(t) = e^{-2\kappa t} + 8e^{-\kappa t} - 6\kappa t$$
 (128)

$$F(t,t') = \frac{3\kappa}{8} \operatorname{sech}^2 \frac{\kappa t}{2} \operatorname{sech}^2 \frac{\kappa t'}{2}, \qquad (129)$$

F(t, t') is the product of the normalized zero mode functions ϕ_0 with the explicit form given in Eq.52, The differential equation for G_{κ} together with boundary and symmetry conditions, readily follows:

$$\hat{\mathscr{L}}G_{\kappa}(t,t') = \delta(t-t') - F(t,t')$$
(130)

$$G_{\kappa}(\pm T/2, \pm T/2) = 0.$$
 (131)

$$G_{\kappa}(t,t') = G_{\kappa}(t',t). \tag{132}$$

In deriving Eqs. 130-132 we have used completeness of $\{\phi_n\}$ and that they vanish at the boundaries. Hence,

$$G_{\kappa}(t,t')\big|_{t^{+}=t'} = G_{\kappa}(t,t')\big|_{t^{-}=t'}$$
(133)

$$\frac{dG}{dt}\Big|_{t^+=t'} - \frac{dG}{dt}\Big|_{t^-=t'} = -1 \tag{134}$$

The symmetrized particular solution of $\hat{\mathscr{L}}G_{\kappa}(t,t') = -F(t,t')$ is,

$$G_{\kappa}(t,t') = \frac{1}{12\kappa^2} F(t,t') \begin{cases} f(t) + f(-t') & t > t' \\ f(-t) + f(t') & t < t' \end{cases}$$
(135)

To the above one may arbitrarily add solutions of the homogeneous equation $\hat{\mathscr{L}}G_{\kappa}(t,t') = 0$. These have the form,

$$[c_0 + c_1[f(t) - f(-t)]][(f(t') - f(-t')]F(t,t').$$
 (136)

The constants c_0, c_1 can be adjusted so that the propagator vanishes at the boundary. But since ϕ_0 never vanishes and exists only in the strict $T \to \infty$ limit, the condition that ϕ_0 is orthogonal to ϕ_n for $n \neq 0$ reduces to the requirement,

$$\int_{-\infty}^{\infty} dt G_{\kappa}(t,t')\phi_0(t') = 0.$$
(137)

This yields $c_0 = -8$, $c_1 = 0$, completing the propagator calculation.

VII. COMPUTING F

With the propagator now in hand, it is fairly straightforward to calculate the seven terms of the correction factor F_c in Eq.124 for U, U^2 terms, for V, V^2 , and W^2 with $p_c q_c \rightarrow p_c q_c - 1$. Prior to executing this calculation, a few remarks are in order. First, for any kernel k(t) a single sum (zero mode excluded!) converts into an integral with a single propagator. This is picturized in Fig.5a while Fig.5b is its square (disconnected diagram).



FIG. 5. Perturbative corrections to the functional determinant. a)First order term where each vertex and line corresponds to one of two interactions and propagators; b)Second order disconnected term; c)Second order connected.

$$\sum_{n} \frac{\langle \phi_n k \phi_n \rangle}{\lambda_n} = \int_{-T/2}^{T/2} dt \ k(t) G_\kappa(t,t).$$
(138)

Since f(t) has finite support only up to $t \sim \epsilon^{-1}$ and $T \gg \epsilon^{-1}$ one may push the integration limits to infinity. The resulting integrals cannot be performed analytically but they can be suitably approximated in the limit $\kappa \gg \epsilon$. Much the same applies to the double sum in Fig.5c which involves two propagators,

$$\sum_{nm} \frac{\langle \phi_n k \phi_m \rangle \langle \phi_n k \phi_m \rangle}{\lambda_n \tilde{\lambda}_m}$$

$$= \int_{-\frac{T}{2}}^{\frac{T}{2}} \int_{-\frac{T}{2}}^{\frac{T}{2}} k(t) G_{\kappa}(t,t') G_{\kappa}(t,t') k(t') dt' dt.$$
(139)

In effect the integrations extend to a distance ϵ^{-1} where $G_{\kappa}(t,t')$ has attained its asymptotic form. Similar remarks can be made for V, V^2 with the difference that f in this case has support for $t \sim \kappa^{-1}$. As for W: without subtracting away the harmonic oscillator contribution we would have been faced with a divergent integral in the $T \to \infty$ limit but after the subtraction it is well behaved.

$$F_P = 1 + \frac{5\nu^2}{8\kappa\epsilon} - \frac{2\mu^2\nu^2}{\kappa^2\epsilon^2} + \frac{75\nu^4}{128\kappa^2\epsilon^2}$$
(140)

$$F_Q = 1 + \frac{\mu^2}{\kappa\epsilon} + \frac{\mu^4}{2\kappa^2\epsilon^2} + \frac{\mu^4}{6\kappa^3\epsilon} - \frac{2\mu^2\nu^2}{\kappa^2\epsilon^2}$$
(141)

$$F_{R} = 1 + \frac{\mu^{2}}{\kappa\epsilon} + \frac{\nu^{2}}{\kappa\epsilon} + \frac{\mu^{*}}{2\kappa^{2}\epsilon^{2}} + \frac{57\nu^{*}}{64\kappa^{2}\epsilon^{2}} + \frac{\mu^{4}}{6\kappa^{3}\epsilon} - \frac{9\mu^{2}\nu^{2}}{2\kappa^{2}\epsilon^{2}} + \frac{2\mu^{2}\nu^{2}}{\kappa^{3}\epsilon} + \frac{5\mu^{2}\nu^{2}\log 4}{2\kappa^{2}\epsilon^{2}} (142)$$

With this the single instanton Feynman amplitude in Eqs.122-123 for all three flavors P, Q, R stands fully determined.

VIII. DILUTE 3-FLAVOR INSTANTON GAS

The classical EOMs admit solutions beyond those considered so far. For one, reversing t gives the antiinstanton of that flavor. For another, any number of well separated instantons and anti-instantons is also a solution if it satisfies the boundary conditions. Extending from the single flavor dilute gas model to three flavors is now our goal. It is picturized in Fig.6.



FIG. 6. A chain of 2-D instantons as they journey from start to end. The edges of a square are the equilibrium points $(p,q) = (\pm 1, \pm 1)$. Each slice has a small but finite thickness corresponding to the instanton width.

The semi-classical prescription requires that one ob-

tain all multi-instanton solutions of the classical EOM's which satisfy the BC's and add up the corresponding amplitudes. A typical multi-instanton has been picturized in Fig.6. If the number of P, Q, R instantons is N = n+m+l then, for sufficiently well separated instantons, the classical action is additive:

$$S_0 = nS_{0P} + mS_{0Q} + lS_{0R}, (143)$$

and the number of possible combinations is,

$$\binom{N}{n m l}.$$
 (144)

This fully takes care of the purely classical part of the action in Eq.35 - no functional integral had to be performed here.

The quadratic fluctuations need more thought. Let $\mathbf{U} = \{U_1, \cdots U_N\}$ be the disjoint, time ordered collection of N time intervals, each interval being roughly one instanton wide. With reference to Eq.37 these are those narrow intervals where p^2, q^2 differ substantially from one. Then the complement \mathbf{U} is the union of those intervals where $p^2 \approx q^2 \approx 1$, i.e. where the time evolution occurs via the SHO Hamiltonian for the p, q dof's. Obviously $\mathbf{U} \cup \mathbf{\bar{U}} = [-T/2, T/2]$. The integration over the fluctuations can be separated into different domains:

$$\int [d\eta d\xi] \exp\left[-\int_{-\frac{T}{2}}^{\frac{T}{2}} dt L[\eta,\xi]\right] = \int [d\eta d\xi] \exp\left[-\sum_{i} \int_{t \in U_{i}} dt L[\eta,\xi]\right] \exp\left[-\sum_{i} \int_{t \in \bar{U}_{i}} dt L[\eta,\xi]\right]$$
(145)
$$\approx \prod \int [d\eta d\xi]_{i} \exp\left[-\int_{t \in U_{i}} dt L[\eta,\xi]\right] \int [d\eta d\xi]_{i} \prod \exp\left[-\int_{t \in \bar{U}_{i}} dt L[\eta,\xi]\right]$$
(146)

$$= J_P^n J_Q^m J_R^l \int [d\eta d\xi] \exp\left[-\int_{t\in\bar{\mathbf{U}}} dt L[\eta,\xi]\right].$$
(147)

The J_i 's with i = P, Q, R are defined as,

$$J_i = \int [d\eta d\xi]_i \exp\left[-\int_{t \in U_i} dt L[\eta, \xi]\right]$$
(148)

The equality in Eq.145 trivially follows from $e^{a+b} = e^a e^b$ and that the entire integration domain [-T/2, T/2] is covered by **U** and its complement. The subsequent approximation assumes that a vast distance separates one energy packet from the next and that, correspondingly, the fluctuations around one instanton cannot have any effect on the other.

The action Eq.31 is symmetric under $p \rightleftharpoons -p$ and $q \rightleftharpoons -q$, and so the transition amplitude from any one initial vertex in the p-q plane to any other vertex (within the same time slice) is independent of the particular starting vertex. This means we can limit our attention to any one chosen vertex and consider horizontal, vertical, and

diagonal transitions to the other three vertices (Fig.7).



FIG. 7. Horizontal, vertical, and diagonal transitions correspond to P,Q,R instantons. In graph theoretic language this is known as a K_4 graph.

Let P_i, P_f be column/row vectors corresponding to the initial and final states respectively and $\mathbb K$ be the matrix below.

$$\mathbb{K} = \begin{bmatrix} 0 & K_P & K_Q & K_R \\ K_P & 0 & K_R & K_Q \\ K_Q & K_R & 0 & K_P \\ K_R & K_Q & K_P & 0 \end{bmatrix}.$$
 (149)

In the language of graph theory this is the weighted adjacency matrix of the graph K_4 (fully connected with four vertices and six edges). The element K_{ij} is the term contributed by the single instanton that takes minimum i to minimum j. As an example choose below $P_I = P_1$, i.e.all entries are zero except the first,

$$\begin{bmatrix} 0 & K_P & K_Q & K_R \\ K_P & 0 & K_R & K_Q \\ K_Q & K_R & 0 & K_P \\ K_R & K_Q & K_P & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ K_P \\ K_Q \\ K_Q \end{bmatrix}.$$
 (150)

At the next time instant, i.e. when the second instanton

"fires", the above will be multiplied by \mathbb{K} until the N'th one is reached. The amplitude matrix can be constructed from the basic quantum mechanical rule of multiplying together amplitudes along a particular path. Each \mathbbm{K} matrix occurs sequentially, i.e. the instantons are time ordered. This is easily taken care of by the identity,

$$\int_{-\frac{T}{2}}^{\frac{T}{2}} \mathbb{K} dt_1 \int_{t_1}^{\frac{T}{2}} \mathbb{K} dt_2 \cdots \int_{t_{N-1}}^{\frac{T}{2}} \mathbb{K} dt_N = \frac{(\mathbb{K}T)^N}{N!}.$$
 (151)

When the above is summed over all N we get, of course, $\exp(\mathbb{K}T)$. Since \mathbb{K} is a real symmetric matrix with a nonvanishing determinant it can be diagonalized and the amplitude matrix becomes,

$$\mathbb{A}_{fi} = P_f^T e^{\mathbb{K}T} P_i = P_f^T C^{-1} e^{\Lambda T} C P_i, \qquad (152)$$

C is the matrix that diagonalizes \mathbb{K} , i.e. $C^{-1}\mathbb{K}C = \Lambda$,

$$\lambda_P = -K_P + K_Q - K_R, \ \lambda_Q = K_P - K_Q - K_R, \ \lambda_R = -K_P - K_Q + K_R, \ \lambda_S = K_P + K_Q + K_R.$$
(154)

Note that $\sum \lambda_i = 0$, a consequence of Tr $\mathbb{K} = 0$. If the vertices of the square, i.e. the minima of the potential, are labelled a, b, c, d then the tunneling amplitudes between them are,

$$\begin{bmatrix} \mathscr{A}_{aa} \\ \mathscr{A}_{ab} \\ \mathscr{A}_{ac} \\ \mathscr{A}_{ad} \end{bmatrix} = \frac{R_0}{4} \begin{bmatrix} e^{\lambda_P T} + e^{\lambda_Q T} + e^{\lambda_R T} + e^{\lambda_S T} \\ e^{\lambda_P T} - e^{\lambda_Q T} + e^{\lambda_R T} - e^{\lambda_S T} \\ -e^{\lambda_P T} + e^{\lambda_Q T} + e^{\lambda_R T} - e^{\lambda_S T} \\ -e^{\lambda_P T} - e^{\lambda_Q T} + e^{\lambda_R T} + e^{\lambda_S T} \end{bmatrix}$$
(155)

With R_0 from Eq.116,

$$R_{0} = \frac{\sqrt[4]{2a_{1}a_{2}}}{\sqrt{\pi}x_{0}} \frac{\sqrt[4]{2b_{1}b_{2}}}{\sqrt{\pi}y_{0}} \exp\left[-(\kappa+\epsilon)\frac{T}{2} + \frac{\mu^{2}\nu^{2}T}{\kappa\epsilon(\kappa+\epsilon)}\right]$$
(156)

the tunneling amplitude Eq.155 is the central result of this paper.

To make contact with a single dof we can set $K_Q =$ $K_R = 0$, and $K_P = K$. Reverting to more standard notation, R_0 (as in Eq.30) becomes,

$$R_0 \to \sqrt{\frac{m\omega}{\pi\hbar}} e^{-\frac{1}{2}\omega T}.$$
 (157)

This recovers the usual result for 1 dof,

$$\begin{bmatrix} \mathscr{A}_{a \to a} \\ \mathscr{A}_{a \to -a} \end{bmatrix} = \frac{R_0}{2} \begin{bmatrix} e^{KT} + e^{-KT} \\ e^{KT} - e^{-KT} \end{bmatrix}$$
$$= \sqrt{\frac{m\omega}{\pi\hbar}} e^{-\frac{1}{2}\omega T} \begin{bmatrix} \cosh KT \\ \sinh KT \end{bmatrix}. \quad (158)$$

ENERGY SPLITTINGS IX.

If the barrier around each of the four wells was infinitely high, a particle would be forever confined within that well. There would be a four-fold degeneracy,

$$E_i = \frac{\hbar}{2}(\kappa + \epsilon) - \frac{\hbar\mu^2\nu^2}{\kappa\epsilon(\kappa + \epsilon)} + \hbar\Delta_i, \quad \Delta_i = 0.$$
(159)

However for any finite height there will be leakage of the wavefunction into the other three wells with rates determined in the last section. To investigate how these leakages affect the spectrum of the Hamiltonian, note first that H commutes with the p and q parity operators Π_p, Π_q . Therefore its eigenfunctions transform under $Z_2 \times Z_2$ and so these nearly degenerate energy eigenstates can be labeled by their parity eigenvalues as E_S, E_P, E_Q, E_R . The unit operator in this truncated space is,

$$\mathbf{1} = |++\rangle\langle++|+|+-\rangle\langle+-|+|-+\rangle\langle-+|+|--\rangle\langle--|.$$

The above can be inserted into the amplitudes in Eq.155. So, for example,

$$\mathcal{A}_{aa} = \left\langle aa, T/2 | e^{-\frac{H}{\hbar}t} | aa, -T/2 \right\rangle$$

$$= \left| \left\langle + + | aa \right\rangle \right|^2 \left(e^{-\frac{\epsilon_P T}{\hbar}} + e^{-\frac{\epsilon_Q T}{\hbar}} + e^{-\frac{\epsilon_R T}{\hbar}} + e^{-\frac{\epsilon_S T}{\hbar}} \right)$$

$$= \frac{R_0}{4} \left(e^{-\frac{\epsilon_P T}{\hbar}} + e^{-\frac{\epsilon_Q T}{\hbar}} + e^{-\frac{\epsilon_R T}{\hbar}} + e^{-\frac{\epsilon_S T}{\hbar}} \right). \quad (160)$$

We have used here relations that follow from symmetries of the wavefunction,

$$\begin{aligned} |\langle + + |aa\rangle|^2 &= |\langle + - |aa\rangle|^2 = \langle - + |aa\rangle|^2 \\ &= |\langle - - |aa\rangle|^2 = \frac{1}{4}R_0. \end{aligned} (161)$$

With reference to Eq.159, the energy splittings can be immediately read off for the totally symmetric, Psymmetric, Q-symmetric, and PQ-antisymmetric states in the order below:

$$\Delta_P = -\lambda_P, \ \Delta_Q = -\lambda_Q, \ \Delta_R = -\lambda_R, \ \Delta_S = -\lambda_S.$$
(162)

As remarked earlier, the center of gravity of the splittings is zero.

X. COMPOSITE TUNNELING

With all ingredients in place for the quartic well problem, it is straightforward to specialize to the very example that motivated this work. From Eqs.24-28 one can readily read off the parameters to be inputted into Eq.31.

$$a_{1} = \frac{m\tilde{\Omega}x_{0}^{2}}{4\hbar}, \quad a_{2} = \frac{m\tilde{\Omega}x_{0}^{4}}{8\hbar L^{2}}, \quad b_{1} = \frac{my_{0}^{2}\tilde{\Omega}}{\hbar},$$
$$b_{2} = \frac{m\omega^{2}y_{0}^{4}}{2\hbar\tilde{\Omega}a^{2}}, \quad c = \frac{3m\omega^{2}x_{0}^{2}y_{0}^{2}}{8\hbar\tilde{\Omega}a^{2}}.$$
(163)

We remind the reader that Lagrangian contains the parameters m, a, ω, Ω, L and all other quantities are expressible in terms of these including the minima $\pm x_0, \pm y_0$. The single parameter assumed large is $\Omega \gg \omega$ (hence, from Eq.28, $\tilde{\Omega} \gg \omega$) while the derived parameters $\kappa, \epsilon, \mu, \nu$ are:

$$\kappa = \frac{x_0}{L} = 1 - \left(1 - \frac{L^2}{a^2}\right)\frac{\omega^2}{\Omega^2} + \cdots$$
 (164)

$$\epsilon = \frac{y_0\omega}{a\tilde{\Omega}} = f\frac{\omega}{\Omega} + O(\omega^3/\Omega^3)$$
(165)

$$\mu = \sqrt{\frac{3}{2}\epsilon} \tag{166}$$

$$\nu = \sqrt{\frac{3}{8}} \frac{x_0 \omega}{a \tilde{\Omega}} = \sqrt{\frac{3}{8}} \frac{\omega}{\Omega} + O(\omega^3 / \Omega^3)$$
(167)

Although all ingredients are in place for going to higher orders, in the interest of clarity the prefactor R_0 is shown below only to leading order,

$$R_0 = \frac{m\sqrt{f\omega\Omega}}{2\pi\hbar} \exp\left[-(\kappa+\epsilon)\frac{T}{2} + \frac{\mu^2\nu^2}{\kappa\epsilon(\kappa+\epsilon)}T\right] + \cdots$$
(168)

Also to leading order are the K factors for the three flavors:

$$K_P = \sqrt{\frac{12}{\pi}} \frac{f^2 m \omega a L}{\hbar} \exp\left[-\frac{m \Omega a L}{6\hbar}\right]$$
(169)

1

$$K_Q = \sqrt{\frac{12}{\pi}} \frac{m\omega a^2}{\hbar} \sqrt{\frac{\omega}{f\Omega}} \left(1 - \frac{9L^2}{8a^2}\right) \exp\left[-\frac{2m\omega a^2}{3\hbar} \left(1 - \frac{9L^2}{8a^2}\right)\right]$$
(170)

$$K_R = \sqrt{\frac{12}{\pi}} \frac{f^2 m \omega a L}{\hbar} \exp\left[-\frac{m \Omega a L}{6 \hbar} - \frac{2m \omega a^2}{3 \hbar} \left(1 - \frac{9L^2}{8a^2}\right)\right].$$
(171)

From the above K_i the energy splittings can be calculated from Eqs.162. So far it has only been assumed that $\omega/\Omega \ll 1$ but no assumption on L/a was made other than f > 0 (and hence that $L/a < 2/\sqrt{3}$). However one region of physical interest is $L \to 0$ or $f \to 1$, i.e. one seeks insight into how tunneling probabilities change in going from point particle to extended object. To this end it is instructive to examine the ratio between single instanton amplitudes. Recall that the P instanton flips the molecule's orientation without cm tunneling while the Q instanton mediates cm tunneling without flip. The ratio of the two amplitudes is,

$$\frac{K_P}{K_Q} = \frac{L}{a} \sqrt{\frac{\Omega}{\omega}} \exp\left[-\frac{maL\Omega}{6\hbar} \left(1 - \frac{4a\omega}{L\Omega}\right)\right].$$
 (172)

There is competition between two dimensionless factors

here: on the one hand we presumed at the outset that Ω/ω is large while $L/a \sim O(1)$ but now the ratio K_P/K_Q above depends on the product of a large and small number. Nevertheless it is clear for any fixed Ω that $K_P/K_Q \to 0$ as $L \to 0$. Also, for any fixed L, that $K_P/K_Q \to 0$ as $\Omega \to \infty$.

Next we recall that the R instanton simultaneously mediates a flip and cm tunneling. The ratio K_R/K_Q is similar to that above:

$$\frac{K_R}{K_Q} = \frac{L}{a} \sqrt{\frac{\Omega}{\omega}} \exp\left[-\frac{maL\Omega}{6\hbar}\right].$$
 (173)

Both the above ratios show that the relative flip probability first increases from zero with L and then decreases.

XI. SUMMARY

This work has extended the well-explored quantum mechanical concept of the instanton in a 1-D symmetric double well potential to the case of instantons mediating transitions between four wells. In principle this can be extended to any number of wells. As per the usual definition, an instanton is a solution of the classical equations of motion in Euclidean space-time with finite, non-zero action. We motivated the present work by considering a 1-D oriented "diatomic molecule" whose centre of mass can tunnel from one vacuum to another equivalent vacuum together with a second well that allows for the additional possibility of orientation flip. The generic form of the interaction between any two dof's is postulated in Eq.31.

The starting point of any analysis of instantons, including the present one, is necessarily the Feynman path integral in imaginary time and the semi-classical framework. Physically this system corresponds to the simultaneous tunneling of both p, q variables. One may picturize the double instanton as in Fig.6. Each slice can be placed anywhere in the nearly infinitely long time axis without any change of action. This gives rise to a zero mode which, as in the single dof case, requires special treatment. The Faddeev-Popov procedure used in field theory is well suited for dealing with this quantum mechanical system.

In adding an extra dof significant new issues were encountered. First, to find the classical path requires solving the Euler-Lagrange equations. These are coupled non-linear differential equations that generally do not admit exact solutions. However, under the assumption of a hierarchy of scales they may be solved order by order perturbatively. It turns out that there are three kinds/flavors of instantons in the present case namely strong-weak (P and Q) and strong-strong (R). Second, corrections to the fluctuation determinant occur at the quadratic level. This requires summing the contribution from bound and unbound states and hence knowledge of the non-linear one-body propagator. Exact propagators for non-linear systems are rare. Even where they exist their forms are complicated. Fortunately the Poschl-Teller propagator can be expressed in terms of hyperbolic functions only.

In the single dof case, an infinite number of time sequenced instantons need to be summed over to give a finite contribution to the action. This is straightforwardly done and is known as the dilute gas approximation. But for three time-sequenced flavors this poses a challenge. Nevertheless, following the usual quantum mechanical rule for compounding amplitudes, and drawing inspiration from graph-theoretic networking, we arrived at a closed form, analytical expression for tunneling from any vertex to any other. Finally, the formalism developed was applied to the linear diatomic molecule where both cm tunneling and orientation flip are possible, both separately and together. While this is only a caricature of reality, it is likely that other physical systems exist where the model developed here will have relevance.

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