

EXACT DIAGONALIZATION OF THE d – DIMENSIONAL SPATIALLY CONFINED QUANTUM HARMONIC OSCILLATOR

Kunle Adegoke^{*}, Adenike Olatinwo, Henry Otoberise, Funmi Akintujoye, Afees Tihamiyu

Department of Physics and Engineering Physics, Obafemi Awolowo University, 220005 Ile-Ife, Nigeria

^{*}Corresponding author, E -mail: adegoke00@gmail.com

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ABSTRACT. In the existing literature various numerical techniques have been developed to quantize the confined harmonic oscillator in higher dimensions. In obtaining the energy eigenvalues, such methods often involve indirect approaches such as searching for the roots of hypergeometric functions or numerically solving a differential equation. In this paper, however, we derive an explicit matrix representation for the Hamiltonian of a confined quantum harmonic oscillator in higher dimensions, thus facilitating direct diagonalization.

Keywords: matrix, Hamiltonian, quantum harmonic oscillator, direct diagonalization.

INTRODUCTION

The d – dimensional confined harmonic oscillator (cho) of mass m and frequency ω is described by the Hamiltonian

$$H(\mathbf{x}) = -\frac{\hbar^2}{2m} \nabla^2 + \frac{1}{2} m \omega^2 \mathbf{x}^2,$$

where $\mathbf{x} = (x_1, x_2, \dots, x_d)$ with $|x_i| \leq L$, $\mathbf{x}^2 = \mathbf{x}^t \mathbf{x}$ and ∇ is the d – dimensional cartesian gradient operator. $H(\mathbf{x})$ being a Kronecker sum, we can also write

$$H(\mathbf{x}) = \sum_{i=1}^d H_i(x_i),$$

where

$$H_i(x_i) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_i^2} + \frac{1}{2} m \omega^2 x_i^2, \quad |x_i| \leq L.$$

We also note that $H(\mathbf{x}) = T(\mathbf{x}) + V(\mathbf{x})$, where

$$T(\mathbf{x}) = \sum_{i=1}^d T_i(x_i) \quad \text{and} \quad V(\mathbf{x}) = \sum_{i=1}^d V_i(x_i),$$

with

$$T_i(x_i) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_i^2} \quad \text{and} \quad V_i(x_i) = \frac{1}{2} m \omega^2 x_i^2, \quad (i = 1, 2, \dots, d).$$

Various techniques have been employed by researchers to numerically diagonalize the Hamiltonian of a confined oscillator. These methods usually involve searching for roots of hypergeometric functions, as can be seen for example in references (AL-JABER, 2008) and (MONTGOMERY *et al.* 2010). In (CAMPOY *et al.* 2002) a method based on the expansion of the wavefunction as well as numerical integration of an ordinary differential equation were used to obtain the energy eigenvalues and wavefunctions of a one-dimensional confined oscillator.

In this paper we will derive an explicit matrix representation for the Hamiltonian of the confined d – dimensional harmonic oscillator.

MATRIX REPRESENTATION OF THE OPERATORS

If we consider each operator $T_i(x_i)$ as living in an N – dimensional Hilbert space, then the functions

$$\varphi_r(x_i) = \sqrt{\frac{1}{L}} \cos\left[\frac{\pi}{2} \sin^2\left(\frac{r\pi}{2}\right) - \frac{(r+1)\pi x_i}{2L}\right], \quad r = 0, 1, 2, \dots, N-1, \quad (1)$$

constitute a set of basis vectors of this N – dimensional Hilbert space since they are the non-degenerate, mutually orthogonal and normalized eigenstates of the Hermitian operator T_i , with corresponding eigenvalues

$$\varepsilon_r = (r+1)^2 \varepsilon, \quad r = 0, 1, 2, \dots, N-1, \quad \text{where } \varepsilon = \frac{\pi^2 \hbar^2}{8mL^2}. \quad (2)$$

Thus the operator $T(\mathbf{x})$ lives in an N^d dimensional Hilbert space whose basis vectors can be taken as the direct product vectors

$$\psi_s(\mathbf{x}) = \psi_s(x_1, x_2, \dots, x_d) = \prod_{i=1}^d \varphi_{s_i}(x_i), \quad s = 0, 1, 2, \dots, N^d - 1, \quad (3)$$

where

$$s_i = \left\lfloor \frac{s}{N^{d-i}} \right\rfloor \bmod N, \quad i = 1, 2, \dots, d, \quad (4)$$

where $\lfloor q \rfloor$, the *floor* of q , is the nearest integer not greater than q .

Thus each state $\psi_s(\mathbf{x})$ is uniquely characterized or labelled by a vector $\mathbf{s} = (s_1, s_2, \dots, s_d)$ such that $s_i \in [0, 1, 2, \dots, N-1]$.

Denoting the eigenvalues of $T(\mathbf{x})$ by e_s , we have

$$e_s = \sum_{i=1}^d \varepsilon_{s_i} = \varepsilon \sum_{i=1}^d (s_i + 1)^2, \quad s = 0, 1, 2, \dots, N^d - 1,$$

with s_i as defined in (4) and ε as given in (2).

Since the cho Hamiltonian $H(\mathbf{x})$ lives in the same Hilbert space as $T(\mathbf{x})$, the complete set of functions $\{\psi_s\}$, with ψ_s as given in (3), will be used as the basis vectors for the matrix representation of H .

Thus, for $s = 0, 1, 2, \dots, N^d - 1$ and $t = 0, 1, 2, \dots, N^d - 1$ and with s_i and t_i as given in (4), the N^{2d} matrix elements of H are given by

$$\begin{aligned}
H_{st} &= \langle \psi_s | H | \psi_t \rangle \\
&= \sum_{i=1}^d \langle \psi_s | H_i | \psi_t \rangle \\
&= \sum_{i=1}^d \left\{ \prod_{j=0}^{d-1} \langle \varphi_{s_{d-j}}(x_{d-j}) | H_i \prod_{j=1}^d \varphi_{t_j}(x_j) \rangle \right\} \\
&= \sum_{i=1}^d \left\{ \left(\prod_{\substack{j=1 \\ j \neq i}}^d \delta_{s_j t_j} \right) \langle \varphi_{s_i} | H_i | \varphi_{t_i} \rangle \right\} \\
&= \sum_{i=1}^d c_{i_{st}} H_{i_{s_i t_i}},
\end{aligned} \tag{5}$$

where we have introduced a d -dimensional vector \mathbf{c} whose components are $N^d \times N^d$ symmetric binary matrices, c_i with elements given by

$$c_{i_{st}} = \prod_{\substack{j=1 \\ j \neq i}}^d \delta_{s_j t_j}, \tag{6}$$

so that $c_{i_{st}} = 1$ if either the two vectors \mathbf{s} and \mathbf{t} are one and the same vector, $\mathbf{s} = \mathbf{t}$, or they differ only at the i^{th} component, otherwise $c_{i_{st}} = 0$.

We note that

$$\delta_{s_i t_i} c_{i_{st}} = \delta_{st}. \tag{7}$$

In (5), $H_i, i = 1, 2, \dots, d$ are $N^d \times N^d$, symmetric matrices with elements

$$\begin{aligned}
H_{i_{s_i t_i}} &= \langle \varphi_{s_i} | H_i | \varphi_{t_i} \rangle \\
&= \langle \varphi_{s_i} | T_i | \varphi_{t_i} \rangle + \langle \varphi_{s_i} | V_i | \varphi_{t_i} \rangle \\
&= T_{i_{s_i t_i}} + V_{i_{s_i t_i}},
\end{aligned} \tag{8}$$

so that (5) can now be written as $H_{st} = T_{st} + V_{st}$ with

$$T_{st} = \sum_{i=1}^d c_{i_{st}} T_{i_{s_i t_i}}, \quad V_{st} = \sum_{i=1}^d c_{i_{st}} V_{i_{s_i t_i}} \tag{9}$$

We introduce yet another d -dimensional vector, $\boldsymbol{\alpha}$, whose components, α_i , are $N^d \times N^d$ symmetric binary matrices, in terms of which the c_i matrices may also be expressed. The α_i matrices are defined through their elements by $\alpha_{i_{st}} = \delta_{s_i t_i}$.

Properties of the auxilliary matrices c_i and α_i

It is straightforward to verify the following property for the α_i matrices:

$$\alpha_i \alpha_j = \alpha_j \alpha_i = N^{d-1} \delta_{ij} \alpha_i + N^{d-2} (1 - \delta_{ij}) J_{N^d}, \tag{10}$$

where

$$J_{N^d} = \begin{pmatrix} 1 & 1 & \vdots & 1 \\ 1 & 1 & \vdots & 1 \\ \vdots & \vdots & \vdots & \vdots \\ 1 & 1 & \vdots & 1 \end{pmatrix}$$

is the $N^d \times N^d$ all-ones matrix. The α_i matrices are singular and have trace equal to N^d . The eigenvalues of α_i are N^{d-1} repeated N times and 0 repeated $N^d - N$ times. Finally using multinomial expansion theorem and (10), it is readily established that the matrix $\alpha = \sum_{i=1}^d \alpha_i$ satisfies

$$\alpha^2 = N^{d-1}\alpha + N^{d-2}d(d-1)J_{N^d}.$$

From (6) it follows that

$$c_{i_{st}} = \delta_{st} + (1 - \alpha_{i_{st}})\delta_{\alpha_{st}, d-1} \quad (11)$$

and

$$c_{st} = \sum_{i=1}^d c_{i_{st}} = \delta_{st}d + \delta_{\alpha_{st}, d-1}.$$

Explicitly

$$c_{i_{st}} = \begin{cases} \cos^2(\alpha_{i_{st}} \pi/2) & \text{if } \alpha_{st} = d-1 \\ 0 & \text{if } \alpha_{st} < d-1 \\ 1 & \text{if } s = t \end{cases}$$

and

$$c_{st} = \begin{cases} 0 & \text{if } \alpha_{st} < d-1 \\ 1 & \text{if } \alpha_{st} = d-1 \\ d & \text{if } s = t \end{cases}.$$

From the definition of the c_i matrices the following further properties are evident:

1. $c_i^n = N^{n-1}c_i$, for $n \in \mathbf{Z}^+$.
2. The eigenvalues of c_i are 0 and N , each being N^{d-1} – fold degenerate.
3. The c_i matrices are singular and have trace N^d .

Representation for T

Since $T_i = \langle \varphi_{s_i} | T_i | \varphi_{t_i} \rangle$, from (9) we have

$$\begin{aligned} T_{st} &= \sum_{i=1}^d c_{i_{st}} \varepsilon(s_i + 1)^2 \delta_{s_i t_i} \\ &= \varepsilon \delta_{st} \sum_{i=1}^d (s_i + 1)^2, \end{aligned} \quad (12)$$

where we have used (1), (2) and (7).

Representation for V

Since $V_i = \langle \varphi_{s_i} | V_i | \varphi_{t_i} \rangle$, performing the indicated integrations, with φ_{s_i} and φ_{t_i} as given in (1) and noting that the only non-zero matrix elements of V_i are those for which s_i and t_i are of the same parity, we obtain

$$V_{i,s_i,t_i} = \frac{\lambda^2 \varepsilon}{2} \left[\frac{(1 - \delta_{s_i,t_i})}{(s_i - t_i)^2 + \delta_{s_i,t_i}} - \frac{(1 - \delta_{s_i,t_i})}{(s_i + t_i + 2)^2} \right] \cos^2 \left[(s_i - t_i) \frac{\pi}{2} \right] + \frac{\lambda^2 \varepsilon}{8} \delta_{s_i,t_i} \left[\frac{\pi^2}{6} - \frac{1}{(s_i + 1)^2} \right],$$

where $\lambda = \omega \hbar / \varepsilon = \varepsilon_\omega / \varepsilon$.

Substituting for V_{i,s_i,t_i} in the second of (9) and using (7) and (11), we obtain

$$V_{st} = \frac{\lambda^2 \varepsilon}{8} \delta_{st} \left[\frac{\pi^2 d}{6} - \sum_{i=1}^d \frac{1}{(s_i + 1)^2} \right] + \frac{\lambda^2 \varepsilon}{2} \delta_{\alpha_{st}, d-1} \sum_{i=1}^d \left\{ \left[\frac{(1 - \delta_{s_i,t_i})}{(s_i - t_i)^2 + \delta_{s_i,t_i}} - \frac{(1 - \delta_{s_i,t_i})}{(s_i + t_i + 2)^2} \right] \cos^2 \left[(s_i - t_i) \frac{\pi}{2} \right] \right\}.$$

We therefore see that off-diagonal survival of V_{st} is possible (but not guaranteed due to the presence of the \cos^2 term) only if $\alpha_{st} = d - 1$, that is only if there exists a $k \in [1, d]$ such that $s_i = t_i$ if $i \neq k$ but $s_k \neq t_k$, so that the vectors \mathbf{r} and \mathbf{s} differ *only* at the k^{th} entry.

Thus,

$$V_{st} = \frac{\lambda^2 \varepsilon}{8} \delta_{st} \left[\frac{\pi^2 d}{6} - \sum_{i=1}^d \frac{1}{(s_i + 1)^2} \right] + \frac{\lambda^2 \varepsilon}{2} \delta_{\alpha_{st}, d-1} \left[\frac{1}{(s_k - t_k)^2} - \frac{1}{(s_k + t_k + 2)^2} \right] \cos^2 \left[(s_k - t_k) \frac{\pi}{2} \right],$$

where

$$k = \sum_{j=1}^d j (1 - \delta_{s_j,t_j}) = \sum_{j=1}^d j (1 - \alpha_{j,st}).$$

Representation for H

Adding the matrix elements T_{st} and V_{st} we find that the matrix elements for the Hamiltonian of the d -dimensional oscillator, with the direct product of eigenstates of the particle in a one dimensional box as basis, are given by

$$H_{st} = \varepsilon \delta_{st} \sum_{i=1}^d (s_i + 1)^2 + \frac{\lambda^2 \varepsilon}{8} \delta_{st} \left[\frac{\pi^2 d}{6} - \sum_{i=1}^d \frac{1}{(s_i + 1)^2} \right] + \frac{\lambda^2 \varepsilon}{2} \delta_{\alpha_{st}, d-1} \left[\frac{1}{(s_k - t_k)^2} - \frac{1}{(s_k + t_k + 2)^2} \right] \cos^2 \left[(s_k - t_k) \frac{\pi}{2} \right],$$

where

$$k = \sum_{j=1}^d j(1 - \delta_{s_j t_j}) = \sum_{j=1}^d j(1 - \alpha_{j_{st}})$$

APPLICATION: APPROXIMATE ANALYTIC EXPRESSION FOR THE ENERGY SPECTRUM OF THE 1-DIMENSIONAL CHO

Based on our discussion in the previous sections culminating in the derivation of the explicit matrix elements of the d -dimensional confined harmonic oscillator, it is now straightforward, in principle, to find the eigenvalues of the oscillator. In practice however, the quantization remains a formidable task because of the exponential growth of the size of the Hamiltonian matrix with d . However, since the matrix elements are available in explicit form, they can be gainfully employed, for example in perturbation calculations, to obtain approximate analytical results.

It is our aim in the remaining part of this paper to derive an approximate analytic expression for the energy spectrum of the 1-dimensional confined harmonic oscillator. We will treat the potential energy of the confined oscillator as a perturbation of the kinetic energy term, the latter being the exactly solvable particle in a box Hamiltonian, with the non-degenerate eigenstates given in (1). Results from perturbation calculations, in the one dimensional case, can also be found in references BAIJAL and SINGH (1955), PADNOS (1965) and GUEORGUIEV *et al.* (2006).

Energy spectrum of the 1-dimensional cho

For the discussion of the confined harmonic oscillator in one dimension, it is convenient to drop the subscripts on s and t . Also we shall refer to H_i , V_i , T_i and x_i simply as H , V , T and x respectively. The eigenvalue problem is therefore

$$H|E_r\rangle = E_r|E_r\rangle, \quad r = 0, 1, 2, \dots, N-1.$$

Since the eigenstates of $T(x)$ are known, being the $\varphi_r(x)$ of (1), it is convenient, for small values of the classical oscillator frequency, ω , to treat $V(x)$ as a perturbation of the exactly solvable particle in a box Hamiltonian, $T(x)$, with ω^2 as the perturbation parameter.

By noting that $\delta_{\alpha_{st}^{d-1}} = \delta_{\alpha_{st}^0} = 1 - \delta_{st}$ we have

$$\begin{aligned} V_{st} &= \frac{\lambda^2 \varepsilon}{8} \delta_{st} \left[\frac{\pi^2}{6} - \frac{1}{(s+1)^2} \right] \\ &+ \frac{\lambda^2 \varepsilon}{2} \left[\frac{(1-\delta_{st})}{(s-t)^2 + \delta_{st}} - \frac{(1-\delta_{st})}{(s+t+2)^2} \right] \cos^2 \left[(s-t) \frac{\pi}{2} \right] \end{aligned} \quad (13)$$

and

$$\begin{aligned} H_{st} &= \varepsilon \delta_{st} (s+1)^2 + \frac{\lambda^2 \varepsilon}{8} \delta_{st} \left[\frac{\pi^2}{6} - \frac{1}{(s+1)^2} \right] \\ &+ \frac{\lambda^2 \varepsilon}{2} \left[\frac{(1-\delta_{st})}{(s-t)^2 + \delta_{st}} - \frac{(1-\delta_{st})}{(s+t+2)^2} \right] \cos^2 \left[(s-t) \frac{\pi}{2} \right]. \end{aligned}$$

Since the states $|E_r\rangle$ are non-degenerate, E_r can be approximated, using standard perturbation

theory, as

$$E_r \approx E_r^{(0)} + E_r^{(1)} + E_r^{(2)} + E_r^{(3)}.$$

The zeroth order correction to the energy of the one dimensional confined harmonic oscillator, $E_r^{(0)}$, being the energy of the one dimensional particle in a box and the first order correction, $E_r^{(1)}$, being the expectation value of the perturbation $V(x)$, in each state $\phi_r(x)$, are straightforward to calculate:

$$\begin{aligned} E_r^{(0)} &= \varepsilon_r = \varepsilon(r+1)^2, \quad \text{from} \\ &\text{and} \\ E_r^{(1)} = V_{rr} &= \frac{\lambda^2 \varepsilon}{8} \left[\frac{\pi^2}{6} - \frac{1}{(r+1)^2} \right], \quad \text{from} \\ &= \frac{\lambda^2 \varepsilon}{8} \left[\zeta(2) - \frac{1}{(r+1)^2} \right], \end{aligned}$$

where $\zeta(m)$ is the Riemann zeta function defined by

$$\zeta(m) = \sum_{r=1}^{\infty} \frac{1}{r^m}.$$

The second order correction to the energy of the one dimensional confined harmonic oscillator, $E_r^{(2)}$, is given by

$$E_r^{(2)} = \sum_{\substack{s=0 \\ s \neq r}}^{\infty} \frac{V_{rs} V_{sr}}{\varepsilon_{rs}} = \sum_{s=0}^{r-1} \frac{V_{rs} V_{sr}}{\varepsilon_{rs}} + \sum_{s=r+1}^{\infty} \frac{V_{rs} V_{sr}}{\varepsilon_{rs}}, \quad (14)$$

where

$$\varepsilon_{rs} = \varepsilon_r - \varepsilon_s = \varepsilon(r+s+2)(r-s), \quad (15)$$

so that

$$\begin{aligned} \frac{2\varepsilon(r+1)}{\varepsilon_{rs}} &= \frac{1}{(r+s+2)} + \frac{1}{(r-s)} \\ &\text{and} \\ \frac{2\varepsilon(s+1)}{\varepsilon_{rs}} &= -\frac{1}{(r+s+2)} + \frac{1}{(r-s)}. \end{aligned} \quad (16)$$

Since V is a real symmetric matrix, (14) is simply

$$E_r^{(2)} = \sum_{s=0}^{r-1} \frac{V_{rs}^2}{\varepsilon_{rs}} + \sum_{s=r+1}^{\infty} \frac{V_{rs}^2}{\varepsilon_{rs}}. \quad (17)$$

We note that the matrix elements occurring in (17) are necessarily off-diagonal ($s \neq r$). Furthermore the only surviving elements V_{rs} , according to (13), are those for which r and s are both odd or both even. It therefore follows from (13) that

$$\begin{aligned} V_{rs} &= \frac{\lambda^2 \varepsilon}{2} \left[\frac{1}{(r-s)^2} - \frac{1}{(r+s+2)^2} \right] \cos^2 \left[(s-t) \frac{\pi}{2} \right] \\ &= \frac{\lambda^2 \varepsilon}{2} \left(\frac{1}{(r-s)} - \frac{1}{(r+s+2)} \right) \left(\frac{1}{(r-s)} + \frac{1}{(r+s+2)} \right) \cos^2 \left[(r-s) \frac{\pi}{2} \right], \end{aligned}$$

and using (16) we have

$$V_{rs} = 2\lambda^2 \varepsilon^3 \frac{(r+1)(s+1)}{\varepsilon_{rs}^2} \cos^2 \left[(r-s) \frac{\pi}{2} \right], \quad s \neq r. \quad (18)$$

From (15) and (18) and noting that

$$\cos^4\left[(r-s)\frac{\pi}{2}\right] \equiv \cos^2\left[(r-s)\frac{\pi}{2}\right]$$

we have

$$\frac{V_{rs}^2}{\mathcal{E}_{rs}} = 4\lambda^4 \mathcal{E} \frac{(r+1)^2(s+1)^2}{(r-s)^5(r+s+2)^5} \cos^2\left[(r-s)\frac{\pi}{2}\right]$$

and thus (17) now becomes

$$\begin{aligned} E_r^{(2)} &= 4\lambda^4 \mathcal{E}(r+1)^2 \sum_{s=0}^{r-1} \frac{(s+1)^2}{(r-s)^5(r+s+2)^5} \cos^2\left[(r-s)\frac{\pi}{2}\right] \\ &\quad + 4\lambda^4 \mathcal{E}(r+1)^2 \sum_{s=r+1}^{\infty} \frac{(s+1)^2}{(r-s)^5(r+s+2)^5} \cos^2\left[(r-s)\frac{\pi}{2}\right]. \end{aligned} \quad (19)$$

Classifying the energy corrections in (19) by parity of r we have

$$E_q^{(2)} = 4\lambda^4 \mathcal{E}(q+1)^2 (A_q + B_q), \quad (20)$$

with

$$\begin{aligned} A_q &= \sum_{s=0}^{q-1} \frac{(s+1)^2}{(q-s)^5(q+s+2)^5} \cos^2\left[(q-s)\frac{\pi}{2}\right] \\ &\text{and} \\ B_q &= \sum_{s=q+1}^{\infty} \frac{(s+1)^2}{(q-s)^5(q+s+2)^5} \cos^2\left[(q-s)\frac{\pi}{2}\right], \end{aligned}$$

where $q = 2r$ for even levels and $q = 2r+1$ for odd levels.

Choosing

$$f_s = \frac{(s+1)^2}{(2r-s)^5(2r+s+2)^5} \cos^2\left[(2r-s)\frac{\pi}{2}\right]$$

in the following summation identity (see section 2.1.1 of GOULD 2011) for more general formulas)

$$\sum_{s=0}^M f_s = \sum_{s=0}^{(M-(M \bmod 2))/2} f_{2s} + \sum_{s=0}^{(M+(M \bmod 2))/2-1} f_{2s+1}, \quad (21)$$

allows us to write (noting that $f_{2s+1} = 0$ with the present choice of f_s)

$$\begin{aligned} A_{2r} &= \sum_{s=0}^{2r-1} \frac{(s+1)^2}{(2r-s)^5(2r+s+2)^5} \cos^2\left[(2r-s)\frac{\pi}{2}\right] \\ &= \sum_{s=0}^{r-1} \frac{(2s+1)^2}{(2r-2s)^5(2r+2s+2)^5} \\ &= \frac{1}{2^{10}} \sum_{s=0}^{r-1} \frac{(2s+1)^2}{(r-s)^5(r+s+1)^5} \end{aligned} \quad (22)$$

and

$$B_{2r} = \frac{1}{2^{10}} \sum_{s=r+1}^{\infty} \frac{(2s+1)^2}{(r-s)^5(r+s+1)^5}. \quad (23)$$

Similarly, taking identity (21) into consideration, we have

$$\begin{aligned} A_{2r+1} &= \sum_{s=0}^{2r} \frac{(s+1)^2}{(2r-s+1)^5(2r+s+3)^5} \cos^2\left[(2r-s+1)\frac{\pi}{2}\right] \\ &= \sum_{s=0}^{r-1} \frac{(2s+2)^2}{(2r-2s)^5(2r+2s+4)^5} \\ &= \frac{4}{2^{10}} \sum_{s=0}^{r-1} \frac{(s+1)^2}{(r-s)^5(r+s+2)^5} \end{aligned} \quad (24)$$

and

$$B_{2r+1} = \frac{4}{2^{10}} \sum_{s=r+1}^{\infty} \frac{(s+1)^2}{(r-s)^5 (r+s+2)^5}. \quad (25)$$

We note that the above results can be combined into

$$A_q = \sum_{s=0}^{r-1} \frac{(2s+1+q \bmod 2)^2}{(2r-2s)^5 (q+2s+2+q \bmod 2)^5}$$

and

$$B_q = \sum_{s=r+1}^{\infty} \frac{(2s+1+q \bmod 2)^2}{(2r-2s)^5 (q+2s+2+q \bmod 2)^5},$$

where $q = 2r$ or $q = 2r+1$.

The finite sums A_{2r} and A_{2r+1} as given in (22) and (24) as well as the infinite sums B_{2r} and B_{2r+1} as given in (23) and (25) are expressible in closed form, in terms of the well-studied polygamma functions; a computer algebra system, such as Waterloo Maple, comes in handy for this purpose. Putting the results together in (20), the final result is (see the Appendix for the Maple code)

$$E_r^{(2)} = \frac{\lambda^4 \varepsilon}{128} \left(\frac{\zeta(4)}{(r+1)^2} - \frac{5\zeta(2)}{(r+1)^4} + \frac{7}{(r+1)^6} \right), \quad r = 0, 1, 2, \dots$$

We remark that an equivalent result to ours, for $E_r^{(2)}$, can also be found in reference BAIJAL and SINGH (1955). The sum was however left unevaluated in that paper.

In standard non-degenerate perturbation theory, the third order correction to the energy of the one dimensional confined harmonic oscillator, $E_r^{(3)}$, is given by

$$E_r^{(3)} = \sum_{s=0}^N \sum_{t=0}^N \frac{V_{rs} V_{st} V_{tr}}{\varepsilon_{rs} \varepsilon_{rt}} - V_{rr} \sum_{s=0}^N \frac{V_{rs} V_{sr}}{\varepsilon_{rs}^2}.$$

Working exactly as in computing the second order corrections, while taking note of the following summation identity

$$\sum_{s=a}^N \sum_{t=a}^N f_{st} = \sum_{s=a}^N f_{ss} + \sum_{s=a}^{N-1} \sum_{t=s+1}^N (f_{st} + f_{ts}),$$

we find that $E_r^{(3)}$ is expressible in closed form, in terms of the polygamma functions. In the limit of $N \rightarrow \infty$ the result is

$$E_r^{(3)} = \frac{\lambda^6 \varepsilon}{2048} \left(\frac{\zeta(6)}{(r+1)^4} - \frac{60\zeta(4)}{(r+1)^6} + \frac{186\zeta(2)}{(r+1)^8} - \frac{242}{(r+1)^{10}} \right).$$

Thus, the energy corrections can be written as

$$E_r^{(m)} = \frac{\lambda^{2m} \varepsilon}{2^{4m-1}} \sum_{n=0}^m \frac{(-1)^n \zeta(2m-2n) c_n^{(m)}}{((r+1)^2)^{m+n-1}}, \quad m = 0, 1, 2, 3,$$

where

$$\begin{aligned}
c_0^{(0)} &= -1, \\
c_0^{(1)} &= 1, c_1^{(1)} = -2, \\
c_0^{(2)} &= 1, c_1^{(2)} = 5, c_2^{(2)} = -14 \\
&\text{and} \\
c_0^{(3)} &= 1, c_1^{(3)} = 60, c_2^{(3)} = 186, c_3^{(3)} = -484.
\end{aligned} \tag{26}$$

To the sixth order in the classical oscillator frequency, ω , therefore, the one dimensional cho has the energy spectrum

$$E_r \approx \sum_{m=0}^3 E_r^{(m)} = \sum_{m=0}^3 \left\{ \frac{\lambda^{2m} \varepsilon}{2^{4m-1}} \sum_{n=0}^m \frac{(-1)^n \zeta(2m-2n) c_n^{(m)}}{(r+1)^{m+n-1}} \right\}, \tag{27}$$

with $c_n^{(m)}$ as given in (26).

The form of (27) allows to conjecture the existence of an exact formula for the energy spectrum of the one dimensional confined harmonic oscillator, in the form

$$E_r = \sum_{m=0}^{\infty} E_r^{(m)} = \sum_{m=0}^{\infty} \left\{ \frac{\lambda^{2m} \varepsilon}{2^{4m-1}} \sum_{n=0}^m \frac{(-1)^n \zeta(2m-2n) c_n^{(m)}}{(r+1)^{m+n-1}} \right\}, \quad c_n^{(m)} \in \mathbf{Z} \setminus \{0\}.$$

SUMMARY

We have derived an explicit matrix representation for the d – dimensional confined harmonic oscillator, using the eigenstates of the kinetic energy operator as basis vectors.

We showed that the Hamiltonian

$$H(\mathbf{x}) = -\frac{\hbar^2}{2m} \sum_{i=1}^d \frac{\partial^2}{\partial x_i^2} + \frac{1}{2} m \omega^2 \sum_{i=1}^d x_i^2, \quad |x_i| \leq L,$$

has the explicit $N^d \times N^d$ matrix representation

$$\begin{aligned}
H_{st} &= \varepsilon \delta_{st} \sum_{i=1}^d (s_i + 1)^2 + \frac{\lambda^2 \varepsilon}{8} \delta_{st} \left[\frac{\pi^2 d}{6} - \sum_{i=1}^d \frac{1}{(s_i + 1)^2} \right] \\
&+ \frac{\lambda^2 \varepsilon}{2} \delta_{\alpha_{st}, d-1} \left[\frac{1}{(s_k - t_k)^2} - \frac{1}{(s_k + t_k + 2)^2} \right] \cos^2 \left[(s_k - t_k) \frac{\pi}{2} \right],
\end{aligned}$$

with

$$\varepsilon = \frac{\pi^2 \hbar^2}{8mL^2}, \quad \lambda = \omega \hbar / \varepsilon = \varepsilon_\omega / \varepsilon, \quad \alpha_{st} = \sum_{i=1}^d \alpha_{i_{st}} = \sum_{i=1}^d \delta_{s_i t_i}$$

and

$$k = \sum_{j=1}^d j \left(1 - \delta_{s_j t_j} \right) = \sum_{j=1}^d j \left(1 - \alpha_{j_{st}} \right),$$

where $s, t = 0, 1, 2, \dots, N^d - 1$ and

$$s_i = \left\lfloor \frac{s}{N^{d-i}} \right\rfloor \bmod N, \quad i = 1, 2, \dots, d$$

and

$$t_i = \left\lfloor \frac{t}{N^{d-i}} \right\rfloor \bmod N, \quad i = 1, 2, \dots, d.$$

In particular, for the one-dimensional confined harmonic oscillator, we have an $N \times N$ representation with the matrix elements given by

$$H_{st} = \varepsilon \delta_{st} (s+1)^2 + \frac{\lambda^2 \varepsilon}{8} \delta_{st} \left[\frac{\pi^2}{6} - \frac{1}{(s+1)^2} \right] \\ + \frac{\lambda^2 \varepsilon}{2} \left[\frac{1}{(s-t)^2 + \delta_{st}} - \frac{1}{(s+t+2)^2} \right] (1 - \delta_{st}) \cos^2 \left[(s-t) \frac{\pi}{2} \right],$$

for $s, t = 0, 1, 2, \dots, N-1$.

Finally, we derived the following approximate analytic expression for the energy spectrum of the 1-dimensional cho, to the sixth order in the oscillator frequency ω ,

$$E_r \approx \sum_{m=0}^3 E_r^{(m)} = \sum_{m=0}^3 \left\{ \frac{\lambda^{2m} \varepsilon}{2^{4m-1}} \sum_{n=0}^m \frac{(-1)^n \zeta(2m-2n) c_n^{(m)}}{(r+1)^{m+n-1}} \right\}, \quad r = 0, 1, 2, \dots, N,$$

with $c_n^{(m)}$ as given in (26).

APPENDIX

Maple code to determine $E_r^{(2)}$

```
=====
>summand:=q->(2*s+1+modp(q,2))^2/(2*r-2*s)^5/(q+2*s+2+modp(q,2))^5;
      summand := q -> \frac{(2s+1+\text{modp}(q,2))^2}{(2r-2s)^5(q+2s+2+\text{modp}(q,2))^5}
>A2r:=sum(summand(2*r),s=0..r-1):
# replace the last ":" with ";" to see the polygamma sums
>B2r:=sum(summand(2*r),s=r+1..infinity):
# replace ":" with ";" to see the polygamma sums
>E2r:=expand(simplify(4*(2*r+1)^2*(A2r+B2r))):
# we suppress the factor [lambda^4*epsilon]
># collect terms of the same order in Pi
E2r:=collect(% ,Pi):
>E2r:=factor(coeff(E2r,Pi^4))*Pi^4+factor(coeff(E2r,Pi^2))*Pi^2+op(3,E2r);
      E2r := \frac{\pi^4}{11520(2r+1)^2} - \frac{5\pi^2}{768(2r+1)^4} + \frac{7}{128(2r+1)^6}
># we now include the lambda^4*epsilon
E2r:=lambda^4*epsilon*E2r;
      E2r := \lambda^4 \varepsilon \left( \frac{\pi^4}{11520(2r+1)^2} - \frac{5\pi^2}{768(2r+1)^4} + \frac{7}{128(2r+1)^6} \right)
=====
```

Since $\zeta(2) = \pi^2/6$ and $\zeta(4) = \pi^4/90$ it follows that

$$E_{2r}^{(2)} = \frac{\lambda^4 \varepsilon}{128} \left(\frac{\zeta(4)}{(2r+1)^2} - \frac{5\zeta(2)}{(2r+1)^4} + \frac{7}{(2r+1)^6} \right). \quad (\text{A1})$$

Similarly running the above code with $\text{summand}(2r+1)$ gives

$$E_{2r+1}^{(2)} = \frac{\lambda^4 \varepsilon}{128} \left(\frac{\zeta(4)}{(2r+2)^2} - \frac{5\zeta(2)}{(2r+2)^4} + \frac{7}{(2r+2)^6} \right). \quad (\text{A2})$$

From (A1) and (A2) we conclude that

$$E_r^{(2)} = \frac{\lambda^4 \varepsilon}{128} \left(\frac{\zeta(4)}{(r+1)^2} - \frac{5\zeta(2)}{(r+1)^4} + \frac{7}{(r+1)^6} \right).$$

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