1. INTRODUCTION

In this paper we introduce a generalization of the characteristic function theory for the time-dependent Schrödinger equation. This approach enables us to evaluate global and local quantum properties of the system.

In order to do this we introduce a new formulation of the time-dependent Schrödinger equation, which is based on a new variational principle. This principle is derived from the variational principle of the time-dependent Schrödinger equation.

We then define a new function, the characteristic function, which is a function of the time-dependent Schrödinger equation. This function is defined as the exponential of the time-dependent Schrödinger equation.

The characteristic function is then used to define a new functional, the characteristic functional, which is a function of the time-dependent Schrödinger equation. This functional is defined as the integral of the time-dependent Schrödinger equation.

The characteristic functional is then used to define a new variational principle, the characteristic principle, which is a principle of the time-dependent Schrödinger equation. This principle is defined as the minimization of the characteristic functional.

By applying the characteristic principle to the time-dependent Schrödinger equation, we obtain a new formulation of the time-dependent Schrödinger equation, which is based on a new variational principle.

This new formulation of the time-dependent Schrödinger equation is then used to derive a new set of quantum properties of the system.

We then apply this new formulation of the time-dependent Schrödinger equation to the case of a single quantum system, and we compare our results with those obtained by other methods.

We find that our results are in good agreement with those obtained by other methods, and we conclude that our new formulation of the time-dependent Schrödinger equation is a useful tool for the study of quantum systems.
II. PATH INTEGRAL REPRESENTATION

The path integral representation for the imaginary-time evolution amplitude of a particle of mass $M$ moving in a one dimensional potential $V(x)$ reads [5]

$$\langle x_0 | x \rangle = \int_{x(0)=x_0}^{x(t)=x} \mathcal{D}x \exp \left\{ - \frac{i}{\hbar} \int_0^t d\tau \left[ M \dot{x}^2(\tau) + V(x(\tau)) \right] \right\}. \quad (1)$$

For the anharmonic oscillator potential

$$V(x) = \frac{M}{2} \omega^2 x^2 + gx^4 \quad (2)$$

the imaginary-time evolution amplitude (1) can be expanded in powers of the coupling constant $g$. Thus we obtain the perturbation series

$$\langle x_0 | x \rangle = \langle x_0 | x \rangle \omega + \cdots \quad (3)$$

where we have introduced the harmonic imaginary-time evolution amplitude

$$\langle x_0 | x \rangle \omega \equiv \int_{x(0)=x_0}^{x(t)=x} \mathcal{D}x \langle \omega \rangle \quad (4)$$

and the harmonic path expectation value for an arbitrary functional $F[x]$

$$\langle F[x] \rangle \omega \equiv \langle x_0 | x \rangle \omega \int_{x(0)=x_0}^{x(t)=x} \mathcal{D}x F[x] \quad (5)$$

The latter is evaluated with the help of the generating functional for the harmonic oscillator, whose path integral representation reads

$$\langle x_0 | x \rangle \omega \omega \equiv \int_{x(0)=x_0}^{x(t)=x} \mathcal{D}x \exp \left\{ - \frac{i}{\hbar} \int_0^t d\tau \left[ M \dot{x}^2(\tau) + \frac{M}{2} \omega^2 x^2(\tau) - j\dot{x}(\tau)x(\tau) \right] \right\}. \quad (6)$$

leading to [5]

$$\langle x_0 | x \rangle \omega \omega = \langle x_0 | x \rangle \omega \omega$$

$$\exp \left\{ - \frac{i}{\hbar} \int_0^t d\tau \left[ \frac{M}{2} \dot{x}^2(\tau) + \frac{M}{2} \omega^2 x^2(\tau) - j\dot{x}(\tau)x(\tau) \right] \right\}. \quad (7)$$

with the harmonic imaginary-time evolution amplitude

$$\langle x_0 | x \rangle \omega = \sqrt{\frac{M \omega}{2 \pi \hbar \sinh h \beta \omega}} \exp \left\{ - \frac{M \omega}{2 \hbar \sinh h \beta \omega} \left[ (x_0^2 + x_0^2) \cosh h \beta \omega - 2x_0 x_0 \right] \right\}. \quad (8)$$

In equation (7) we have introduced the classical path $x_c(\tau) \equiv \langle x_0 | x \rangle \omega \omega$, and the Dirichlet Green’s function

$$G^{(D)}(\tau_1, \tau_2) \equiv \frac{1}{M \omega \sinh h \beta \omega} \left[ \theta(\tau_1 - \tau_2) \sinh (h \beta - \tau_1) \sinh \omega \tau_2 - \theta(\tau_1 - \tau_2) \sinh (h \beta - \tau_2) \sinh \omega \tau_1 \right]. \quad (9)$$

We follow Ref. [3, 4] and evaluate harmonic path expectation values of polynomials in $x$ arising from the generating functional (7) according to Wick’s theorem. Let us illustrate the procedure to reduce the power of polynomials by the example of the harmonic path expectation value $\langle x^n(\tau) x^n(\tau) \rangle \omega$.

(i) Contracting $x(\tau)$ with $x^{n-1}(\tau)$ and $x^m(\tau)$ leads to Green’s functions $G^{(D)}(\tau_1, \tau_2)$ and $G^{(D)}(\tau_2, \tau_1)$ with multiplicity $n-1$ and $m$, respectively.

(ii) If $n > 1$, extract one $x(\tau)$ from the path expectation value giving $x_c(\tau)$ multiplied by $\langle x^{n-1}(\tau) x^{m-1}(\tau) \rangle \omega$.

(iii) Add the terms from (i) and (ii).

(iv) Repeat the previous steps until only products of path expectation values $\langle x(\tau) \rangle \omega = x_c(\tau)$ remain.

With the help of this procedure, we obtain to first order

$$\langle x^n(\tau) \rangle \omega = x_c^n(\tau) + 6 x_c(\tau) G^{(D)}(\tau_1, \tau) + 3 G^{(D)}(\tau_1, \tau). \quad (11)$$

III. FEYNMAN DIAGRAMS

These contractions can be illustrated by Feynman diagrams with the following rules: A vertex represents the integration over $\tau$

$$\times = \int_0^{\beta} d\tau. \quad (12)$$
a line denotes the Dirichlet Green’s function
\[ 1 \longrightarrow 2 = G^{(D)}(\tau_1, \tau_2), \] \hspace{1cm} \text{(13)}
and a cross or a “current” pictures a classical path
\[ \times \longrightarrow 1 = x_{cl}(\tau_1). \hspace{1cm} \text{(14)} \]
Inserting the harmonic path expectation value (11) into the perturbation expansion (3) leads in first order to the diagrams
\[
\int_0^{h\beta} d\tau_1 \langle x^4(\tau_1) \rangle_\omega = \times + 6 \times + 3 \bigcirc \bigcirc.
\hspace{1cm} \text{(15)}
\]
We now evaluate the first-order Feynman diagrams in (15) for finite temperatures and arbitrary \( x_0, x_b \). Thus we will get a first-order result for the imaginary-time evolution amplitude in (3). The first diagram leads to
\[
\times = \frac{1}{32\omega \sinh^4 h/\beta \omega} \left[ (x_0^4 + x_b^4) (\sinh 4h/\beta \omega - 8 \sinh 2h/\beta \omega + 12h/\beta \omega) + (x_0^3 x_b + x_0 x_b^3) (4 \sinh 3h/\beta \omega + 36 \sinh h/\beta \omega - 48h/\beta \omega \cosh h/\beta \omega) + x_0^2 x_b^2 (-36 \sinh 2h/\beta \omega + 48h/\beta \omega + 24h/\beta \omega \cosh 2h/\beta \omega) \right],
\hspace{1cm} \text{(16)}
\]
whereas the last diagram turns out to be
\[
\bigcirc \bigcirc = \frac{h^2}{16M^2 \omega^3 \sinh^2 h/\beta \omega} (-3 \sinh 2h/\beta \omega + 4h/\beta \omega + 2h/\beta \omega \cosh 2h/\beta \omega).
\hspace{1cm} \text{(18)}
\]
So all in all we get the following first-order result for the imaginary-time evolution amplitude
\[
(x_b, h/\beta | x_0, 0) = (x_b, h/\beta | x_0, 0) \omega \times \left( 1 - \frac{g}{h} \left[ \frac{h^2}{M^2 \omega^3 \sinh^2 h/\beta \omega} \left[ -\frac{9}{16} \sinh 2h/\beta \omega + \frac{3}{4} h/\beta \omega + \frac{3}{8} h/\beta \omega \cosh 2h/\beta \omega \right] + \frac{h}{M^2 \omega^3 \sinh^2 h/\beta \omega} \left[ x_0^2 + x_b^2 \right] \left( \frac{3}{16} \sinh 3h/\beta \omega + \frac{27}{16} \sinh h/\beta \omega - \frac{9}{4} h/\beta \omega \cosh h/\beta \omega \right) + x_0 x_b \left( -\frac{9}{4} \sinh 2h/\beta \omega + 3h/\beta \omega + \frac{3}{2} h/\beta \omega \cosh 2h/\beta \omega \right) \right] + \frac{1}{\omega} \sinh^4 h/\beta \omega \left[ \left( x_0^4 + x_b^4 \right) \left( \frac{1}{32} \sinh 4h/\beta \omega - \frac{1}{4} \sinh 2h/\beta \omega + \frac{3}{8} h/\beta \omega \right) + \left( x_0^3 x_b + x_0 x_b^3 \right) \left( \frac{1}{8} \sinh 3h/\beta \omega + \frac{9}{8} \sinh h/\beta \omega - \frac{3}{2} h/\beta \omega \cosh h/\beta \omega \right) + x_0^2 x_b^2 \left( -\frac{9}{8} \sinh 2h/\beta \omega + \frac{3}{2} h/\beta \omega + \frac{3}{4} h/\beta \omega \cosh 2h/\beta \omega \right) \right] \right) \right) \bigg). \hspace{1cm} \text{(19)}
\]
The imaginary-time evolution amplitude thus has the time reversal behaviour
\[
(x_b, h/\beta | x_0, 0) = (x_a, h/\beta | x_0, 0)^*,
\hspace{1cm} \text{(20)}
\]
while it is known that the imaginary-time evolution amplitude is real for one-dimensional problems.
IV. PARTIAL DIFFERENTIAL EQUATION

Consider the Schrödinger equation for the real-time evolution amplitude

\begin{equation}
\frac{i\hbar}{\partial t} \langle x_b | \xi | x_a 0 \rangle = \frac{\hbar^2}{2M} \frac{\partial^2}{\partial x_b^2} \langle x_b | \xi | x_a 0 \rangle + V(x_b) \langle x_b | \xi | x_a 0 \rangle . \tag{21}
\end{equation}

In order to get a corresponding quantum statistical Schrödinger equation we now have to change from the real time to imaginary time, i.e. we have to perform the Wick rotation \( t \to -i\tau \). Thus the Schrödinger equation (21) becomes

\begin{equation}
-\frac{\hbar}{\partial \tau} \langle x_b | \xi | x_a 0 \rangle = -\frac{\hbar^2}{2M} \frac{\partial^2}{\partial x_b^2} \langle x_b | \xi | x_a 0 \rangle + V(x_b) \langle x_b | \xi | x_a 0 \rangle . \tag{22}
\end{equation}

For both the real and the imaginary-time evolution amplitude the initial condition reads

\begin{equation}
(\xi, 0) = \delta(x_b - x_a) . \tag{23}
\end{equation}

Plugging the anharmonic oscillator potential (2) into the Schrödinger equation (22) we finally get

\begin{equation}
\left\{ -\frac{\hbar}{\partial \tau} + \frac{\hbar^2}{2M} \frac{\partial^2}{\partial x_b^2} - \frac{M}{2} \omega^2 x_b^2 - g x_b \right\} \langle x_b | \xi | x_a 0 \rangle = 0 . \tag{24}
\end{equation}

Making the ansatz

\begin{equation}
(\xi, 0) = (\xi, 0) |_{\omega} A(x_b, x_a, \tau) , \tag{25}
\end{equation}

we conclude from (24) a partial differential equation for \( A(x_b, x_a, \tau) \):

\begin{equation}
\left\{ \frac{\partial}{\partial \tau} - \frac{\hbar^2}{2M} \frac{\partial^2}{\partial x_b^2} + \frac{x_a \cosh \omega \tau - x_b}{\sinh \omega \tau} \frac{\partial}{\partial x_b} + g x_b \right\} A(x_b, x_a, \tau) = 0 . \tag{26}
\end{equation}

We now choose our ansatz for \( A(x_b, x_a, \tau) \) by introducing three expansions in \( g \), in \( x_a \), and in \( x_b \), respectively. Also we take out the factor \( \sinh^{-1} \omega \tau \), such that the ordinary differential equations for the expansion coefficients become as simple as possible:

\begin{equation}
A(x_b, x_a, \tau) = \sum_{n=0}^{\infty} \sum_{k=0}^{\infty} g^n c_{2k+1}^{(n)}(\tau) x_a^{2k+1} x_b . \tag{27}
\end{equation}

In order to obtain the unperturbed result \( A(x_b, x_a, \tau) = 1 \) for \( g = 0 \) we need \( c_{2k+1}^{(n)}(\tau) = 1 \). The superscript \( n \) in equation (27) denotes the perturbative order, whereas \( 2k \) counts the (even) powers of the various products \( x_a x_b \). The summations over the coordinates \( x_a \), \( x_b \) can be truncated at \( k = 4n \), because we learn from Feynman diagrammatic considerations that the diagram with the most currents \( x \) in the \( n \)th order looks like

\begin{equation}
\cdots \times \times \times \times \times \cdots . \tag{28}
\end{equation}

Inserting the new ansatz (27) into the Schrödinger equation (26) and arranging the indices in such a way that each term is proportional to \( x_a^{2k+1} x_b \) we get for the different powers of \( g \) and for \( n > 0 \):

\begin{equation}
\sum_{k=0}^{2n} \sum_{l=0}^{2k} \frac{2k-l}{\sinh^2 \omega \tau} c_{2k+l}^{(n)}(\tau) = -\frac{\hbar}{2M} \sum_{k=0}^{2n-1} \sum_{l=0}^{2k-1} (l+1)(l+1) \frac{c_{2k+4l+4}^{(n)}(\tau)}{\sinh^2 \omega \tau} x_a^{2k+1} x_b + \sum_{k=0}^{2n} \sum_{l=0}^{2k} \frac{(n-l)}{\sinh^2 \omega \tau} x_a^{2k+l} x_b = 0 . \tag{29}
\end{equation}

Thus the sums over \( k \) and over \( l \) collapse and we determine the master equation for our coefficients \( c_{2k+l}^{(n)}(\tau) \)

\begin{equation}
\frac{\partial}{\partial \tau} c_{2k+l}^{(n)}(\tau) = (l+1)(l+1) \frac{\hbar}{2M} c_{2k+4l+4}^{(n)}(\tau) \sinh^2 \omega \tau + (l+1) \omega c_{2k+l}^{(n)}(\tau) - \frac{1}{\hbar} c_{2k+4l+4}^{(n)}(\tau) \sinh^2 \omega \tau(\tau) \tag{30}
\end{equation}

which is solved by

\begin{equation}
c_{2k+l}^{(n)}(\tau) = (l+1)(l+1) \frac{\hbar}{2M} \int d\tau' c_{2k+4l+4}^{(n)}(\tau') \sinh^2 \omega \tau' + (l+1) \omega \int d\tau' c_{2k+l}^{(n)}(\tau') \sinh^2 \omega \tau' - \frac{1}{\hbar} \int d\tau' c_{2k+4l+4}^{(n-1)}(\tau') \sinh^2 \omega \tau' + c_{2k+l}^{(n)} . \tag{31}
\end{equation}

Here the $c^{(n)}_{2k,l}$ denote the integration constants which are fixed by applying the initial condition

$$\lim_{\tau \rightarrow 0} \left| \frac{c^{(n)}_{2k,l}(\tau)}{\sinh \omega \tau} \right| < \infty \quad \Rightarrow \quad c^{(n)}_{2k,l}(0) \neq 0 \quad (32)$$

However the above master equation (30) is not valid for all $k$ and $l$. Therefore we now introduce a set of empirical rules telling us which of the coefficients $c^{(n)}_{2k,l}(\tau)$ have to be dropped once we write down (31) for any order $n$:

(i) Drop all terms containing a $c^{(n)}_{2k,l}(\tau)$ where $2k > 4n$

(ii) Drop all terms containing a $c^{(n)}_{2k,l}(\tau)$ with $l > 2k$

(iii) Neglect all terms containing a $c^{(n)}_{2k,l}(\tau)$ with any negative indices $k$ and $l$.

To convince the reader that equation (31) together with this procedure leads to the correct results we now recollect our first-order result from (19). To that end we set $n = 1$, such that $k$ runs from 0 to 2 and $l$ from 0 to 4. Fixing $k = 2$ and counting down from $l = 4$ to $l = 0$ we get

\[
\begin{align*}
c^{(1)}_{44}(\tau) &= -\frac{1}{h} \int d\tau c^{(0)}_{44}(\tau) \sinh^4 \omega \tau + d^{(1)}_{44} = \frac{1}{h \omega} \left( \frac{3}{32} \sinh 4\omega \tau - \frac{1}{4} \sinh 2\omega \tau + \frac{3}{8} \sinh \omega \tau \right), \\
c^{(1)}_{43}(\tau) &= 4\omega \int d\tau \frac{c^{(0)}_{44}(\tau)}{\sinh^2 \omega \tau} + d^{(1)}_{43} = \frac{1}{h \omega} \sinh \omega \tau \left( \frac{3}{2} \sinh 2\omega \tau + \frac{9}{8} \sinh \omega \tau \right), \\
c^{(1)}_{42}(\tau) &= 3\omega \int d\tau \frac{c^{(0)}_{44}(\tau)}{\sinh^2 \omega \tau} + d^{(1)}_{42} = \frac{1}{h \omega} \sinh \omega \tau \left( -\frac{9}{8} \sinh 2\omega \tau - \frac{3}{2} \sinh \omega \tau \right), \\
c^{(1)}_{41}(\tau) &= 2\omega \int d\tau \frac{c^{(0)}_{44}(\tau)}{\sinh^2 \omega \tau} + d^{(1)}_{41} = \frac{1}{h \omega} \sinh \omega \tau \left( \frac{9}{8} \sinh \omega \tau - \frac{3}{2} \sinh \omega \tau \right), \\
c^{(1)}_{40}(\tau) &= \omega \int d\tau \frac{c^{(0)}_{44}(\tau)}{\sinh^2 \omega \tau} + d^{(1)}_{40} = \frac{1}{h \omega} \sinh \omega \tau \left( \frac{3}{16} \sinh 4\omega \tau - \frac{1}{4} \sinh 2\omega \tau + \frac{3}{8} \sinh \omega \tau \right).
\end{align*}
\]

Correspondingly, for $k = 1$ we obtain

\[
\begin{align*}
c^{(1)}_{34}(\tau) &= 6h \int \frac{c^{(0)}_{34}(\tau)}{\sinh^2 \omega \tau} + d^{(1)}_{34} = \frac{1}{M \omega^3 \sinh \omega \tau} \left( \frac{3}{16} \sinh 3\omega \tau + \frac{27}{16} \sinh \omega \tau - \frac{9}{4} \omega \tau \cosh \omega \tau \right), \\
c^{(1)}_{33}(\tau) &= 3h \int \frac{c^{(0)}_{34}(\tau)}{\sinh^2 \omega \tau} + 2\omega \int \frac{c^{(0)}_{33}(\tau)}{\sinh^2 \omega \tau} + d^{(1)}_{33} = \frac{1}{M \omega^3 \sinh \omega \tau} \left( -\frac{9}{4} \sinh 2\omega \tau + 3\omega \tau + \frac{3}{2} \omega \tau \cosh 2\omega \tau \right), \\
c^{(1)}_{32}(\tau) &= \frac{h}{M} \int \frac{c^{(0)}_{34}(\tau)}{\sinh^2 \omega \tau} + \omega \int \frac{c^{(0)}_{32}(\tau)}{\sinh^2 \omega \tau} + d^{(1)}_{32} = \frac{1}{h \omega^3 \sinh^3 \omega \tau} \left( \frac{3}{16} \sinh 3\omega \tau + \frac{27}{16} \sinh \omega \tau - \frac{9}{4} \omega \tau \cosh \omega \tau \right), \\
c^{(1)}_{31}(\tau) &= \frac{h}{M} \int \frac{c^{(0)}_{34}(\tau)}{\sinh^2 \omega \tau} + \omega \int \frac{c^{(0)}_{31}(\tau)}{\sinh^2 \omega \tau} + d^{(1)}_{31} = \frac{h}{M^2 \omega^3 \sinh^3 \omega \tau} \left( -\frac{9}{16} \sinh 2\omega \tau + \frac{3}{4} \omega \tau + \frac{3}{8} \omega \tau \cosh 2\omega \tau \right).
\end{align*}
\]

Finally for $k = 0$ we get the equation

\[
\begin{align*}
c^{(1)}_{24}(\tau) &= \frac{h}{M} \int \frac{c^{(0)}_{24}(\tau)}{\sinh^2 \omega \tau} + d^{(1)}_{24} = \frac{h}{M^2 \omega^3 \sinh^3 \omega \tau} \left( -\frac{9}{16} \sinh 2\omega \tau + \frac{3}{4} \omega \tau + \frac{3}{8} \omega \tau \cosh 2\omega \tau \right).
\end{align*}
\]

The path of recursion which follows from this procedure is shown in Fig. 1.

**V. EXPLORING THE SYMMETRIES**

As seen above we already have to solve nine ordinary differential equations for the first-order imaginary-time
evolution amplitude. For any order \( n \) the number \( p \) of integrals to solve is

\[ p = \sum_{j=1}^{2n+1} (2j - 1) = 4n^2 + 4n + 1. \tag{42} \]

Due to the time reversal behaviour (20), the coefficients \( c_{2k+l}^{(n)}(\tau) \) show a symmetry, namely:

\[ \frac{c_{2k+l}^{(n)}(\tau)}{\sinh^k \omega \tau} = \frac{-c_{2k-2l}^{(n)}(\tau)}{\sinh^k \omega \tau}. \tag{43} \]

Exploiting the symmetry (43), we can cut down the number (42) considerably. At first sight it is reduced to

\[ p' = \sum_{j=1}^{2n+1} j = 2n^2 + 3n + 1. \tag{44} \]

so there are only six integrals left for the first order. But we can go even further. Employing these symmetries we can eventually change almost all recursive differential equations into purely algebraic ones leaving only \( 2^n \leq (2n+1) \) integrations. So for the first order we are left with three integrations only, namely with equations (33), (38), and (41). These coefficients \( c_{4l}^{(1)}(\tau) \), \( c_{4l}^{(1)}(\tau) \), and \( c_{4l}^{(1)}(\tau) \) are integrated recursively. The other coefficients can then be obtained algebraically: Once we have \( c_{4l}^{(1)}(\tau) \) we also know \( c_{4l}^{(1)}(\tau) \) because of the symmetry (43). Comparing equation (30) for \( k = 2, l = 4 \) and \( k = 2, l = 0 \) we then obtain an algebraic equation for \( c_{4l}^{(1)}(\tau) \). The knowledge of \( c_{4l}^{(1)}(\tau) \) gives us \( c_{4l}^{(1)}(\tau) \) because of the symmetry (43) and by comparing (30) this time for \( k = 2, l = 3 \) on the one hand and \( k = 2, l = 1 \) on the other hand we are left with an algebraic equation for \( c_{4l}^{(1)}(\tau) \). Thus we get all the coefficients for \( k = 2 \) only by solving one differential equation, namely the one for \( c_{4l}^{(1)}(\tau) \). For \( k = 1 \) the procedure is similar, \( k = 0 \) only generates one coefficient anyway, namely \( c_{4l}^{(1)}(\tau) \), which still has to be solved by evaluating one integral. The new path of recursion is shown in Fig. 2.

So finally three out of the nine first-order coefficients are obtained by integration, three more are clear for symmetry reasons and three come from an algebraic recursion. We now generalize the algebraic part of our recursion. Consider again the symmetry property (43). Differentiation on both sides yields

\[
\frac{\partial c_{2k+l}^{(n)}(\tau)}{\partial \tau} = \frac{1}{\sinh^{2k+2l} \omega \tau} \left( 1 \frac{\partial c_{2k-2l}^{(n)}(\tau)}{\partial \tau} - 2(k-l) \cos \omega \tau \frac{c_{2k+l-2}^{(n)}(\tau)}{\sinh^{2k+2l+2} \omega \tau} \right). \tag{45}
\]

Now we substitute for the two partial derivatives according to equation (30). Solving for the \((l+1)\)-st coefficient and shifting the index \( l \) down by one we obtain

\[
c_{2k+l}^{(n)}(\tau) = \frac{(l+1)h}{2M \omega} c_{2k+3l+1}^{(n)}(\tau) + \frac{c_{2k-4l+3}^{(n)}(\tau)}{h \omega l} \sinh^4 \omega \tau
\]

+ \[
\frac{(2k-l+3)(2k-l+2)h}{2M \omega l} \frac{c_{2k-2l+3}^{(n)}(\tau)}{\sinh^{2k+2l+2} \omega \tau} + \frac{2k-l+2}{h} \frac{c_{2k-4l+7}^{(n)}(\tau)}{\sinh^{2k+2l+4} \omega \tau}
\]

- \[
\frac{1}{h \omega l} \frac{c_{2k-4l-1}^{(n-1)}(\tau)}{\sinh^{2k+2l+4} \omega \tau} - \frac{(2k-l+2) \cos \omega \tau \frac{c_{2k-4l+1}^{(n+1)}(\tau)}{\sinh^{2k+2l+4} \omega \tau}}{l}
\] \tag{46}

which is the algebraic recursion relation for any non-diagonal coefficient \( c_{2k+l}^{(n)}(\tau) \) with \( 0 < l < k \). (The coefficients with \( k < l < 2k \) are then clear for symmetry reasons.) The diagonal coefficients \( c_{2k+2}^{(n)}(\tau) \) still have to be integrated.

VI. COMBINED DIFFERENTIAL AND ALGEBRAIC EQUATION

We now combine the differential recursion with the algebraic one. As only the diagonal coefficients have to be evaluated by integrating the differential recursive equation, we can even further simplify the solution (31) to our master equation (30). We only need it for the diagonal coefficients, for which \( l+1 = 2k+1 \) is always greater than \( 2k \). And according to our index rule (ii), coefficients of the shape \( c_{2k+2l+4}^{(n)}(\tau) \) have to be neglected. We get

\[
c_{2k+2l}^{(n)}(\tau) = (2k+2)(2k+1) \frac{h}{2M \omega} \int d\tau \frac{c_{2k+2l+3}^{(n)}(\tau)}{\sinh^{2k+2l+3} \omega \tau}
\]

- \[
\frac{1}{h} \int d\tau \frac{c_{2k-4l+1}^{(n-1)}(\tau)}{\sinh^{2k+2l+4} \omega \tau} + \frac{c_{2k+2l}^{(n)}(\tau)}{h \omega l} \sinh^4 \omega \tau \] \tag{47}
Fig. 1: This diagram depicts the path of recursion for $n = 1$. We start in the top right hand side corner, which is to be identified with the coefficient $c_{n}^{(1)}$ and follow the arrows until reaching the bottom left hand side corner with the coefficient $c_{0}^{(1)}$.

Index rules (i) and (iii) still have to be applied, $k$ runs from 0 to $2n$.

Let us quickly summarize the combined differential and algebraic recursion relation considering the first order as an example. Fig. 2 shows all first-order coefficients for the imaginary-time evolution amplitude. Each coefficient is represented by a little circle. Now the coefficients on the diagonal line $2k = l$ have to be obtained by referring to equation (47) together with rules (i) and (iii). These two rules tell us which of the coefficients either from the the same order $n$ or from the previous order $n - 1$ have to be integrated and which ones can be put to zero.

Once we have the diagonal coefficients $c^{(1)}_{2n}(\tau)$ we can calculate the off-diagonal ones with $l \leq k$ with the help of equation (46). The coefficients with $k < l < 2k$ are then clear for symmetry reasons.

Using the computer algebra programme Maple V R7 we managed to calculate seven perturbative orders of the imaginary-time evolution amplitude which can be found at [12].

VII. FREE ENERGY

In this section we obtain perturbative results for the partition function by integrating the diagonal elements of our perturbative expression for the imaginary-time evolution amplitude from the previous sections:

$$ Z = \int_{-\infty}^{+\infty} dx (x \hbar \beta | \tau = 0) . \quad (48) $$

From the partition function we then compute the free energy perturbatively:

$$ F = -\frac{1}{\beta} \log Z . \quad (49) $$

We have to expand the logarithm in order to obtain a perturbation expansion for the free energy $F$. For the first order we insert (19) together with (8) into (48) and evaluate the integral for the second order we use, correspondingly, the data from Ref. [12]. By taking the logarithm we get with (49) and with the expansion for the logarithm for the free energy to second order

$$ F^{(2)}(\beta) = \frac{1}{\beta} \log 2 \sinh \frac{h \beta \omega}{2} \quad (50) $$

$$ + \frac{3gh^2}{4M^2\omega^2} \cosh \frac{h \beta \omega}{2} - \frac{g^2h^3}{64M^4\omega^3} \left( \frac{54h \beta \omega}{\sinh^4 \frac{h \beta \omega}{2}} 
+ \frac{36h \beta \omega \cosh h \beta \omega + 60 \sinh h \beta \omega + 21 \sinh 2h \beta \omega}{\sinh^4 \frac{h \beta \omega}{2}} \right). $$

The higher orders are omitted for the sake of keeping the type face clear.

With Maple we have as high as the fifth variational order which is two orders more than what has been obtained in previous work [14].

VIII. DIAGRAMMATICAL CHECK

It is possible to check the perturbative results for the free energy for all temperatures. Namely, we can expand $Z$ in terms of harmonic expectations in a similar way as for the imaginary-time evolution amplitude in (3). To that end we need the generating functional

$$ Z[\hat{g}(\tau)] = \int_{-\infty}^{+\infty} dx (x \hbar \beta | \tau = 0) \hat{g}|Z[\hat{g}] \quad (51) $$

which we get from (7)-(10). It is of the form

$$ Z[\hat{g}(\tau)] = Z[0] $$

$$ \times \exp \left[ \frac{1}{2h^2} \int_{0}^{h^2} d\gamma_1 \int_{0}^{h^2} d\gamma_2 \langle G^{(1)}(\gamma_1, \gamma_2) \hat{g}(\gamma_1) \hat{g}(\gamma_2) \rangle \right]. $$
where the harmonic partition function reads
\[
Z[0] = \frac{1}{2\sinh \frac{\beta \omega}{2}}
\] (53)
and
\[
G^{(\delta)}(\tau_1, \tau_2) = \frac{\hbar}{2M\omega} \cosh \left( \frac{\beta \hbar \omega}{2} - |\tau_1 - \tau_2| \omega \right)
\] (54)
denotes the periodic Green’s function of the harmonic oscillator. We now obtain the partition function \(Z\) of the anharmonic oscillator from the generating functional \(Z[j(\tau)]\) by differentiating with respect to the current \(j(\tau)\) while setting \(j(\tau) = 0\) afterwards:
\[
Z = \exp \left\{ -\frac{1}{\hbar} \int_0^{\beta \hbar} d\tau \frac{\hbar}{\delta j(\tau)} \left( \frac{\hbar}{\delta j(\tau)} \right)^4 \right\} Z[j(\tau)] \bigg|_{j=0}. \tag{55}
\]
Thus we get
\[
Z = Z[0] \left( 1 - \frac{3g}{h} \int_0^{\beta \hbar} d\tau_1 G^{(\delta)}(\tau_1, \tau_1) + \frac{g^2}{4h^2} \int_0^{\beta \hbar} d\tau_1 \int_0^{\beta \hbar} d\tau_2 \left[ gG^{(\delta)}(\tau_1, \tau_1)G^{(\delta)}(\tau_2, \tau_2) + 72G^{(\delta)}(\tau_1, \tau_1)G^{(\delta)}(\tau_2, \tau_1)G^{(\delta)}(\tau_1, \tau_2) + 24G^{(\delta)^4}(\tau_1, \tau_2) \right] + \ldots \right). \tag{56}
\]
In terms of Feynman diagrams this reads
\[
Z = Z[0] \left( 1 - \frac{3g}{h} \int_0^{\beta \hbar} d\tau_1 G^{(\delta)}(\tau_1, \tau_1) + \frac{g^2}{4h^2} \int_0^{\beta \hbar} d\tau_1 \int_0^{\beta \hbar} d\tau_2 \left( 72 \int_0^{\beta \hbar} d\tau_1 G^{(\delta)}(\tau_1, \tau_1) + 24 \int_0^{\beta \hbar} d\tau_1 G^{(\delta)}(\tau_1, \tau_2) \right) + \ldots \right). \tag{57}
\]
where we have introduced the symbol
\[
\frac{1}{2} \bigg\{ \bigg\} \equiv \log Z[0]. \tag{59}
\]
Once we rewrite the partition function \(Z\) in the form of the cumulant expansion as on the right hand side of equation (57), the disconnected Feynman diagrams disappear [5]. Now we can easily take the logarithm. Following (49) we obtain for the free energy
\[
F = -\frac{1}{\beta} \int_0^{\beta \hbar} \frac{1}{\frac{1}{2}} - \frac{3g}{h} \int_0^{\beta \hbar} d\tau_1 G^{(\delta)}(\tau_1, \tau_1) + \frac{g^2}{2h^2} \int_0^{\beta \hbar} d\tau_1 \int_0^{\beta \hbar} d\tau_2 \left( 72 \int_0^{\beta \hbar} d\tau_1 G^{(\delta)}(\tau_1, \tau_1) + 24 \int_0^{\beta \hbar} d\tau_1 G^{(\delta)}(\tau_1, \tau_2) \right) + \ldots \right). \tag{60}
\]
The above Feynman diagrams are of course constructed with the help of the same rules for the imaginary-time evolution amplitude (12), (13), and (14), but instead of the Dirichlet’s Green’s function (10) we have to use the periodic Green’s function (54). We now want to evaluate the four diagrams (60) so that we get a second-order expression for the free energy for finite temperatures. According to (53) and (59) we get for the zeroth-order contribution
\[
\frac{1}{2} \bigg\{ \bigg\} = \log \left( \frac{1}{2\sinh \frac{\beta \omega}{2}} \right), \tag{61}
\]
whereas the first-order diagram becomes
\[
\frac{1}{2} \bigg\{ \bigg\} = \frac{g^2 \beta}{4M^2\omega^2} \coth^2 \frac{\beta \omega}{2} \tag{62}
\]
The integration in (62) is trivial, because \(G^{(\delta)}(\tau_1, \tau_1)\) does not depend on \(\tau\) any more according to (54). For the second order the integrations become more sophisticated:
\[
\frac{1}{2} \bigg\{ \bigg\} = \frac{g^2 \beta}{256M^4\omega^6} \sinh^4 \frac{\beta \omega}{2} \tag{63}
\]
\[
\times (h\beta\omega + \sinh h\beta\omega). \tag{65}
\]
So all in all we get for the free energy (60) up to second order in the coupling constant \(g\) the result (50). It shows the correct low-temperature behaviour
\[
\lim_{\beta \to 0} F^{(2)}(\beta) = \frac{h\omega}{2} + \frac{3g\hbar^2}{4M^2\omega^2} - \frac{21g^2\hbar^4}{8M^4\omega^4}, \tag{66}
\]
which is the ground state energy and can be found for instance in [1, 5].

IX. VARIATIONAL PERTURBATION THEORY

Variational perturbation theory is a method that enables us to resum divergent Borel-type perturbation series in such a way that they converge even for infinitely large values of the perturbative coupling. To this end we add and subtract a trial harmonic oscillator with trial frequency \(\Omega\) to our anharmonic oscillator (2):
\[
V(x) = \frac{M}{2} \Omega^2 x^2 + g \frac{M}{2} \omega^2 - \Omega^2 x^2 + gx^4. \tag{67}
\]
Now we treat the second term as if it was of the order of the coupling constant \(g\). The result is obtained most simply by substituting for the frequency \(\omega\) in the original
anharmonic oscillator potential (2) according to Kleinert’s square-root trick [5]
\[ \omega \rightarrow \Omega \sqrt{1 + gr} , \]  
(68)
where
\[ r \equiv \frac{\omega^2 - \Omega^2}{2g\Omega^2} . \]  
(69)
These substitutions are not the most general ones. The square root is just a special case for the anharmonic oscillator.
We now apply the trick (68) to our first order series representation for the free energy \( F \) found in (50). Substituting for the frequency \( \omega \) according to (68), expanding for fixed \( r \) up to the first order in \( g \) and re-substituting for \( r \) according to (69) we get
\[ F^{(1)}(\beta, \Omega) = \frac{1}{\beta} \log \left( \frac{1}{2} \frac{\hbar^2}{2M^2 \Omega^2} \coth^2 \frac{\hbar \beta \Omega}{2} \right) + \frac{\hbar \Omega}{4} \left( \frac{\omega^2}{2} - \Omega^2 \right) \coth \frac{\hbar \beta \Omega}{2} . \]  
(70)
So the free energy (70) now depends on the trial frequency \( \Omega \) which is of no physical relevance. In order to get rid of it, we have to minimize its effect by employing the principle of least sensitivity [13]. This principle suggests to search for local extrema of \( F(\beta, \Omega) \) with respect to \( \Omega:\)
\[ \frac{\partial F^{(1)}(\beta, \Omega)}{\partial \Omega} = 0 . \]  
(71)
For the first order \( F^{(1)}(\beta, \Omega) \) it turns out that there are several extrema for each \( \beta \). As we seek a curve \( \Omega^{(1)}(\beta) \) that is as smooth as possible the choice is easy — we take the lowest branch for the others are not bounded (see Fig. 3). Moreover the other branches lead to diverging results.
To second order, we proceed in a similar way and we find that there are no extrema at all for \( F^{(2)}(\beta, \Omega) \). In accordance with the principle of least sensitivity we look for inflection points instead, i.e. we look for solutions to the equation
\[ \frac{\partial^2 F^{(2)}(\beta, \Omega)}{\partial \Omega^2} = 0 . \]  
(72)
In general we try to solve the equation
\[ \frac{\partial^p F^{(N)}(\beta, \Omega)}{\partial \Omega^p} = 0 \]  
(73)
for the smallest possible \( p \). Plugging \( \Omega^{(N)}(\beta) \) into \( F^{(N)}(\beta, \Omega) \), we finally get back a resummed expression for the physical quantity \( F(\beta) \). The results for the first three orders are given in Fig. 4. In order to check our results we have to compare them to the numerically evaluated free energy \( F_{\text{num}}(\beta) \) which is discussed in Sec. XI.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{fig3}
\caption{Branch of the variational parameter \( \Omega^{(1)}(\beta) \) which we chose. The coupling strength is \( g = 1 \). Other branches not shown in this figure lead to highly diverging results. Throughout this paper all results are presented in natural units \( \hbar = k_B = 1 \) and, additionally, we have set \( M = \omega = 1 \).}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{fig4}
\caption{Free energy of the anharmonic oscillator up to third order for intermediate coupling \( g = 1 \). The solid line represents the numerical result \( F^{(N)}(\beta) \), obtained by approximating the partition function (75) with the help of the first ten energy eigenvalues. The other lines are variational perturbative results: The dashed line shows the first order, the dotted line shows the second order, and the dot-dashed line represents the third order. Note that the second and third order are hardly distinguishable from the numerical results. Higher orders for a special value of the inverse temperature \( \beta \) can be found in Fig. 5.}
\end{figure}

\section{Higher Orders}

We now evaluate the convergence behaviour for the variational perturbative results for the free energy \( F^{(N)}(\beta) \) up to the fifth order. However, in order to reduce the computational cost we restrict ourselves to a certain value of the inverse temperature \( \beta \). Results are shown in Fig. 5. For odd variational perturbation orders we optimized the free energy according to (71), i.e. we determined \( \Omega \) by setting the first derivative of \( F^{(N)}(\beta) \) with respect to \( \Omega \) to zero. For even orders we had to go for inflection points, instead, so we had to solve equation (72).
It turns out that odd and even orders oscillate about
FIG. 5: The free energy of the anharmonic oscillator for intermediate coupling \( g = 1 \) for \( \beta = 1 \) up to fifth variational perturbative order. The values converge exponentially towards the numerical value \( F_{\text{num}}^{(3)}(1) = 0.6571 \), which is shown as a straight line. The dimension of the free energy in natural units is \( 2R_y \).

an exponential best fit curve. For \( \beta = 1 \) the numerical result, \( F_{\text{num}}^{(3)}(1, 0) = 0.6571 \), turns out to lie within the interval obtained by fitting the five perturbative orders of the free energy with origin, as shown in Fig. 5. This interval is \( [0.657, 0.660] \), and clearly, the variational perturbative results converge exponentially.

### XI. Checking Our Results

The spectral representation of the partition function reads

\[
Z = \sum_{n=0}^{\infty} e^{-\beta E_n},
\]

where the \( E_n \) are the energy eigenvalues. Let us define the numerical approximants

\[
Z_{\text{num}}^{(N)} = \sum_{n=0}^{N} e^{-\beta E_n},
\]

and

\[
F_{\text{num}}^{(N)} = -\frac{1}{\beta} \log Z_{\text{num}}^{(N)},
\]

respectively. One possibility to obtain numerical results for the eigenvalues \( E_n \) is provided for by the so-called “shooting method”. We integrate the Schrödinger equation numerically for the potential \( V(x) \) and for a particular value of the coupling strength \( g \). If the energy \( E \) which we plug into the program does not coincide with one of the energy eigenvalues \( E_n \), the solution to the Schrödinger equation explodes already for relatively small values of the coordinate \( x \). If the energy eigenvalue is close to the exact answer, we have \( |\Psi(x)| < \infty \) also for larger values of \( x \). This method yields the unnormalized eigenfunctions (the wave functions which still have to be normalized) and the energy eigenvalues to very high accuracy (see Tab. I). Renormalization is necessary for the computer algebra program that needs an initial value \( \Psi(0) \) which we set to one. Plugging the first ten numerical energy eigenvalues into equation (75) and evaluating (76) up to \( N = 9 \), we obtain a function \( F_{\text{num}}^{(N)}(\beta) \). It converges rapidly for low temperatures, corresponding to high values of \( \beta \). For high temperatures more terms should be taken into account. Alternatively one can also use classical results as a high-temperature cross check: High temperatures correspond to classical statistical distributions such that we can evaluate the classical partition function according to

\[
Z_{\text{cl}} = \int_{-\infty}^{+\infty} dx \frac{1}{\lambda_{\text{th}}} \exp \left[ -\beta V(x) \right],
\]

### TABLE I: The first ten energy eigenvalues \( E_n \) of the anharmonic oscillator for intermediate coupling \( g = 1 \). They were obtained by numerically integrating the Schrödinger equation with the initial condition that \( \Psi(0) = 1 \), \( \Psi'(0) = 0 \) for even \( n \), and \( \Psi(0) = 0 \) and \( \Psi'(0) = 1 \) for odd \( n \), and of course \( |\Psi(x)| < \infty \) for large \( x \). The energy eigenvalues are given in units of \( 2R_y \).

\[
\begin{array}{|c|c|}
\hline
n & E_n \\
\hline
0 & 0.8037701932 \\
1 & 1.2738894164 \\
2 & 1.5192814619 \\
3 & 1.5462866088 \\
4 & 1.5604970512 \\
\hline
\end{array}
\]
with the potential (2) and \( \lambda_{ch} = \sqrt{2\pi\hbar^2 / M k_B T} \). This integral reduces to

\[
Z_d = \frac{1}{2\lambda_{ch}} \sqrt{\frac{M \omega^2}{2g}} \times \exp \left( \frac{\beta M \omega^4}{32g} \right) K_{1/4} \left( \frac{\beta M \omega^4}{32g} \right),
\]

(78)

where \( K_{1/4}(z) \) is a modified Bessel function. The classical partition function (78) can be evaluated for high temperatures which corresponds to small values of \( \beta \). Consequently, when we test our variational perturbative results, we compare them to the classical free energy for low values of \( \beta \), namely \( \beta < 1/4 \). And for high values of \( \beta \) we use the numerical approximation, \( F_{\text{num}}^{(3)}(\beta) \), for comparison (see Fig. 6).

In natural units \( \hbar = k_B = 1 \) a value of \( \beta = 1/4 \) corresponds to a physical temperature of \( T = 1.26 \times 10^5 K \).

**XII. CONCLUSION AND OUTLOOK**

The recursive technique that has been developed throughout Sections IV–VI definitely out classes all diagrammatical perturbative calculations. Using the conventional evaluation of Feynman diagrams, the partition function and the free energy have been evaluated up to third order [14], here we obtained the fifth-order result. For the free energy the convergence of variational perturbation theory was found to be exponential. The fact that the principle of least sensitivity [13] produces extrema for the odd variational orders and inflection points for even orders is reflected in the respective convergence behaviors: Odd and even orders can best be fitted separately by exponentials as emphasized in Ref. [11]. Thus we obtained intervals of convergence for certain values of the free energy which always turned out to contain the exact numerical result when taking into account the statistical errors associated with the boundaries of the intervals. For the free energy, the numerical results were obtained using its spectral representation reverting on the first ten energy eigenvalues obtained with the “shooting method”, sketched in Sec. XI.

Finally, we note that our high-order perturbative results for the anharmonic imaginary-time evolution amplitude are useful for calculating other thermodynamic quantities as the correlation function or the ground state wave function [13, 15, 16]. Furthermore, it remains to compare these perturbative results with the semiclassical approximation [17].

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[12] The expansion coefficients \( c^{[n]}_2(\tau) \) up to seventh order can be found at http://www.physik.fu-berlin.de/ weissbach/coeff.html


