Path integrals for difficult actions

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Abstract

In some theories, one can't find the hamiltonian because the time derivatives of the fields occur in ways that make the required Legendre transformation intractable. In some other theories, one has a hamiltonian, but one can't integrate over the momenta to get the usual euclidian-space path integral, whose weight function is positive.

This paper solves both problems. We first show how to construct path integrals when one can't find the hamiltonian because the first time derivatives of the fields occur in ways that make the required Legendre transformation intractable. We then show how to combine the Monte Carlo method with numerical integration and a look-up table so as to compute the desired euclidian-space path integrals. The present paper therefore is a partial solution to the sign problem.

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I. INTRODUCTION

Despite the success of renormalization, infinities remain a major problem in quantum field theory, one that has grown more important as cosmological observations have confirmed the reality of dark energy [1]. For if dark energy is the energy of the vacuum, then we need to be able to compute energies in finite theories. The ground-state energy of a theory with hamiltonian H is the limit of

$$E(\beta) = -\frac{d \ln Z(\beta)}{d\beta} = -\frac{d \ln \mathrm{Tr}\, e^{-\beta H}}{d\beta} = \frac{\mathrm{Tr}\, H\, e^{-\beta H}}{\mathrm{Tr}\, e^{-\beta H}} \tag{1}$$

as $\beta = 1/kT \to \infty$. We can study the ground-state energy if we can compute the euclidian path integral for the partition function $Z(\beta)$.

If the action is quadratic in the time derivatives of the fields, then the hamiltonian is a simple Legendre transform of the action density, and we can use the hamiltonian as usual to construct the path integral in spacetime and in euclidian space. But the actions of string theory and of some quantum field theories with finite Green's functions and finite euclidian action densities [2] are not quadratic in the time derivatives of the fields. In such theories, the Legendre transformation may be impossible and the hamiltonian inaccessible. Even if the Legendre transformation is feasible, one's hamiltonian may be so complicated a function of the momenta that one cannot perform the required momentum integral. In this case, the exponential in the euclidian path integral for the partition function $Z(\beta)$

$$Z(\beta) = \mathrm{Tr}\, e^{-\beta H} = \int \exp\left\{ \int_0^\beta \int \left[i\, \dot{\phi}\, \pi - H(\phi, \pi) \right] dt\, d^3x \right\} D\phi\, D\pi. \tag{2}$$

is complex. It therefore is not a probability distribution, and the usual Monte Carlo methods do not work. This is an example of the sign problem [3].

This paper solves both problems. We first show how to construct path integrals when one can't find the hamiltonian because the first time derivatives of the fields occur in ways that make the required Legendre transformation intractable. We then show how to compute complex euclidian-space path integrals (2) by combining the Monte Carlo method with numerical integration and a look-up table.

In section II, we review the classical Legendre transformation. In section III, we derive and illustrate with four ? examples our path-integral formula for the partition function in theories without known hamiltonians. While discussing these examples, we note that the oft-repeated recipe according to which one passes from Minkowski path integrals to euclidian path integrals by replacing t by it is wrong for the scalar Born-Infeld theory. In section IV, we show that complex weight functions like the exponential in our formula (2) for the partition function are ill-suited to estimation by Monte Carlo methods. In section V, we solve this problem by combining numerical integration and look-up tables with Monte Carlo methods. In section **??**, we demonstrate this technique in the context of quantum mechanics.

The paper is about scalar fields and does not discuss higher-derivative theories [4] or those in which certain fields have no time derivatives [5].

II. LEGENDRE TRANSFORMATIONS

The lagrangian of a theory tells us about symmetries and equations of motion, but one needs a hamiltonian to construct path integrals and to determine the time evolution of states and their energies. To find the hamiltonian of a theory of scalar fields $\phi = \{\phi_1, \ldots, \phi_n\}$, one defines the conjugate momenta $\pi = \{\pi_1, \ldots, \pi_n\}$ as the derivatives of the action density

$$\pi_j = \frac{\partial L}{\partial \dot{\phi}_j}, \tag{3}$$

and inverts these equations so as to write the time derivatives $\dot{\phi}_j = \dot{\phi}_j(\phi, \pi)$ of the fields in terms of the fields ϕ_ℓ and their momenta π_ℓ. The hamiltonian density then is

$$H = \sum_{j=1}^{n} \pi_j \dot{\phi}_j(\phi, \pi) - L(\phi, \dot{\phi}(\phi, \pi)). \tag{4}$$

When the action is quadratic in all the time derivatives, this Legendre transformation is easy to do, but in most other cases no solution is known even in the absence of constraints.

Once one has a hamiltonian, one inserts complete sets of eigenstates of the fields ϕ_j and of their conjugate momenta π_j into the Boltzmann operator $\exp(-\beta H) = (\exp(-\beta H/n))^n$ and writes the partition function as the complex path integral

$$Z(\beta) = \operatorname{Tr} e^{-\beta H} = \int \langle \phi | e^{-\beta H} | \phi \rangle D\phi = \int \exp\left\{ \int_0^\beta \int \left[i \dot{\phi}_j \pi_j - H(\phi, \pi) \right] dt\, d^3x \right\} D\phi D\pi. \tag{5}$$

If one can integrate over the momentum π_j, then one gets the classic formula

$$Z(\beta) = \int \exp\left[\int_0^\beta \int -L_e(\phi, \dot{\phi})\, dt\, d^3x \right] D\phi \tag{6}$$

in which L_e is the euclidian action density. In many theories, L_e is real and positive, and the exponential $\exp[-L_e(\phi, \dot{\phi})]$ is a probability distribution well-suited to Monte Carlo methods.

This procedure is straightforward when the action is quadratic in its time derivatives, and the integral over the momenta is gaussian. But in most other theories, one can't express the time derivatives $\dot{\phi}_j$ in terms of the fields ϕ_j and their momenta π_j, and so the hamiltonian is unknown. We solve this problem in section III.

III. A PATH-INTEGRAL LEGENDRE TRANSFORMATION

Our proposed solution to the problem of making a path integral when one lacks a hamiltonian is to use functional integration to perform Legendre's transformation implicitly by means of delta functionals that impose the required relation (3) between the time derivatives $\dot{\phi}_j$ and the fields ϕ_j and their momenta π_j. Our formula for the partition function is the double path integral

$$Z(\beta) = \int \exp\left\{ \int_0^\beta \int \left[(i\dot{\phi}_\ell - \dot{\psi}_\ell) \frac{\partial L(\phi, \dot{\psi})}{\partial \dot{\psi}_\ell} + L(\phi, \dot{\psi}) \right] dt d^3x \right\} \left| \det\left(\frac{\partial^2 L(\phi, \dot{\psi})}{\partial \dot{\psi}_k \partial \dot{\psi}_\ell} \right) \right| D\phi D\dot{\psi} \tag{7}$$

in which the determinant converts $D\dot{\psi}$ into $D\pi$, and the term

$$E(\phi, \dot{\psi}) = \dot{\psi}_\ell \, \frac{\partial L(\phi, \dot{\psi})}{\partial \dot{\psi}_\ell} - L(\phi, \dot{\psi}) \tag{8}$$

is the hamiltonian when $\dot{\psi} = \dot{\phi}$ and when the time derivatives $\dot{\psi}_\ell = \dot{\phi}_\ell$ are expressed in terms of the ϕ_ℓ and π_ℓ. Like the hamiltonian, it is conserved in time when $\dot{\psi}_\ell = \dot{\phi}_\ell$ and when the equations of motion are obeyed.

The double integral (7) for the partition function $Z(\beta)$ is complex and so is ill-suited to estimation by Monte Carlo methods. We solve this problem is sections V & **??**.

To derive our formula (7), we write the path integral (5) as

$$\begin{aligned} Z(\beta) = & \int \exp\left\{ \int_0^\beta \int \left[i\, \dot{\phi}_j \pi_j - (\pi_k \dot{\psi}_k - L(\phi, \dot{\psi})) \right] dt d^3x \right\} \\ & \times \exp\left[i \int \left(\pi_\ell - \frac{\partial L}{\partial \dot{\psi}_\ell} \right) a_\ell \, d^4x \right] \left| \det\left(\frac{\partial^2 L}{\partial \dot{\psi}_k \partial \dot{\psi}_\ell} \right) \right| D\phi D\pi D\dot{\psi} Da \end{aligned} \tag{9}$$

in which the integration over the n auxiliary fields a_ℓ makes the second exponential a delta functional $\delta(\pi - \partial L/\partial\dot{\psi})$ that enforces the definition (3) of the momentum π_j as the derivative of the action density L with respect to the time derivative $\dot{\phi}_j$. The jacobian is an $n \times n$ determinant that converts $D\dot{\psi}$ to $D\pi$. The integration is over all fields that are periodic with period β. Integrating first over a, we get

$$Z(\beta) = \int \exp\left\{\int_0^\beta \int \left[i\dot{\phi}_j \pi_j - (\pi_k \dot{\psi}_k - L(\phi, \dot{\psi}))\right] dt d^3x\right\} \times \prod_{\ell=1}^{n} \left[\delta\left(\pi_\ell - \frac{\partial L}{\partial \dot{\psi}_\ell}\right)\right] \left|\det\left(\frac{\partial^2 L}{\partial \dot{\psi}_k \partial \dot{\psi}_\ell}\right)\right| D\phi D\pi D\dot{\psi}. \tag{10}$$

Let us recall the delta-function formula

$$\int \delta^n(g_1(x_1, \ldots, x_n), \ldots, g_n(x_1, \ldots, x_n)) \left|\det\left(\frac{\partial g_k(x)}{\partial x_\ell}\right)\right| d^n x = g(x_{10}, \ldots, x_{n0}) \tag{11}$$

in which we took g to have a unique zero x_0. Thus if we integrate the triple path integral (10) over $\dot{\psi}$, then the delta functional and the jacobian force $\dot{\psi}_0(\phi, \pi)$ to satisfy Legendre's formula (3), and we get the path integral (5) over ϕ and π

$$Z(\beta) = \int \exp\left\{\int_0^\beta \int \left[i\dot{\phi}\pi - (\pi\dot{\psi}_0 - L(\phi, \dot{\psi}_0))\right] dt d^3x\right\} D\phi D\pi. \tag{12}$$

On the other hand, if we integrate the triple path integral (10) over π, then we get our proposed formula (7)

$$Z(\beta) = \int \exp\left\{\int_0^\beta \int \left[(i\dot{\phi}_\ell - \dot{\psi}_\ell)\frac{\partial L(\phi, \dot{\psi})}{\partial \dot{\psi}_\ell} + L(\phi, \dot{\psi})\right] dt d^3x\right\} \left|\det\left(\frac{\partial^2 L(\phi, \dot{\psi})}{\partial \dot{\psi}_k \partial \dot{\psi}_\ell}\right)\right| D\phi D\dot{\psi}. \tag{13}$$

This functional integral generalizes the path integral to theories of scalar fields in which the action is not quadratic in the time derivatives of the fields. A similar formula should work in theories of vector and tensor fields, apart from the issue of constraints.

Our first example is a free scalar field with action density

$$L = \frac{1}{2}\,\partial_\mu \phi\, \partial^\mu \phi - \frac{1}{2} m^2 \phi^2 \tag{14}$$

and the determinant is unity because

$$\frac{\partial^2 L(\phi, \dot{\psi})}{\partial \dot{\psi}^2} = 1. \tag{15}$$

To simplify many of the subsequent formulas, we will use the compact notation

$$\int_0^\beta dt \int d^3x \equiv \int^\beta d^4x. \tag{16}$$

In this notation, the proposed path integral (13) for the free field theory (14) is

$$
\begin{aligned}
Z(\beta) &= \int \exp\left\{\int^{\beta} \left[L(\phi,\dot\psi) + \dot\psi(i\dot\phi - \dot\psi)\right] d^4x\right\} D\phi D\dot\psi \\
&= \int \exp\left\{\int^{\beta} \left[\frac{1}{2}\dot\psi^2 - \frac{1}{2}(\nabla\phi)^2 - \frac{1}{2}m^2\phi^2 + \dot\psi(i\dot\phi - \dot\psi)\right] d^4x\right\} D\phi D\dot\psi \\
&= \int \exp\left\{\int^{\beta} \left[-\frac{1}{2}\left(\dot\psi - i\dot\phi\right)^2 - \frac{1}{2}\dot\phi^2 - \frac{1}{2}(\nabla\phi)^2 - \frac{1}{2}m^2\phi^2\right] d^4x\right\} D\phi D\dot\psi \qquad (17) \\
&= \int \exp\left\{\int^{\beta} \left[-\frac{1}{2}\dot\phi^2 - \frac{1}{2}(\nabla\phi)^2 - \frac{1}{2}m^2\phi^2\right] d^4x\right\} D\phi \\
&= \int \exp\left[-\int^{\beta} L_e(\phi,\dot\phi)\, d^4x\right] D\phi
\end{aligned}
$$

which is the standard result.

Our second example is the scalar Born-Infeld theory with action density

$$
L = M^4\left(1 - \sqrt{1 - M^{-4}\left(\dot\phi^2 - (\nabla\phi)^2 - m^2\phi^2\right)}\right) \qquad (18)
$$

and conjugate momentum

$$
\pi = \frac{\partial L(\phi,\dot\phi)}{\partial\dot\phi} = \frac{\dot\phi}{\sqrt{1 - M^{-4}\left(\dot\phi^2 - (\nabla\phi)^2 - m^2\phi^2\right)}}. \qquad (19)
$$

The proposed path integral (13) is

$$
Z(\beta) = \int \exp\left\{\int^{\beta}\left[(i\dot\phi - \dot\psi)\frac{\partial L(\phi,\dot\psi)}{\partial\dot\psi} + L(\phi,\dot\psi)\right] d^4x\right\} \left|\frac{\partial^2 L(\phi,\dot\psi)}{\partial\dot\psi^2}\right| D\phi D\dot\psi \qquad (20)
$$

in which

$$
\frac{\partial L(\phi,\dot\psi)}{\partial\dot\psi} = \frac{\dot\psi}{\sqrt{1 - M^{-4}\left(\dot\psi^2 - (\nabla\phi)^2 - m^2\phi^2\right)}} \qquad (21)
$$

and

$$
\frac{\partial^2 L(\phi,\dot\psi)}{\partial\dot\psi^2} = \frac{1 + M^{-4}\left((\nabla\phi)^2 + m^2\phi^2\right)}{\left[1 - M^{-4}\left(\dot\psi^2 - (\nabla\phi)^2 - m^2\phi^2\right)\right]^{3/2}}. \qquad (22)
$$

Substituting these formulas into (20) gives

$$Z(\beta) = \int \exp\left\{ \int^{\beta} \left[\frac{(i\dot{\phi} - \dot{\psi})\dot{\psi}}{\sqrt{1 - M^{-4}\left(\dot{\psi}^2 - (\nabla\phi)^2 - m^2\phi^2\right)}} \right.\right.$$
$$\left.\left. + M^4 \left(1 - \sqrt{1 - M^{-4}\left(\dot{\psi}^2 - (\nabla\phi)^2 - m^2\phi^2\right)}\right) \right] d^4x \right\} \tag{23}$$
$$\times \frac{1 + M^{-4}\left((\nabla\phi)^2 + m^2\phi^2\right)}{\left[1 - M^{-4}\left(\dot{\psi}^2 - (\nabla\phi)^2 - m^2\phi^2\right)\right]^{3/2}} \, D\phi D\dot{\psi}.$$

We can set

$$\pi = \frac{\partial L(\phi, \dot{\psi})}{\partial \dot{\psi}} = \frac{\dot{\psi}}{\sqrt{1 - M^{-4}\left(\dot{\psi}^2 - (\nabla\phi)^2 - m^2\phi^2\right)}} \tag{24}$$

and so absorb the jacobian in

$$d\pi = \frac{\partial \pi}{\partial \dot{\psi}} \, d\dot{\psi} = \frac{\partial^2 L(\phi, \dot{\psi})}{\partial \dot{\psi}^2} \, d\dot{\psi} = \frac{1 + M^{-4}\left((\nabla\phi)^2 + m^2\phi^2\right)}{\left[1 - M^{-4}\left(\dot{\psi}^2 - (\nabla\phi)^2 - m^2\phi^2\right)\right]^{3/2}} \, d\dot{\psi}. \tag{25}$$

The partition function (23) then is

$$Z(\beta) = \int \exp\left[\int^{\beta} (i\dot{\phi} - \dot{\psi})\pi + M^4 \left(1 - \sqrt{1 - \left(\dot{\psi}^2 - (\nabla\phi)^2 - m^2\phi^2\right)/M^4}\right) d^4x \right] D\phi D\pi \tag{26}$$

where now $\dot{\psi}$ is a function of ϕ and π defined by (24).

This theory is one of the few in which we can solve (21) or equivalently (24) for the time derivative $\dot{\psi}$

$$\dot{\psi} = \frac{\pi}{\sqrt{1 + M^{-4}\pi^2}} \sqrt{1 + M^{-4}\left((\nabla\phi)^2 + m^2\phi^2\right)} \tag{27}$$

and find as the hamiltonian density

$$\begin{aligned}
\mathcal{H}(\phi, \pi) &= \pi\dot{\psi} - L(\phi, \dot{\psi}) \\
&= \frac{\pi^2 \sqrt{1 + M^{-4}\left((\nabla\phi)^2 + m^2\phi^2\right)}}{\sqrt{1 + M^{-4}\pi^2}} - M^4 \\
&\quad + M^4 \sqrt{1 - M^{-4}\left(\frac{\pi^2\left(1 + M^{-4}\left((\nabla\phi)^2 + m^2\phi^2\right)\right)}{1 + M^{-4}\pi^2} - (\nabla\phi)^2 - m^2\phi^2\right)} \qquad (28) \\
&= \frac{\pi^2 \sqrt{M^4 + (\nabla\phi)^2 + m^2\phi^2}}{\sqrt{M^4 + \pi^2}} + M^4 \sqrt{\frac{M^4 + (\nabla\phi)^2 + m^2\phi^2}{M^4 + \pi^2}} - M^4 \\
&= \sqrt{\left(M^4 + \pi^2\right)\left(M^4 + (\nabla\phi)^2 + m^2\phi^2\right)} - M^4.
\end{aligned}$$

Thus for this theory, the standard formula (2) is

$$Z(\beta) = \int \exp\left\{\int^{\beta} \left[i\dot{\phi}\pi - \sqrt{(M^4+\pi^2)\,(M^4+(\nabla\phi)^2+m^2\phi^2)} + M^4\right] d^4x\right\} D\phi D\pi. \quad (29)$$

One may check that the proposed double path integral (23) leads to this standard formula (29) by using the formula (27) to change variables in (23) from $\phi, \dot{\psi}$ to ϕ, π.

Our third example is the theory defined by the action density

$$L = M^4 \exp(L_0/M^4) \quad (30)$$

in which L_0 is the action density (14) of the free field. The derivatives of L are

$$\frac{\partial L}{\partial \dot{\psi}} = M^{-4}\dot{\psi}\, L \quad \text{and} \quad \frac{\partial^2 L}{\partial \dot{\psi}^2} = M^{-4}(1 + M^{-4}\dot{\psi}^2)\, L. \quad (31)$$

So the proposed path integral is

$$\begin{aligned} Z(\beta) &= \int \exp\left\{\int^{\beta} \left[L(\phi,\dot{\psi}) + \frac{\partial L(\phi,\dot{\psi})}{\partial\dot{\psi}}(i\dot{\phi} - \dot{\psi})\right] d^4x\right\} \left|\frac{\partial^2 L(\phi,\dot{\psi})}{\partial\dot{\psi}^2}\right| D\phi D\dot{\psi} \\ &= \int \exp\left\{\int^{\beta} \left[1 + \frac{\dot{\psi}(i\dot{\phi} - \dot{\psi})}{M^4}\right] L(\phi,\dot{\psi})\, d^4x\right\} M^{-4}(1 + M^{-4}\dot{\psi}^2)\, L\, D\phi D\dot{\psi}. \end{aligned} \quad (32)$$

Our fourth example is the Nambu-Gotō action density

$$L = -\frac{T_0}{c}\int_0^{\sigma_1} \sqrt{\left(\dot{X}\cdot X'\right)^2 - \left(\dot{X}\right)^2 (X')^2} \quad (33)$$

in which the tau or time derivatives of the coordinate fields X^μ do not occur quadratically [6]. The momenta are

$$\mathcal{P}^{\tau}_{\mu} = \frac{\partial L}{\partial \dot{X}^\mu} = -\frac{T_0}{c}\frac{(\dot{X}\cdot X')X'_\mu - (X')^2\dot{X}_\mu}{\sqrt{\left(\dot{X}\cdot X'\right)^2 - \left(\dot{X}\right)^2 (X')^2}} \quad (34)$$

and the second derivatives of the Lagrange density are

$$\begin{aligned} \frac{\partial^2 L}{\partial\dot{X}^\mu\partial\dot{X}^\nu} = \frac{T_0}{c}\Bigg[&\frac{\delta_{\mu\nu}X'^2 - X'_\mu X'_\nu}{\sqrt{\left(\dot{X}\cdot X'\right)^2 - \left(\dot{X}\right)^2 (X')^2}} \\ &- \frac{\left((\dot{X}\cdot X')X'_\mu - (X')^2\dot{X}_\mu\right)\left((\dot{X}\cdot X')X'_\nu - (X')^2\dot{X}_\nu\right)}{\left[\left(\dot{X}\cdot X'\right)^2 - \left(\dot{X}\right)^2 (X')^2\right]^{3/2}}\Bigg]. \end{aligned} \quad (35)$$

The proposed partition function (13) for the Nambu-Gotō action is then

$$Z(\beta) = \int \exp\left\{ \int^{\beta} \left[(i\dot{X}^{\mu} - \dot{Y}^{\mu}) \frac{\partial L(X,\dot{Y})}{\partial \dot{Y}^{\mu}} + L(X,\dot{Y}) \right] d^4x \right\} \left| \det\left[\frac{\partial^2 L(X,\dot{Y})}{\partial \dot{Y}^{\mu} \partial \dot{Y}^{\nu}} \right] \right| DXD\dot{Y} \tag{36}$$

in which the formulas (34) and (35) (with $\dot{X}^{\mu} \to \dot{Y}^{\mu}$) are to be substituted for the first and second derivatives of the action density L with respect to the tau derivatives $\dot{Y}^{\mu}$.

Here's an example from quantum mechanics of a hamiltonian with a difficult momentum integration

$$H(q,p) = M \left\{ \exp\left[\frac{1}{M} \left(\frac{p^2}{2m} + \frac{m\omega^2 q^2}{2} \right) \right] - 1 \right\} \tag{37}$$

which we can write as

$$H = M \left[\exp\left(\frac{\omega(a^{\dagger}a + \frac{1}{2})}{M} \right) - 1 \right]. \tag{38}$$

So the energies are

$$E_n = M \left[\exp\left(\frac{\omega(n + \frac{1}{2})}{M} \right) - 1 \right], \tag{39}$$

and the ground-state energy is

$$E_0 = M \left[\exp\left(\frac{\omega}{2M} \right) - 1 \right]. \tag{40}$$

$$\begin{aligned} L = {} & \frac{\dot{q} \sqrt{M \left(2m \left(\frac{\sqrt[3]{2}\, 3^{2/3}}{\sqrt[3]{\sqrt{3}\sqrt{\frac{m^3\dot{q}^6(4M+27m\dot{q}^2)}{M^4}} + \frac{9m^2\dot{q}^4}{M^2}}} + 3 \right) - \frac{2^{2/3} M \sqrt[3]{3\sqrt{3}\sqrt{\frac{m^3\dot{q}^6(4M+27m\dot{q}^2)}{M^4}} + \frac{27m^2\dot{q}^4}{M^2}}}{\dot{q}^2} \right)}}{\sqrt{6}} \\ & - M \left(\frac{\sqrt[3]{6}}{\sqrt{\frac{\sqrt[3]{2} M \left(\sqrt{3}\sqrt{\frac{m^3\dot{q}^6(4M+27m\dot{q}^2)}{M^4}} + \frac{9m^2\dot{q}^4}{M^2} \right)^{2/3} - 2\sqrt[3]{3} m\dot{q}^2}{m\dot{q}^2 \sqrt[3]{\sqrt{3}\sqrt{\frac{m^3\dot{q}^6(4M+27m\dot{q}^2)}{M^4}} + \frac{9m^2\dot{q}^4}{M^2}}}}} - 1 \right) - V(q) \end{aligned} \tag{41}$$

IV. PROBLEMS IN EUCLIDIAN SPACE

The mean value of an observable $A[\phi]$ at maximum entropy and inverse temperature β is

$$\begin{aligned}\langle A[\phi]\rangle &= \frac{\mathrm{Tr}\, A[\phi]e^{-\beta H}}{\mathrm{Tr}\, e^{-\beta H}} \\ &= \int A[\phi] \exp\left[\int \left(i\,\dot\phi_j - \dot\psi_j\right)\frac{\partial L}{\partial \dot\psi_j} + L(\phi,\dot\psi)\, d^4x\right] \left|\det\left(\frac{\partial^2 L}{\partial\dot\psi_k \partial\dot\psi_\ell}\right)\right| D\phi D\dot\psi \\ &\quad \Bigg/ \int \exp\left[\int \left(i\,\dot\phi_j - \dot\psi_j\right)\frac{\partial L}{\partial \dot\psi_j} + L(\phi,\dot\psi)\, d^4x\right] \left|\det\left(\frac{\partial^2 L}{\partial\dot\psi_k \partial\dot\psi_\ell}\right)\right| D\phi D\dot\psi \,.\end{aligned} \tag{42}$$

The complex action

$$S = \int \left(i\,\dot\phi_j - \dot\psi_j\right)\frac{\partial L}{\partial \dot\psi_j} + L(\phi,\dot\psi)\, d^4x \tag{43}$$

oscillates and does not give us a probability distribution unless we can integrate over $D\dot\psi$. One can write the mean value (42) as a ratio of mean values

$$\begin{aligned}\langle A[\phi]\rangle &= \left\langle A[\phi] \exp\left[\int i\,\dot\phi_j \frac{\partial L}{\partial \dot\psi_j}\, d^4x\right]\right\rangle \Bigg/ \left\langle \exp\left[\int i\,\dot\phi_j \frac{\partial L}{\partial \dot\psi_j}\, d^4x\right]\right\rangle \\ &= \int A[\phi] \exp\left[\int i\,\dot\phi_j \frac{\partial L}{\partial \dot\psi_j}\, d^4x\right] P(\phi,\dot\psi) D\phi D\dot\psi \\ &\quad \Bigg/ \int \exp\left[\int i\,\dot\phi_j \frac{\partial L}{\partial \dot\psi_j}\, d^4x\right] P(\phi,\dot\psi)\, D\phi D\dot\psi\end{aligned} \tag{44}$$

each of which one can estimate in principle by Monte Carlo simulation [7] in the normalized probability distribution

$$\begin{aligned}P(\phi,\dot\psi) =& \exp\left[\int \left(L(\phi,\dot\psi) - \dot\psi_j \frac{\partial L}{\partial \dot\psi_j}\right) d^4x\right] \left|\det\left(\frac{\partial^2 L}{\partial\dot\psi_k \partial\dot\psi_\ell}\right)\right| \\ & \Bigg/ \int \exp\left[\int \left(L(\phi,\dot\psi) - \dot\psi_j \frac{\partial L}{\partial \dot\psi_j}\right) d^4x\right] \left|\det\left(\frac{\partial^2 L}{\partial\dot\psi_k \partial\dot\psi_\ell}\right)\right| D\phi D\dot\psi \,.\end{aligned} \tag{45}$$

Although the functional (75) is a normalized probability distribution, the mean value (44) of an observable $A[\phi]$ is a ratio N/D of path integrals of functionals that are complex and that oscillate. In many if not most cases of interest, both N and D are smaller than the measurement errors δN and δD in computations of reasonable lengths. The error in an observable

$$\delta\langle A[\phi]\rangle = \delta\frac{N}{D} = \frac{\delta N}{D} - \frac{N}{D^2}\delta D = \frac{\delta N}{D} - \langle A[\phi]\rangle\frac{\delta D}{D}. \tag{46}$$

To make matters worse, in many cases, both N and D are zero in the limit in which $\beta \to \infty$. For instance, if we apply the technique (44–75) to the computation of the ground-state energy of the harmonic oscillator, where we know the hamiltonian H and can use q and p, then we get

$$\langle H \rangle = \frac{N}{D} \tag{47}$$

in which the numerator is

$$\begin{aligned} N = & \int \left(\frac{p^2}{2m} + \frac{1}{2} m\omega^2 q^2 \right) \exp \left[\int \left(i\dot{q}p - \frac{p^2}{2m} - \frac{1}{2} m\omega^2 q^2 \right) dt \right] DpDq \\ & \Big/ \int \exp \left[\int \left(-\frac{p^2}{2m} - \frac{1}{2} m\omega^2 q^2 \right) dt \right] DpDq \end{aligned} \tag{48}$$

and the denominator D is

$$\begin{aligned} D = & \int \exp \left[\int \left(i\dot{q}p - \frac{p^2}{2m} - \frac{1}{2} m\omega^2 q^2 \right) dt \right] DpDq \\ & \Big/ \int \exp \left[\int \left(-\frac{p^2}{2m} - \frac{1}{2} m\omega^2 q^2 \right) dt \right] DpDq \end{aligned} \tag{49}$$

and the measure $DpDq$ is

$$DpDq = \prod_{j=1}^{n} \frac{1}{2\pi} dp_j dq_j. \tag{50}$$

In the continuum limit ($n \to \infty$, $dt \to 0$, with $\beta = n\, dt$ fixed), the numerator $\mathcal{N}$ of the denominator $D \equiv \mathcal{N}/\mathcal{D}$ of the ratio (49) is the partition function

$$\begin{aligned} \mathcal{N} &= Z(\beta) = \operatorname{Tr} e^{-\beta H} \\ &= \int \exp \left[\int \left(i\dot{q}p - \frac{p^2}{2m} - \frac{1}{2} m\omega^2 q^2 \right) dt \right] DpDq \\ &= \frac{1}{2 \sinh(\beta\omega/2)}. \end{aligned} \tag{51}$$

The denominator is

$$\begin{aligned} \mathcal{D} &= \int \exp \left[\int \left(-\frac{p^2}{2m} - \frac{1}{2} m\omega^2 q^2 \right) dt \right] DpDq \\ &= \prod_{j=1}^{n} \int \frac{dp_j dq_j}{2\pi} \exp \left[\sum_{j=1}^{n} \left(-\frac{p_j^2}{2m} - \frac{1}{2} m\omega^2 q_j^2 \right) \frac{\beta}{n} \right] \\ &= \left(\frac{1}{2\pi} \right)^n \left(\frac{2\pi m n}{\beta} \right)^{n/2} \prod_{j=1}^{n} \int dq_j \exp \left[\sum_{j=1}^{n} \left(-\frac{1}{2} m\omega^2 q_j^2 \right) \frac{\beta}{n} \right] \\ &= \left(\frac{1}{2\pi} \right)^n \left(\frac{2\pi m n}{\beta} \right)^{n/2} \left(\frac{2\pi n}{m\omega^2 \beta} \right)^{n/2} = \left(\frac{n}{\beta\omega} \right)^n. \end{aligned} \tag{52}$$

This denominator goes to infinity as $n \to \infty$ and $\beta/n \to 0$ for any $\beta \neq 0$. So the denominator D vanishes

$$D = \frac{1}{2\sinh(\beta\omega/2)\,\mathcal{D}} = 0. \tag{53}$$

The numerator also vanishes, so the expression (47) is hard to estimate, being 0/0.

So the double ratio method (44–75)) is not a good way to estimate the mean value of an observable (42) in which either the hamiltonian is unknown or the integration over momentum cannot be done analytically.

V. MONTE CARLOS WITH NUMERICAL INTEGRATION AND LOOK-UP TABLES

When we can't analytically integrate over the momentum or can't find the hamiltonian, we usually can't use the double ratio (44–75) either. We can, however, numerically integrate over the momentum or over the auxiliary variable $\dot{\psi}$, make a look-up table of these integrals, and then use the look-up table to perform a Monte Carlo estimate of the partition function or of the desired observable.

To keep things simple, we will restrict the discussion in the remainder of this paper to problems in quantum mechanics and in this section and the next to problems in which we know the hamiltonian but can't analytically integrate over the momentum.

Suppose that we know the hamiltonian $H(q,p)$ but can't integrate over the momentum p analytically. Then the partition function $Z(\beta)$ is

$$\begin{aligned} Z(\beta) = \mathrm{Tr}\, e^{-\beta H} &= \int \exp\left\{\int_0^\beta [i\dot{q}p - H(q,p)]\,dt\right\} DpDq \\ &= \prod_{j=1}^{n} \int \frac{dp_j dq_j}{2\pi} \exp\left[\sum_{\ell=0}^{\beta/a} i(q_{\ell+1} - q_\ell)p_\ell - aH(q_\ell, p_\ell)\right]. \end{aligned} \tag{54}$$

We know that

$$P[q,\beta] = \int \exp\left\{\int_0^\beta [i\dot{q}p - H(q,p)]\,dt\right\} Dp \tag{55}$$

is a functional probability distribution that assigns a number $P[q,\beta]$ to every path $q(t)$. It is the limit as $n \to \infty$ and $a = \beta/n \to 0$ of the multiple integral

$$P_n[q,\beta] = \prod_{j=1}^{n} \int \frac{dp_j}{\sqrt{2\pi}} \exp\left[\sum_{\ell=0}^{n} i(q_{\ell+1} - q_\ell)p_\ell - aH(q_\ell, p_\ell)\right]. \tag{56}$$

If the hamiltonian is even in the momentum, then the probability distribution is

$$P_n[q,\beta] = \prod_{j=1}^{n} \int \frac{dp_j}{\sqrt{2\pi}} \prod_{k=1}^{n} \cos((q_{k+1}-q_k)p_k) e^{-aH(q_k,p_k)}. \tag{57}$$

The partition function $Z(\beta)$ is

$$Z(\beta) = \int P[q,\beta]\, Dq = \int \prod_{j=1}^{n} \frac{dq_j}{\sqrt{2\pi}} P_n[q,\beta]. \tag{58}$$

The mean value of the energy at inverse temperature β is

$$\langle H \rangle_\beta = \frac{\mathrm{Tr}\, H\, e^{-\beta H}}{\mathrm{Tr}\, e^{-\beta H}} = -\frac{1}{Z(\beta)} \frac{dZ(\beta)}{d\beta} = -\frac{1}{Z(\beta)} \int \prod_{j=1}^{n} \frac{dq_j}{\sqrt{2\pi}} \frac{dP_n[q,\beta]}{d\beta}. \tag{59}$$

The derivative of the probability distribution with respect to $\beta = n\,a$ is

$$-\frac{dP_n[q,\beta]}{d\beta} = \frac{1}{n} \sum_{k=1}^{n} \int \prod_{j=1}^{n} \frac{dp_j}{\sqrt{2\pi}} H(q_k,p_k) \exp\left[\sum_{\ell=0}^{n} i(q_{j+1}-q_j)p_j - aH(q_\ell,p_\ell)\right]. \tag{60}$$

So the mean value of the hamiltonian at inverse temperature β is

$$\begin{aligned} \langle H \rangle_\beta = \frac{1}{n} \sum_{k=1}^{n} \int \prod_{j=1}^{n} dq_j\, dp_j\;\, H(q_k,p_k) \exp\left[\sum_{\ell=0}^{n} i(q_{j+1}-q_j)p_j - aH(q_\ell,p_\ell)\right] \\ \Big/ \int \prod_{j=1}^{n} dq_j\, dp_j\; \exp\left[\sum_{\ell=0}^{n} i(q_{\ell+1}-q_\ell)p_\ell - aH(q_\ell,p_\ell)\right]. \end{aligned} \tag{61}$$

We do the p integrations numerically, setting

$$I(q_{\ell+1},q_\ell) = \langle q_{\ell+1} | e^{-aH(q_\ell,p)} | q_\ell \rangle = \int_{-\infty}^{\infty} \frac{dp}{\sqrt{2\pi}} \exp\left[i(q_{\ell+1}-q_\ell) - a\, H(q_\ell,p)\right]. \tag{62}$$

and

$$HI(q_{\ell+1},q_\ell) = \int_{-\infty}^{\infty} \frac{dp}{\sqrt{2\pi}} H(q_\ell,p) \exp\left[i(q_{\ell+1}-q_\ell) - a\, H(q_\ell,p)\right]. \tag{63}$$

In terms of these numerical integrals, the mean value of the hamiltonian is

$$\langle H \rangle_\beta = \frac{1}{n} \sum_{k=1}^{n} \int dq_k \prod_{j=1,\, j\neq k}^{n} dq_j\, HI(q_{k+1},q_k)\, I(q_{j+1},q_j) \Big/ \int \prod_{j=1}^{n} dq_j\, I(q_{j+1},q_j) \tag{64}$$

which we may write as

$$\langle H \rangle_\beta = \frac{1}{n} \sum_{k=1}^{n} \int \prod_{j=1}^{n} dq_j \frac{HI(q_{k+1},q_k)}{I(q_{k+1},q_k)} I(q_{j+1},q_j) \Big/ \int \prod_{j=1}^{n} dq_j\, I(q_{j+1},q_j)\,. \tag{65}$$

We do a Monte Carlo over the probability distribution

$$P(q) = \prod_{j=1}^{n} I(q_{j+1}, q_j) \bigg/ \int \prod_{j=1}^{n} dq_j \, I(q_{j+1}, q_j) \tag{66}$$

and measure the ratio

$$\langle H \rangle_\beta = \left\langle \frac{1}{n} \sum_{k=1}^{n} \frac{H I(q_{k+1}, q_k)}{I(q_{k+1}, q_k)} \right\rangle = \int \frac{1}{n} \sum_{k=1}^{n} \frac{H I(q_{k+1}, q_k)}{I(q_{k+1}, q_k)} \, P(q) \, Dq. \tag{67}$$

The probability distribution $P[q, \beta]$ is positive. For instance, the quantity

$$\langle q^2(t) \rangle = \mathrm{Tr}\, e^{-(\beta - t)H} q^2 e^{-tH} = \int q^2(t) P[q, \beta] \, Dq \tag{68}$$

is positive for every t and every path $q(t)$. In most problems of interest, the hamiltonian is an even function of the momentum, $H(q, -p) = H(q, p)$, and the integrals (62 & 63) are real

$$\begin{aligned} I(q_{\ell+1}, q_\ell) &= \sqrt{\frac{2}{\pi}} \int_0^\infty dp \, \cos\left[(q_{\ell+1} - q_\ell)\, p\right] \, e^{-a\, H(q_\ell, p)} \\ H I(q_{\ell+1}, q_\ell) &= \sqrt{\frac{2}{\pi}} \int_0^\infty dp \, H(q_\ell, p) \, \cos\left[(q_{\ell+1} - q_\ell)\, p\right] \, e^{-a\, H(q_\ell, p)}. \end{aligned} \tag{69}$$

We use these explicitly real forms in our Monte Carlos.

In most problems of interest, the hamiltonian increases monotonically with the momentum when the momentum is positive

$$\frac{\partial H(q, p)}{\partial p} > 0 \quad \text{when} \quad p > 0 \tag{70}$$

and so the exponential $\exp[-a\, H(q_\ell, p)]$ in the integral (69) decreases monotonically with p for $p > 0$

$$\frac{\partial}{\partial p} e^{-a\, H(q_\ell, p)} = -\, a \, \frac{\partial H(q, p)}{\partial p} \, e^{-a\, H(q_\ell, p)} < 0 \quad \text{for} \quad p > 0. \tag{71}$$

Now let us divide the domain of the integration (69) into the successive intervals

$$I_n = \left[\frac{n\pi}{2|q_{\ell+1} - q_\ell|}, \frac{(n+1)\pi}{2|q_{\ell+1} - q_\ell|} \right] \tag{72}$$

for $n = 0, 1, \ldots$. Because the exponential decreases monotonically with p, it follows that the integral over any pair of intervals $I_{4n} \cup I_{4n+1}$ for $n \geq 0$ is positive. Invoking the inequality (71) once again, we see that the integral over any quartet of intervals $I_{4n} \cup I_{4n+1} \cup I_{4n+2} \cup I_{4n+3}$ for $n \geq 0$ also is positive. Thus the integral (62) is positive as long as the hamiltonian is a monotonically increasing, even function of the momentum.

For instance, when H represents a harmonic oscillator

$$H = \frac{p^2}{2m} + \frac{m\omega^2 q^2}{2}, \tag{73}$$

the integral (62) is obviously positive

$$I(q_{\ell+1}, q_\ell) = \sqrt{\frac{m}{a}} \exp\left\{ - a \left[\frac{m(q_{\ell+1} - q_\ell)^2}{2a^2} + \frac{m\omega^2 q_\ell^2}{2} \right] \right\}. \tag{74}$$

To take a Metropolis step, we pick a new q_j' and look up the value of the probability distribution

$$P(q_j') = I(q_{j+1}, q_j')\, I(q_j', q_{j-1}) \tag{75}$$

If $P(q_j') \geq P(q_j)$, then we accept the new q_j'. If $P(q_j') < P(q_j)$, then we accept the new q_j' with probability

$$P(q_j \to q_j') = P(q_j')/P(q_j). \tag{76}$$

VI. APPLICATION OF THE HYBRID METHOD TO THE QUANTUM-MECHANICAL BORN-INFELD MODEL

We now use numerical integration and look-up tables to perform a Monte Carlo estimate of the ground-state energy of the quantum-mechanical Born-Infeld model. Its lagrangian is

$$L = Mc^2 - Mc^2 \left[1 - \frac{m}{Mc^2} \left(\dot{q}^2 - \omega^2 q^2 \right) \right]^{1/2}. \tag{77}$$

The momentum is

$$p = \frac{m\dot{q}}{\sqrt{1 - m\left(\dot{q}^2 - \omega^2 q^2\right)/(Mc^2)}}, \tag{78}$$

and the velocity is

$$\dot{q} = \frac{p}{m} \frac{\sqrt{1 + m\omega^2 q^2/Mc^2}}{\sqrt{1 + p^2/(mMc^2)}}. \tag{79}$$

The quantum-mechanical Born-Infeld hamiltonian is

$$H = \sqrt{\frac{p^2}{m} + Mc^2}\, \sqrt{Mc^2 + m\omega^2 q^2} - Mc^2. \tag{80}$$

In terms of the harmonic-oscillator variables

$$a = \sqrt{\frac{m\omega}{2}} \left(q + \frac{ip}{m\omega} \right) \quad \text{and} \quad a^\dagger = \sqrt{\frac{m\omega}{2}} \left(q - \frac{ip}{m\omega} \right), \tag{81}$$

the operators q and p are $q = \left(a^\dagger + a\right)/\sqrt{2m\omega}$ and $p = i\sqrt{m\omega/2}\left(a^\dagger - a\right)$, and so the hamiltonian (80) is

$$H = \sqrt{Mc^2 - \frac{\omega}{2}\left(a^\dagger - a\right)^2}\sqrt{Mc^2 + \frac{\omega}{2}\left(a^\dagger + a\right)^2} - Mc^2. \tag{82}$$

Like the hamiltonian of the simple harmonic oscillator, it is independent of the mass m.

With $c = 1$ and $\beta = n\,a$, the partition function is

$$\begin{aligned} Z(\beta) = \mathrm{Tr}\, e^{-\beta H} &= \int \exp\left\{\int_0^\beta \left[i\dot{q}p - H(q,p)\right] dt\right\} DpDq \\ &= \prod_{j=1}^n \int \frac{dp_j dq_j}{2\pi} \exp\left[\sum_{\ell=0}^n i(q_{\ell+1} - q_\ell)p_\ell - aH(q_\ell, p_\ell)\right] \\ &= \prod_{j=1}^n \int \frac{dp_j dq_j}{2\pi} \exp\left[\sum_{\ell=0}^n i(q_{\ell+1} - q_\ell)p_\ell - a\left(\sqrt{p_\ell^2/m + M}\ \sqrt{M + m\omega^2 q_\ell^2} - M\right)\right], \end{aligned} \tag{83}$$

and the mean value of the hamiltonian at inverse temperature β is

$$\begin{aligned} \langle H\rangle_\beta = -\frac{\mathrm{Tr}\, H\, e^{-\beta H}}{\mathrm{Tr}\, e^{-\beta H}} &= -\frac{1}{Z(\beta)}\frac{dZ(\beta)}{d\beta} \\ &= \prod_{j=1}^n \int \frac{dp_j dq_j}{2\pi} \left[\frac{1}{n}\sum_{\ell=0}^n \left(\sqrt{p_\ell^2/m + M}\ \sqrt{M + m\omega^2 q_\ell^2} - M\right)\right] \\ &\quad \times \exp\left[\sum_{\ell=0}^n i(q_{\ell+1} - q_\ell)p_\ell - a\left(\sqrt{p_\ell^2/m + M}\ \sqrt{M + m\omega^2 q_\ell^2} - M\right)\right] \\ &\quad \Bigg/ \prod_{j=1}^n \int \frac{dp_j dq_j}{2\pi} \exp\left[\sum_{\ell=0}^n i(q_{\ell+1} - q_\ell)p_\ell - a\left(\sqrt{p_\ell^2/m + M}\ \sqrt{M + m\omega^2 q_\ell^2} - M\right)\right]. \end{aligned} \tag{84}$$

We wrote Fortran90 codes to compute the integrals

$$\begin{aligned} I(q_{\ell+1}, q_\ell) = \langle q_{\ell+1}|e^{-aH(q_\ell,p_\ell)}|q_\ell\rangle &= \int_{-\infty}^\infty \frac{dp}{\sqrt{2\pi}} \exp\left[i(q_{\ell+1} - q_\ell)\,p - a\,H(q_\ell, p)\right] \\ &= \int_0^\infty \frac{dp}{\sqrt{\pi}} \cos\left[(q_{\ell+1} - q_\ell)\,p\right] \exp\left[-a\,H(q_\ell, p)\right] \\ &= \int_0^\infty \frac{dp}{\sqrt{\pi}} \cos\left[(q_{\ell+1} - q_\ell)p\right] \exp\left[-a\left(\sqrt{p^2/m + M}\sqrt{M + m\omega^2 q_\ell^2} - M\right)\right] \end{aligned} \tag{85}$$

and

$$\begin{aligned} HI(q_{\ell+1}, q_\ell) = &\int_0^\infty \frac{dp}{\sqrt{\pi}} \left(\sqrt{p_\ell^2/m + M}\ \sqrt{M + m\omega^2 q_\ell^2} - M\right) \\ &\times \cos\left[(q_{\ell+1} - q_\ell)p\right] \exp\left[-a\left(\sqrt{p^2/m + M}\sqrt{M + m\omega^2 q_\ell^2} - M\right)\right] \end{aligned} \tag{86}$$

for a suitably large set of values of q_ℓ and $q_{\ell+1}$ and used them to estimate the mean value

$$\langle H \rangle_\beta = \left\langle \frac{1}{n} \sum_{k=1}^{n} \frac{HI(q_{k+1}, q_k)}{I(q_{k+1}, q_k)} \right\rangle = \int \frac{1}{n} \sum_{k=1}^{n} \frac{HI(q_{k+1}, q_k)}{I(q_{k+1}, q_k)} P_n[q, \beta] \, Dq. \tag{87}$$

We made look-up tables for $m = \omega = 1$ and $0.1 \le M \le 10$ and for $m = M = 1$ and $0.1 \le \omega \le 1$. We also wrote Monte Carlo codes that use these look-up tables. All the work is in making the look-up tables. The Monte Carlo codes run fast.

We used Matlab to compute the exact eigenvalues of the Born-Infeld hamiltonian (82) by making a 1000×1000 matrix a as diag(sqrt([1:Nmax]),1) with Nmax $= 1000$ and $a^\dagger$ as its transpose.

The exact values and our hybrid Monte Carlo results for $m = \omega = 1$ and $0.1 \le M \le 10$ are listed in table I and plotted in figure 1.

TABLE I: Exact and Monte Carlo results for the ground-state energy E_0 of the Born-Infeld hamiltonian (80) for $\omega = m = 1$ and $0.1 \le M \le 10$.

ω	m	M	E_0 exact	E_0 Monte Carlo
1	1	0.1	0.1881	0.1759
1	1	0.5	0.3155	0.3191
1	1	1.0	0.3702	0.3746
1	1	2.5	0.4288	0.4308
1	1	5.0	0.4587	0.4603
1	1	7.5	0.4708	0.4723
1	1	10.0	0.4774	0.4781

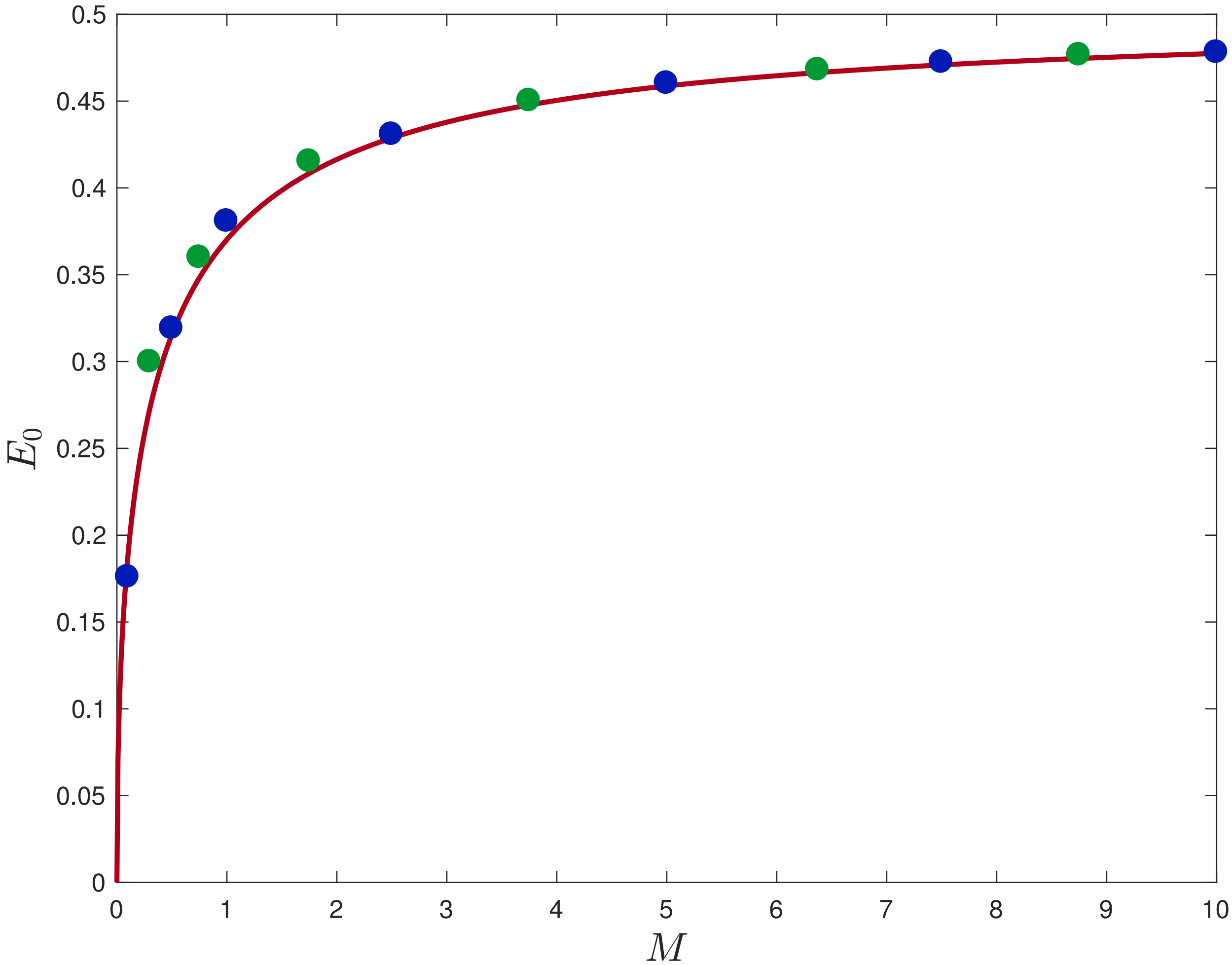

FIG. 1: The hybrid Monte Carlo estimates (85–87, blue dots) and (90–92, green dots) of the ground-state energies of the Born-Infeld model are plotted along with the exact values (red curve) for $0.1\,m \le M \le 10\,m$ and $m = \omega = 1$.

The exact values and our hybrid Monte Carlo results for $0.1 \le \omega \le 1$ and $m = M = 1$ are listed in table II and plotted in figure 2.

TABLE II: Exact and Monte Carlo results for the ground-state energy E_0 of the Born-Infeld hamiltonian (80) for $0.1 \leq \omega \leq 1.0$ and $m = M = 1$.

ω	m	M	E_0 exact	E_0 Monte Carlo
0.1	1	1	0.0477	0.0471
0.2	1	1	0.0917	0.0953
0.3	1	1	0.1328	0.1354
0.4	1	1	0.1715	0.1749
0.5	1	1	0.2082	0.2130
0.6	1	1	0.2432	0.2493
0.7	1	1	0.2768	0.2843
0.8	1	1	0.3090	0.3197
0.9	1	1	0.3401	0.3528
1.0	1	1	0.3702	0.3746

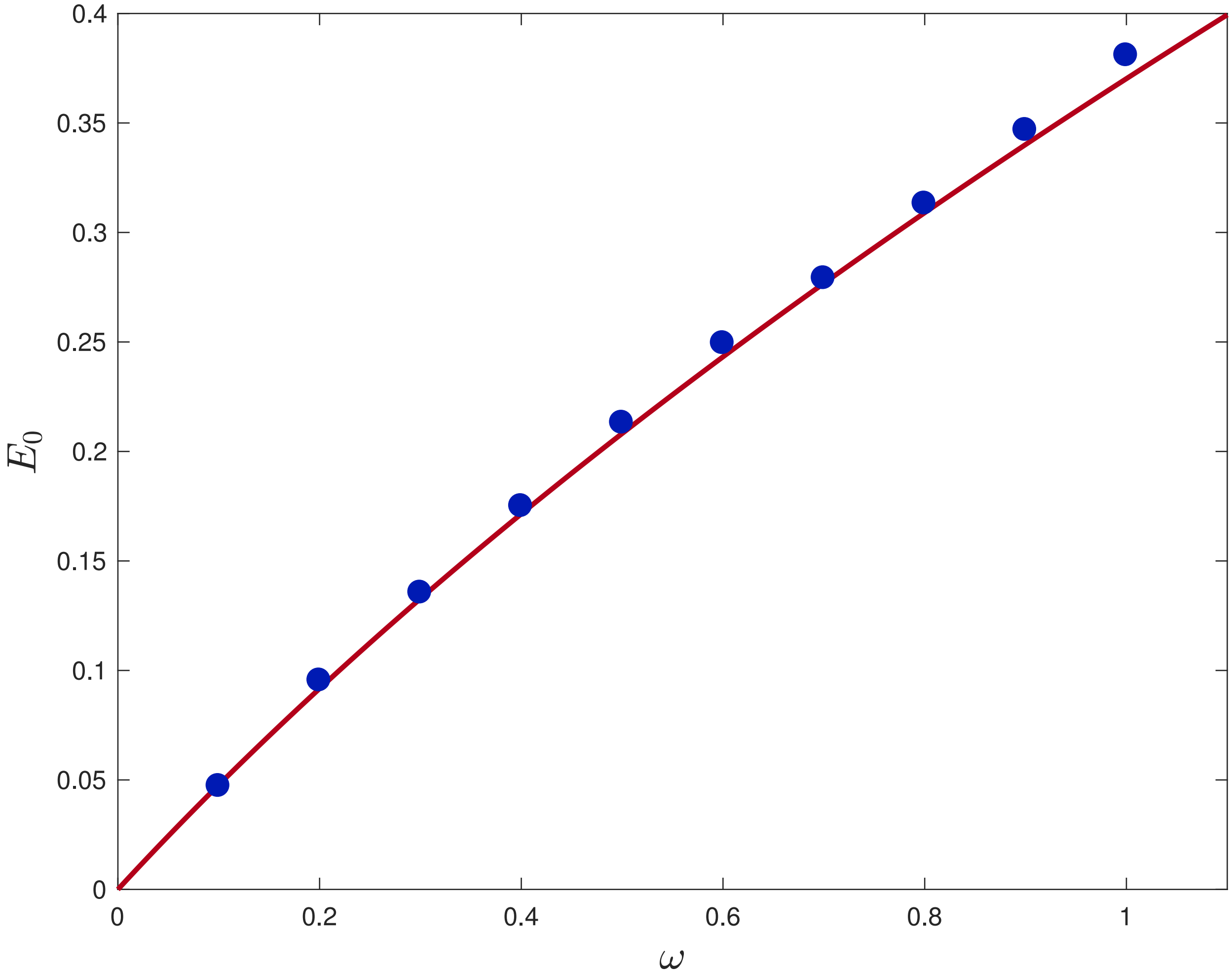

FIG. 2: The hybrid Monte Carlo estimates (blue dots) of the ground-state energies of the Born-Infeld model are plotted along with the exact values (red curve) for $0.1 \le \omega \le 10$ and $m = M = 1$.

We may apply our hybrid technique to other quantum-mechanical models, but our real goal is to apply it to field theories like those of the papers [2].

VII. WHEN ONE CAN'T FIND THE HAMILTONIAN

When one can't find the hamiltonian, one may use the complex path-integral formula (7). We now test this formula by applying it to the quantum-mechanical Born-Infeld model (18). Now instead of the partition function (23) of the field theory, we have the partition function

$$\begin{aligned}Z(\beta) &= \int \exp\left\{\int^{\beta}\left[(i\dot{q}-\dot{s})\frac{\partial L(q,\dot{s})}{\partial \dot{s}} + L(q,\dot{s})\right] d^4x\right\} \left|\frac{\partial^2 L(q,\dot{s})}{\partial \dot{s}^2}\right| DqD\dot{s} \\ &= \int \exp\left\{\int^{\beta}\left[\frac{mi\dot{q}\dot{s} - m\omega^2 q^2 - M}{\sqrt{1-m\left(\dot{s}^2-\omega^2 q^2\right)/M}} + M\right] dt\right\} \\ &\quad \times \frac{m + m^2\omega^2 q^2/M}{\left[1-m\left(\dot{s}^2-\omega^2 q^2\right)/M\right]^{3/2}} DqD\dot{s}.\end{aligned} \tag{88}$$

We approximate this path integral on an $n \times n$ lattice of lattice spacing $a = \beta/n$ as the multiple integral

$$\begin{aligned}Z(\beta) = \prod_{j=1}^{n} \int \frac{d\dot{s}_j dq_j}{2\pi} \exp\left\{\sum_{\ell=1}^{n}\left[\frac{i\, m(q_{\ell+1}-q_\ell)\dot{s}_\ell - am\omega^2 q_\ell^2 - aM}{\sqrt{1-m\left(\dot{s}_\ell^2-\omega^2 q_\ell^2\right)/M}} + aM\right]\right. \\ \times \frac{m + m^2\omega^2 q_j^2/M}{\left[1-m\left(\dot{s}_j^2-\omega^2 q_j^2\right)/M\right]^{3/2}}.\end{aligned} \tag{89}$$

Apart from the phase factor, the integrand is even in $\dot{s}$. So setting $\dot{s} = r$ and $R(q_j) = \sqrt{M/m + \omega^2 q_j^2}$, we numerically compute the integrals

$$\begin{aligned}I(q_{j+1}, q_j) = \int_{-R(q_j)}^{R(q_j)} dr\, \cos\left[\frac{m(q_{j+1}-q_j)r}{\sqrt{1+m\left(\omega^2 q_j^2 - r^2\right)/M}}\right] \\ \times \exp\left[aM - \frac{am\omega^2 q_j^2 + aM}{\sqrt{1+m\left(\omega^2 q_j^2 - r^2\right)/M}}\right] \frac{\left(m + m^2\omega^2 q_j^2/M\right)}{\left[1+m\left(\omega^2 q_j^2 - r^2\right)/M\right]^{3/2}}.\end{aligned} \tag{90}$$

and

$$\begin{aligned}HI(q_{j+1}, q_j) = \int_{-R(q_j)}^{R(q_j)} dr \left[\frac{m\omega^2 q_j^2 + M}{\sqrt{1+m\left(\omega^2 q_j^2 - r^2\right)/M}} - M\right] \cos\left[\frac{m(q_{j+1}-q_j)r}{\sqrt{1+m\left(\omega^2 q_j^2 - r^2\right)/M}}\right] \\ \times \exp\left[aM - \frac{am\omega^2 q_j^2 + aM}{\sqrt{1+m\left(\omega^2 q_j^2 - r^2\right)/M}}\right] \frac{\left(m + m^2\omega^2 q_j^2/M\right)}{\left[1+m\left(\omega^2 q_j^2 - r^2\right)/M\right]^{3/2}}\end{aligned} \tag{91}$$

and make a look-up table. We then use the look-up table to estimate the mean value

$$\langle H \rangle_\beta = \left\langle \frac{1}{n} \sum_{k=1}^{n} \frac{HI(q_{k+1}, q_k)}{I(q_{k+1}, q_k)} \right\rangle. \tag{92}$$

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