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Phase transition in quantum tunneling and exact statistical mechanics for a model of parametrized double-well potential

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Summary

A model for one-dimensional bistable systems characterized by a deformable double-well energy landscape, is introduced in order to investigate the effect of shape deformability on the order of phase transition in quantum tunneling, and on the quasi-exact integrability of the classical statistical mechanics of these systems. The deformable double-well energy landscape is modelled by a parametrized double-well potential possessesing two fixed degenerate minima and a constant barrier height, but a tunable shape of its walls which affects the confinement of the two wells. It is found that unlike bistable models involving the standard ϕ^4-field model for which the transition in quantum tunneling is predicted to be strictly of second order, a parametrization of the double-well potential also favors a first-order transition occurring above a universal critical value of the shape deformability parameter. The partition function of the model is constructed within the framework of the transfer-integral formalism, with emphasis on low-lying eigenstates of the transfer-integral operator. A criteria for quasi-exact integrability of the partition function is formulated, in terms of the condition for possible existence of exact eigenstates of the transfer-integral operator. The quasi-exact solvability condition is obtained analytically and from this, some exact eigenstates are derived at several temperatures. The exact probability densities obtained from the analytical expressions of the ground-state wavefunctions at different temperatures, are found to be in excellent agreement with the probability density obtained from numerical simulations of the Langevin equation.

KEYWORDS:
Quantum equilibrium statistical mechanics, Quantum field theory; related classical field theories, Transition in quantum tunneling, bistable systems, solitons, Langevin equation.

1 | INTRODUCTION

In systems with multiple equilibrium states, the transition between metastable states separated by energy barriers arise either in the classical regime via thermal activation, or in the quantum regime via tunneling processes. At high temperature, thermal activation governs the transition which usually occurs as a hopping over the potential barrier. However, at low enough temperature (i.e. near quantum criticality $T \to 0$), the transition is governed by quantum tunnelings through the potential barrier. In this second context the system dynamics is characterized by classical configurations called instantons [1,2], which are expected to

dominate the thermal rate at low temperature[3,4]. As the temperature increases, the thermally-induced crossover becomes more and more important and at some critical temperature, a phenomenon known as "phase transition in quantum tunneling"[5] can take place. This phenomenon has recently attracted a great deal of interest, in particular it was demonstrated that some physical systems can exhibit not only a smooth second-order transition at a critical temperature T_0, but also a first-order transition[6,7,8,9,10,11,12] at some different temperature.

Another aspect of interest in the study of displacive elementary excitations in condensed matter physics, is their dominant contribution in the low-temperature statistical mechanics of the systems[13,14,15,16,17]. In the early eighties a soliton-gas phenomenology was proposed[15] to address the problem of low-temperature statistical mechanics of condensed matter systems admitting kin and solitary-wave solutions in general. This phenomenology, then called transfer-integral formalism, was later generalized to kink-bearing systems for which kink-phonon interactions lead to reflectionless scattering potentials[18]. The transfer-integral formalism has gained a constantly growing attention over the four last years, because of the universal framework it offers in the study of a wide-range of thermodynamics-based processes including in quantum systems[19,20,21,22,23]. In kinetic theory the formalism has been used to develop nontrivial (i.e. quasi-exact) approaches to escape-rate problems in both classical and quantum regimes[24,25], and so on.

The above mentioned studies, however, rest mainly on the assumption of two universal models namely the sine-Gordon[26,27] model, assumed to describe systems with periodic one-site potentials, and the ϕ^4[28,29] model intended for systems with double-well (DW) energy landscapes. Yet real physical systems to which these models and studies address are actually far more complex, sometimes also displaying a rich diversity with unique structural features. For instance the sine-Gordon and ϕ^4 potentials both have fixed extrema, in addition to their shape profiles that are rigid and hence restrict their applications to only very few physical contexts. Nonetheless, it has been shown that these weaknesses can be overcomed by envisaging a parametrization of these two universal models. Indeed the sine-Gordon model was generalized by Remoissenet and Peyrard[3,30,31] into a parametrized periodic potential (the so-called Remoissenet-Peyrard potential)[30,31,32], and the ϕ^4 potential was parametrized[33,34,35,36] into a DW potential model with a tunable shape profile. It is worthwhile to stress that although some other parametric DW potentials exist in the literature[37,38,39], the family of DW potentials proposed in refs.[33,34,35,36] is peculiar in that it groups three different classes with distinct shape deformability features, but the three classes admit the ϕ^4 potential as a specific limit.

The importance of shape deformability in the context of bistable systems lies in two issues related to their structural properties. The first issue is linked with the problem of symmetry breaking, for which the ϕ^4 model predicts the transition in quantum tunneling to be strictly of second order[9,10,11,12]. The second issue is related to observations[13,15] that the transfer-integral formalism always reduces the classical statistical mechanics of a one-dimensional (1D) ϕ^4-field theory, to a time-dependent quantum-mechanical problem for which no exact solution exists. The first issue was recently addressed by Zhou et al.[40], who formulated the problem of transitions in quantum tunneling for one[34] among the three existing classes of parametrized DW potentials[33,34,35,36]. Thus, Zhou et al.[40] obtained that due to the extra degree of freedom accounting for shape deformability, bistable systems which can be described by the parametrized DW potential could exhibit a first-order transition occurring at a finite critical value of the shape deformability parameter, besides the second-order transition predicted by the ϕ^4 model. As for the second issue, given that the classical statistical mechanics of a field-theoretical system can be fully analyzed with just the knowledge of its low-lying eigenstates, parametrized DW models are quite likely to introduce the possibility for quasi-exactly solvable (QES) systems in field theory[41,42,43,44,45,46].

In the work of Zhou et al.[40], the parametrized DW potential was one for which the height of the potential barrier could be varied continuously by varying a shape deformability parameter, leaving unchanged the positions of the two degenerate minima[34]. In the present work we wish to examine the possible occurrence of a first-order transition in quantum tunneling, for a new family of DW potential which is parametrized in such a way that the barrier height and positions of the two minima are always fix, but the the steepness of the potential walls can be tuned which affects the confinement of the two potential wells. We shall see that this model too leads to a first-order transition in quantum, besides the second-order transition predicted within the framework of the ϕ^4 theory. We will also discuss the issue of exact integrability of the statistical-mechanical problem for this new parametrized DW model. In this purpose the low-temperature partition function will be expressed in terms of a transfer-integral operator eigenvalue problem[18], for which exact low-lying eigenstates will be shown to exist provided under a specific condition. Analytical expressions of some exact low-lying eigenfunctions, together with the corresponding energy eigenvalues, will be derived and results for the probability density functions discussed both analytically and via numerical simulations of the Langevin equation with a Gaussian white noise.

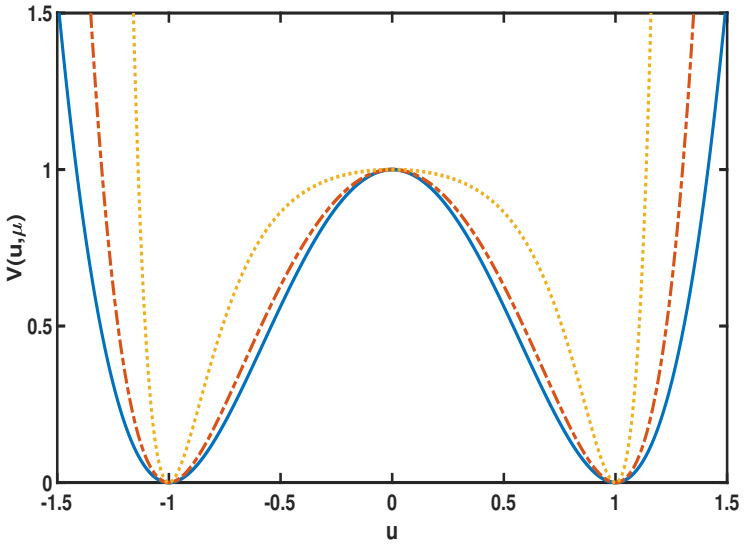

FIGURE 1 (Color online) Profiles of the parametrized DW potential $V(u,\mu)$, for different values of the shape deformability parameter μ: $\mu \to 0$ (Solid line), $\mu = 1.0$ (Dot-dashed line), $\mu = 4.0$ (Dotted line). $a_0 = 1$.

2 | THE MODEL OF PARAMETRIZED DW POTENTIAL

We are interested in $1D$ systems for which the bistable energy landscape is represented by a DW potential of the general form:

$$V(u,\mu) = a(\mu)\left[\frac{\sinh^2(\alpha(\mu)u)}{\mu^2} - 1\right]^2, \quad \mu > 0, \tag{1}$$

where $a(\mu) > 0$ and $\alpha(\mu)$ are two functions of the shape deformability parameter μ. $V(u,\mu)$ given by (1) belongs to a family of parametric DW potentials[33,34,35,36] whose shape profiles can be tuned differently, but which admit a common asymptotic limit which is the ϕ^4 potential when $\mu \to 0$. For the new member the two functions $a(\mu)$ and $\alpha(\mu)$ are defined as:

$$\alpha(\mu) = sinh^{-1}\mu, \quad a(\mu) = a_0, \tag{2}$$

in which case $V(u,\mu)$ is a DW potential with two degenerate minima fixed at $u = \pm 1$, and a barrier height also fixed at a constant value a_0. However a variation of μ changes the steepness of the potential walls, and consequently the sharpness (or confinement) of the potential wells. In fig. 1 , $V(u,\mu)$ is sketched for some arbitrary values of μ. When μ tends to zero, the parametrized DW potential reduces to $V(u) = a_0\left(u^2-1\right)^2$ [13,15]. When μ is varied, the slope of the potential walls gets steeper. Hence the narrowest part of the potential barrier broadens while the flatness of the barrier top beocomes more pronounced, resulting in an enhancement of the confinement of the potential wells. Quite instructively, a variation of the barrier shape observed in fig. 1 is consistent with the experimentally observed rates and experimentally observed kinetic isotope effects, when studying vibrationally assisted hydrogen tunneling in enzyme-catalyzed reactions[47]. Indeed in these biophysical processes, the effect of the catalyzer becoming less efficient results in a progressive broadening of the narrowest part of the barrier, with the shoulder shape of the barrier peak becoming increasingly less pronounced. The patrametrized DW potential eqs. (1)-(2) is infinite at the boundaries of the final interval and therefore is suitable for modelling hydrogen bonds in enzyme-catalyzed reactions. Also worthwhile to note, for significant values of the shape deformability parameter μ the DW potential eqs. (1)-(2) displays features similar to the double-Morse potential, used[39] to describe proton motion in the hydrogen bond $O-H\cdots O$ in KDP ferroelectrics. In these specific materials[39] the one-body proton potential rises steeply in the vicinity of the oxygen atoms, with a gentler slope at the sides of the potential barrier. The parametric DW potential eqs. (1)-(2) can reproduce some of these peculiar features, namely by taking the proton displacement u from the center of the hydrogen bond and using μ to mimic the rate of variation of the $O-O$ bond distance. Last but not least, a confinement of potential wells in bistable systems has recently been shown to hold a crucial role in the occurrence of stochastic resonance in these systems[48].

3 | FIRST-ORDER TRANSITION IN QUANTUM TUNNELING

Consider a $1D$ quantum system with an Euclidean action (in dimensionless form):

$$S = \int d\tau \left(\frac{1}{2} \left(\frac{du}{d\tau} \right)^2 + V(u, \mu) \right), \tag{3}$$

where u is a scalar field in one time and zero space dimension, $\tau = it$ is the imaginary time and $V(u, \mu)$ is the parametrized DW potential energy. The integral is taken over the period τ_p of the path. In statistical mechanics this period is related to temperature T through the relation $\tau_p = \hbar/(k_B T)$, where k_B is the Boltzmann constant. Without loss of generalities we will take $\hbar \equiv 1$. The decay rate of the system in the semiclassical limit is of the form:

$$\Gamma \sim \exp^{-F_{min}/T}, \tag{4}$$

where F_{min} is the minimum of the effective "free energy"[10] $F \equiv E + TS(E) - E_{min}$. E is the energy of a classical pseudo-particle in the system, while $E_{min} = 0$ corresponds to the bottom of the potential. The minimum of the effective Euclidean action i.e. S_{min}, is obtained by minimizing (3) along the trajectories $\phi(\tau)$ satisfying the energy-integral equation:

$$\left(\frac{du_c}{dt} \right)^2 = 2 \left(V(u_c, \mu) - E \right). \tag{5}$$

When $E = 0$, corresponding to $\tau_p = \infty$ and $T = 0$, the particle is at rest at the bottom of one of the two degenerate potential wells. The solution to eq. (5) in this case is a regular vacuum instanton (kink soliton) given by:

$$u_c(\tau) \to \frac{1}{\alpha(\mu)} \tanh^{-1} \left[\frac{\mu}{\sqrt{1+\mu^2}} \tanh \frac{\tau}{\sqrt{2} d(\mu)} \right], \tag{6}$$

where $d(\mu) = \mu \left[a_0 \alpha^2(\mu)(1+\mu^2) \right]^{-1/2}$ is the kink width. Imposing periodic boundary conditions, with τ_p the period of motion, leads instead to the following expression for the trajectory $u_c(\tau)$ with energy $E \geq 0$:

$$u_c(\tau) = \frac{1}{\alpha(\mu)} \tanh^{-1} \left[C_1 \cdot sn \left(C_2 \tau, \kappa \right) \right], \tag{7}$$

with $sn(\tau, \kappa)$ a Jacobi elliptic function[49] the modulus κ of which is given by:

$$\kappa = \sqrt{\frac{\left(1 - \sqrt{E/a_0}\right) \left[1 + \mu^2 \left(1 + \sqrt{E/a_0}\right)\right]}{\left(1 + \sqrt{E/a_0}\right) \left[1 + \mu^2 \left(1 - \sqrt{E/a_0}\right)\right]}}. \tag{8}$$

The two parameters C_1 and C_2 appearing in formula (7) were defined as:

$$C_1 = \sqrt{\frac{\mu^2 \left(1 - \sqrt{E/a_0}\right)}{1 + \mu^2 \left(1 - \sqrt{E/a_0}\right)}}, \tag{9}$$

$$C_2 = \frac{\alpha(\mu)}{\mu} \sqrt{2a_0 \left(1 + \sqrt{\frac{E}{a_0}}\right) \left[1 + \mu^2 \left(1 - \sqrt{\frac{E}{a_0}}\right)\right]}. \tag{10}$$

The trajectory (7) possesses real periods for values of its argument equal to $4m\mathcal{K}(\kappa)$, where m is an integer and $\mathcal{K}(\kappa)$ is the quarter period determined by the complete elliptic integral of the first kind[49]. Eq. (7) therefore describes a periodic trajectory which we can refer to as periodon, the period of which is ($m = 1$):

$$\tau_p = \frac{4}{C_2} \mathcal{K}(\kappa). \tag{11}$$

The classical action corresponding to the periodon eq. (7) is obtained as:

$$S_p(E) = E\, \tau_p + W \left(u_c(\tau_p)/2, E \right), \tag{12}$$

where:

$$W \left(u_c(\tau_p)/2, E \right) = \frac{2C_2}{(\alpha(\mu) C_1)^2} [(C_1^4 - \kappa^2)\Pi(C_1, \kappa) + \kappa^2 \mathcal{K}(\kappa) + C_1^2 (\mathcal{K}(\kappa) - \mathcal{E}(\kappa))].$$

$\mathcal{E}(\kappa)$ and $\Pi(C_1, \kappa)$ in the last formula are the complete elliptic integrals of the second and third kinds, respectively[49].
At $E = a_0$, which corresponds to the top of the potential barrier, the solution to eq. (5) is the trivial configuration $u_c(\tau) = 0$. This trajectory is a sphaleron[50] and its action is the thermodynamic action namely:

$$S_0(\mu) = a_0\tau. \tag{13}$$

For the sphaleron the escape rate has the Boltzmann signature, characteristic of a pure thermal activation i.e.:

$$\Gamma_c \sim \exp\left(-a(\mu)\tau_p\right) = \exp\left(-a(\mu)/k_BT\right). \tag{14}$$

From the above results we can conclude that a periodon interpolates between the sphaleron $u_c(\tau) = 0$, and the instanton given by eq. (6). Hence the escape rate in the preriodon sector will be:

$$\Gamma \sim \exp\left(-S_{min}(E)\right), \tag{15}$$

where $S_{min}(E) = min\left\{S_0, S_p(E)\right\}$.
To examine the possible occurrence and characteristic features of the transition(s) in quantum tunneling, for the $1D$ quantum system with the action given by formula (3), it is useful to start with the remark that for periodic problems in classical statistical mechanics, the derivative of the action with respect to the energy is equivalent to the oscillation time τ of the system with this energy. Since the oscillation time τ is proportional to the inverse temperature, with the action corresponding to motion in the periodon sector we can readily define the period of motion as:

$$\tau_p(E) = \frac{1}{k_BT} = \frac{dS_p(E)}{dE}, \quad \frac{dS_0}{d\tau_p} = a(\mu). \tag{16}$$

Taking (16) together with (11) and (12), it is possible to analyze the influence of the shape deformability parameter μ on the temperature dependence of S_{min}, based upon the energy dependence of the period of periodon $\tau_p(E)$. In particular these equations will enable us obtain the critical value of μ at which a first-order transition from quantum to thermal regime, can be expected.
Two well-established criteria are known[5,8] which determine conditions for occurrence of transitions in quantum tunnelings, in the general problem of decay of a metastable state[5,8,9,10,51]. The first criteria states that the transition will be of first order if the period $\tau_p(E)$ decreases to a minimum, and next increases again when E increases from the potential bottom to the barrier height. If $\tau_p(E)$ instead decreases monotonically with increasing E, the transition will be of second order. The second criteria states that if at some critical temperature the first derivative of $S_{min}(T)$ is discontinuous, and an abrupt change is observed in the temperature dependence of the action, then the transition from quantum to thermal regime is a first-order transition in temperature. The first criteria is equivalent to solving the equation:

$$\frac{d}{dE}\tau_p(E) = 0, \tag{17}$$

where one seeks for nontrivial solutions with the temperature dependence of $\tau_p(E)$ given by (16). We solved the last equation numerically by setting $a_0 = 1/2$, and evaluated the energy E_1 corresponding to the minimum of $\tau_p(E)$ for some values of μ. Results are shown in table 1 .

TABLE 1 Numerical computation of critical values of E_1.

μ^2	Energy E_1 at minimun of $\tau_p(E)$	$E_0 = a_0$ (barrier height)
9	0.1503	0.5
4	0.2278	0.5
2	0.3817	0.5
1.6	0.4691	0.5
1.501	0.4994	0.5

The table indicates the quantity E_1 approaching the maximum energy E_0, when μ tends to $\sqrt{3/2}$. Therefore the critical value of μ for a transition in quantum tunneling would be $\mu_c = \sqrt{3/2}$, and smaller values of μ should correspond to unphysical

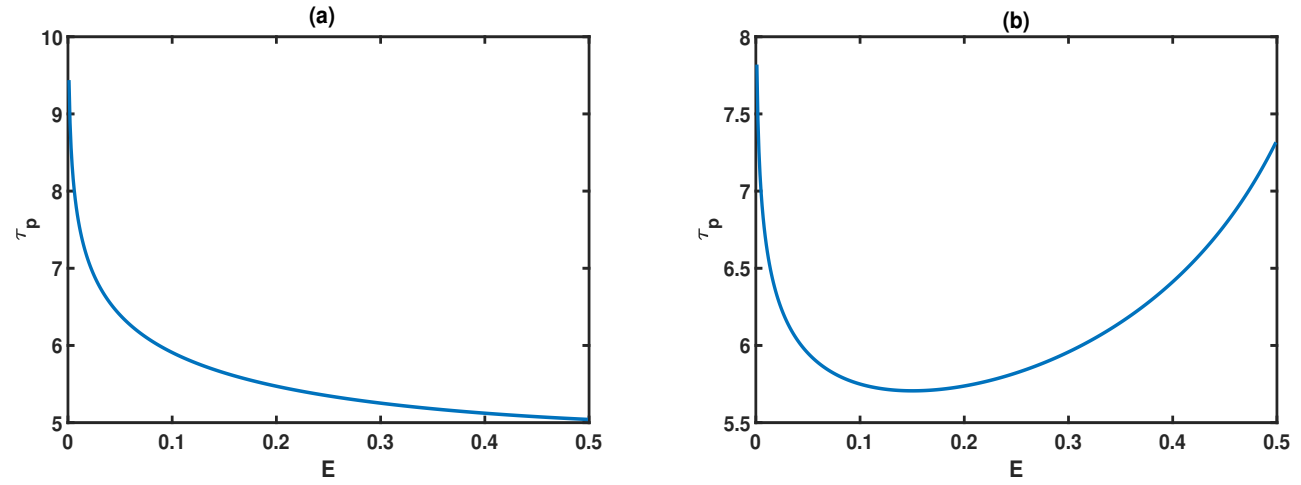

FIGURE 2 (Color online) Variation of the instanton period with the energy E for (a) $\mu = 1$, and (b) $\mu = 3$. Here $a_0 = 0.5$.

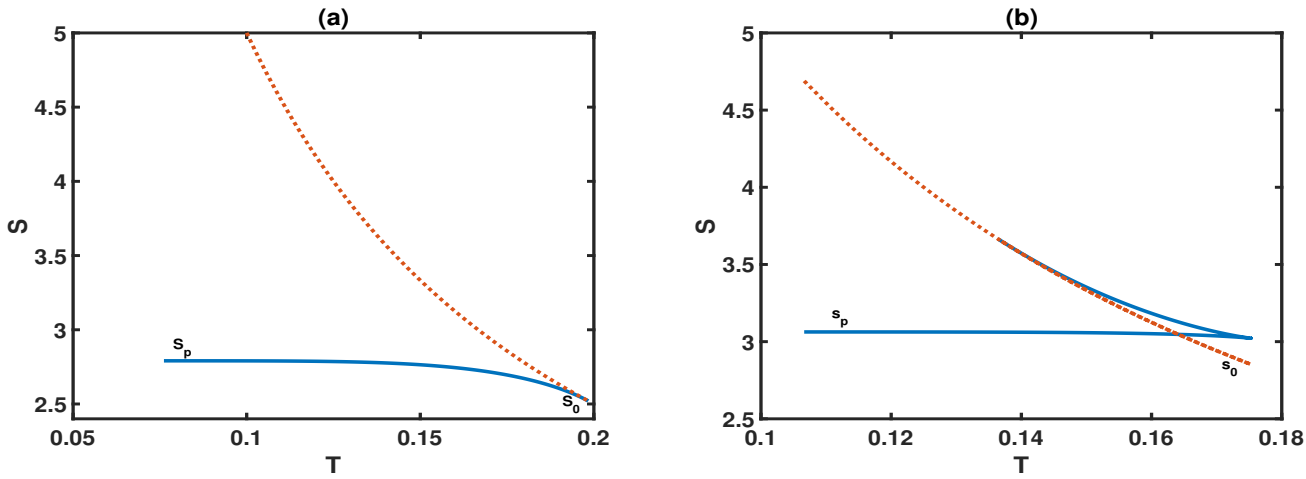

FIGURE 3 (Color online) Plots of the action versus temperature, the dashed line corresponds to the thermodynamic action and the solid line to the periodon action: (a) $\mu = 1$, second-order transition from quantum to thermal regimes, (b) $\mu = 3$, First-order transition from quantum to thermal regimes.

values of the energy E. Clearly, a first-order quantum-classical transition will occur in the parametrized DW model when the deformability parameter lies in the range $\mu > \sqrt{3/2}$. For values of μ far above the critical threshold μ_c, we should have $E_1 \approx 0$ and $E_1 \to E_0$ as μ decreases to μ_c. So to say, increasing the deformability parameter above the critical value μ_c should result in a sharper first-order transition in quantum tunneling[52].

Fig. 2 represents the energy dependence of the periodon period τ_p for two values of the shape deformability parameter μ, selected respectively below and above the critical value μ_c. Fig. 2 (a) suggests a monotonic decrease of the periodon period with increasing energy, for $\mu = 1$ lower than μ_c. However for $\mu = 3$, which is a value greater than μ_c, the period has a re-entrant behaviour afer decreasing untill a critical value of the energy as evidenced in fig. 2 (b). This re-entrant behaviour of the period actually reflects a favorable condition for a first-order transition. The physical behaviours just discussed and emerging from fig. 2 , can also be observed in the corresponding plots of the periodon and thermodynamic actions shown in fig. 3 , here also for $\mu = 1$ and $\mu = 3$ respectively. When the temperature increases we observe a smooth change from S_p to S_0 in fig. 3 (a), characteristic of a second-order transition. In fig. 3 (b) the change from quantum to classical regime is abrupt, this abrupt change in the temperature dependence of the minimum action fulfills the second criterion proposed by Chudnovsky[8], for a first-order phase transition in temperature.

For the purpose of mathematical simplicity, it can be useful to be able to determine analytically the critical value μ_c of μ for a first-order transition. In this purpose we exploit the proposal of ref.[11], who extended the criteria for determining the order of transition in quantum tunneling, to the dependence of the Euclidean action with the instanton period. Indeed the authors proposed that provided the period $\tau_p(E \to V_0)$ of the periodon close to the barrier peak is accessible, the condition $\tau_p(E \to V_0) - \tau_s < 0$ or $\omega^2 - \omega_s^2 > 0$ will be sufficient for a first-order transition. Here V_0 and τ_s denote respectively, the barrier height and period of small oscillations around the sphaleron, ω and ω_s are the corresponding frequencies. In our context the last criteria translates to:

$$V''''(u_{sph}, \mu) - \frac{5\left[V'''(u_{sph}, \mu)\right]^2}{3V''(u_{sph}, \mu)} < 0, \tag{18}$$

where $u_{sph} = 0$ corresponds to position of the sphaleron solution. The potential beeing symmetric, we have $V'''(0, \mu) = 0$ such that the criteria reduces to $V''''(0, \mu) < 0$. Using the general expression of the potential given by formula (1), the criteria can be expressed more generally as:

$$4\left(\frac{3}{\mu^2} - 2\right)\frac{\alpha(\mu)^4 a(\mu)}{\mu^2} < 0, \tag{19}$$

which suggests a critical value of $\mu_c^2 = 3/2$ irrespective of the specific forms of $\alpha(\mu)$ and $a(\mu)$. This is in agreement with the results of ref.[40], where the phase transition in quantum tunneling was investigated with different forms of $a(\mu)$ and $\alpha(\mu)$ corresponding to the complete hierarchy of Dikandé-Kofané DW potentials.

To close this section, we wish to underline that the parametrized DW potential considered in this study is member of the family of potentials changing slowly near the top and the bottom, which were recently designated to stand for ideal candidates for a first order transition[46]. When $\mu \to 0$, the parametrized DW potential reduces to the ϕ^4 model that can account only for second-order transition. As μ increases, the concave shoulders of the barrier become less pronounced and the narrowest part of the barrier enlarges progressively. Therefore, as the shape deformability parameter approaches a critical value μ_c, the barrier top becomes similar to that of a rectangular barrier and the probability of thermally assisted tunneling, just below the top of the barrier, decreases gradually due to the increase of the tunneling distance. In the region $\mu > \mu_c$ this tunneling becomes unfavorable, a first-order transition occurs as a consequence of a direct competition between the groundstate tunneling and thermal activation. The independence of μ_c on the barrier height highlights the critical role of the shape of the top of the potential barrier, in the occurrence and the nature of the transition from quantum to thermal regime.

4 | STATISTICAL MECHANICS AND QUASI-EXACT SOLVABILITY CONDITION

We now turn to the low-temperature statistical mechanics of the parametrized DW potential model given in (1)-(2), paying attention to the canonical partition function using the transfer-integral formalism[14,15,16,17,18]. The (dimensionless) Hamiltonian governing the continuum dynamics of the system reads:

$$H = \int dx \left[\frac{1}{2}\pi^2 + \frac{1}{2}(\partial_x u)^2 + V(u, \mu)\right], \tag{20}$$

where π is the momentum conjugate to the displacement field u. The solitary-wave solution to the equation of motion, i.e.:

$$\frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} + V(u, \mu) = 0, \tag{21}$$

derived from the Hamilonian (20), can be shown to express:

$$u_c(s, \mu) = \pm\frac{1}{\alpha(\mu)}\tanh^{-1}\left[\frac{\mu}{\sqrt{1+\mu^2}}\tanh\frac{s}{\sqrt{2}d(\mu)}\right], \qquad s = x - vt, \tag{22}$$

and corresponds to the vacuum instanton already obtained in formula (6). This solution describes a kink (+) or an antikink (-) with a rest mass:

$$M_0(\mu) = \frac{\sqrt{2a(\mu)}}{2\alpha(\mu)\mu^2}\left[2\alpha(\mu)(1+\mu^2) - sinh(2\mu)\right]. \tag{23}$$

For the low-temperature statistical mechanics, we apply the transfer-integral formalism and with the Hamiltonian given in eq. (20), we find a Schrödinger-like equation for eigenstates of the transfer-integral operator:

$$-\frac{1}{2\beta^2}\frac{\partial^2}{\partial u^2}\psi_j + a(\mu)\left(\frac{\sinh^2(\alpha(\mu)u)}{\mu^2} - 1\right)^2 \psi_j = \epsilon_j \psi_j. \tag{24}$$

In the thermodynamic limit, the lowest eigenstate with eneregy ϵ_0 brings the most relevant contribution to the partition function In this context Z can readily reduce to the classical partition function;

$$Z_c = (2\pi/\beta h)^N \exp\left(-\beta N \epsilon_0\right), \tag{25}$$

where $\beta = (k_B T)^{-1}$ and N ($\to \infty$) is the total number of particles in the system.
Most generally, finding exact values of the partition function Z depends on the solvability of the eigenvalue problem (24). To transform this eigenvalue problem into a form for which the exact solvability is established[38,53,54], we use the variable change $z = \alpha(\mu)u$ and introduce $\xi = (1+2\mu^2)^{-1}$, $E_j = 4\mu^4\xi^2\epsilon_j/a(\mu)$. With these new variables the eigenvalue problem (24) becomes:

$$\frac{1}{2\beta^2}\frac{\partial^2}{\partial z^2}\psi_j + \frac{a(\mu)}{4\mu^4(\alpha(\mu)\xi)^2}\left[E_j - (\xi\cosh(2z) - 1)^2\right]\psi_j = 0. \tag{26}$$

Remark that by taking $2\beta = 1$, and rescaling the parameter $E_j \to E_j/\eta^2$ with $\eta = \sqrt{a(\mu)}/[2\mu^2\alpha(\mu)\xi] = n+1$, $n = 0, 1, 2, ...$, the eigenvalue problem (26) turns exactly to the equation treated in ref.[38]. In this last work the author obtained exact expressions of eigenfunctions and energy eigenvalues of the corresponding eigenvalue problem, for some energy levels n. By following a similar idea in our context, this will mean taking one energy level at a fixed temperature which yields the value of μ for which the system is quasi-exactly solvable. However, what we really want is instead to obtain eigenstates at different temperatures for each value of μ. This is possible by considering a distinct picture in which the temperature is related to the shape deformability parameter through:

$$\beta^2 = \frac{2\mu^4(\alpha(\mu)\xi)^2}{a(\mu)}q^2, \tag{27}$$

where q is a positive integer hereafter referred to as "temperature order". Substituting (27) into (26) we obtain:

$$\frac{\partial^2}{\partial z^2}\psi_j + q^2\left[E_j - (\xi\cosh(2z) - 1)^2\right]\psi_j = 0. \tag{28}$$

Equation (28) describes a quasi-exactly solvable system similar to the one studied in refs.[38,53,54], for the energy level $n = 1$. We are interested in solutions which vanish in the limit $z \to \pm\infty$, in this respect we can readily define:

$$\psi(z) = r(z)\exp\left[-z_0\cosh(2z)\right], \tag{29}$$

where the function $r(z)$ is a polynomial expressed as a linear combination of $\cosh m_p z$ or $\sinh m_p z$ and their powers, with z_0 and m_p ($p = 0, 1, 2, ...$) being constant quantities to be determined.
The exact expressions for the (unnormalized) groundstate wavefunctions, and of the associated energy eigenvalues, are found for the first four values of q and are list bellow:

$q = 1$:

$$\begin{aligned}\psi_0(u) &= \exp\left[-\frac{\cosh(2\alpha(\mu)u)}{2(1+2\mu^2)}\right],\\ \epsilon_0 &= \frac{a(\mu)}{4\mu^4}\left[1 + (1+2\mu^2)^2\right].\end{aligned} \tag{30}$$

$q = 2$:

$$\begin{aligned}\psi_0(u) &= \cosh(\alpha(\mu)u)\exp\left[-\frac{\cosh(2\alpha(\mu)u)}{1+2\mu^2}\right],\\ \epsilon_0 &= \frac{a(\mu)}{16\mu^4}\left[3(1+2\mu^2)^2 - 8\mu^2\right].\end{aligned} \tag{31}$$

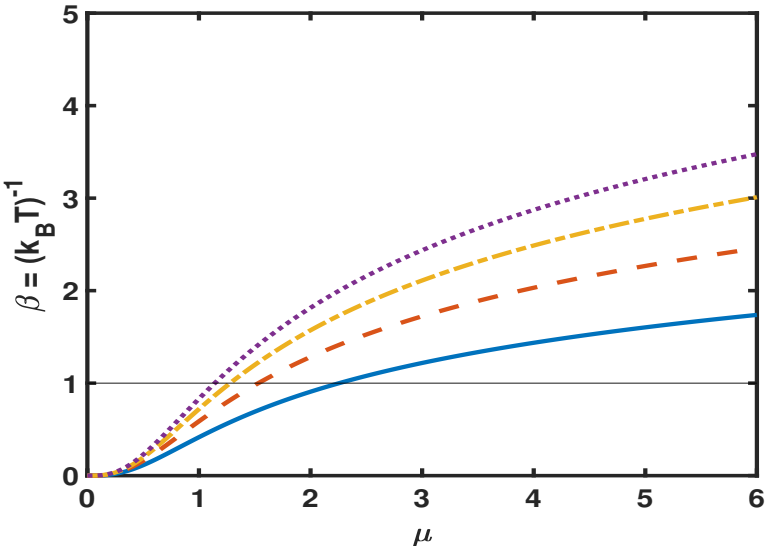

FIGURE 4 (Color online) Variation of the inverse temperature β as a function of the shape deformability parameter μ, for four different values of q according to the quasi-exact solvability condition (27): $q = 1$ (Solid line), $q = 2$ (Dashed line), $q = 3$ (Dash-dotted line), $q = 4$ (Dotted line). The horizontal line stands for the energy barrier taken to be $a_0 = 1$.

$q = 3$:

$$\psi_0(u) = [\frac{6}{1+2\mu^2} + \left(1 + \sqrt{1 + \frac{36}{(1+2\mu^2)^2}}\right)\cosh(2\alpha(\mu)u)]\exp\left[-\frac{3\cosh(2\alpha(\mu)u)}{2(1+2\mu^2)}\right],$$
$$\epsilon_0 = \frac{a(\mu)}{36\mu^4}[9 - 2(1+2\mu^2)\sqrt{(1+2\mu^2)^2+36} + 7(1+2\mu^2)^2]. \tag{32}$$

$q = 4$:

$$\psi_0(u) = 2[\frac{6\cosh(\alpha(\mu)u)}{1+2\mu^2} + \left(2\mu^2 - 1 + \sqrt{12 - 8\mu^2 + (1+2\mu^2)^2}\right)\frac{\cosh(3\alpha(\mu)u)}{1+2\mu^2}]$$
$$\times \exp\left[-\frac{2\cosh(2\alpha(\mu)u)}{1+2\mu^2}\right],$$
$$\epsilon_0 = \frac{a(\mu)}{16\mu^4}[2 - 4\mu^2 - (1+2\mu^2)\sqrt{(1+2\mu^2)^2 - 8\mu^2 + 12} + \frac{11}{4}(1+2\mu^2)^2]. \tag{33}$$

Eigenfunctions and eigenvalues for some higher energy levels are given in the appendix.

The condition for quasi-exact solvability of the system at several temperatures, is defined by relation (28). This relation sets the dependence of the temperature (in unit of the Boltzmann constant) on the shape deformability parameter μ and is illustrated in Fig. 4 . It is particularly remarkable that in the limit $\mu \to 0$, the quasi-exact solvability condition requires $T \to \infty$. This is in excellent agreement with the transfer-operator prediction relative to the absence of exact solutions at finite temperatures, for the ϕ^4 model. We can also conclude from fig. 4 that for small values of μ, the four temperatures are far greater than the energy barrier a_0. As μ gradually increases the temperatures obtained from the largest to the lowest q steadily decrease, and go far below the energy barrier. For sufficiently larga values of μ, the exact solvability condition thus holds at four tempratures lying below the symmetry-breaking temperature.

The free energy is strongly related to the groundstate energy, the influence of μ on the groundstate energies and on their relative positions with respect to the energy barrier is illustrated in fig. 5 . The groundstate energies are infinitely large for $\mu \to 0$, and decrease with an increase of μ irrespective of q. However, combining the influence of μ together with the choice of q affects the position of the energy level with respect to the energy barrier. Taking $q = 1$ for illustration, the groundstate energy decreases drastically but will always remain above the energy barrier. This drastic decrease is also observed for higher values of q, but when μ rises beyond a specific value namely $\mu_s = \sqrt{3/2}, \sqrt{3/4}$ and $\mu_s \simeq 0.717$ for $q = 2, q = 3$ and $q = 4$ respectively, the grounstate

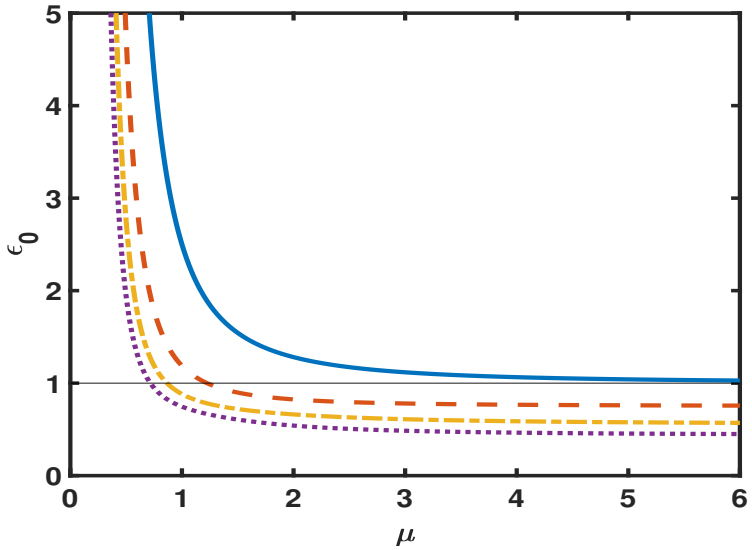

FIGURE 5 (Color online) Variation of the groundstate energy ϵ_0 with the shape deformability parameter μ, for four different values of q (corresponding to four different temperatures) namely: $q = 1$ (Solid line), $q = 2$ (Dashed line), $q = 3$ (Dash-dotted line), $q = 4$ (Dotted line). The horizontal line stands for the energy barrier a_0 here fixed as $a_0 = 1$.

energy drops below the energy barrier and tends to a finite value i.e. $\epsilon_0(\mu \to \infty) = (3/4)a_0$ for $q = 2$, $\epsilon_0(\mu \to \infty) = (5/9)a_0$ for $q = 3$ and $\epsilon_0(\mu \to \infty) = (7/16)a_0$ for $q = 4$. Moreover for a fixed value of μ, lower energy levels are obtained by increasing the temperature order q.

With the expressions of the exact groundstate wavefunctions and energy eigenvalues at several temperatures, for arbitrary values of the deformability parameter μ, quantities such as the probability density which are relevant in the formulation of correlation functions and correlation lengths at low temperatures, turn out to be easily formulated analytically. In effect the probability density associated with the classical field u, is nothing but the square of the normalized groundstate wavefunction. For this reason we expect the influence of shape deformability on the probability density, to be qualitatively the same as the influence of the same parameter on the groundstate wavefunction. The groundstate wavefunctions (unnormalized), for four different temperatures, are plotted in fig. 6 considering different values of the shape deformability parameter μ. To capture the physics lying in the difference in profiles of the probability density which emerges from fig. 6 , it is useful to combine features related to the deformability and general properties of probability densities for bistable systems. To this last point, in fig. 5 we have seen that for small values of μ, the groundstate energies were higher than the energy barrier a_0 and hence correspond to a high-temperature regime. Thus in this regime the Schrödinger pseudo-particles have sufficient energy to cross the energy barrier, and move freely from one well to another behaving as if trapped instead by a single-well potential. The full state space is then covered with power law and the whole space is probable, with a maximum probability density at the barrier peak. As μ increases the probability density at the four temperatures increases in amplitude and a decrease in width, but is still dominated by a single peak. This is actually justified by the fact that an increase of μ enhances the potential confinement by strengthening the steepness of the reflective walls, thus restricting the attainable space to the region covered by just the valleys and the energy barrier. The groundstate energy beeing high the energy barrier remains the most probable state. For $q = 1$ the groundstate energy lies above the energy barrier independently of μ. It turns out that even a lowering of temperature by increase in μ will still yield a probability density with a single peak, located at the barrier (top graph in fig. 6). However, for choices of q greater than one, this behaviour is observed only for $\mu \leq \mu_S$. When μ increases in the range $\mu > \mu_S$, the groundstate energy falls below the energy barrier a_0 and a decrease in temperature below the transition temperature restricts the transitions form one well to another. The pseudo-particles are consequently more confined in the potential wells, such that the valleys become more probable. In fig. 6 this is illustrated by the probability density showing two peaks, each located in the neighborhood of the degenerate minima of the parametrized DW potential. To enrich our understanding of the temperature dependence of the probability density for a fixed μ, but at different temperatures, in fig. 7 we represented the groundstate probability density for $\mu = 2$ and for three distinct temperatures at which the quasi-exactly solvable condition holds. We note a continuous shift from a single peak feature to a

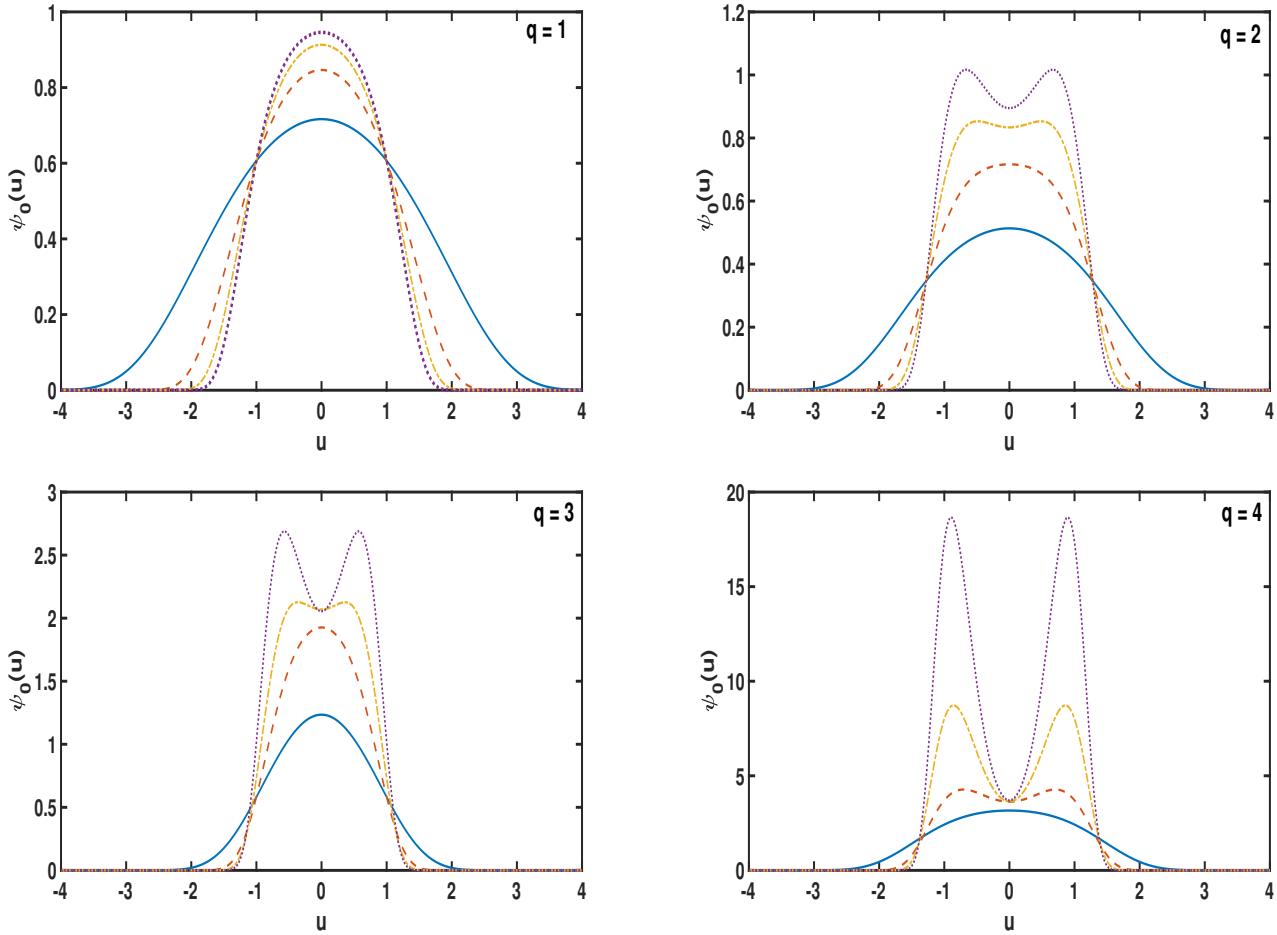

FIGURE 6 (Color online) Groundstate wavefunctions in position space at four different temperatures, for $\mu = 0.5$ (Solid line), $\mu = 1$ (Dashed line), $\mu = 1.5$ (Dot-dashed line), $\mu = 2$ (Dashed line).

two-peak feature, with decreasing temperature. Remark that the change in the peak width with temperature is different from that of the ϕ^4 model. Instructively the exact probability densities, are superimposed with those obtained from numerical simulations of the following additive-noise Langevin equation associated to the model:

$$\partial_{tt}^2 u - \partial_{xx}^2 u + \eta \partial_t u + dV(u,\mu)/du = F(x,t), \tag{34}$$

where the Gaussian white noise $F(x,t)$, and the viscosity η, are related by the fluctuation-dissipation theorem:

$$\langle F(x,t)F(x',t')\rangle = 2\eta\beta^{-1}\delta(x-x')\delta(t-t'). \tag{35}$$

We used standard techniques[55] to solve the discrete version of the above Langevin equation, and sampled the results in time to obtain time-averaged probability densities after random initial conditions had been driven to equilibrium. In the simulations we employed both Euler and Runge-Kutta schemes, with a lattice size of typically 350K points taking a lattice spacing of $d = 0.02$ and a time step of $h = 0.001$. As evidenced by fig. 7 , the exact (i.e. analytical) probability density and the results from numerical simulations, show excellent agreement. This agreement between the analytical and numerical results suggests that the groundstate energies can be numerically computed using the corresponding probability densities, at any temperature where quasi-exactly solvable condition holds for a wide range of values of the shape deformability parameter μ. A relevant implication of this is the possibility to compute exactly, thermodynamic quantities such as the enthalpy, the internal energy, the entropy and so on.

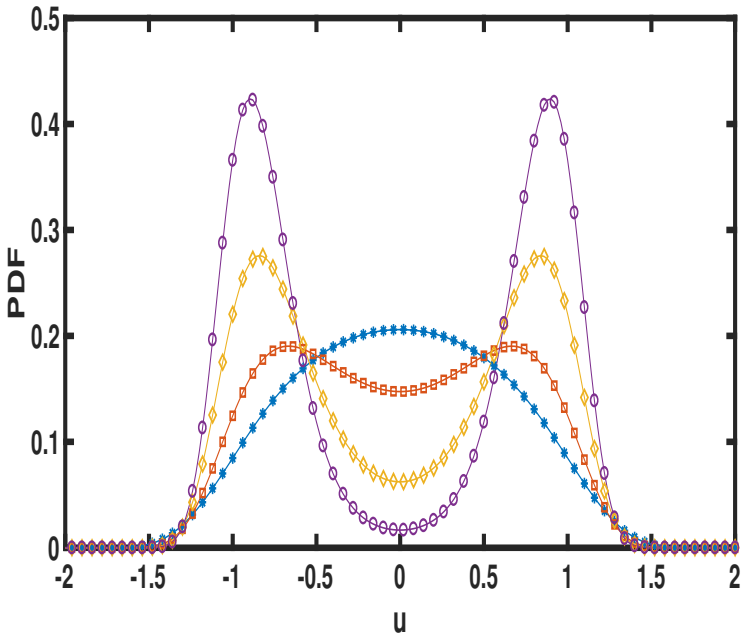

FIGURE 7 (Color online) Comparision of the exact (Solid Line) probability density function (PDF) and the results from numerical simulations of he Langevin equation, for $\mu = 2$ and for values of β obtained for $q = 1$ (stars), $q = 2$ (squares), $q = 3$ (diamonds) and $q = 4$ (circles). Note the excellent agreement between exact PDFs and numerical simulations.

5 | CONCLUSION

We have investigated the influence of shape deformability on the occurrence and orders of transitions in quantum tunneling, and on the statistical mechanics of a bistable system characterized by a parametrized DW potential. Systems with this feature abound in nature, ranging from biology to soft matters such as lipid membranes[56], linear polymer chains, molecular crystals and hydrogen-bonded ferroelectrics and antiferroelectrics. In these systems chemical processes such as the effects of catalyzers or solvants, isotopic substitutions or simply the intrinsic structure of molecular chains (e.g. flexible chain backbones and soft interactions) can favor changes in bond lengths and characteristic parameters of the double-well energy landscape as for instance the height of the potential barrier, positions of the potential wells, the steepness of the potential walls, etc. These characteristic parameters are well known to govern symmetry-breaking instabilities in low-dimensional systems.

We have established the existence of a critical value of the shape deformability parameter μ aobve which a first-order transition in quantum tunneling would occur, besides the second-order transition inherent to the Ginzburg-Landau feature of the DW potential energy. We explored the possibility to study the statistical mechanics of the system via the transfer-integral operator method, with emphasis on conditions for quasi-exact solvability of the associated pseudo-particle's Schrödinger equation. We determined the condition, and obtained groundstate wavefunctions and the corresponding energy eigenvalues for temperatures determined by the quasi-exact solvability condition. Concerning the dependence of these wavefunctions and energy eigenvalues on the shape deformability parameter, we found that for each value of μ the quasi-exact solvability of the model allows exact computation of the eigenstates at various temperatures. These temperatures were obtained above and below the transition temperature, depending on values of the shape deformability parameter. The influence of shape deformability on the probability density was also examined. Analytical results showed a striking agreement with large-scale Langevin simulations, implying that the study of probability density-based thermodynamics via Langevin simulations is feasable for bistable systems with the parametrized DW potential.

Author contributions

F. Naha Nzoupe carried out the analytical calculations and the numerical simulations, Alain M. Dikandé proposed the topic, assisted in the simulations and drafted the manuscript, C. Tchawoua contributed in the analytical calculations and in the writeup of the manuscript.

Financial disclosure

None reported.

Conflict of interest

The authors declare no potential conflict of interests.

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