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Path Integral Estimates of the Quantum Fluctuations of the Relative Soliton-Soliton Velocity in a Gross-Pitaevskii Breather

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Abstract: In this paper, the quantum fluctuations of the relative velocity of constituent solitons in a Gross-Pitaevskii breather are studied. The breather is confined in a weak harmonic trap. These fluctuations are monitored, indirectly, using a two-body correlation function measured at a quarter of the harmonic period after the breather creation. The results of an ab initio quantum Monte Carlo calculation, based on the Feynman-Kac path integration method, are compared with the analytical predictions using the recently suggested approach within the Bogoliubov approximation, and a good agreement is obtained.

Keywords: solitons; breathers; quantum fluctuations; Feynman-Kac path integration; Gross-Pitaevskii breather

1. Introduction

A purely solitonic solution focusing on nonlinear Schrödinger equation (NLSE) consists of a finite number of solitons, each parameterized by the norm, velocity, initial position, and initial phase. A single stationary soliton is known as the fundamental soliton. When a solution consists of two or more solitons that are at rest relative to each other and have the same initial positions, it is commonly known as a breather. The name comes from the fact that the density profile of this kind of solution periodically oscillates in time (provided the constituent solitons have unequal amplitudes). Certain kinds of breathers can be produced by quenching the strength of the nonlinear interaction. Mathematically, this means the following: let $\psi(x)$ be the fundamental soliton of an NLSE, at some point of time. Suppose this $\psi(x)$ is used as the initial condition for time propagation under an NLSE whose interaction strength is four times that of the original NLSE. Then, one would find that the propagated solution is a 2-breather whose constituent solitons have norms that are in a ratio of 3:1. Experimentally, this means that a sudden increase of the interaction strength by a factor of 4 converts a fundamental soliton to a 3:1 breather. This was analytically predicted by Satsuma and Yajima [1] in 1974 and recently experimentally verified in dilute Bose-Einstein condensates (BECs) [2,3]. Now, in experiments, there is always a background trapping potential, so that the relevant equation for BEC experiments is the NLSE plus external harmonic confinement. The resulting equation is called the one-dimensional Gross-Pitaevskii equation (GPE). Corresponding to the NLSE breathers, there are Gross-Pitaevskii (GP) breathers. In this paper, a correlation function, associated with a GP breather, corresponding to the 3:1 NLSE breather, is computed using a path integral technique.

Yurovsky et al. [4] showed that quantum many-body effects cause an NLSE breather to disassociate into its constituent solitons. Recall that the 3:1 breather consists of two solitons of norms $N/4$ and $3N/4$ (where N is the number of atoms in the condensate), which, in the mean-field approximation (i.e., at the level of the GPE), sit on the top of each other and do not move. Using the Bethe ansatz, in [4], it was found that quantization leads to a



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drift in the relative position of the constituent solitons. Unfortunately, this method cannot be applied to more than $N = 23$ atoms, and the prediction for experimentally relevant, larger N was an extrapolation. Nevertheless, it was predicted that the relative soliton-soliton velocity in a GP breather may become experimentally observable, for empirically realistic propagation times. Further investigations corroborated this prediction using two different kinds of approximation: the Bogoliubov approach [5] and the truncated Wigner approximation [6]. The predicted quantum fluctuations of macroscopic variables still to be observed but the breather itself is already observed experimentally. From the theory side, however, one can find that there is a need for a nonperturbative, fully quantum-mechanical approach for building a quantum counterpart of the GP breather, an approach that can be applied to a number of particles N that is substantially larger than 23.

In order to estimate the quantum fluctuations of the relative soliton-soliton velocity in a GP breather, we adopt a quantum Monte Carlo method based on the Feynman-Kac path integration [7]. An ab initio confirmation of the observability of the quantum fluctuations of the relative soliton-soliton velocities is presented here using this path integral method [7].

Metropolis and Ulam [8] were the first to exploit a relationship between the Schrödinger equation for imaginary time and the random-walk solution of the general diffusion equation. Let us consider the initial-value problem,

$$\begin{aligned}\frac{\partial\psi(x,t)}{\partial t} &= \left(\frac{\Delta}{2} - V\right)\psi(x,t), \\ \psi(x,0) &= f(x),\end{aligned}\tag{1}$$

where $x \in \mathbb{R}^d$, d denotes the dimension, and t is the time. The solution of Equation (1) can be written in FK representation as

$$\psi(x,t) = E_x \left[e^{-\int_0^t V(X(s))ds} f(X(t)) \right],\tag{2}$$

where $X(t)$ is a Brownian motion trajectory, E_x is the average value of the exponential term with respect to these trajectories, and f is the initial value of ψ , the latter being the sought-after solution of the above Cauchy problem. This classical representation of the time-dependent solution to the Schrödinger equation involves a Wiener measure [9] (i.e., the probability measure on the space of continuous functions) and, unlike the ordinary path integration, provides a rigorous mathematical justification. The above representation is used to calculate the energies and any correlation properties associated with any particular solution.

It is straightforward to implement numerically and does not require a trial function. This method was first applied to calculate energy eigenvalues of simple systems by Donsker and Kac [10] (see also [11]) and was eventually extended to atomic systems by Korzeniowski et al. [12].

It is also known that the classical FK formula provides a rather slow rate of convergence due to the fact that the underlying diffusion process—Brownian motion (Wiener process)—is non-recurrent. Specifically, in dimensions higher than two, the trajectories of the process escape to infinity with the probability one [13]. Mathematically speaking, for $d \geq 3$, the probability $P(\lim_{t \rightarrow \infty} R_t = \infty) = 1$ (where R_t is the distance of the Brownian particle from the origin) and $\lim_{t \rightarrow \infty} P[X(t) \in B] = 0$. Here B is a Borel set, i.e., the set of all Brownian processes $X(t)$. As a result, the sampling within the quantum-mechanical region of intersection occurs only during a small fraction of the total simulation time and the rate of convergence becomes prohibitively slow.

Another path integral method, known as the generalized Feynman-Kac (GFK) method, was initiated by Soto-Equibar and Claverie [14] and was subsequently extended to the full GFK method by Caffarel and Claverie [15]. These procedures can be considered an application of importance sampling to the FK integral, along with the transformation of Equation (1) into a Wiener path integral over a distribution determined by both the diffusion

and drift terms. This transforms the difficult-to-handle branching (potential energy) term into a more manageable path integral. The GFK method is mathematically more convenient because the limiting distribution exists, i.e., $\lim_{t \rightarrow \infty} P[X(t) \in B] = \int_B \phi_T^2(x) dx$.

In this paper, the GFK method is used to calculate the two-body correlation functions as a measure of the quantum fluctuation of the soliton-soliton relative velocity in a GP breather. It is found that the numerical estimate for the quantum fluctuations compares favorably with the preliminary theoretical estimates and is consistent with the Bogoliubov prediction [5].

2. The Model

For calculating the two-body correlation function, let us first consider the ground state of a solitonic system consisting of bosonic atoms (for example, ⁷Li) with a negative scattering length. We assume that a 2-soliton breather is created at $t = 0$ by quenching the interaction strength of the initial Hamiltonian.

We would like to perform a time propagation of the time-dependent Schrödinger equation:

$$i \frac{\partial}{\partial t} |\psi(t)\rangle = \hat{H}_0 |\psi(t)\rangle, \tag{3}$$

with the initial condition given by the ground state of the initial Hamiltonian

$$\hat{H}_0 = -\frac{1}{2} \Delta + V_0(x), \tag{4}$$

where

$$\Delta = \sum_{i=1}^N \frac{\partial^2}{\partial x_i^2} \tag{5}$$

$$V_0 = V_{\text{int},0} + V_{\text{trap}}$$

$$V_{\text{int},0} = -\tilde{g}_0 \sum_{i < j} \delta_{\tilde{\sigma}}(x_i - x_j),$$

$$V_{\text{trap}} = \frac{1}{2} \sum_i x_i^2. \tag{6}$$

Here and elsewhere below, the system of units, $\hbar = m = \omega = 1$, is used (unlike otherwise given), where \hbar is the reduced Planck constant, m is the atomic mass, ω is the frequency of the harmonic confinement. $\delta_{\tilde{\sigma}}(x_i - x_j)$ is the Dirac delta function, $\tilde{\sigma}$ denotes the width of the Gaussian potential, and

$$\tilde{g}_0 \equiv \frac{|g_0| \sqrt{m}}{\hbar^{\frac{3}{2}} \sqrt{\omega}}$$

is the dimensionless form of the absolute value of the initial coupling constant, g_0 , and N is the number of bosonic particles. We assume that a 2-soliton breather is created at $t = 0$. For that to happen, the pre- and post-quench values of the coupling constant have to satisfy the relation

$$g_0 = \frac{1}{4} g. \tag{7}$$

To estimate the quantum fluctuations of the relative velocity of the constituent solitons in a GP breather, a path integral approach [16–18] is adopted based on the FK integral

formalism. To find the path integral solution, let us first consider the Cauchy problem related to the time-dependent Schrödinger equation (3):

$$i\frac{\partial\psi(x,t)}{\partial t} = \left(-\frac{\Delta}{2} + V\right)\psi(x,t),$$

$$\psi(x,0) = f(x),$$

with a Hamiltonian,

$$H = -\Delta/2 + V(x).$$

The solution of the above equation in the FK representation reads:

$$\psi(x,t) = E_x \left[e^{-\int_0^t V(X(s))ds} f(X(t)) \right], \tag{8}$$

where E_x is the expectation value of the random variables. Numerical implementation of Equation (8) is given in Appendix A.

As was mentioned in the introduction, even though the FK formalism provides a basis for rigorous and accurate calculations of ground-state and excited-state properties of many-particle systems, it suffers from a slow convergence rate as soon as the underlying diffusion process—Brownian motion (Wiener process)—is non-recurrent. To speed up the convergence, one needs to apply the GFK formalism, as described below.

The GFK formalism employs an Ornstein-Uhlenbeck process $Y(t)$, which has a stationary distribution and the convergence becomes much faster. The solution in the FK representation holds for any potential V which belongs to the Kato class [19]. All the ordinary potentials fall under this category.

One can obtain the GFK formalism from the raw FK representation by allowing a large class of diffusions that, unlike Brownian motion, have stationary distributions. Specifically, for any twice-differentiable positive $\phi(x)$, one defines a new potential U as a perturbation of the potential V :

$$U(x) = V(x) - \frac{1}{2} \frac{\Delta\phi(x)}{\phi(x)}. \tag{9}$$

Then:

$$\frac{\partial w(x,t)}{\partial t} = \frac{1}{2} \Delta w(x,t) + \frac{\nabla\phi(x)}{\phi(x)} \nabla w(x,t) - U(x)w(x,t) \tag{10}$$

$$= -Lw(x,t),$$

$$w(x,0) = h(x),$$

where h is the initial value of w . Equation (10) has the solution

$$w(x,t) = E_x \left[e^{-\int_0^t U(Y(s))ds} h(Y(t)) \right], \tag{11}$$

where the new diffusion $Y(t)$ has an infinitesimal generator, $A = \frac{\Delta}{2} + \frac{\nabla\phi}{\phi} \nabla$ with adjoint, $A^*(\cdot) = \frac{\Delta}{2} - \nabla \left[\frac{\nabla\phi}{\phi}(\cdot) \right]$. Here, $\phi^2(x)$ is a stationary density of $Y(t)$, or equivalently, $A^*(\phi^2) = 0$.

To see the connection between $w(x,t)$ and $\psi(x,t)$, observe that for $f = 1$ and $h = 1$,

$$w(x,t) = \frac{\psi(x,t)}{\phi(x)} \tag{12}$$

because $w(x,t)$ satisfies Equation (10). The diffusion $Y(t)$ solves the following stochastic differential equation, $dY(t) = \nabla\phi(Y(t))/\phi(Y(t)) + dX(t)$.

For numerical calculations, the Gaussian representation for the delta-function potential,

$$\delta_{\tilde{\sigma}}(x_i - x_j) = \frac{1}{\sqrt{2\pi\tilde{\sigma}}} \exp\left[-\frac{(x_i - x_j)^2}{2\tilde{\sigma}^2}\right], \tag{13}$$

is used. The justification for choosing the negative Gaussian potential is given in Appendix B.

For the purpose of the path-integral Monte Carlo, the system is represented by a d -dimensional particle, with $d = N$, subject to the boundary conditions,

$$\begin{aligned} \psi|_{\vec{x}=\pm\infty} &= 0, \\ \frac{\partial\psi}{\partial\vec{x}}|_{\vec{x}=\pm\infty} &= 0. \end{aligned}$$

The raw FK equation [7] provides a Cauchy-type solution and a guided random walk is adopted here using a trial function that satisfies the required boundary conditions. Using Equation (10) and the GFK path integral representation [15], the solution for Equation (3) can be represented as [16]

$$\psi(x, t) = w(x, t)\phi(x) = \phi(x)E_x\left[e^{-U(Y(s))ds}\right]. \tag{14}$$

Equation (14) contains the two sums: the modified potential $U(Y(s))$ is summed over all the steps in a given trajectory, and then, $\exp[-U(Y(s))ds]$ is summed over all the trajectories. Here, in this computational problem, a soliton can be viewed as a bound state of ${}^7\text{Li}$ atoms interacting through a strong attractive potential, described in Equation (13). The nonnegative function $\phi(x)$ can be chosen as a trial function consistent with the symmetry of the problem. In the present case, the following function is used for $\phi(x)$ and is denoted as $\phi_0(x)$:

$$\phi_0(x) = Ce^{-bx^2}, \tag{15}$$

where C is a normalization constant and b is a variational parameter. Let us now introduce a new perturbed potential,

$$V_p(x) = e_0 - U(x) = e_0 - V(x) - \frac{1}{2} \frac{\Delta\phi_0(x)}{\phi_0(x)}, \tag{16}$$

in terms of $U(x)$ and the energy e_0 , associated with the trial function ϕ_0 .

The Ornstein-Uhlenbeck process $Y(t)$ is related to the Brownian process $X(t)$ as follows:

$$dY(t) = \nabla\phi(Y(t))/\phi(Y(t)) + dX(t). \tag{17}$$

In Equation (17), the first and second terms represent the drift and diffusion, respectively, and the presence of these terms enables the trajectory $Y(t)$ to be highly localized. As a result, the important regions of the potential are frequently sampled and Equation (14) converges rapidly. Similarly, the expectation value of the operator A is given by [15]

$$\langle Y|A|Y \rangle = \frac{\lim_{t \rightarrow \infty} \int dY(t) A(Y(t)) e^{-\int V_p(Y(s))ds}}{\int dY(t) e^{-\int V_p(Y(s))ds}}. \tag{18}$$

Equation (18) is the key formula used here to calculate the quantum fluctuations of the soliton-soliton velocity.

The goal is to compute the second moment of the two-body relative distance at $t = T/4$:

$$\langle \psi(t = T/4) | (x_1 - x_2)^2 | \psi(t = T/4) \rangle.$$

The reason we are interested in is that this particular correlator is sensitive to the quantum fluctuations of the relative soliton-soliton velocity being itself a macroscopic variable. The large- N analytic predictions for the velocity fluctuations is [5]:

$$\langle \psi(t = 0) | V_{\text{rel}}^2 | \psi(t = 0) \rangle = 0.0429 \tilde{g}^2 N ,$$

where the numerical prefactor comes from a numerically computed integral. This expression neglects the zero-point quantum fluctuations that are induced by the harmonic confinement. In turn, the variance of the relative distance between the centers of mass of the two solitons, after a quarter of a period, is given by

$$\langle \psi(t = T/4) | X_{\text{rel}}^2 | \psi(t = T/4) \rangle = \langle \psi(t = 0) | V_{\text{rel}}^2 | \psi(t = 0) \rangle .$$

The mean occupations of the two constituent solitons are $N/4$ and $3N/4$. Therefore, the probability that two detected particles 1 and 2 of the two different solitons is $6/16$. Furthermore, assume that at $T/4$, the distance between the solitons exceeds their width, and therefore the 1 to 2 distance will be dominated by the distance between the centers of mass of the two solitons. Since $(6/16) \times 0.0429 = 0.0161$, one obtains:

$$\langle \psi(t = T/4) | (x_1 - x_2)^2 | \psi(t = T/4) \rangle \approx 0.0161 \tilde{g}^2 N . \tag{19}$$

As mentioned above, this estimate assumes that (a) the interaction-induced fluctuations in the relative velocity of the solitons exceed those generated by the zero-point fluctuations of the trap, and (b) the soliton-soliton separation at the quarter of the period exceeds the size of the initial density distribution. Let us check the validity of these assumptions.

For (a), the separation (19) is compared with the zero-point fluctuations of the relative distance, $\sqrt{(8/3)/N}$. For (b), the worst-case scenario is considered and it is assumed that the detected atoms 1 and 2 were found on the opposite wings of their respective solitons. That would require that the soliton-soliton distance, given by (19), exceeds the resulting correction to the distance, $\ell_{N/4} + \ell_{3N/4}$, where $\ell_{N'} \equiv 2/(\tilde{g}N')$ is the size of a soliton with N' atoms. One gets:

$$\frac{1}{(\tilde{g}N)^2} \ll 0.06 , \tag{20}$$

$$\frac{1}{(\tilde{g}N)^2} \ll \frac{0.01}{\sqrt{N}} , \tag{21}$$

for the conditions (a) and (b), respectively.

The left-hand side of Equation (19) is numerically calculated here using Equation (18), where $A = (x_1 - x_2)^2$ is set. Here, $T \equiv 2\pi$ is the dimensionless form of the trapping period.

3. Results

The variance in the particle-particle distance that is of interest here is shown in Table 1. The agreement between the theoretical predictions and the numerical results is good, with the exception of the $\tilde{g} = 0.78$ case. Meantime, the condition (21) is barely satisfied, and it is likely that the solitons' width still contributes to the variance in the interparticle distance.

Table 1. Quantum fluctuations of the relative velocity of constituent solitons obtained from numerical calculations and from theory. N is the number of atoms, “scale” represents $\sqrt{(\text{number of steps})/t}$ with t being the simulation time, “npi” stays for the number of trajectories, \tilde{g} and $\tilde{\sigma}$ denote the dimensionless forms of the interaction strength and the width of the Gaussian potential, respectively. See text for details.

N	Scale	npi	\tilde{g}	$\tilde{\sigma}$	$\langle (x_i - x_j)^2 \rangle$ (Numerics)	$\langle (x_i - x_j)^2 \rangle$ (Theory)
100	30	50	0.5	0.016	0.5884 ± 0.1647	0.4025
			0.55	0.015	0.5309 ± 0.1486	0.487
			0.61	0.015	0.6209 ± 0.1738	0.599
			0.78	0.012	0.4389 ± 0.1229	0.9795
			0.83	0.01	1.6773 ± 0.4696	1.1091
			0.85	0.01	1.8155 ± 0.5083	1.632

In order to make a connection with experiments with ${}^7\text{Li}$ [3], it was assumed that the mass of an individual atom is $m = 7.016$ u (in unified atomic mass units), the post-quench scattering length, $a_{\text{sc}} = -16.2 a_0$ (a_0 is the Bohr radius), and the frequency of the radial trapping potential, $\omega_r = 2\pi \times 297$ Hz. The coupling constant is given by $g = 2\hbar\omega_r a_{\text{sc}}$. This set reproduces the conditions of the Rice experiment [3] verbatim, with the exception of the scattering length a_{sc} . The different value of a_{sc} accounts for the difference between the number of atoms in the experiment and that in the current study. In particular, a_{sc} is adjusted so that the ratio between the number of atoms and the condensate collapse threshold, $N_c = 0.67a_r/|a_{\text{sc}}|$ [20], is the same as it was in the experiment. The second line of Table 1, $\tilde{g} = 0.55$, would correspond to a one-dimensional trapping frequency of $\omega = g^2 m / (\tilde{g}^2 \hbar^3) = 3.7 \times 10^{-3}$ Hz with a propagation time of $T/4 = 4.3 \times 10^2$ s.

The propagation time obtained appears to be much larger than the estimate of 4.7 s in [5], for $N = 3 \times 10^3$. However, the former corresponds to a conservative estimate, based on a soliton-soliton separation exceeding six half-widths of the broader soliton. For a less conservative requirement, used in [5], the propagation time will be as short as $T/4 = 0.83$ s, reached with $\omega = 1.9$ Hz (accordingly, $\tilde{g} = 0.024$) and other experimental conditions kept intact.

4. Conclusions and Outlook

In the study presented here, it is justified that quantum fluctuations of a macroscopic observable—represented by the relative velocity of two solitons in a harmonically trapped Gross-Pitaevskii breather—can be observed in a predominantly mean-field environment. The scheme involves a harmonic quarter-period propagation of the breather: this time turns out to be sufficient for the breather to dissociate through purely quantum effects. As a computational method, the path integral Monte Carlo is used, the numerical results of which are consistent with the earlier predictions, based on the Bogoliubov approximation [5].

In further studies, stronger interactions to be considered both to move closer to the experimental conditions and to suppress the residual effects of the soliton width. We expect that then Table 1 will exhibit a closer correspondence between the theory predictions and the numerical calculations.

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Appendix A. Details of Numerical Calculations

The formalism, described in Section 2, can include any generalized potential [21] and is valid for any arbitrary dimension d ($d = 3N$). To implement Equation (3) numerically, the $3N$ -dimensional Brownian motion can be replaced by properly scaled one-dimensional random walks as follows [12,17,22]:

$$W(l) \equiv W(t, n, l) = w_1^1(t, n, l), w_2^1(t, n, l), w_3^1(t, n, l), \dots, w_1^N(t, n, l), w_2^N(t, n, l), w_3^N(t, n, l), \tag{A1}$$

where

$$w_j^i(t, n, l) = \sum_{k=1}^l \frac{\epsilon_{jk}^i}{\sqrt{n}}, \tag{A2}$$

with $w_j^i(0, n, l) = 0$ for $i = 1, 2, \dots, N, j = 1, 2, 3$, and $l = 1, 2, \dots, nt$. Here, ϵ s denote the binomially distributed random variables, which are chosen independently and randomly with probability P for all i, j, k such that $P(\epsilon_{jk}^i = 1) = P(\epsilon_{jk}^i = -1) = 1/2$, and t is the simulation time. It is known (from an invariance principle [23]) that for every ν and $W(l)$, defined in Equation (A2),

$$\lim_{n \rightarrow \infty} P \left[\frac{1}{n} \sum_{l=1}^{nt} V(W(l)) \right] = P \left[\int_0^t V[X(s)] ds \right] \leq \nu. \tag{A3}$$

Consequently, for large n ,

$$P \left\{ \exp \left[- \int_0^t V(X(s)) ds \right] \right\} \approx P \left\{ \exp \left[- \frac{1}{n} \sum_{l=1}^{nt} V(W(l)) \right] \right\} \leq \nu. \tag{A4}$$

Finally, by generating N_{rep} independent realization $Z_1, Z_2, \dots, Z_{N_{\text{rep}}}$ of

$$Z_m = \exp \left\{ - \left[- \frac{1}{n} \sum_{l=1}^{nt} V(W(l)) \right] \right\}, \tag{A5}$$

and using the law of large numbers, with regard to Equation (A3), one concludes that

$$(Z_1 + Z_2 + \dots + Z_{N_{\text{rep}}}) / N_{\text{rep}} = Z(t) \tag{A6}$$

is an approximation of Equation (8). Here, $W^m(l)$, $m = 1, 2, \dots, N_{\text{rep}}$, denotes the m^{th} realization of $W(l)$ out of N_{rep} independently run simulations. In the limit of large t and N_{rep} , this approximation approaches an equality and forms the basis of a computational scheme for the lowest energy of a many-particle system with a prescribed symmetry.

Appendix B. Validity of the Gaussian Approximation for the δ -Function

To ensure that the pairwise Gaussian potential correctly describes the intended delta potential, the following has to be checked: (i) the potential supports only one bound state, and (ii) the energy of the bound state is less than the potential depth. To prove that the Gaussian potential with the parameters chosen in the current study supports only one bound state the prescriptions in [24] was followed. In one dimension, the Wentzel–Kramers–Brillouin (WKB) integral for the energy E is given by $\int_{x_1}^{x_2} \sqrt{2[E - V(x)]} dx = (n - \frac{1}{2})\pi$ [25], where x_1 and x_2 are the turning points of the classical motion. For the Gaussian potential, the quantum number N of the last bound state can be obtained by using the above WKB

equation for $E = 0$: $\sqrt{2V_0} \int_{-\infty}^{+\infty} e^{-\alpha x^2/2} dx = (N - \frac{1}{2})\pi$, $V = V_0 e^{-\alpha x^2}$ (α is a parameter related to width of the Gaussian potential), which leads to $N = (2/\sqrt{\pi})\sqrt{V_0/\alpha} + 1/2$. For finite V_0 and α , N is also finite. Therefore, the number of bound states is finite for the Gaussian well.

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