Semiclassical solutions in statistical quantum mechanics: second-order corrections and applications to nuclear matter

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Abstract: We consider the Feynman path integral formalism applied to different quantum systems at finite temperature under the semiclassical approximation. To refine previous results, we first develop its second-order correction by implementing the Gel'fand-Yaglom method numerically and apply it to the 1D nonperturbative anharmonic oscillator. Then, we extend the semiclassical approach to a generic two-body potential, $V(r)$, and apply it to the 3D spherical harmonic oscillator and to the nucleon-nucleon interaction to obtain thermodynamical properties of nuclear matter.
Keywords: Quantum mechanics, path integral, nucleon-nucleon potential, virial coefficient
SDGs: 4. Quality Education. 9. Industry, Innovation and Infrastructure.

I. Introduction

An alternative formulation of Schrödinger's quantum mechanics is the one developed by Richard Feynman: the path integral formalism [1]. In this approach, instead of the wavefunction, the object of interest is the "kernel", which is the sum of all possible trajectories that the system can follow, each of them weighted by the imaginary exponential of the action associated to the path. This kernel allows us to define a probability distribution.

On the one hand, our goal is to expand upon the results of the TFG [2], where the classical solution of the path integral in imaginary time (the so-called flucton [3, 4]) was applied to the one-dimensional (1D) harmonic (HO) and anharmonic oscillators (AHO) in quantum mechanics (QM). Here, we also study the 1D AHO, but go beyond the flucton solution and apply second-order corrections to test the convergence of the semiclassical expansion and compare it to the solution of the Schrödinger equation combined within the thermal density matrix.

For this goal, we adapt the so-called Gel'fand-Yaglom (GY) method [5]. It allows us to obtain the determinant of a differential operator by solving a differential equation with initial conditions instead of an eigenvalue problem. This alternative requires much less computation time, as it is easier to solve numerically. We test this method for the AHO potential in the nonperturbative regime,

$$V(x) = m\omega^2 x^2/2 + g^2 x^4/2 \ , \quad g \sim 1 \ . \tag{1}$$

On the other hand, we extend the semiclassical method to the two-body problem, specifically, to two particles interacting through a pairwise potential, $V(r)$, whose relative motion turns out to be, in fact, one dimensional.

After a consistency check in the 3D spherically symmetric harmonic oscillator (which we discuss in detail in App. C), we consider two nucleons interacting through a very simple potential, the Serot-Walecka model. The study of the two-body problem using the flucton path allows us to extract the radial distribution function, $g(r)$, and the second virial coefficient, $B_2(T)$, of nuclear matter at finite temperature. In contrast to the standard classical calculations [6], our approach incorporates not only thermal, but also quantum fluctuations.

We use natural units consisting of $\hbar = k_{\mathrm{B}} = c = 1$ throughout the following sections.

II. Theoretical background

In this section, we review the path integral formalism applied to a 1D potential in QM as well as the two-body problem. We also introduce the radial distribution function, $g(r)$, and the second virial coefficient, $B_2(T)$.

A. Path integrals in statistical mechanics

In the path integral formalism, the probability amplitude for a particle in 1D of going from $a = (x_a, t_a)$ to $b = (x_b, t_b)$ is defined as the kernel [1],

$$K(b;a) = K(x_b, t_b; x_a, t_a) = \int_{x(t_a)=x_a}^{x(t_b)=x_b} \mathcal{D}x(t)\ \mathrm{e}^{\mathrm{i}S[x(t)]} \ , \tag{2}$$

where $\mathcal{D}x(t)$ and the limits of integration indicate that we are summing over all possible trajectories starting at a and ending at b. The action associated to a given trajectory, $x(t)$, in a potential, $V(x)$, is defined as

$$S[x(t)] = \int_{t_a}^{t_b} \mathrm{d}t \left(\frac{1}{2} m \dot{x}(t)^2 - V(x(t)) \right) \ , \tag{3}$$

where $\dot{x}(t)$ is the time derivative of the trajectory.

Alternatively, we can also express the kernel in Eq. (2) in terms of its spectral decomposition [1],

$$K(b;a) = \sum_n \phi_n(x_b)\phi_n^*(x_a)\mathrm{e}^{-\mathrm{i}E_n(t_b - t_a)} \ , \tag{4}$$

where the $\phi_n(x)$ and the E_n are, respectively, the eigenfunctions and the energy eigenvalues obtained from the time-independent Schrödinger equation.

Equation (4) formally coincides with the density matrix at temperature $T = 1/\beta$ used in statistical QM [1],

$$\rho(x_a, x_b) = \sum_n \phi_n(x_b)\phi_n^*(x_a)\mathrm{e}^{-E_n\beta} \ . \tag{5}$$

Thus, it is possible to establish a connection between these two quantities if we perform a Wick rotation of the time coordinate, $t = -\mathrm{i}\tau$. In this imaginary time, Eqs. (4) and (2) can be rewritten, respectively, as

$$K(x_b, \tau_b; x_a, \tau_a) = \sum_n \phi_n(x_b)\phi_n^*(x_a)\mathrm{e}^{-E_n(\tau_b-\tau_a)} \tag{6}$$

$$= \int_{x(\tau_a)=x_a}^{x(\tau_b)=x_b} \mathcal{D}x(\tau)\ \mathrm{e}^{-S_\mathrm{E}[x(\tau)]} \ , \tag{7}$$

where the weighting factor is a real exponential and $S_\mathrm{E}[x(\tau)]$ is the so-called Euclidean action,

$$S_\mathrm{E}[x(\tau)] = \int_{\tau_a}^{\tau_b} \mathrm{d}\tau \left(\frac{1}{2}m\dot{x}(\tau)^2 + V(x(\tau))\right) \ . \tag{8}$$

The comparison of Eqs. (5) and (6) allows us to identify the time interval with the temperature: $\tau_b - \tau_a = \beta$. We take $\tau_a = 0$ and $\tau_b = \beta$ to study the thermal density matrix of a quantum system and compute it using the path integral in Eq. (7).

We eventually want to assign a probability density function to the system to perform spatial averages. This can be achieved by considering the diagonal elements of the thermal density matrix in Eq. (5),

$$\tilde{P}(x) := \rho(x, x) = \sum_n |\phi_n(x)|^2\mathrm{e}^{-E_n\beta} \ . \tag{9}$$

Notice that the integral of $\tilde{P}(x)$ over all $x \in (-\infty, \infty)$ is not one, but the well-known partition function,

$$Z(\beta) = \sum_n \mathrm{e}^{-E_n\beta} \ . \tag{10}$$

In the path integral, to evaluate the diagonal elements, we need to consider closed paths, i.e., trajectories starting and ending at the same point in space, which we call the "observation point", $x_0 := x_a = x_b$. From Eqs. (6),(9) and (7), we can define a normalized probability density function by $P(x) = Z(\beta)^{-1}\tilde{P}(x)$, where

$$\tilde{P}(x_0) = \int_{x(\tau=0)=x_0}^{x(\tau=\beta)=x_0} \mathcal{D}x(\tau)\ \mathrm{e}^{-S_\mathrm{E}[x(\tau)]} \ . \tag{11}$$

B. Semiclassical approximation and flucton

The semiclassical approach relies on the assumption that the trajectories which contribute the most to the path integral are those near the one that minimizes the Euclidean action. For this reason, we search for closed-path solutions that make this action stationary. In the present context, such a solution is called the "flucton", $x_\mathrm{fl}(\tau)$ [7]. It satisfies the following differential equation deduced from the corresponding stationary action principle,

$$m\ddot{x}_\mathrm{fl}(\tau) = V'(x_\mathrm{fl}(\tau)) \quad \leftrightarrow \quad \frac{\delta S_\mathrm{E}}{\delta x(\tau)}\Big|_{x=x_\mathrm{fl}} = 0 \ , \tag{12}$$

where V' is the first derivative of V with respect to x. Note the opposite sign relative to Newton's equation.

If we consider trajectories around the classical solution, $x(\tau) = x_\mathrm{fl}(\tau) + y(\tau)$, and make a functional expansion of the Euclidean action, we obtain [1, 8],

$$S_\mathrm{E}[x(\tau)] = S_\mathrm{E}[x_\mathrm{fl}(\tau) + y(\tau)] = S_\mathrm{E}[x_\mathrm{fl}(\tau)] + \\ + \frac{1}{2}\int_0^\beta \mathrm{d}\tau\ y(\tau)\frac{\delta^2 S_\mathrm{E}}{\delta x(\tau)^2}\Big|_{x=x_\mathrm{fl}} y(\tau) + \cdots \ , \tag{13}$$

where the linear term is zero because of Eq. (12).

At zeroth order, the action is simply given by the flucton path, $S_\mathrm{E}[x(\tau)] \approx S_\mathrm{E}[x_\mathrm{fl}(\tau)] =: S_\mathrm{fl}(x_0)$, depending only on the observation point, x_0. Then, we obtain a normalized density, $P(x)$, by using Eq. (11) for $S_\mathrm{fl}(x)$, and normalizing to one:

$$P(x) = \frac{\mathrm{e}^{-S_\mathrm{fl}(x)}}{\int_{-\infty}^{\infty}\mathrm{d}x_0\ \mathrm{e}^{-S_\mathrm{fl}(x_0)}} \ . \tag{14}$$

This approximation was used in Ref. [2] to solve the 1D HO and AHO at zeroth order. In this TFG, we aim to go to the next non-trivial order in the expansion (13).

C. Second-order corrections

To manipulate the second-order corrections to $P(x)$ in Eq. (13), we define the functional operator

$$\mathcal{O}(x_\mathrm{fl}) := \frac{\delta^2 S_\mathrm{E}}{\delta x(\tau)^2}\Big|_{x=x_\mathrm{fl}} = -m\frac{\mathrm{d}^2}{\mathrm{d}\tau^2} + V''(x_\mathrm{fl}(\tau)) \tag{15}$$

and insert the second-order term of the action into the exponential of the path integral (11). We arrive at the following form for the probability density function [8],

$$\tilde{P}(x) \approx \mathrm{e}^{-S_\mathrm{fl}(x)}\int_{y(\tau=0)=0}^{y(\tau=\beta)=0} \mathcal{D}y(\tau)\ \mathrm{e}^{-\frac{1}{2}\int_0^\beta \mathrm{d}\tau\ y(\tau)\mathcal{O}(x_\mathrm{fl})y(\tau)} \\ = C\mathrm{e}^{-S_\mathrm{fl}(x)}[\det(\mathcal{O}(x_\mathrm{fl}))]^{-1/2} \ , \tag{16}$$

where C is a constant appearing after the Gaussian integration that needs to be renormalized by matching the result which uses $V = 0$ to the free case, whose partition function is finite and well known [1]. The remaining task is to find the value of the determinant, which can be expressed as the infinite product

$$\det(\mathcal{O}(x_\mathrm{fl})) = \prod_n \lambda_n \ , \tag{17}$$

where the λ_n are the eigenvalues of the operator,

$$\mathcal{O}(x_{\rm fl})\ \psi_n(\tau) = \lambda_n \psi_n(\tau)\ , \tag{18}$$

with boundary conditions $\psi_n(0) = \psi_n(\beta) = 0$, since these are the path's boundary conditions that the deviations from the fluctón solution, $y(\tau)$, must satisfy.

Instead of solving Eq. (18) (which is a problem of similar complexity to solving the original Schrödinger equation for $V(x)$), we adapt the GY method [5]. This method replaces the eigenvalue equation (18) with a related initial value problem with the same differential operator,

$$\mathcal{O}(x_{\rm fl})\ \psi(\tau) = 0\ , \tag{19}$$

with $\psi(0) = 0$ and $\dot{\psi}(0) = 1$. By obtaining the solution, $\psi(\tau)$, the functional determinant simply reads [5],

$$\det\left(\mathcal{O}(x_{\rm fl})\right) = \psi(\beta)\ , \tag{20}$$

so we have reduced the problem to solving Eq. (19), whose numerical scheme is described in App. B.

We conclude by noting that, for the HO, the second-order correction to $\tilde{P}(x)$ is just a constant [1, 8], while, for the AHO, we obtain an x-dependent factor, which will be presented in Sec. III A. Our numerical method is general, so it can be applied to any 1D potential.

D. The two-body problem: application to nuclear matter

In this section, we implement, with some minor differences, the fluctón procedure on a pair of particles interacting via a central force in 3D. In the absence of external forces, the kernel can be decoupled and expressed as the product of the contribution of the center of mass (CM) coordinate, $\mathbf{R}$, and the relative coordinate, $\mathbf{r}$ [1],

$$K(b;a) = K_{\mathbf{r}}(\mathbf{r}_b, t_b; \mathbf{r}_a, t_a) K_{\mathbf{R}}(\mathbf{R}_b, t_b; \mathbf{R}_a, t_a)\ . \tag{21}$$

Thus, by factorizing the CM and relative motion, and ignoring the CM movement, we focus on the radial coordinate, as commonly done in classical mechanics, and reduce the system to a 1D problem for the variable r, which takes values in the interval $(0, \infty)$ instead of $(-\infty, \infty)$.

In order to explore a more physical situation, we study a system of two nucleons interacting through a simple pair potential, $V(r)$. The treatment of this two-body problem allows us to obtain two different fluid quantities for a gas of interacting nucleons under such potential.

The first one is the radial distribution function, $g(r)$. It is a measure of the probability of finding a nucleon at distance r from another one. In the classical, dilute limit, it has the form [6],

$$g(r) = \mathrm{e}^{-V(r)/T}\ , \tag{22}$$

with normalization $4\pi \int_0^\infty \mathrm{d}r\ r^2 g(r) = \Omega$, where Ω is the volume of the system.

We recall that, for ideal gases, $g(r) = 1$ and the probability of finding a particle at a given point does not depend on the position of the others. For interacting gases, liquids and solids, $g(r)$ presents a nontrivial structure that lets us infer the most probable mutual distances between particles in a fluid or a solid.

For a thermal quantum system, we can use the fluctón solution to approximate the path integral. The value of $g(r)$ coincides with that of $\tilde{P}(r)$ at this order [9],

$$g(r) = \mathrm{e}^{-S_{\rm fl}(r)}\ . \tag{23}$$

In addition, the equation of state for a non-ideal gas or fluid can be expressed in terms of the virial expansion, in powers of the particle density, $\rho = N/\Omega$,

$$p/T = \rho + B_2(T)\rho^2 + B_3(T)\rho^2 + \cdots\ , \tag{24}$$

where p is the pressure and the quantities $B_n(T)$ are the second, third, etc. virial coefficients. We are interested in $B_2(T)$, which is the first correction to the ideal gas behavior. In the classical, dilute limit [6],

$$B_2(T) = -2\pi \int_0^\infty \mathrm{d}r\ \left(\mathrm{e}^{-V(r)/T} - 1\right) r^2\ , \tag{25}$$

but in our approach (including quantum fluctuations through the fluctón at zeroth order) we use [9],

$$B_2(T) = -2\pi \int_0^\infty \mathrm{d}r\ \left(\mathrm{e}^{-S_{\rm fl}(r)} - 1\right) r^2\ . \tag{26}$$

III. Results

In this section, we present the results of this TFG. In Sec. III A, we consider the 1D AHO and show the fluctón trajectories and the second-order probability density function, $P(x)$, for different temperatures. In Sec. III B, we deal with the nucleon-nucleon interaction, and show how $g(r;T)$ and $B_2(T)$ depend on temperature.

The uncertainty associated with the numerics has been minimized by choosing a very fine discretization in the codes, but the systematic error caused by truncating the semiclassical expansion is very difficult to estimate since it depends on $V(r)$, T and r in a complex way. For this reason, we do not assign error bars to our figures.

A. 1D AHO potential

We start with a 1D system under the potential (1) with $\omega = 1$ (without loss of generality) and $g = 1$, since this method allows us to treat the nonperturbative regime. We also set $m = 1$, so that all physical quantities, with mass dimension, carry no units. The fluctón trajectories have been calculated by solving Eq. (12) numerically (see details in App. A). We show some examples in Fig. 1 for different values of $\beta = 0.75, 1, 1.25$, where we compare them with the analytical solutions given in Ref. [10].

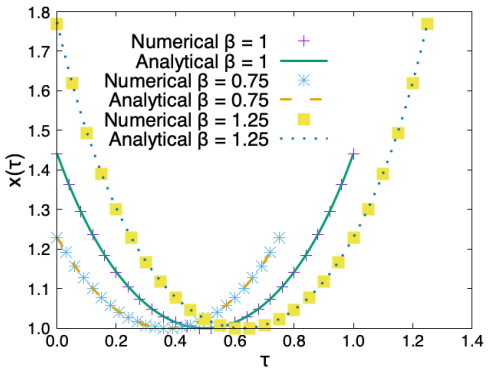

FIG. 1. Symbols: our numerical flucton path solutions of the AHO for three different values of β, each of them, with a different value of x_0. Lines: analytical solutions given in [10] for the AHO. All paths start at $\tau = 0$ and end at $\tau = \beta$.

For a given β, we compute the action of each flucton path as in (8) and the corresponding $\tilde{P}(x_0) = \exp(-S_{\text{fl}}(x_0))$. In order to add the second-order correction, we include the calculation of the determinant to the classical approximation as detailed in Sec. II C. Then, we repeat for all values of x_0 and normalize the probability distribution to obtain $P(x)$. We do this for $\beta = 1/T = 10$, 1 and 0.1, corresponding to low, medium and high temperatures, respectively. These results are shown in Fig. 2, where we compare them with the solution obtained by solving the Schrödinger equation for 200 eigenvalues and then applying Eq. (9) and normalizing.

We observe that the second-order semiclassical correction (GY method) improves over the zeroth-order calculation (flucton), especially at low temperatures ($\beta \gtrsim 1$), improving over the results of Ref. [2]. Next orders (third and fourth) are needed to describe the low temperature case around $x = 0$.

We expect our numerical method to work well with other potentials, since it is already written to use a generic $V(x)$.

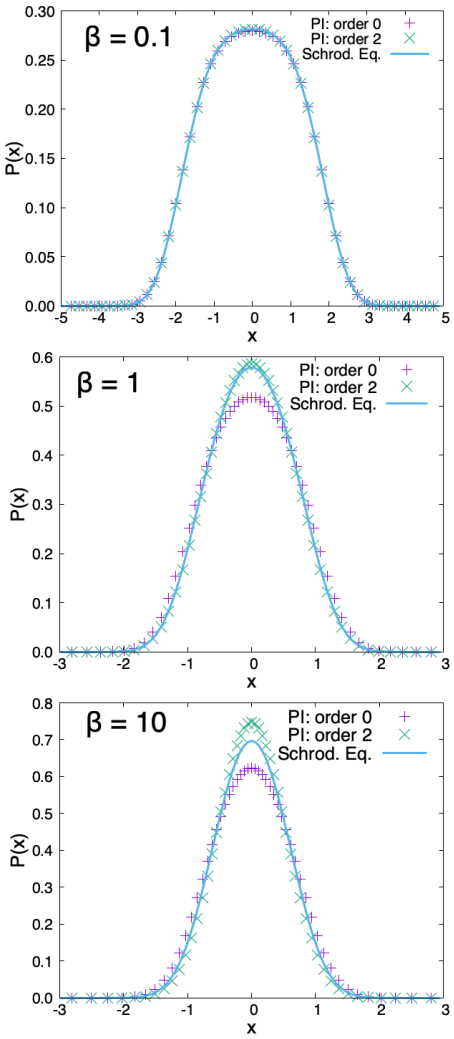

FIG. 2. Normalized probability distribution, $P(x)$, for the AHO with $\omega = g = m = 1$ for high (top panel), medium (middle) and low (bottom) temperatures. We compare the path integral result (PI) at 0th and 2nd order and the solution to the Schrödinger equation (Sch. Eq.) together with Eq. (9).

B. Application to nuclear matter

In this section, we turn to a 3D spherically symmetric potential. The simplest, exactly solvable potential is the 3D HO, but it is formally very similar to the 1D solution given in [2]. For this reason, and due to space limitation, we summarize this case in App. C, where we demonstrate the excellent numerical performance of our code.

In order to present a more applied result, we turn to the two-nucleon case and consider the Serot-Walecka (SW) potential [11] as the simplest model for the NN interaction (we do not try to tackle precision physics in this TFG, but to explore the capability of the semiclassical approach in a toy model). The SW potential reads [7, 11],

$$V(r) = -\alpha_\sigma \frac{\mathrm{e}^{-m_\sigma r}}{r} + \alpha_\omega \frac{\mathrm{e}^{-m_\omega r}}{r} \,, \tag{27}$$

where the attractive part corresponds to the exchange of a scalar mode with strength $\alpha_\sigma = 6.04$ and mass $m_\sigma = 500$ MeV, and the repulsive part, with $\alpha_\omega = 15.17$ and $m_\omega = 782$ MeV, all parameters chosen to reproduce the binding energy per nucleon in infinite nuclear matter [11].

To implement this potential, we need to restore the mass units in our code (fixing the overall scale of the problem). We present the results for the function $g(r)$ in Fig. 3, where we consider temperatures of $T = 25$ MeV (blue), $T = 50$ MeV (orange) and $T = 75$ MeV (green), typical for low-energy heavy-ion collisions [7, 12] or the medium formed in neutron star mergers [12]. In the inset, we show the SW potential of Eq. (27).

At high T, the flucton calculation (lighter-colored symbols) reproduces the classical expectation (darker-colored lines), only with differences at low r (where the potential increases). The differences become larger as we decrease

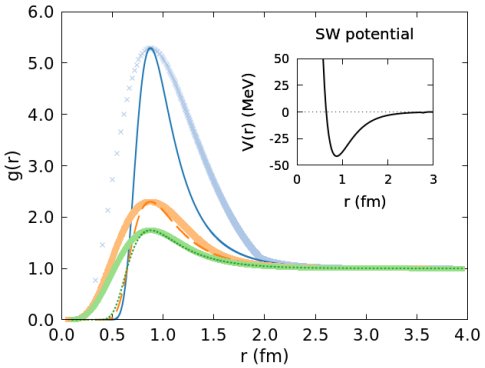

FIG. 3. Radial distribution function of a gas of nucleons. We show 3 temperatures: $T = 25$ MeV (blue), $T = 50$ MeV (orange) and $T = 75$ MeV (green). Data points show the numerical flucton solution, and lines, the classical expectation in Eq. (22). In the inset, we show the SW potential for the NN interaction.

the temperature, indicating that they are of quantum origin. Since the flucton solution also considers quantum fluctuations, the additional probability in the classical-forbidden area is due to quantum penetration into the potential. We also observe that the maximum of $g(r)$ at 0.9 fm coincides with the minimum of the potential, but quantum and thermal fluctuations can slightly shift it.

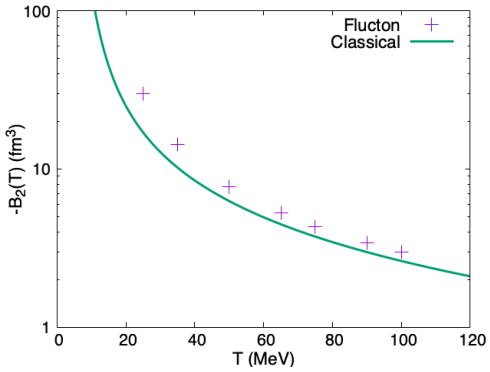

FIG. 4. Second virial coefficient versus temperature for a gas of nucleons interacting with the SW potential. We show the results using the flucton solution and the classical expectation.

Finally, we compare, in Fig. 4, the values obtained for the coefficient $B_2(T)$ using the flucton method of Eq. (26) with the classical expectation in Eq. (25). We observe that both the classical and the flucton values are negative, which means, in accordance with Eq. (24), that the actual pressure is lower than that of the ideal gas, due to the net attractive character of the potential. This effect is more pronounced in the flucton case, where quantum fluctuations are included, in line with the results of $g(r)$. Especially at low temperatures, our flucton solution can be used to account for corrections to the ideal Fermi gas approximation of infinite nuclear matter.

IV. Conclusions

In this TFG, we have studied the 1D AHO in QM using the semiclassical approximation. We have improved the previous results in Ref. [2] by adding second-order corrections with functional analysis and the GY method. To the best of our knowledge, this is the first numerical application of the GY method in QM in the literature. Additionally, we have also applied the semiclassical approximation to the two-body problem. Specifically, we considered two nucleons that interact through the SW potential, allowing us to access the nuclear matter radial distribution function and the second virial coefficient.

Our results could be helpful to explore the equation of state of nuclear matter, for example, in neutron star mergers. Some other possible extensions could be the use of the flucton method to atomic systems to study the properties of a quantum gas of interacting atoms, for example, through a Lennard-Jones potential.

We are currently working on the application of the second-order corrections into the two-body problem, to combine the two main results of this TFG and quantify the size of the corrections to the results of Figs. 3 and 4.

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Solucions semiclàssiques en mecànica quàntica estadística: correccions de segon ordre i aplicacions a matèria nuclear

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Resum: Considerem el formalisme de la integral de camins de Feynman aplicat a diversos sistemes quàntics a temperatura finita sota l'aproximació semiclàssica. Per millorar resultats anteriors, primer desenvolupem la correcció a segon ordre implementant, numèricament, el mètode de Gel'fand-Yaglom i l'apliquem a l'oscil·lador anharmònic en una dimensió. Després, estenem el mètode semiclàssic a un potencial de dos cossos genèric, $V(r)$, i l'apliquem a l'oscil·lador harmònic en tres dimensions esfèricament simètric, així com a la interacció nucleó-nucleó, per obtenir diverses propietats termodinàmiques de la matèria nuclear.
Paraules clau: Mecànica quàntica, integral de camins, potencial nucleó-nucleó, coeficient del virial

ODSs: Aquest TFG està relacionat amb els Objectius de Desenvolupament Sostenible (SDGs) 4. Educació de qualitat. 9. Indústria, innovació, infraestructures.

Objectius de Desenvolupament Sostenible (ODSs o SDGs)

1. Fi de la es desigualtats		10. Reducció de les desigualtats	
2. Fam zero		11. Ciutats i comunitats sostenibles	
3. Salut i benestar		12. Consum i producció responsables	
4. Educació de qualitat	X	13. Acció climàtica	
5. Igualtat de gènere		14. Vida submarina	
6. Aigua neta i sanejament		15. Vida terrestre	
7. Energia neta i sostenible		16. Pau, justícia i institucions sòlides	
8. Treball digne i creixement econòmic		17. Aliança pels objectius	
9. Indústria, innovació, infraestructures	X		

El contingut d'aquest TFG, centrat en aspectes teòrics de la mecànica quàntica i la metodologia de la integral de camins, es relaciona amb l'ODS 4, i, en particular, amb la fita 4.4, ja que contribueix a l'educació avançada en l'àmbit universitari, fomentant competències d'alt nivell en ciència i tecnologia. A més, pot vincular-se amb l'ODS 9, fita 9.5, ja que la recerca en física teòrica fomenta el desenvolupament científic i tecnològic i impulsa les capacitats d'investigació en camps amb aplicacions potencialment transformadores.

Appendices

A. Numerical application of the flucton solution

As explained in Sec. II B, the flucton trajectory, $x_{\text{fl}}(\tau)$, is the solution of the classical equation of motion,

$$m\ddot{x}_{\text{fl}}(\tau) = V'(x_{\text{fl}}(\tau)) \ , \tag{A1}$$

in the interval $\tau = (0, \beta)$ and subjected to the boundary conditions $x_{\text{fl}}(0) = x_{\text{fl}}(\beta) = x_0$. In order to make the problem numerically simpler, we make some slight modifications to the approach.

Let us first prove that the solution of Eq. (A1) subjected to $x_{\text{fl}}(0) = x_{\text{fl}}(\beta) = x_0$ automatically implies that $\dot{x}_{\text{fl}}(\beta/2) = 0$.

We define an auxiliary function, $\tilde{x}_{\text{fl}}(\tau) := x_{\text{fl}}(\beta - \tau)$. For values of τ in $(0, \beta)$, the variable $\beta - \tau$ must also be in the same interval. So the domain of the new function is the same as the original. From Eq. (A1), we have

$$m\ddot{\tilde{x}}_{\text{fl}}(\tau) = m\ddot{x}_{\text{fl}}(\beta - \tau) = V'(x_{\text{fl}}(\beta - \tau)) = V'(\tilde{x}_{\text{fl}}(\tau)) \ , \tag{A2}$$

that is, $\tilde{x}_{\text{fl}}(\tau)$ is also solution of the same differential equation (this is nothing but the invariance of the equations of motion under temporal translations and reflection). Finally, $\tilde{x}_{\text{fl}}(0) = x_{\text{fl}}(\beta) = x_0$ and $\tilde{x}_{\text{fl}}(\beta) = x_{\text{fl}}(0) = x_0$. Since the solution of a second-order differential equation with two boundary conditions is unique, and both solutions (fluctons) satisfy the same equation with the same conditions in the same interval, they must be the same function: $\tilde{x}_{\text{fl}}(\tau) = x_{\text{fl}}(\tau)$, or

$$x_{\text{fl}}(\tau) = x_{\text{fl}}(\beta - \tau) \ , \tag{A3}$$

which shows its symmetry around the midpoint $\tau = \beta/2$. From this condition, we arrive at

$$\dot{x}_{\text{fl}}(\tau) = -\dot{x}_{\text{fl}}(\beta - \tau) \ , \tag{A4}$$

which is the antisymmetry property of the velocity around $\beta/2$. Substituting $\tau = \beta/2$, one obtains $\dot{x}_{\text{fl}}(\beta/2) = -\dot{x}_{\text{fl}}(\beta/2)$, which implies the condition that we were trying to prove, $\dot{x}_{\text{fl}}(\beta/2) = 0$.

In view of this, we transform the second-order ordinary differential equation into a system of two first-order ordinary differential equations via the introduction of $v_{\text{fl}}(\tau) := \dot{x}_{\text{fl}}(\tau)$,

$$\begin{cases} \dot{x}_{\text{fl}}(\tau) = v_{\text{fl}}(\tau) \ , \\ \dot{v}_{\text{fl}}(\tau) = \frac{1}{m} V'(x_{\text{fl}}(\tau)) \ , \end{cases} \tag{A5}$$

where the mixed boundary conditions are $x_{\text{fl}}(\beta) = x_0$ and $v_{\text{fl}}(\beta/2) = 0$.

Although the probability distribution $P(x_0)$ is a function of the observation point, x_0, it is much easier to leave it unfixed and instead start at the value $x_{\text{ext}} := x(\beta/2)$.

Now, we can solve the differential equation from $\tau = \beta/2$ to $\tau = \beta$ using the initial conditions $x_{\text{fl}}(\beta/2) = x_{\text{ext}}$ and $v_{\text{fl}}(\beta/2) = 0$. Once we have computed the values in this interval, we can obtain the ones in $(0, \beta/2)$ using the symmetry condition in Eq. (A3). With this method, the value of x_0 will be determined *a posteriori*, as the value $x_0 = x(\beta)$.

The numerical implementation uses a finite difference approximation for both derivatives,

$$\begin{cases} \dot{x}(\tau) \approx \frac{x(\tau+h) - x(\tau-h)}{2h} \\ \dot{v}(\tau) \approx \frac{v(\tau+h) - v(\tau-h)}{2h} \end{cases} , \tag{A6}$$

from which we obtain an algorithm to solve the differential equation numerically,

$$\begin{cases} x_{\text{fl}}(\tau + h) \approx x_{\text{fl}}(\tau - h) + 2h v_{\text{fl}}(\tau) \\ v_{\text{fl}}(\tau + h) \approx v_{\text{fl}}(\tau - h) + \frac{2h}{m} V'(x_{\text{fl}}(\tau)) \end{cases} \tag{A7}$$

where h is the time step that determines the numerical precision of the method.

Given a number of steps n, we define $h := \beta/n$. We have used $n = 50$ for the calculation of the fluctons in Fig. 1, $n = 1000$ for the results of the AHO potential in Fig. 2 and $n = 100$ for Figs. 3 and 4.

Once the numerical flucton has been calculated, we can obtain the probability density function in Eq. (14). Both numerical integrals needed in the action in Eq. (8) and for the normalization of $P(x)$ as in Eq. (14) have been computed using the trapezoidal rule.

B. Numerical application of Gel'fand-Yaglom method

As seen in Sec. II C, the Gel'fand Yaglom method requires to solve the differential equation in Eq. (19),

$$\left[-m\frac{\mathrm{d}^2}{\mathrm{d}\tau^2} + V''(x_{\text{fl}}(\tau)) \right] \psi(\tau) = 0 \ . \tag{A8}$$

For example, for the AHO potential, this equation takes the particular form

$$m\ddot{\psi}(\tau) = \left(m\omega^2 + 6g^2 x_{\text{fl}}(\tau)^2 \right) \psi(\tau) \tag{A9}$$

with the initial conditions $\psi(0) = 0$ and $\dot{\psi}(0) = 1$. Notice that in Eq. (A9), the flucton path, $x_{\text{fl}}(\tau)$, is a complicated function of τ which is known numerically. Even employing the analytical solution found in [10] for the flucton of the AHO, the resulting differential equation is highly intricate and we only hope to obtain a numerical solution.

In order to solve this equation, we introduce $\phi(\tau) := \dot{\psi}(\tau)$ and formally use the same method of finite difference approximation as in the previous section,

$$\begin{cases} \psi(\tau + h) \approx \psi(\tau - h) + 2h\phi(\tau) \\ \phi(\tau + h) \approx \phi(\tau - h) + \frac{2h}{m} \left(m\omega^2 + 6g^2 x_{\text{fl}}(\tau)^2 \right) \psi(\tau) \end{cases} \tag{A10}$$

We start the method at $\tau = 0$ and run it until we reach $\tau = \beta$. The determinant of the differential operator in Eq. (15) is given as the value $\psi(\beta)$.

C. Solution of 3D spherical harmonic oscillator

As stated in Sec. III B, the simplest, exactly-solvable potential for the two-body problem is the 3D spherically-symmetric HO potential,

$$V(r) = \frac{1}{2}\mu\omega^2 r^2 \ , \tag{A11}$$

where μ is the reduced mass of the two-body system and r is the radial variable, taking values in $(0, \infty)$. In the case of two identical particles, $\mu = m/2$, where m is their individual mass.

In this situation, the analytical solution of the equation of motion

$$\mu\ddot{r}_{\text{fl}}(\tau) = V'(r_{\text{fl}}(\tau)) = \mu\omega^2 r_{\text{fl}}(\tau) \ , \tag{A12}$$

for $r_{\text{fl}}(0) = r_{\text{fl}}(\beta) = r_0$ is really easy to obtain,

$$r_{\text{fl}}(\tau) = r_0 \frac{e^{(\beta-\tau)\omega} + e^{\tau\omega}}{e^{\beta\omega} + 1} \ . \tag{A13}$$

From this analytical expression, we proceed as detailed in Sec. II B by computing the Euclidean action and the probability distribution, $P(r)$. We normalize it so that

$$\int_0^\infty dr P(r) = 1 \tag{A14}$$

and finally arrive at the probability density function,

$$P(r) = \frac{4}{\sqrt{\pi}} \left[\mu\omega \tanh(\omega\beta/2)\right]^{3/2} \ r^2 e^{-\mu\omega r^2 \tanh(\omega\beta/2)} \ . \tag{A15}$$

This is the analytical result for $P(r)$ using the flucton solution (or zeroth-order approximation in the semiclassical expansion). It is easy to see that in this case, the second-order contribution is a constant (and therefore can be absorbed in the normalization), and that higher orders vanish. Therefore, we expect this expression to be the exact analytical solution for the thermal 3D HO case.

In Fig. 5, we observe an excellent agreement between the probability density function obtained from our numerical flucton and the analytical result in Eq. (A15), demonstrating that our code works properly.

On the other hand, we can alternatively approach $P(r)$ using the spectral decomposition in Eq. (9) with the known wavefunctions of the 3D HO potential. The equivalent expression in spherical coordinates is (we have integrated over the angles using the spherical harmonics)

$$P(r) = \frac{1}{\sum_{n,l} e^{-E_{n,l}\beta}} \sum_{n,l} (2l+1) r^2 (R_{n,l}(r))^2 e^{-E_{n,l}\beta} \ , \tag{A16}$$

with $l = 0, 1, 2, 3...$ (with degeneracy $g_l = 2l + 1$) and $n = l, l + 2, l + 4, l + 6...$

The eigenvalues (energies) of the exact solutions of the 3D spherical HO from the Schrödinger equation are

$$E_n = \omega\left(n + \frac{3}{2}\right) \ , \tag{A17}$$

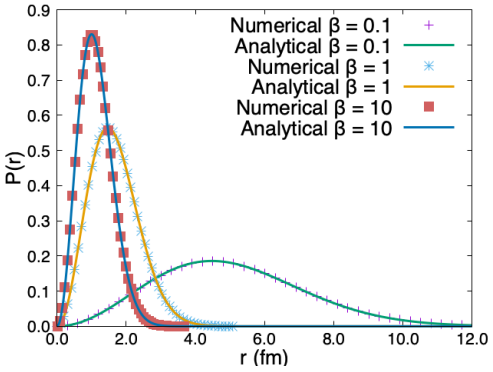

FIG. 5. Symbols: $P(r)$ obtained from the numerical flucton path solution of the 3D HO for three different values of β. Lines: analytical solutions of $P(r)$ obtained from the analytical flucton, and given in Eq. (A15).

and the eigenfunctions,

$$R_{n,l}(r) = \left[\frac{\left(\frac{n-l}{2}\right)!\left(\frac{n+l}{2}\right)!\ 2^{n+l+2}}{(n+l+1)!\ \sqrt{\pi}\alpha^{2l+3}}\right]^{1/2} r^l e^{-\frac{r^2}{\alpha^2}} L_{\frac{n-l}{2}}^{l+\frac{1}{2}}\left(\frac{r^2}{\alpha^2}\right) \ , \tag{A18}$$

where $\alpha = 1/\sqrt{\mu\omega}$, and the $L_{\frac{n-l}{2}}^{l+\frac{1}{2}}\left(\frac{r^2}{\alpha^2}\right)$ are the generalized Laguerre polynomials. Eqs. (A17), (A16) and (A18) have been extracted from the book *Quantum Mechanics, vol. 1* by A. Messiah, North Holland Publishing Company, Amsterdam (1967).

It seems impressive that Eq. (A15) should be equal to Eq. (A16). While we were not able to analytically prove the equality between them, we have numerically checked the agreement to a very high precision for different values of m, ω and $\beta = 1/T$. This can be seen in Fig. 6 for $m = \omega = 1$, where we observe a precise alignment between the numerical $P(r)$ obtained from the flucton path and the solution given by Eq. (A16), where the energy level sum has been carried out up to high enough values of n and l.

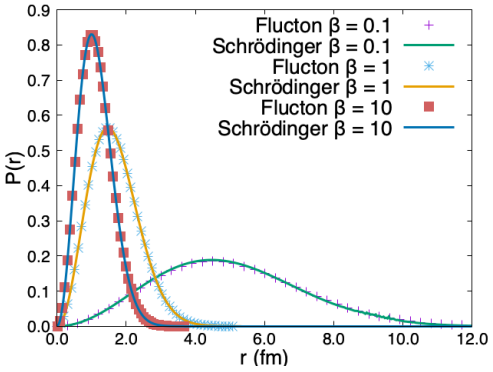

FIG. 6. Symbols: $P(r)$ obtained from the numerical flucton path solution of the 3D HO for three different values of β. Lines: analytical solutions of $P(r)$ obtained from the solution of the Schrödinger equation.