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Carlos Handy
Texas Southern University, carlos.handy@tsu.edu

Daniel Vrinceanu
Texas Southern University, daniel.vrinceanu@tsu.edu

C. B. Marth
Dulles High School

R. Gupta
Lawrence E. Elkins High School

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C. R. Handy[1], D. Vrinceanu[1], C. B. Marth[2] and R. Gupta[3]

[1]Department of Physics, Texas Southern University, Houston, Texas 77004
[2]Dulles High School, Sugar Land, Texas 77459
[3]Science Department, Lawrence E. Elkins High School, Missouri City, Texas 77459

E-mail: `handycr@tsu.edu`

Abstract. The Orthogonal Polynomial Projection Quantization (OPPQ) is an algebraic method for solving Schrödinger's equation by representing the wave function as an expansion $\Psi(x) = \sum_n \Omega_n P_n(x) R(x)$ in terms of polynomials $P_n(x)$ orthogonal with respect to a suitable reference function $R(x)$, which decays asymptotically not faster than the bound state wave function. The expansion coefficients Ω_n are obtained as linear combinations of power moments $\mu_p = \int x^p \Psi(x) \, dx$. In turn, the μ_p's are generated by a linear recursion relation derived from Schrödinger's equation from an initial set of low order moments. It can be readily argued that for square integrable wave functions representing physical states $\lim_{n\to\infty} \Omega_n = 0$. Rapidly converging discrete energies are obtained by setting Ω coefficients to zero at arbitrarily high order. This paper intruduces an extention of OPPQ in momentum space by using the representation $\Phi(k) = \sum_n \Xi_n Q_n(k) T(k)$, where $Q_n(k)$ are polynomials orthogonal with respect to a suitable reference function $T(k)$. The advantage of this new representation is that it can help solving problems for which there is no coordinate space moment equation. This is because the power moments in momentum space are the Taylor expansion coefficients, which are recursively calculated via Schrödinger's equation. We show the convergence of this new method for the sextic anharmonic oscillator and an algebraic treatment of Gross-Pitaevskii nonlinear equation.

1. Introduction

The Hill Determinant Quantization (HDQ) ansatz studied by Banerjee [1], and more recently by Killingbeck and Grosjean [2], represents bound state solutions of Schrödinger's equation in terms of a non-orthogonal basis,

$$\Psi(x) = \sum_n a_n x^n R(x), \tag{1}$$

where the positive reference function $R(x)$ should match the asymptotic behavior of the wave function. The coefficients a_n are obtained recursively as polynomials in the energy

parameter and bound state energies are obtained algebraically from the truncation of the HDQ series (1) at a finite order N.

It was pointed out [3] that although this approach produces the correct local representation of the wave function at the origin, it fails in certain cases to provide a global representation because it can not easily discriminate between the bound (physical) and the un-bounded (non-physical) linearly independent solutions. This is because the forward recursion for a_n picks up the dominant solution, and not the subdominant solution.

The failure of HDQ was studied by Tater and Turbiner [4] in the context of the sextic anharmonic oscillator with potential energy $V(x) = gx^6 + bx^4 + mx^2$. They show that when the reference function $R(x) = e^{-\sqrt{g}x^4/4}$ coincides with the leading asymptotic form of the wave function for a bound state, HDQ does not converge, or converges to the wrong answer, for certain potential energy parameters.

These difficulties are addressed through the Orthogonal Polynomial Projection Quantization (OPPQ) method proposed by Handy and Vrinceanu [5]. This original OPPQ formulation (in contrast to the alternative formulation presented in this work) depends on a momentum space local analysis as defined by the power moments of the configuration space solution. For the class of systems considered, the power moments in turn are generated through a moment equation, recursion relation which filters out un-bounded wave functions that have infinite power moments. As such, OPPQ is predisposed to only generate the discrete state solutions. This OPPQ formulation generates the exact local expansion in momentum space. Empirical evidence [6] also suggests that it leads to a very good local approximation (i.e. pointwise convergence) in the configuration space.

The basic structure of the one-dimensional OPPQ method is briefly explained below, although its extension to two-dimensional examples has also yielded very good results [7, 8]. In this algebraic method the wave function is represented as

$$\Psi(x) = \sum_n \Omega_n P_n(x) R(x), \tag{2}$$

where polynomials $P_n(x)$ are orthogonal with respect to the chosen reference function $R(x)$. Explicitly

$$P_n(x) = \sum_{k=0}^{n} \pi_k^{(n)} x^k \tag{3}$$

and

$$\int P_i(x) P_j(x) R(x)\, dx = \mathcal{N}_i \delta_{ij} \tag{4}$$

Such representations fall under the more general heading of "weighted polynomial expansions" [9]. The expansion coefficients Ω_n are calculated from the power moments of the wave function $\mu_p = \int x^p \Psi(x)\, dx$ because

$$\mathcal{N}_n \Omega_n = \int P_n(x) \Psi(x)\, dx = \sum_{k=0}^{n} \pi_k^{(n)} \mu_k \tag{5}$$

The power moments can be calculated through a linear recursive relation that is obtained by multiplying Schrödinger's equation with x^p and integrating over the configuration space coordinate, implicitly assuming a square-integrable bound state wave function. This moment equation allows calculation of any power moment providing a small number s of lower moments $\mu_0, \mu_1, \ldots, \mu_{s-1}$ are given. Together with the energy E parameter, these "missing" moments form a set of $(s+1)$ parameters that completely define a bound state, because each coefficient Ω_n is a linear combination of the "missing" moments. The un-physical, non-integrable, solutions are automatically eliminated because their power moments are infinite and do not satisfy the moment equation.

Schrödinger's equation does not provide information about the "missing moments", which have to be eliminated by imposing supplementary constrains. In the case of exactly, or quasi-exactly solvable problems (such as the harmonic oscillator, Coulomb problem, Morse potential, etc) a simple examination of the consistency of a related moment equations directly provide the exact energy eigenvalues [10], and the lack of knowledge of "missing moments" is irrelevant. More generally, positivity conditions for the "missing moments" lead to converging upper and lower bounds for the ground state energy, as demonstrated by Handy in pioneering results [11, 12, 13].

In OPPQ, the extra constrains that allow elimination of the missing moments are obtained by observing that if the reference function $R(x)$ is chosen such that

$$\int \frac{|\Psi(x)|^2}{R(x)}\, dx = \sum_n \mathcal{N}_n |\Omega_n|^2 < \infty \tag{6}$$

then it must be true that

$$\lim_{n\to\infty} \Omega_n = 0. \tag{7}$$

Equation (6) limits the choice of $R(x)$ to functions that decay no faster that the leading asymptotic form of the square of the wave function. This includes functions for which $\lim_{|x|\to\infty} |\Psi(x)|/R(x) < \infty$. Clearly, taking $R(x)$ to be the asymptotic form of the physical wave function is consistent with Eq. (6).

The asymptotic condition Eq. (7) justifies that, given a truncation order N, one can set $\Omega_N = 0, \Omega_{N+1} = 0, \ldots \Omega_{N+s-1} = 0$ as a system of s linear equations in the "missing" moments $\mu_0, \mu_1, \ldots, \mu_{s-1}$. The determinant of this system is a polynomial in energy E, and its roots converge to the energy eigenvalues in the $N \to \infty$ limit. This completes the OPPQ analysis, and unlike HDQ, the un-bounded wave functions are automatically eliminated.

We note that the above formalism works for a large class of problems, and applies even for non-hermitian (pseudo-hermitian) bound state problems with complex wave functions [5]. Details about the implementation and numerical examples are in [5].

It is important to note that OPPQ method works differently than the variational Rayleigh-Ritz (RR) method. In RR the wave function is searched within a target finite subspace spanned by a basis set $B_n(x)$, with the representation $\Psi(x) = \sum_n c_n B_n(x)$ and through minimizing the symmetrical energy functional $\langle \Psi | H | \Psi \rangle$. For this reason one

can chose $B_n(x) = \tilde{P}_n(x)R(x)$, where the new polynomials $\tilde{P}_n$ (different from the P_n polynomials considered in OPPQ) are orthogonal with respect to $R(x)^2$

$$\int \tilde{P}_i(x)\tilde{P}_j(x)R(x)^2 \, dx \sim \delta_{ij}. \tag{8}$$

On the other hand, in OPPQ the moment equation is obtained by "testing" Schrödinger's equation $H\Psi = E\Psi$ with power functions x^p, which are not even in the Hilbert target space,

$$\langle x^p|H\Psi\rangle = E\langle x^p|\Psi\rangle \tag{9}$$

The target space of solutions consists of functions that have a (given) finite number of moments, while the test space consist of non-normalizable polynomials. In RR method the target and the test spaces are both L^2.

If formulated as an RR problem, the coefficients $\Omega_n = \langle B_n|\Psi\rangle$ are obtained as projection coefficients for the function $\psi(x) = \Psi(x)/\sqrt{R(x)}$ with respect to the orthogonal basis $B_n(x) = P_n(x)\sqrt{R(x)}$. If the expansion of ψ is L^2 convergent

$$\lim_{N\to\infty} \int dx |\psi(x) - \sum_{n=0}^{N} \Omega_n B_n(x)|^2 = 0 \tag{10}$$

then, because

$$\int dx |\psi(x) - \sum_{n=0}^{N} \Omega_n B_n(x)|^2 \geq \inf_x \{1/R(x)\} \times \int dx |\Psi(x) - \sum_{n=0}^{N} \Omega_n P_n(x)R(x)|^2 \tag{11}$$

we can conclude that the OPPQ expansion is also L^2:

$$\lim_{N\to\infty} \int dx |\Psi(x) - \sum_{n=0}^{N} \Omega_n P_n(x)R(x)|^2 = 0. \tag{12}$$

2. OPPQ in Momentum Space

The configuration space OPPQ method requires that a moment equation can be derived from Schrödinger's equation. A way to avoid this requirement is to formulate OPPQ in the Fourier transformed momentum space. The corresponding power moments in momentum space are the Taylor expansion coefficients in the coordinate space, and therefore the momentum space moment equation is the recursion relation for coordinate space power expansion coefficients.

If $\Phi(k) = 1/\sqrt{2\pi} \int dx \, e^{-ikx}\Psi(x)$ defines the momentum space wave function, then the Momentum Space Orthogonal Polynomial Projection Quantization (MSOPPQ) representation of the momentum wave function becomes

$$\Phi(k) = \sum_n \Xi_n Q_n(k)T(k) \tag{13}$$

where the polynomials $Q_n(k) = \sum_{j=0}^{n} q_j^{(n)} k^j$ are orthogonal with respect to the momentum space reference function $T(k)$, which is chosen in relation to the asymptotic form of the momentum wave function $\Phi(k \to \infty)$.

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Following a similar formalism as in the configuration space OPPQ analysis, summarized in the previous section, the expansion coefficients Ξ_n result from

$$\mathcal{N}_n \Xi_n = \int \Phi(k) Q_n(k) \, dk = \sum_{j=0}^{n} q_j^{(n)} \nu_j \tag{14}$$

where $\mathcal{N}_n$ is the norm of polynomial $Q_n(k)$ and ν_j are the k-space power moments defined by

$$\nu_j = \int \Phi(k) k^j \, dk = \sqrt{2\pi}(-i)^j \, j! \, c_j \tag{15}$$

involving the power series expansion coefficients of the configuration space wave function

$$\Psi(x) = \sum_{j=0}^{\infty} c_j x^j. \tag{16}$$

The power series coefficients satisfy a second order finite difference recursion relation:

$$c_j = M_j^{(0)}(E) c_0 + M_j^{(1)}(E) c_1 \tag{17}$$

Any coefficient c_j is then a linear combination of c_0 and c_1 with factors M that are polynomials in energy parmeter E. This is also true for expansion coefficients Ξ_n because of equations (14) and (15).

Similar arguments as in the coordinate space OPPQ require that

$$\int \frac{|\Phi(k)|^2}{T(k)} = \sum_n \mathcal{N}_n |\Xi_n|^2 < \infty \tag{18}$$

so that the expansion (13) can be truncated at a finite order and the two quantization conditions imposed: $\Xi_N = 0$ and $\Xi_{N+1} = 0$. These two conditions represent a system of two linear equations in c_0 and c_1, for which the determinant, a polynomial in energy, has to be set to zero. The roots of this determinant polynomial converge to energy eigenvalues in the $N \to \infty$ limit.

Once the energy approximations are obtained, the coefficients c_j, ν_j and Ξ_n can be calculated and an expression for the coordinate space wave function is obtained by inverse Fourier transform

$$\Psi(x) = \sum_{n=0}^{N-1} \sum_{j=0}^{n} \Xi_n q_j^{(n)} \frac{1}{\sqrt{2\pi}} \int e^{ikx} k^j T(k) \, dk \tag{19}$$

For a reference function $T(k)$ with an analytic inverse transform, $R(x)$, one obtains

$$\Psi(x) = \sum_{n=0}^{N-1} \Xi_n Q_n(-i\frac{d}{dx})^n R(x), \tag{20}$$

where $R(x) \equiv \frac{1}{\sqrt{2\pi}} \int e^{ikx} k^j T(k)$.

There has been significant interest in understanding the class of functions whose Fourier transforms are positive. This also includes cases where both the configuration space expression and its Fourier transform are both positive, as developed by Giraud and Peschanski [14]. These studies are of relevance to us, but not exploited here. Also, as will be shown for the sextic case considered here, the Fourier space weight need not

be differentiable (at the origin) in order for Eq.(19) to yield good approximants to the wave function.

Of considerable significance we note that the above configuration space expansion exactly recovers the power series expansion of $\Psi(x)$. This is because (as in the configuration space case) $\int dk\ k^p Q_n(k)T(k) = 0$, for $n > p$. Accordingly

$$
\begin{aligned}
c_p &= \frac{i^p}{\sqrt{2\pi}p!} \int dk\ k^p \Phi(k), \\
&= \frac{i^p}{\sqrt{2\pi}p!} \sum_{n=0}^{p} \Xi_n \int dk\ k^p Q_n(k)T(k), \\
&= \frac{1}{p!}(\partial_x)^p \sum_{n=0}^{p} \Xi_n Q_n\left(-i\frac{d}{dx}\right)R(x)\Bigg|_{x=0}.
\end{aligned}
\tag{21}
$$

Thus the Fourier space OPPQ formulation allows us to work with systems not admitting a moment equation representation, and if one can find a suitable weight that captures the asymptotic form of the physical states, in the momentum space, then the representation in Eq. (13) will not only generate the exact local expansion at $x = 0$ but also incorporate the desirable physical asymptotic behavior (in x-space as well). These are the objectives of the original HDQ representation.

3. MSOPPQ for the $V(x) = gx^6 + mx^2$ potential

In this section we apply the MSOPPQ method to the sextic anharmonic oscillator problem described by Schrödinger's equation

$$
-\frac{d^2\Psi}{dx^2} + (gx^6 + mx^2)\Psi(x) = E\Psi(x).
\tag{22}
$$

The recursion relation for power series coefficients is obtained by using $\Psi(x) = \sum_n c_n x^n$ in Eq. (22) resulting in

$$
(p+1)(p+2)c_{p+2} = -Ec_p + mc_{p-2} + gc_{p-6},
\tag{23}
$$

with $p \geq 0$ and $c_j = 0$ for $j < 0$, in terms of the unknown coefficients c_0 and c_1. Exploiting the parity symmetry of the potential energy in equation (22) one can select even and odd states with the choice $(c_0 = 1, c_1 = 0)$ or $(c_0 = 0, c_1 = 1)$, respectively.

We choose as a momentum space reference function $T(k) = \exp(-s|k|^{4/3})$. This choice can be motivated in two ways: by calculating the asymptotic form of the momentum wave function and by Fourier transforming the coordinate space asymptotic form.

The momentum space representation of Eq. (22) is obtained by taking the Fourier transform to get

$$
k^2\Phi(k) - g\frac{d^6\Phi}{dk^6} - m\frac{d^2\Phi}{dk^2} = E\Psi,
\tag{24}
$$

for the momentum space wave function $\Phi(k) = 1/\sqrt{2\pi} \int e^{-ikx} \Psi(x) \, dx$. A JWKB analysis is obtained by replacing $d/dk \rightarrow \epsilon d/dk$ to get the expansion $\Phi(k) = \exp(\sum_{j=0} \epsilon^{j-1} S^{(j)}(k))$, and then the leading asymptotic behavior of the solution

$$g\left(\frac{dS^{(0)}}{dk}\right)^6 + m\left(\frac{dS^{(0)}}{dk}\right)^2 - k^2 = -E \tag{25}$$

to get

$$\frac{dS^{(0)}}{dk} \approx (k^2/g)^{1/6}, \tag{26}$$

which leads to the result

$$\Phi(k) \sim \exp(e^{-n\pi i/3} \frac{3}{4g^{1/6}} |k|^{4/3}), \quad n = 0, 1, 2, 3, 4, 5 \tag{27}$$

The choices that lead to exponentially decaying configurations are $n = 2, 3, 4$, which corresponds to $s = 3/8g^{1/6}$ and $s = 3/4g^{1/6}$.

A better analysis is provided by a stationary phase analysis of the Fourier transform of the configuration space asymptotic controlling form

$$\mathcal{I}(k) \equiv \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} dx \ e^{-ikx} exp(-\frac{\sqrt{g}}{4} x^4), \tag{28}$$

resulting in

$$\mathcal{I}(k) \sim g^{\frac{1}{6}} \sqrt{\frac{2\pi}{3}} k^{-\frac{1}{3}} exp(-\frac{3}{8g^{1/6}} k^{\frac{4}{3}}) Re\left((\sqrt{3} - i) \times exp(\frac{3\sqrt{3}i}{8g^{1/6}} k^{\frac{4}{3}})\right). \tag{29}$$

This further affirms the choice of $s = 3/8g^{1/6}$.

The monic orthogonal polynomials $Q_n(k)$ for the reference function $T(k) = \exp(-s|k|^{4/3})$ are constructed using the reccurence $Q_0(k) = 1$, $Q_1(k) = k$ and

$$Q_{n+1}(k) = kQ_n(k) - \frac{||Q_n||^2}{||Q_{n-1}||^2} Q_{n-1}(k), \tag{30}$$

where the norms of polynomials can be calculated based on the power moments of the reference function given by

$$\sigma_p = \int_{-\infty}^{\infty} k^p T(k) \, dk = (1 + (-1)^p) \frac{3s^{-3(p+1)/4}}{4} \Gamma\left(\frac{3}{4}(p+1)\right). \tag{31}$$

As a numerical example we take the potential $V(x) = x^6 - 4x^2$ for which the ground state energy has been accurately calculated in [5] to be $E = -0.523268622$. Figure 1 shows the convergence of the ground state energy obtained by using the MSOPPQ method as a function of the truncation order $20 \leq N \leq 160$ for three choices of reference function $T(k) = e^{-3/4|k|^{4/3}}$, $T(k) = e^{-3/8|k|^{4/3}}$ and $T(k) = e^{-k^2/2}$. The fastest convergence is obtained for $s = 3/4$, and not the $s = 3/8$ predicted as the one consistent with the true asymptotic form in momentum space. As expected, the harmonic oscillator choice $e^{-k^2/2}$ does not give convergent results at all. This figure also demonstrate the exponential convergence of MSOPPQ. Other conventional methods, such as Rayleigh-Ritz, finite element, etc, have a slower power-like $\sim 1/N^k$ (with $k = 2 \sim 3$) convergence as a
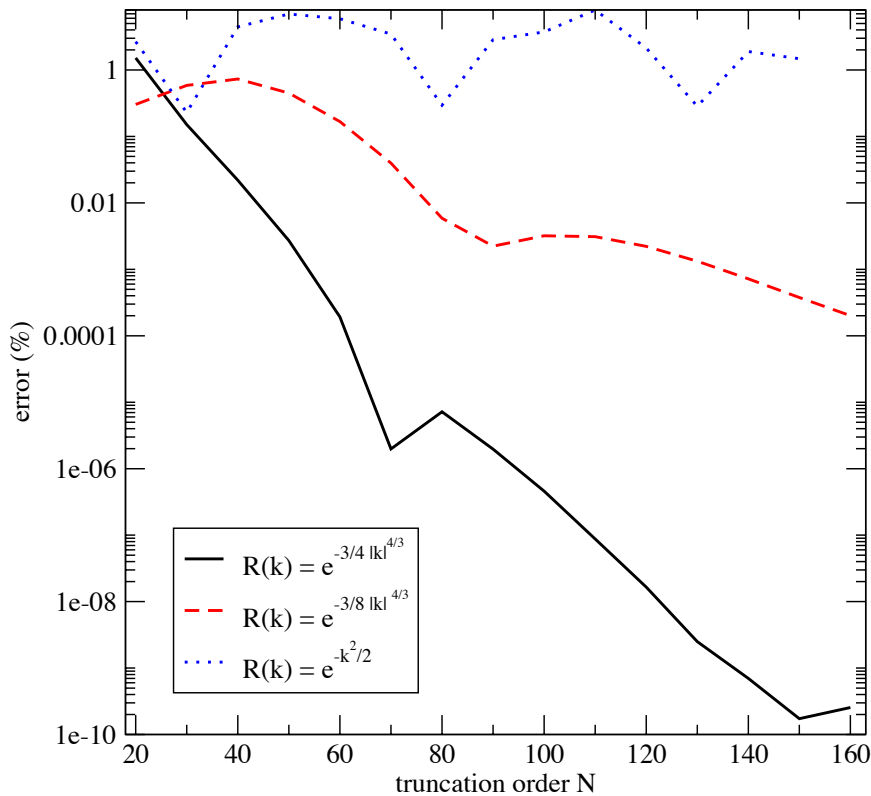
Figure 1. Relative error in calculation the ground state energy of the sextic anharmonic oscillator $V(x) = x^6 - 4x^2$, obtained by using the MSOPPQ method, as a function of truncation order and for three choices of the momentum space reference function. The "exact" value $E = -0.523268622$ is calculated by using the coordinate space OPPQ with $N = 60$.

function of truncation order. It is worth noting a recent publication [15] that reports remarkably accurate results obtained for the sextic anharmonic problem Eq.(22), by using similar algebraic methods.

4. MSOPPQ for Non-linear Schrödinger Equation

A gas of weakly interacting bosons at low temperature can be successfully described by a mean-field theory provided most of the particles occupy the condensate mode. This mode is a solution of a nonlinear Schödinger equation known as the Gross-Pitaevskii equation (GPE):

$$-\frac{\hbar^2}{2m}\nabla^2\Psi + V\Psi + \frac{4\pi\hbar^2 a_s}{m}|\Psi|^2\Psi = \mu\Psi. \tag{32}$$

This is the stationary form of (GPE), with eigenvalue μ being the chemical potential, and the number of particles given by

$$N = \int |\Psi(\mathbf{r})|^2 \, d\mathbf{r}. \tag{33}$$

The (positive) scattering length a_s specifies the interparticle interactions at the mean field level and provides the magnitude of the non-linear density dependent term, and

$V = V(\mathbf{r})$ is an external potential in which the condensate is trapped. In an elongated, quasi-one-dimensional harmonic trap, a_s is replaced by an effective interaction strength that depends on the scattering length and the transverse confinement. The 1D GPE takes a simpler form, after appropriate scaling,

$$-\frac{d^2\Psi}{dx^2} + x^2\Psi + g|\Psi|^2\Psi = E\Psi \quad \text{with} \quad \int |\Psi(x)|^2 \, dx = 1. \tag{34}$$

These equations can only be solved numerically since no analytical solutions are known [16]. For a detailed discussion about existence and stability of solutions for Eq.(34) please see [17] and references therein. Considerable efforts have been made to find appropriate approximations for this problem, see for example recent works [18, 19]. The configuration space OPPQ approach will not work here because there is no moment equation that can be derived for Eq. (34). However, MSOPPQ can be employed to give an algebraic solution to Eq. (34) as shown below.

The recursions for coordinate space expansion $\Psi(x) = \sum_{j=0} c_j x^j$ coefficients is

$$c_{j+2} = (c_{j-2} - Ec_j + g \sum_{j_1+j_2+j_3=j} c_{j_1} c_{j_2} c_{j_3})/[(j+1)(j+2)] \tag{35}$$

with $j \geq 2$ and $c_{-2} = c_{-1} = 0$. The triple summation is over all weak compositions $(j_{1,2,3} \geq 0)$ of j into 3 parts.

The power moments of the Fourier space wave function $\Phi(k)$ can be obtained in terms of Taylor expansion coefficients of $\Psi(x)$ as

$$\nu_p = \int_{-\infty}^{\infty} \Phi(k)k^p \, dk = \sqrt{2\pi}(-i)^p p! c_p. \tag{36}$$

In the limit of a gas on non-interacting particles, when $g = 0$, GPE is the equation of a simple harmonic oscillator which motivates the choice of the reference function $T(k) = e^{-k^2/2}$, for which the orthogonal polynomials are determined by the Hermite polynomials as

$$Q_n(k) = 2^{-n/2} H_n(k/\sqrt{2}). \tag{37}$$

On the other hand, for strongly interacting gases the kinetic energy term in the GPE can be ignored and the Thomas-Fermi ground state solution is obtained as

$$\Psi_{TF}(x) = \sqrt{\frac{E - x^2}{g}}, \tag{38}$$

and corresponds to Fourier space Thomas-Fermi solution

$$\Phi_{TF}(k) = \sqrt{\frac{\pi E}{g}} \frac{J_1(k\sqrt{E})}{k} \tag{39}$$

where J_1 is Bessel function of index 1.

By using the representation (13) for the solution in momentum space, MSOPPQ method requires that for a given truncation order N the expansion coefficient Ξ_N to be zero. This condition is sufficient here because the ground state is even and $c_1 = 0$. One simple way to proceed is to chose a value for E and solve for the corresponding g and c_0 that result from $\Xi_N = 0$ and normalization condition.

It is easy to see that the MSOPPQ condition has the form

$$\Xi_N = c_0 \mathcal{F}(gc_0^2) = 0 \tag{40}$$

where $\mathcal{F}$ is a polynomial of order $N/2 + 1$. Ξ_N for odd orders is 0. By assuming that the MSOPPQ series representation is truncated at the order N, then the normalization condition is

$$\int_{-\infty}^{\infty} |\Phi(k)|^2 \, dk = \sum_{i,j=0}^{N-2} \Xi_i \Xi_j \Gamma_{ij} = c_0^2 \mathcal{Z}(gc_0^2) = 1, \tag{41}$$

where the coefficients $\Gamma_{ij} = \int Q_i(k)Q_j(k)T^2(k) \, dk$ are easily calculated based on the given set of orthogonal polynomials, and where $\mathcal{Z}$ is a polynomial. From this we obtain that

$$g = gc_0^2 \mathcal{Z}(gc_0^2) \tag{42}$$

Therefore, we can carry the calculation of the polynomial $\mathcal{F}$ with the assumption of $c_0 = 1$, solve for its roots G_k and obtain g as the smallest value of $G_k \mathcal{Z}(G_k)$. The corresponding solution for c_0 is obtained as

$$c_0 = \sqrt{\frac{G_k}{g}}. \tag{43}$$

Coefficients Ξ_n, with $n < N$, can then be calculated and the wave function in coordinate space can be obtained after an inverse Fourier transform as:

$$\Psi(x) \approx \frac{1}{q_n} \sum_n \Xi_n \sum_j q_j^{(n)} (-i)^j \frac{d^j T(x)}{dx^j}. \tag{44}$$

When the simple choice of reference function is $T(x) = e^{-x^2/2}$ then

$$\Psi(x) = \sum_n \Xi_n H_n(x/\sqrt{2}) e^{-x^2/2}. \tag{45}$$

Figure 2 shows the ground state of GPE Eq. (34) obtained by using MSOPPQ. The inset table shows the results of calculations, compared with reference results obtained by Majorević [20]. The limit case of $E = 1$ corresponds to the linear case where $g = 0$. This is obtained algebraically exact for $N = 2$. For the other ground state energy considered, $E = 10, 50$ and 80, the corresponding non-linearity parameter g increases as expected. In the same time, the wave function departs considerably from the ideal ground state of the harmonic oscillator (black solid line), spreading over larger and larger regions due to the increase of non-linear pressure. As expected, the agreement with semi-classical Thomas-Fermi approximation becomes better as the non-linear term grows, specially in the center of the trap, while big differences appear at its borders due to quantum tunneling. The reported calculation of g could not be improved by increasing the truncation order, probably, because the reference function does not reproduce correctly the asymptotic form of the wave function for $x \to \infty$. It is clear that the simple reference function $T(k) = e^{-k^2/2}$ decays too fast in comparison with GPE momentum space wave function, for which an approximation is given by the Fourier transform of the Thomas-Fermi solution Eq. (39).
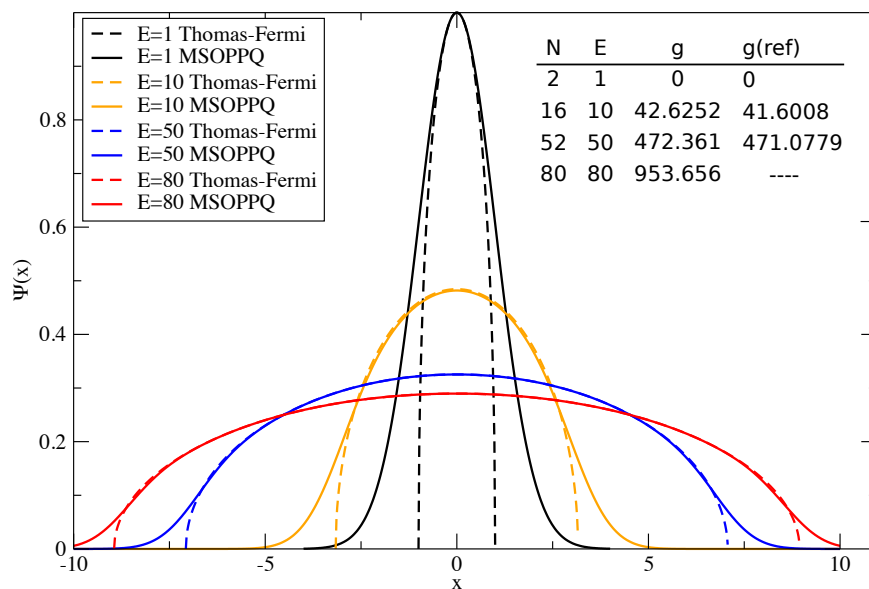
Figure 2. Ground state solutions of GPE using MSOPPQ (solid lines) compared with Thomas-Fermi approximation (dashed lines) for the 4 cases presented in the inset table, where N is the truncation order, E is the energy considered and g is the calculated value by the present method and $g(\text{ref})$ that was obtain in [20].

5. Conclusions

A new algebraic method MSOPPQ is introduced in momentum space to complement the coordinate space OPPQ method. This method succeeds to achieve the same goal, which is to get a representation for the wave function that reproduces exactly the local analytical structure at the origin and preserve at the same time the required global properties such as boundedness over the entire x-axis. Also, in keeping with OPPQ, the computed energy converges exponentially with the truncation order N. However, in contrast to OPPQ, the new method does not require a moment equation, and therefore it can be applied for a larger class of problems, such as the non-linear Schrödinger equation. As with OPPQ, the new method depends crucially on the choice of the reference function and the knowledge of the leading asymptotic form, which in momentum space, may not be as easy to obtain as in coordinate space.

Acknowledgments

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