Equivalence of a complex $\mathcal{PT}$-symmetric quartic Hamiltonian and a Hermitian quartic Hamiltonian with an anomaly

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In a recent paper Jones and Mateo used operator techniques to show that the non-Hermitian $\mathcal{PT}$-symmetric wrong-sign quartic Hamiltonian $H = \frac{1}{2}p^2 - gx^4$ has the same spectrum as the conventional Hermitian Hamiltonian $\tilde{H} = \frac{1}{2}p^2 + 4gx^4 - \sqrt{2g}x$. Here, this equivalence is demonstrated very simply by means of differential-equation techniques and, more importantly, by means of functional-integration techniques. It is shown that the linear term in the Hermitian Hamiltonian is anomalous; that is, this linear term has no classical analog. The anomaly arises because of the broken parity symmetry of the original non-Hermitian $\mathcal{PT}$-symmetric Hamiltonian. This anomaly in the Hermitian form of a $\mathcal{PT}$-symmetric quartic Hamiltonian is unchanged if a harmonic term is introduced into H. When there is a harmonic term, an immediate physical consequence of the anomaly is the appearance of bound states; if there were no anomaly term, there would be no bound states. Possible extensions of this work to $-\phi^4$ quantum field theory in higher-dimensional space-time are discussed.

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I. INTRODUCTION

In this paper we consider the quantum system described by the Hamiltonian

$$H = \frac{1}{2m}p^2 - gx^4, \tag{1}$$

where g is real and positive. The Hamiltonian (1) is of particular interest because the corresponding $-\phi^4$ quantum field theory might be a good model for describing the dynamics of the Higgs sector of the standard model. This is because the $-\phi^4$ theory is asymptotically free and thus nontrivial [1–3]. Furthermore, the one-point Green's function $\langle 0|\phi|0\rangle$ is nonvanishing [4].

While the $-x^4$ potential in (1) appears to be unbounded below and the Hamiltonian H appears to be symmetric under parity reflection, neither of these properties holds because, as we will explain shortly, the eigenfunctions of the Hamiltonian are required to vanish exponentially as $|x| \to \infty$ in a pair of Stokes' wedges in the complex-x plane. These wedges do not include the real-x axis.

The Hamiltonian (1) is not Hermitian in the conventional Dirac sense, where Hermitian conjugation is defined as combined matrix transposition and complex conjugation. Nevertheless, the eigenvalues E_n are all real, positive, and discrete. This is because H possesses an unbroken $\mathcal{PT}$ symmetry [5–7], which means that H and its eigenstates $\psi_n(x)$ are invariant under space-time reflection. Here, $\mathcal{P}$ denotes spatial reflection $p \to -p$ and $x \to -x$, and $\mathcal{T}$ denotes time reversal $p \to -p$, $x \to x$, and $i \to -i$.

Even though H is not Dirac Hermitian, it is possible to construct a state space having a positive inner product with respect to which H is Hermitian and in this Hilbert space, time evolution is unitary (probability conserving) [6]. This positive inner product involves $\mathcal{CPT}$-conjugation, where $\mathcal{C}$ is a linear operator whose square is unity and which commutes with the Hamiltonian. (These mathematical properties are reminiscent of the charge conjugation operator in particle physics.) Given the operator $\mathcal{C}$, we can construct the *positive* operator $e^{\mathcal{Q}} = \mathcal{CP}$, which can in turn be used to construct by means of a similarity transformation an equivalent Hamiltonian $\tilde{H} \equiv e^{-\mathcal{Q}/2}He^{\mathcal{Q}/2}$, where $\tilde{H}$ is Dirac Hermitian [8].

Many quantum-mechanical Hamiltonians that are $\mathcal{PT}$-symmetric have been studied in the recent literature [9]. However, the Hamiltonian (1) is especially interesting because, unlike the $\mathcal{PT}$-symmetric Hamiltonian $\frac{1}{2}p^2 + ix^3$, for example, the boundary conditions on the eigenfunctions are not imposed on the real-x axis. Rather, these boundary conditions hold in the interiors of wedges in the complex-x plane. To identify these wedges we use a WKB approximation to determine the possible asymptotic behaviors of the eigenfunctions. For large $|x|$ the possible exponential behaviors of the solutions to the Schrödinger equation are given by

$$\psi_n(x) \sim e^{\pm i\sqrt{2mg}x^3/3} \qquad (|x| \to \infty). \tag{2}$$

This result shows that the eigenfunctions are purely oscillatory along six lines separated by 60° angles. In particular, the wave functions are oscillatory on the positive and negative real-x axes. These six lines are the boundaries of the six 60° Stokes' wedges in which the solutions in (2) grow or decay exponentially.

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The eigenfunctions for the Hamiltonian (1) are required to decay exponentially in the interiors of a pair of Stokes' wedges in the lower-half x-plane. These wedges, which are symmetrically placed with respect to the imaginary axis, lie below the positive and negative real-x axes with the upper edges of the wedges lying on the real axis.

Note that under space reflection $x \to -x$, the original two-wedge domain changes to the interior of a *different* pair of 60° wedges that lie in the *upper*-half plane. Therefore, while H in (1) may appear to be parity symmetric, it obeys parity-violating boundary conditions. One can also understand the parity violation of H in (1) in a different way. In Ref. [10] it is shown that the real spectrum of H in (1) can be obtained without having to impose boundary conditions in the complex plane. The procedure is simply to require that the $-x^4$ potential be reflectionless. Thus, an incoming plane wave from $x = -\infty$ propagates past the potential and becomes an outgoing plane wave at $x = +\infty$. This configuration is not parity invariant because under parity reflection, the incoming plane wave at $x = -\infty$ becomes an outgoing plane wave and the outgoing plane wave at $x = \infty$ becomes an incoming plane wave. In short, the right-going flow of probability current becomes a left-going flow. (Of course, this configuration is invariant under combined $\mathcal{P}$ and $\mathcal{T}$ reflection.)

This violation of parity symmetry occurs only at the quantum level. At the classical level, the equations of motion are clearly parity symmetric:

$$\dot{x}(t) = \frac{1}{m}p(t), \qquad \dot{p}(t) = 4gx^3(t). \tag{3}$$

In general, it is difficult to construct the operator $\mathcal{C}$, and in the past for nontrivial models this operator has only been determined perturbatively [11]. However, recently Jones and Mateo used perturbative operator methods to construct C in closed form for the Hamiltonian in (1) [12]. They then found the equivalent Hermitian Hamiltonian $\tilde{H}$, whose potential has a positive quartic term and also a linear term. (Using Rayleigh-Schrödinger perturbation theory, Buslaev and Grecchi had already discovered this equivalent Hamiltonian much earlier [13].)

The purpose of this paper is to examine the connection between the $\mathcal{PT}$-symmetric non-Hermitian Hamiltonian (1) and the equivalent Hermitian Hamiltonian $\tilde{H}$, whose potential has a positive quartic term and a linear term. In Sec. II we demonstrate the equivalence between these two Hamiltonians simply and directly by transforming the Schrödinger equation for the former Hamiltonian into the Schrödinger equation for the latter Hamiltonian. We show that the linear term in $\tilde{H}$ is proportional to $\hbar$ and is thus a quantum anomaly. This anomaly arises because the boundary conditions on the $\mathcal{PT}$-symmetric Hamiltonian violate parity. As explained above, this parity violation is not a feature of the classical equations of motion. In Sec. III we generalize the Hamiltonian H in (1) to include a harmonic (quadratic) term and show that the equivalent Hermitian Hamiltonian has an anomaly of exactly the same form. Furthermore, we show that an immediate consequence of the anomaly is the appearance of bound states.

The Schrödinger-equation approach of Sec. II does not readily generalize to quantum field theory, so in Sec. IV we demonstrate the equivalence between H and $\tilde{H}$ by using path-integration techniques in which we treat H as defining a quantum field theory in one-dimensional space-time. We conclude in Sec. V by indicating how path-integral techniques might be extended and used to identify the equivalent Hermitian Lagrangian for a $-\phi^4$ quantum field theory in higher space-time dimensions.

II. DIFFERENTIAL-EQUATION DERIVATION OF THE ANOMALY

In this section we use straightforward differential-equation techniques to establish the equivalence of H and $\tilde{H}$. Consider the one-dimensional Schrödinger eigenvalue problem

$$-\frac{\hbar^2}{2m}\psi''(x) - gx^4\psi(x) = E\psi(x) \tag{4}$$

associated with the non-Hermitian Hamiltonian (1), where the boundary conditions on $\psi(x)$ are that as $\lim_{|x|\to\infty}\psi(x) = 0$ if $-\frac{\pi}{3} < \arg x < 0$ and $-\pi < \arg x < -\frac{2\pi}{3}$. These boundary conditions do not include the real-x axis and they require that the differential equation (4) be solved along a contour whose ends lie in the above wedges in the complex-x plane (see Fig. 1). We will use here the same complex contour that Jones and Mateo employed in their operator analysis of the Hamiltonian (1) [12]:

$$x = -2iL\sqrt{1 + iy/L}, \tag{5}$$

where y runs from $-\infty$ to ∞ along the real axis. This contour is acceptable because as $y \to \pm\infty$, $\arg x$ approaches $-45°$ and $-135°$, so the contour lies inside the Stokes' wedges. In (5) L is an arbitrary positive constant

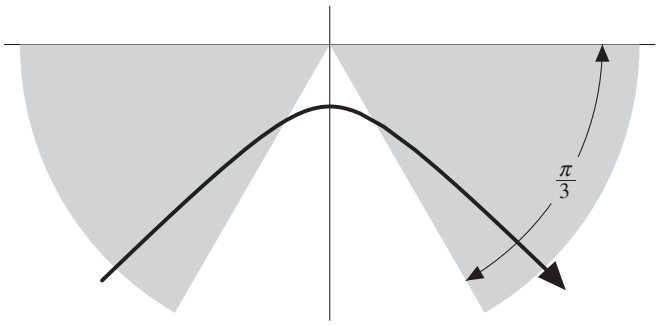

FIG. 1. Stokes' wedges in the lower-half complex-x plane for the Schrödinger equation (4) arising from the Hamiltonian H in (1). The eigenfunctions of H decay exponentially as $|x| \to \infty$ inside these wedges. Also shown is the contour in (5).

having dimensions of length. In terms of the parameters of H in (1) the fundamental unit of length is $[\hbar^2/(mg)]^{1/6}$. Thus,

$$L = \lambda\left(\frac{\hbar^2}{mg}\right)^{1/6}, \tag{6}$$

where λ is an arbitrary positive dimensionless constant. When we change the independent variable in (4) from x to y according to (5), the Schrödinger equation (4) becomes

$$-\frac{\hbar^2}{2m}\left(1+\frac{iy}{L}\right)\phi''(y) - \frac{i\hbar^2}{4Lm}\phi'(y) - 16gL^4\left(1+\frac{iy}{L}\right)^2\phi(y) = E\phi(y). \tag{7}$$

Next, we perform a Fourier transform of (7). We define

$$\tilde{f}(p) \equiv \int_{-\infty}^{\infty} dy e^{-iyp/\hbar} f(y), \tag{8}$$

so that the Fourier transform of $f'(y)$ is $ip\tilde{f}(p)/\hbar$ and the Fourier transform of $yf(y)$ is $i\hbar\tilde{f}'(p)$. Then, the Fourier transform of the Schrödinger equation (7) is

$$\frac{1}{2m}\left(1-\frac{\hbar}{L}\frac{d}{dp}\right)p^2\tilde{\phi}(p) + \frac{\hbar}{4Lm}p\tilde{\phi}(p) - 16gL^4\left(1-\frac{\hbar}{L}\frac{d}{dp}\right)^2\tilde{\phi}(p) = E\tilde{\phi}(p). \tag{9}$$

Expanding and simplifying this equation, we obtain

$$-16gL^2\hbar^2\tilde{\phi}''(p) + \left(-\frac{\hbar p^2}{2mL} + 32gL^3\hbar\right)\tilde{\phi}'(p) + \left(\frac{p^2}{2m} - \frac{3p\hbar}{4mL} - 16gL^4\right)\tilde{\phi}(p) = E\tilde{\phi}(p). \tag{10}$$

[Note that the variable p used here is not the same as the variable p used in (1). Here, considered as an operator, p represents $-i\hbar\frac{d}{dy}$, whereas in (1) p represents $-i\hbar\frac{d}{dx}$.]

This equation is not a Schrödinger equation because there is a one-derivative term. However, we can eliminate this term by performing a simple transformation:

$$\tilde{\phi}(p) = e^{Q(p)/2}\Phi(p). \tag{11}$$

The condition on $Q(p)$ for which the equation satisfied by $\Phi(p)$ has no one-derivative term is a first-order differential equation whose solution is

$$Q(p) = \frac{2L}{\hbar}p - \frac{1}{96gmL^3\hbar}p^3. \tag{12}$$

It is interesting that $e^{Q(p)}$ is precisely the operator found in Ref. [12].[1] Substituting this expression for Q gives the Schrödinger equation satisfied by $\Phi(p)$:

$$-16gL^2\hbar^2\Phi''(p) + \left(-\frac{\hbar p}{4mL} + \frac{p^4}{256gm^2L^4}\right)\Phi(p) = E\Phi(p). \tag{13}$$

Finally, we make the scaling substitution

$$p = zL\sqrt{32mg}, \tag{14}$$

to replace the p variable, which has units of momentum, by z, which is a coordinate variable having units of length. The resulting eigenvalue equation, posed on the real-z axis, is

$$-\frac{\hbar^2}{2m}\Phi''(z) + \left(-\hbar\sqrt{\frac{2g}{m}}z + 4gz^4\right)\Phi(z) = E\Phi(z). \tag{15}$$

We emphasize that, while z has dimensions of length, it is not a conventional coordinate variable because it is odd under the discrete transformation of time reversal.

Observe that the eigenvalue problem (15) is similar in structure to that in (4). [Eq. (15) is not *dual* to (4) because it is still weakly coupled.] However, the potential has acquired a linear term, and since this linear term is proportional to $\hbar$, we may regard it as a quantum anomaly. The linear term has no classical analog because the classical equations of motion are parity symmetric. The breaking of parity symmetry occurs at large values of x where the boundary conditions on the wave function $\psi(x)$ are imposed. Because we have taken a Fourier transform to obtain the Schrödinger equation (15), this parity anomaly now manifests itself at small values of z.

The Hamiltonian $\tilde{H}$ for which (15) is the eigenvalue problem is

$$\tilde{H} = \frac{\tilde{p}^2}{2m} - \hbar\sqrt{\frac{2g}{m}}z + 4gz^4. \tag{16}$$

This Hamiltonian is Hermitian in the Dirac sense and is bounded below on the real-z axis. Furthermore, it is also $\mathcal{PT}$-symmetric. This is because at every stage in the sequence of transformations above, $\mathcal{PT}$ symmetry is preserved. However, while z and $\tilde{p}$ are canonically conjugate operators satisfying $[z, \tilde{p}] = i$, the new variable z behaves like a momentum rather than a coordinate variable because z changes sign under time reversal.

III. BOUND STATES—A DIRECT PHYSICAL CONSEQUENCE OF THE ANOMALY

If we generalize the Hamiltonian (1) to include a harmonic term in the potential,

$$H = \frac{1}{2m}p^2 + \frac{\mu^2}{2}x^2 - gx^4, \tag{17}$$

then the same differential-equation analysis used in Sec. II straightforwardly yields the following equivalent Hermitian Hamiltonian:

[1]Note that $e^{Q(p)}$ is *not* the $\mathcal{CP}$ operator that could, in principle, be used in a similarity transformation to produce the Hermitian Hamiltonian from the non-Hermitian $\mathcal{PT}$-symmetric Hamiltonian (1). One can only use $e^{Q(p)}$ to transform the non-Hermitian Hamiltonian H to Hermitian form if H has first been written in terms of the real variable y.

$$\tilde{H} = \frac{\tilde{p}^2}{2m} - \hbar\sqrt{\frac{2g}{m}}z + 4g\left(z^2 - \frac{\mu^2}{8g}\right)^2. \tag{18}$$

This result is given in Refs. [12,13]. Observe that for these more general Hamiltonians the form of the linear anomaly term remains unchanged from that in (15).

In an earlier paper [14] it was shown that the Hamiltonian (17) exhibits bound states. In a particle physics model a bound state is defined as a state having a negative binding energy. In the context of a quantum-mechanical model we define bound states as follows: Let the energy levels of the Hamiltonian be E_n ($n = 0, 1, 2, \ldots$). The renormalized mass is the mass gap; that is, $M = E_1 - E_0$. The higher excitations must also be measured relative to the vacuum energy: $E_n - E_0$ ($n = 2, 3, 4, \ldots$). We say that the nth higher excitation is a bound state if the binding energy

$$B_n \equiv E_n - E_0 - nM \tag{19}$$

is negative. If B_n is positive, then we regard the state as unbound because this state can decay into n 1-particle states of mass M in the presence of an external field.

It was observed numerically in Ref. [14] that for small positive values of g the first few states of H in (17) are bound. As g increases, the number of bound states decreases until, when g/μ^3 is larger than the critical value 0.0465, there are no bound states. In this paper a rough heuristic argument was given to explain why there is such a critical value. This argument is difficult to formulate because the non-Hermitian Hamiltonian is evaluated for x in the complex plane. When x is complex, one cannot use order relationships such as $>$ or $<$, which only apply to real numbers.

However, now that we have established that H in (17) has the same spectrum as the Hermitian Hamiltonian in (18), it is easy to understand the appearance of bound states. Furthermore, as we will now show, the bound states are a direct consequence of the linear anomaly term. To probe the influence of the anomaly, let us generalize (18) by inserting a parameter ϵ that measures the strength of the anomaly term:

$$\tilde{H} = \frac{\tilde{p}^2}{2} - \epsilon\hbar\sqrt{2g}z + 4g\left(z^2 - \frac{1}{8g}\right)^2, \tag{20}$$

where for simplicity we have set $m = \mu = \hbar = 1$.

If we take $\epsilon = 0$, then there is no anomaly term and the potential is a *symmetric* double well. The mass gap for a double well is exponentially small because it is a result of the tunneling between the wells. Thus, the renormalized mass M is very small. Therefore, B_n in (19) is positive and there are no bound states. In Fig. 2 we display the double-well potential and the first several states of the system for the case $g = 0.046$ and $\epsilon = 0$. Note that the lowest two states have a very small splitting.

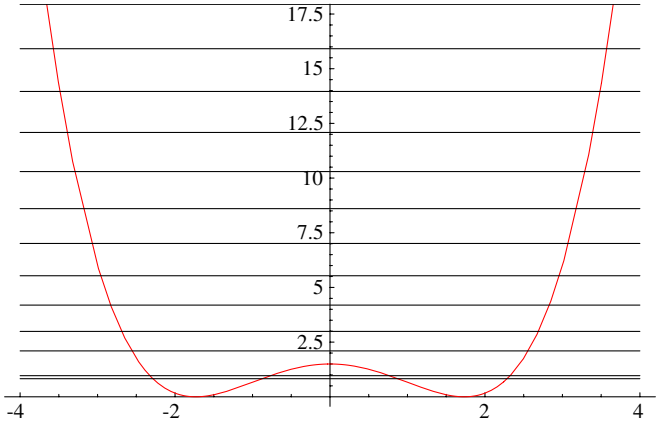

FIG. 2 (color online). Potential of the Hermitian Hamiltonian (20) plotted as a function of the real variable z for the case $\epsilon = 0$ and $g = 0.046$. The energy levels are indicated by horizontal lines. Because $\epsilon = 0$ there is no anomaly, and the double-well potential is symmetric. Therefore, the mass gap is very small and, as a consequence, there are no bound states at all. The occurrence of bound states can be attributed to the anomaly.

If $\epsilon = 1$, the double-well potential is asymmetric and the lowest two states are not approximately degenerate. As a result, bound states can occur near the bottom of the potential well. The higher-energy states eventually become unbound because, as we know from WKB theory, in a quartic well the nth energy level grows like $n^{4/3}$ for large n. As g becomes large, the number of bound states becomes smaller because the depth of the double well decreases. For sufficiently large g there are no bound states. In Fig. 3 we display the potential for $\epsilon = 1$ for $g = 0.046$. For this value of g there is only one bound state.

To display the bound states we simply plot the value of the binding energy B_n as a function of n. For example, in Fig. 4 we display the bound states for $\epsilon = 1$ and $g = 0.008\,333$. Note that for these values there are 23 bound

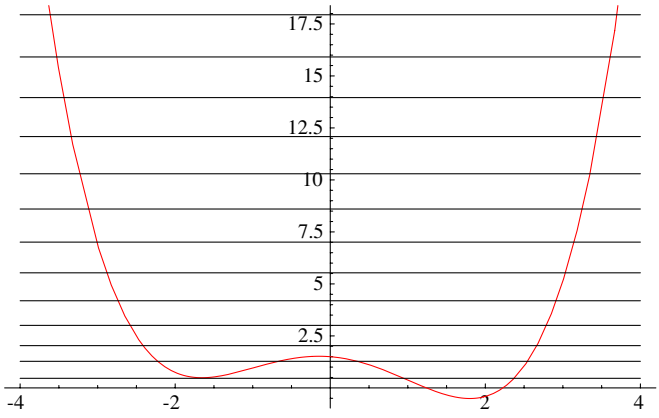

FIG. 3 (color online). Asymmetric potential well plotted as a function of the real variable z for the Hermitian Hamiltonian (20) with $\epsilon = 1$ and $g = 0.046$. The energy levels are indicated by horizontal lines. There is one bound state.

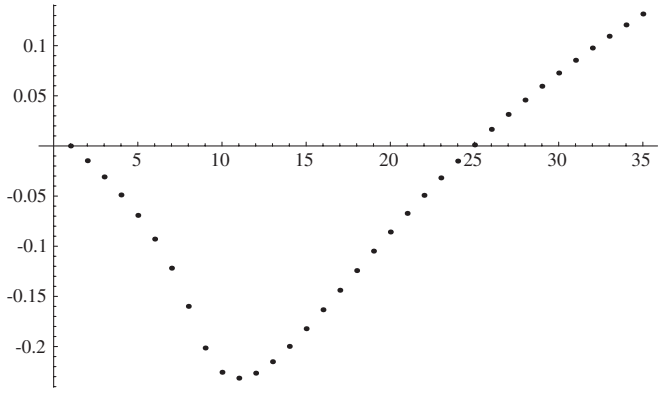

FIG. 4. Binding energies $B_n = E_n - E_0 - nM$ plotted as a function of n for $g = 0.008333$ and $\epsilon = 1$. A negative value of B_n indicates a bound state. Observe that there are 23 bound states for these parameter values. Note that B_n is a smooth function of n.

states. Observe also that the binding energy B_n is a smooth function of n.

It is interesting that the bound-state spectrum depends sensitively on the anomaly term in the Hamiltonian (20). If ϵ is slightly less than 1, the first few states become unbound, as is shown in Fig. 5. In this figure $g = 0.008\,333$ and $\epsilon = 0.9$.

If ϵ is slightly greater than 1, the binding energy B_n is not a smooth function of n for small n. In Fig. 6 we plot B_n as a function of n for $g = 0.008\,333$ and $\epsilon = 1.1$. Note that for these values of the parameters there are 30 bound states. Figs. 4–6 are strikingly different, and demonstrate the extreme sensitivity of the bound-state spectrum to the anomaly term.

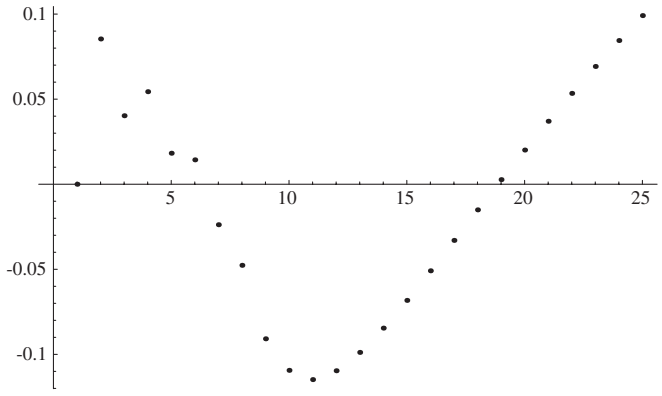

FIG. 5. Binding energies B_n plotted as a function of n for $g = 0.008333$ and $\epsilon = 0.9$. Note that the first five states have now become unbound and B_n is not a smooth function of n for $n \leq 6$. The next 12 states are bound, and in this region B_n is a smooth function of n. A comparison of this figure with Fig. 4 shows that the bound-state spectrum is exquisitely sensitive to the strength of the linear anomaly term.

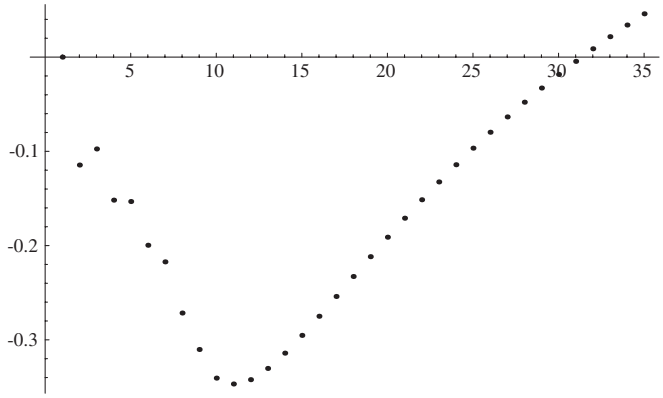

FIG. 6. Binding energies B_n plotted as a function of n for $g = 0.008\,333$ and $\epsilon = 1.1$. Note that there are 30 bound states and that B_n is not a smooth function of n when n is small.

IV. PATH-INTEGRAL DERIVATION OF THE PARITY ANOMALY

A path integral is used to represent the partition function of a quantum field theory. A path integral is much more complicated than a Schrödinger equation, and thus the elementary differential-equation methods applied in Sec. II cannot be used directly for a quantum field theory. To prepare for our study of a $\mathcal{PT}$-symmetric $-\phi^4$ field theory in Sec. V, we need to establish the equivalence of H in (1) and $\tilde{H}$ in (16) by using path-integration methods.

For the Hamiltonian (1) the Euclidean functional integral for the partition function Z is

$$Z = \int_C D\phi \exp\left[-\frac{1}{\hbar}\int dt\left(\frac{m}{2}\dot{\phi}^2 - g\phi^4\right)\right], \qquad (21)$$

where the normalization factor is understood. A functional integral is an infinite product of ordinary integrals, one for each lattice point in the discretized representation. The $g\phi^4$ term in the exponent would cause each of these integrals to diverge if the integration path lay on the real axis. To make these integrals converge, the contour of integration at each lattice point must approach infinity inside a pair of wedges having an angular opening of 45° and centered about the angles $-45°$ and $-135°$ in the lower-half complex plane. The subscript C on the functional integral sign indicates that the path integral is taken along a complex contour.

Our goal is to transform the functional integral (21) into a conventional functional integral in which the contour of integration runs along the real axis rather than in the complex plane. We expect to find that the action in the exponent will correspond to $\tilde{H}$ in (16).

Our approach is as follows: First, in Sec. IV A we transform the continuum functional integral in (21) directly using (5). We discover that if we proceed formally without recognizing that a functional integral is a subtle construct involving the limit of a discrete product of ordinary integrals, the resulting equivalent Hermitian Hamiltonian that

we obtain does not contain the linear anomaly term in $\tilde{H}$ in (16). Thus, this derivation produces the classical ($\hbar \to 0$) limit of $\tilde{H}$. Hence, this derivation is equivalent to the geometrical-optics approximation (zeroth-order WKB). To obtain the anomaly, we must discretize the functional integral, and this discretization requires great care. We explain and motivate the discretization procedure in Sec. IV B and carry it out in Sec. IV C.

A. Formal derivation correct to order $\hbar^0$

We begin by making a substitution analogous to that in (5),

$$\phi(t) = -2iL\sqrt{1 + i\psi(t)/L}. \tag{22}$$

This substitution introduces a functional Jacobian in the form of a square root:

$$D\phi = \frac{D\psi}{\det\sqrt{1 + i\psi/L}}. \tag{23}$$

The new functional integral over the ψ variable is

$$Z = \int \frac{D\psi}{\det\sqrt{1 + i\psi/L}} \exp\Big\{-\frac{1}{\hbar}\int dt\Big[\frac{m}{2}\frac{\dot{\psi}^2(t)}{1 + i\psi(t)/L} - 16gL^4\Big(1 + i\frac{\psi(t)}{L}\Big)^2\Big]\Big\}. \tag{24}$$

This is a conventional functional integral in the sense that the field $\psi(t)$ is real and the path of integration lies on the real axis rather than in the complex plane.

Next, we exploit the functional-integral version of the simple integral identity

$$\frac{1}{A} = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dt e^{-(1/2)A^2(t-B)^2} \qquad (\mathrm{Re}A^2 > 0) \tag{25}$$

and obtain (apart from an overall normalization factor)

$$Z = \int D\psi \int D\pi \exp\Big\{-\frac{1}{\hbar}\int dt\Big[\frac{1 + i\psi(t)/L}{2m} \times (\pi(t) - B(t))^2 + \frac{m}{2}\frac{\dot{\psi}^2(t)}{1 + i\psi(t)/L} - 16gL^4(1 + i\psi(t)/L)^2\Big]\Big\}. \tag{26}$$

This integral converges because $\mathrm{Re}[1 + i\psi(t)/L] = 1$, which is positive. Both functional integrals in (26) are conventional real integrals.

We eliminate the term containing the square of $\dot{\psi}(t)$ by choosing

$$B(t) = \frac{im\dot{\psi}(t)}{1 + i\psi(t)/L}. \tag{27}$$

With this choice the exponential in (26) simplifies to:

$$-\frac{1}{\hbar}\int dt\Big[\frac{1}{2m}\pi^2(t)(1 + i\psi(t)/L) - i\pi(t)\dot{\psi}(t) - 16gL^4(1 + i\psi(t)/L)^2\Big]. \tag{28}$$

Next, we integrate by parts in order to transfer the derivative from $\psi(t)$ to $\pi(t)$ and in doing so discard the surface term:

$$-\int dt\dot{\psi}(t)\pi(t) = \int dt\dot{\pi}(t)\psi(t). \tag{29}$$

After interchanging orders of integration and completing the square, we get

$$Z = \int D\pi \exp\Big[-\frac{1}{\hbar}\int dt\Big(\frac{1}{64gL^2}\dot{\pi}^2(t) + \frac{1}{256gm^2L^4}\pi^4(t) - L\dot{\pi}(t) + \frac{1}{64gmL^3}\pi^2(t)\dot{\pi}(t)\Big)\Big] \times \int D\psi \exp\Big[-\frac{16gL^2}{\hbar}\int dt\Big(\psi(t) - iL + \frac{i}{64gmL^3}\pi^2(t) + \frac{i}{32gL^2}\dot{\pi}(t)\Big)^2\Big]. \tag{30}$$

We integrate the $\dot{\pi}(t)$ and $\pi^2(t)\dot{\pi}(t)$ terms and ignore the surface contributions.

Finally, we rescale π and ψ in analogy with (14):

$$\pi(t) = L\sqrt{32mg}\varphi(t), \qquad \psi(t) = \frac{1}{L\sqrt{32mg}}p(t), \tag{31}$$

and evaluate the Gaussian integral over p. The result is

$$Z = \int D\varphi \exp\Big[-\frac{1}{\hbar}\int dt\Big(\frac{m}{2}\dot{\varphi}^2(t) + 4g\varphi^4(t)\Big)\Big], \tag{32}$$

which is the Euclidean functional integral for the *classical* (anomaly-free) version of the Hamiltonian $\tilde{H}$ in (16).

B. Discretization of the functional integral

Evidently, the analysis in Sec. IVA is not delicate enough to recover the linear anomaly term of $\tilde{H}$ in (16). In order to obtain this anomaly term it is necessary to discretize the functional integral (21). In order to do so, we replace $\dot{\phi}(t)$ by the usual lattice expression $(\phi_{n+1} - \phi_n)/a$, where a is the lattice spacing. Furthermore, we must replace $\phi(t)$ by the average $\frac{1}{2}(\phi_{n+1} + \phi_n)$ to preserve the time independence of the equal-time commutation relation in the underlying quantum-mechanical theory. Our purpose in this subsection is to explain the reason behind this latter substitution.

Consider a one-dimensional quantum-mechanical Hamiltonian of the form

$$H = \frac{1}{2}p^2 + V(q). \tag{33}$$

The Heisenberg equations of motion of the operators $p(t)$ and $q(t)$ have the same form as the classical equations in

(3):

$$\dot{x}(t) = p, \qquad \dot{p}(t) = -V'[q(t)]. \tag{34}$$

To discretize the differential equations in (34), we write

$$\begin{aligned} \frac{x_{n+1} - x_n}{a} &= \frac{p_{n+1} + p_n}{2}, \\ \frac{p_{n+1} - p_n}{a} &= -V'\left(\frac{x_{n+1} + x_n}{2}\right), \end{aligned} \tag{35}$$

where a is the lattice spacing.

One can verify that (35) is correct by following the procedure introduced in Ref. [15]. The right side of the first equation in (35) is a function of $p_{n+1} + p_n$, so the commutator of this equation with $p_{n+1} + p_n$ is

$$[x_{n+1} - x_n, p_{n+1} + p_n] = 0. \tag{36}$$

Also, the right side of second equation in (35) is a function of $x_{n+1} + x_n$. Thus, commuting $x_{n+1} + x_n$ with this equation gives

$$[x_{n+1} + x_n, p_{n+1} - p_n] = 0. \tag{37}$$

Adding (36) and (37) then gives

$$[x_{n+1}, p_{n+1}] = [x_n, p_n]. \tag{38}$$

This establishes the crucial result that the equal-time commutator is *exactly* preserved in time. Thus, the discretization scheme in (35) is exactly unitary. If a discretization scheme other than that in (35) had been used, there would be a small violation of unitarity. Evidently, to avoid violating unitarity on the lattice it is essential to replace a local function of $x(t)$, say $f[x(t)]$ by $f[\frac{1}{2}(x_{n+1} + x_n)]$ rather than by $f(x_n)$. Of course, the violation of unitarity vanishes in the continuum limit $a \to 0$, but we need to preserve unitarity in the lattice version of the theory.

To discretize an action, we follow the same approach as that used to obtain (35). Thus, for the Lagrangian $L = \frac{1}{2}\dot{x}^2(t) - V[x(t)]$ we discretize the action $\int dtL$ as follows:

$$\sum_n \left\{\frac{1}{2a}(x_{n+1} - x_n)^2 - aV\left[\frac{1}{2}(x_{n+1} + x_n)\right]\right\}. \tag{39}$$

To verify that this is the correct way to discretize the action, we vary this discrete action with respect to x_n to obtain the lattice equations of motion:

$$\begin{aligned} &\frac{1}{a}(2x_n - x_{n+1} - x_{n-1}) - \frac{a}{2}V'\left[\frac{1}{2}(x_{n+1} + x_n)\right] \\ &\qquad - \frac{a}{2}V'\left[\frac{1}{2}(x_n + x_{n-1})\right] = 0. \end{aligned} \tag{40}$$

To solve this equation, we substitute

$$\frac{x_{n+1} - x_n}{a} = \frac{p_{n+1} + p_n}{2}, \tag{41}$$

which is the first equation in (35). This reduces (40) to the form

$$b_n + b_{n-1} = 0, \tag{42}$$

where

$$b_n = \frac{p_{n+1} - p_n}{a} + V'\left(\frac{x_{n+1} + x_n}{2}\right). \tag{43}$$

The solution to (42) is

$$b_n = c(-1)^n, \tag{44}$$

where c is an arbitrary constant. However, if c is nonzero, then in the continuum limit where the lattice spacing tends to 0 the solution in (44) becomes infinitely oscillatory. To avoid the appearance of an infinite-energy solution, we must require that $c = 0$. We therefore obtain the result that $b_n = 0$, and we have recovered the second equation in (35). We have reproduced both equations in (35) and hence conclude that the discretization scheme used in (39) is correct. The lattice average used on the right sides of (35) and in the second term of (39) is completely consistent with Moyal ordering [16].

C. Derivation of the parity anomaly

Deriving the Hamiltonian $\tilde{H}$ in (16) from the partition function Z in (21) requires great care. First, we must discretize the functional integral (21) representing Z by following the procedure in Sec. IV B:

$$\begin{aligned} Z = \prod_n \int_C d\phi_n \exp\Big\{-\frac{a}{\hbar}\Big[\frac{m}{2a^2}(\phi_{n+1} - \phi_n)^2 \\ - \frac{g}{16}(\phi_{n+1} + \phi_n)^4\Big]\Big\}, \end{aligned} \tag{45}$$

where a is the lattice spacing. For each of the one-dimensional integrals in (45), the contour C begins in a wedge in the lower complex plane centered about $-135°$ and terminates in the $\mathcal{PT}$-symmetric wedge centered about $-45°$ (see Fig. 7).

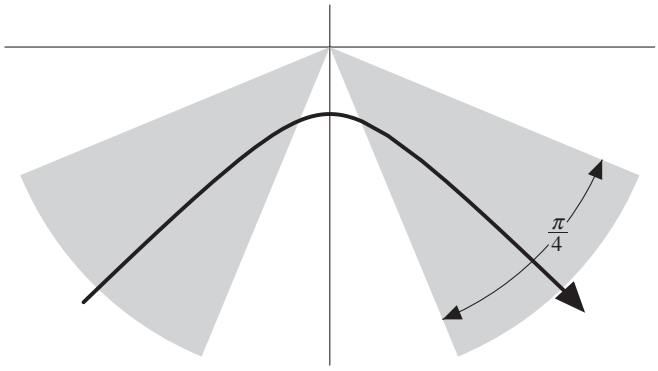

FIG. 7. Stokes' wedges in the lower-half complex-ϕ_n plane for each of the one-dimensional complex integrals used in (45). The integrands of these complex integrals vanish exponentially fast as $|\phi_n| \to \infty$ within these wedges. Also shown is the complex contour in (46).

For each of the complex integrals in (45) we make a substitution analogous to that in (5):

$$\phi_n = -2iL\sqrt{1 + i\psi_n/L}, \tag{46}$$

where L is an arbitrary positive constant having dimensions of length. At each lattice point this substitution introduces a Jacobian in the functional integral;

$$d\phi_n = \frac{d\psi_n}{\sqrt{1 + i\psi_n/L}}. \tag{47}$$

Thus, an exact transcription of (45) is

$$Z = \prod_n \int_{-\infty}^{\infty} \frac{d\psi_n}{\sqrt{1 + i\psi_n/L}} \exp\left[-\frac{a}{\hbar}\left(\frac{m}{2}\frac{\dot{\psi}_n^2}{A_n^2} - 16gL^4A_n^4\right)\right], \tag{48}$$

where we use the shorthand notation

$$\dot{\psi}_n \equiv \frac{1}{a}(\psi_{n+1} - \psi_n) \tag{49}$$

and

$$A_n \equiv \frac{1}{2}(\sqrt{1 + i\psi_{n+1}/L} + \sqrt{1 + i\psi_n/L}). \tag{50}$$

Note that in (48) the path of integration of each of the integrals lies on the real axis.

We now use the integral identity (25) to introduce the conjugate auxiliary field π_n at each lattice site n. To apply this identity we choose

$$A^2 = \frac{a}{m\hbar}A_n^2, \qquad t = \pi_n, \qquad B = B_n, \tag{51}$$

where B_n is as yet unspecified. The result is

$$Z = \prod_n \int_{-\infty}^{\infty} d\psi_n \int_{-\infty}^{\infty} d\pi_n \sqrt{\frac{a}{2\pi\hbar m}} \frac{A_n}{\sqrt{1 + i\psi_n/L}} \times \exp\left\{ -\frac{a}{\hbar}\left[\frac{A_n^2}{2m}(\pi_n - B_n)^2 + \frac{m}{2}\frac{\dot{\psi}_n^2}{A_n^2} - 16gL^4A_n^4\right]\right\}. \tag{52}$$

Making no approximations, we simplify the Jacobian in (52) as follows:

$$\begin{aligned} \frac{A_n}{\sqrt{1 + i\psi_n/L}} &= \frac{\sqrt{1 + i\psi_{n+1}/L} + \sqrt{1 + i\psi_n/L}}{2\sqrt{1 + i\psi_n/L}} \\ &= 1 + \frac{\sqrt{1 + i\psi_{n+1}/L} - \sqrt{1 + i\psi_n/L}}{2\sqrt{1 + i\psi_n/L}} \\ &= 1 + \frac{i(\psi_{n+1} - \psi_n)}{4LA_n\sqrt{1 + i\psi_n/L}} \\ &= 1 + a\frac{i\dot{\psi}_n}{4LA_n\sqrt{1 + i\psi_n/L}}. \end{aligned} \tag{53}$$

Next, we choose B_n:

$$B_n = \frac{im\dot{\psi}_n}{A_n^2}. \tag{54}$$

[Note that the choice of sign on the right side of (54) is arbitrary. If we replace i by $-i$ in this equation, then at the end of the calculation the sign of the linear term in the Hermitian Hamiltonian will be reversed. Reversing this sign has no effect on the energy levels of the Hamiltonian.] With this choice, we can approximate for small lattice spacing a the Jacobian factor in the last line of (53):

$$1 + a\frac{i\dot{\psi}_n}{4LA_n\sqrt{1 + i\psi_n/L}} = 1 + \frac{aB_n}{4mL} + O(a^2). \tag{55}$$

Next, we use the identity

$$\begin{aligned} &\int_{-\infty}^{\infty} d\pi_n \pi_n \exp\left[-\frac{aA_n^2}{2m\hbar}(\pi_n - B_n)^2\right] \\ &\quad = \int_{-\infty}^{\infty} d\pi_n B_n \exp\left[-\frac{aA_n^2}{2m\hbar}(\pi_n - B_n)^2\right], \end{aligned} \tag{56}$$

which holds because the exponent is an even function of $\pi_n - B_n$. This identity implies that (52) with the Jacobian in (55) can be rewritten as

$$\begin{aligned} Z = \prod_n \int_{-\infty}^{\infty} d\psi_n \int_{-\infty}^{\infty} d\pi_n \sqrt{\frac{a}{2\pi\hbar m}}\left[1 + \frac{a\pi_n}{4mL} + O(a^2)\right] \\ \times \exp\left[-\frac{a}{\hbar}\left(\frac{A_n^2\pi_n^2}{2m} - i\pi_n\dot{\psi}_n - 16gL^4A_n^4\right)\right]. \end{aligned} \tag{57}$$

Next we promote the Jacobian factor to the exponent by noting that for any number w, we have $1 + aw = e^{aw}$ with an error of order a^2. We also simplify terms in the exponent by ignoring terms of order a^2. The result is

$$\begin{aligned} Z = \prod_n \int_{-\infty}^{\infty} d\psi_n \int_{-\infty}^{\infty} d\pi_n \sqrt{\frac{a}{2\pi\hbar m}} \exp\left\{ -\frac{a}{\hbar}\left[(1 + i\psi_n/L)\frac{\pi_n^2}{2m}\right.\right. \\ \left.\left. + i\dot{\pi}_n\psi_n - 16gL^4(1 + i\psi_n/L)^2 - \frac{\hbar\pi_n}{4mL} + O(a)\right]\right\}, \end{aligned} \tag{58}$$

where we have performed a summation by parts to obtain the $i\dot{\pi}_n\psi_n$ term.

Next, we perform a scaling like that in (31):

$$\pi_n = \sqrt{32mg}L\varphi_n, \qquad \psi_n = \frac{1}{\sqrt{32mg}L}p_n, \tag{59}$$

and continue as we did in Sec. IVA. After completing the square and integrating over p_n, we obtain the final result for the lattice version of the continuum functional integral:

$$Z = \int D\varphi \exp\left[-\frac{1}{\hbar}\int dt\left(\frac{m}{2}\dot{\varphi}^2 + 4g\varphi^4 - \hbar\sqrt{\frac{2g}{m}}\varphi\right)\right]. \tag{60}$$

This is precisely the functional integral for the theory described by the Hermitian Hamiltonian $\tilde{H}$ in (16).

V. GENERALIZATION TO QUANTUM FIELD THEORY

The Euclidean functional integral for the partition function Z of a d-dimensional $-\phi^4$ quantum field theory is

$$Z = \int_C D\phi \exp\left[- \int d^d x \left(\frac{1}{2}(\nabla\phi)^2 - g\phi^4 \right) \right], \tag{61}$$

where the normalization factor is understood and we have adopted natural units where $\hbar = 1$. As in the one-dimensional quantum field theory in (21), the contour of integration at each space-time point must approach infinity inside a pair of wedges having an angular opening of 45° and centered about the angles −45° and −135° in the lower-half complex plane. The subscript C on the functional integral sign indicates that the path integral is taken along a complex contour.

As in the quantum-mechanical case, our goal is to transform the functional integral (61) into a conventional functional integral in which the contour of integration runs along the real axis rather than in the complex plane. Following the procedures in Sec. IV we make the substitution

$$\phi(x) = -2i\sqrt{1 + i\psi(x)}, \tag{62}$$

where we have set $L = 1$. This substitution introduces a functional Jacobian in the form of a square root:

$$D\phi = \frac{D\psi}{\det\sqrt{1 + i\psi}}. \tag{63}$$

The new functional integral over the ψ variable is

$$Z = \int \frac{D\psi}{\det\sqrt{1 + i\psi}} \exp\left\{ - \int d^d x \left[\frac{(\nabla\psi)^2}{2(1 + i\psi)} - 16g(1 + i\psi)^2 \right] \right\}. \tag{64}$$

This is a conventional functional integral in the sense that the field $\psi(x)$ is real and the path of functional integration lies on the real axis rather than in the complex plane.

From the form of the path integral in (64) we can see that even though the complex number i appears in the integrand, Z is real because the change of variable $\psi \to -\psi$ changes the sign of i. Thus, the ground-state energy density is real.

This same argument implies that the $2n$-point Green's functions are real and the $(2n + 1)$-point Green's functions are imaginary. The n-point Green's function $G_n(x_1, x_2, x_3, \ldots, x_n)$ is constructed from the moments of products of ϕ fields:

$$\langle 0|\phi(x_1)\phi(x_2)\phi(x_3)\cdots\phi(x_n)|0\rangle = \int_C D\phi\, \phi(x_1)\phi(x_2)\phi(x_3)\cdots\phi(x_n) \times \exp\left[- \int d^d x \left(\frac{1}{2}(\nabla\phi)^2 - g\phi^4 \right) \right]. \tag{65}$$

After making the substitution (62), we can apply the above symmetry argument to show that G_n is real when n is even and imaginary when n is odd.

Even though we have shown that the partition function Z in (64) is real, we are still unable to identify a Hermitian field-theoretic Lagrangian that is equivalent to the $-\phi^4$ non-Hermitian Lagrangian. This is because the functional integral (64) has a Jacobian factor, and this factor is complex. By following the procedure in Sec. IV, we were able to eliminate this Jacobian factor for the case of a one-dimensional quantum field theory. It is not obvious how to proceed in the case of higher dimensions. We now propose three possible approaches to solving this problem.

(1) The simplest approach is to follow Sec. IV and introduce a new field $\pi(x)$ by using the identity (25). The advantage of this procedure is that, at least at the classical level where we do not perform the point-splitting described in Sec. IV C, the Jacobian factor in the functional integral cancels. We obtain the d-dimensional analog of (26):

$$Z = \int D\psi \int D\pi \exp\left\{ - \int d^d x \left[\frac{1 + i\psi}{2}(\pi - B)^2 + \frac{(\nabla\psi)^2}{2(1 + i\psi)} - 16g(1 + i\psi)^2 \right] \right\}. \tag{66}$$

There are now several possibilities for the choice of B. The choice

$$B(x) = \frac{i\nabla_1\psi(x)}{1 + i\psi(x)} \tag{67}$$

eliminates the $[\nabla_1\psi(x)]^2$ term from (66) but the resulting action is nonpolynomial in ψ and thus the integral over ψ cannot be evaluated analytically. Furthermore, the resulting action is not manifestly Lorentz covariant. The more symmetric choice

$$B(x) = \frac{i\sqrt{(\nabla\psi)^2}}{1 + i\psi(x)} \tag{68}$$

eliminates the $(\nabla\psi)^2/(1 + i\psi)$ term completely, but again the resulting action is nonpolynomial and it is impossible to perform the ψ integral.

(2) A second approach is to introduce the d-dimensional vector field π_μ ($\mu = 1, \ldots d$). Now, using the identity (25) d times, we obtain an action that is a quadratic polynomial in ψ. However, we still cannot perform the ψ integration because the Jacobian factor no longer cancels. Indeed, there are now $d - 1$ functional determinant factors of

$\sqrt{1+i\psi}$ in the numerator. Furthermore, had we kept the scale factor L in the change of variables (62), the resulting Jacobian would have explicit L dependence, even though the partition function is clearly independent of L. Therefore, this integral representation of the partition function is clumsy and is likely to be intractable.

(3) We believe that the most promising approach is to introduce a single scalar field $\rho(x)$ by formally rewriting Z in (64) as

$$Z = \int D\psi \frac{\det\sqrt{\nabla_\mu(1+i\psi)\nabla_\mu}}{\det\sqrt{1+i\psi}} \times \int D\rho \exp\left\{-\int d^dx\left[\frac{1}{2}(\nabla\rho)^2(1+i\psi) - i\nabla_\mu\rho\nabla_\mu\psi - 16g(1+i\psi)^2\right]\right\}. \quad (69)$$

The advantage of this representation of Z is that the action is quadratic in ψ and is Lorentz covariant. The Jacobian remains complicated, but it may become analytically tractable if we introduce a Grassmann integration variable η to promote the functional determinant to the action. After integrating out the ψ field, the action will now depend on the scalar boson field ρ and the fermion field η. The resulting Hermitian action will bear a strong resemblance to supersymmetric actions. This is not surprising because, even in the one-dimensional case, the equivalent Hermitian Hamiltonian $\tilde{H}$ in (16) strongly resembles a supersymmetric quantum theory. In a future paper we hope to present a thorough analysis of this quantum theory.

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