On the diagonalization of quadratic Hamiltonians

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Abstract
A new procedure to diagonalize quadratic Hamiltonians is introduced. We show that one can establish the diagonalization of a quadratic Hamiltonian by changing the frame of reference by a unitary transformation. We give a general method to diagonalize an arbitrary quadratic Hamiltonian and derive a few of the simplest special cases in detail.

Keywords: quadratic Hamiltonian, coupled harmonic oscillators, entanglement

1. Introduction

Quadratic Hamiltonian plays a special role in the history of quantum physics. Not only being a famous solvable example at the dawn of quantum mechanics, it is exact physical Hamiltonian for such fundamental quantum systems as a quantized electromagnetic field in a vacuum and a free electron in a uniform magnetic field. The range of validity of the quadratic Hamiltonian is vast. For instance, the Hamiltonians of this form appear whenever one studies the nuclear contribution in the Born–Oppenheimer (BO) approximation [1, 2] and in the description of nuclear dynamics beyond the BO approximation [3, 4]. Therefore these Hamiltonians play a central role in the study of phonon spectrum in crystals [5–9], conventional superconductivity [10–12], thermal conductivities [13–15] and molecular vibrations [16]. Further, these Hamiltonians are also relevant in the study of quantum entanglement [17–27], in the field of quantum optics [28] and in the analysis of light–matter interaction within full quantum description [29, 30].

The exact diagonalization of the quadratic Hamiltonian is a standard procedure which can be done with different approaches. From these available approaches, one can choose the most
suitable one for the problem at hand. For instance, the phonon representation is useful in the field of lattice dynamics [2] and normal coordinates in the study of molecular vibrations [16]. Yet another way is to use symplectic transformations [31, 32] to establish the diagonalization which has turned out to be useful in the study of entanglement [22, 33, 34]. What unites these approaches is that after the transformation the Hamiltonian is diagonal in the new coordinates which in turn are some collective coordinates of the original position and momentum variables.

In this work, we take yet another root and diagonalize the quadratic Hamiltonian by changing the frame of reference [35, 36] by a unitary transformation. Similar transformations were introduced in reference [37]. The transformed Hamiltonian is diagonal, but this time in the original position and momentum variables the difference of the original and transformed Hamiltonians being in the masses and coupling constants.

This paper is organized as follows. In section 2, the generic quadratic Hamiltonian is given, we discuss some of its properties and how the diagonalization is usually established. We introduce a transformation to diagonalize generic \( n \)-body quadratic Hamiltonians in section 3 and discuss the physical interpretation of our results. A special case of two-body system is discussed in section 4.1 and one dimensional chain with nearest neighbour interactions in section 4.2. We consider the three-body case in appendix A.

2. Quadratic Hamiltonians

The object of our study is the quadratic Hamiltonian of the form

\[
H = \sum_{i} \frac{p_i^2}{2m_i} + \sum_{i,j} \frac{\Phi_{ij} \mu_i \mu_j}{\sqrt{m_im_j}},
\]

where \( m_i \) is the mass of the \( i \)th particle, \( u_i \) the position operator of the particle \( i \) and \( p_i = -i\hbar \partial / \partial u_i \) the corresponding momentum. The quantities \( \Phi_{ij} \) are the coupling constants and will be considered as real parameters. For example, in the BO context, the quantities \( \Phi_{ij} \) are the so-called interatomic force constants, the second-order derivatives of the BO energy surface with respect to the nuclear equilibrium positions. There are many alternative approaches to diagonalize quadratic Hamiltonians like \( H \) and here we provide a summary of them. By doing so, we obtain some central results to be compared with those obtained in this work.

From the structure of the Hamiltonian \( H \) it follows that we can write the potential part in terms of symmetric parameters. Sometimes the parameters \( \Phi_{ij} \) are symmetric themselves. For such symmetric matrices, the diagonalization can be established by an orthogonal coordinate transformation. For the sake of clarity we summarize the diagonalization procedure [2]. We assume that the parameters are symmetric \( \Phi_{ij} = \Phi_{ji} \). The symmetric matrix \( D_{ij} \equiv \Phi_{ij}/\sqrt{m_im_j} \) satisfies

\[
\omega_s^2 e_{is} = \sum_j D_{ij} e_{js}, \quad s = 1, \ldots, n,
\]

where the eigenvectors have the following properties

\[
\sum_i e_{is} e_{it} = \delta_{st}, \quad \sum_s e_{is} e_{ts} = \delta_{it}.
\]
We transform the Hamiltonian to mass scaled coordinates \( w_i \equiv \sqrt{m_i} u_i \) and then transform these coordinates with the eigenvectors as

\[
    w_i = \sum_s e_{is} q_s.
\]

(4)

After establishing the corresponding transformations for momentum we obtain the diagonal form of the Hamiltonian

\[
    H = \frac{1}{2} \sum_{s=1}^n \left( -\hbar^2 \frac{\partial^2}{\partial q^2_s} + \omega_s^2 q^2_s \right).
\]

(5)

and thus the eigenfunctions of \( H \) can be written as \( \psi(q) = \psi(q_1) \ldots \psi(q_n) \), each of the functions \( \psi(q_s) \) being of a simple harmonic oscillator form (here we use \( q \) for all the normal coordinates). By solving equation (4) for \( q_s \), we see that each of the functions \( \psi(q_s) \) involve a linear combination of the original coordinates \( u_i \). We can further write equation (5) in terms of creation and annihilation operators as

\[
    H = \sum_{s=1}^n \hbar \omega_s \left( \frac{1}{2} + b_s^{\dagger} b_s \right).
\]

(6)

Here, the creation operator is defined as \( b_s^{\dagger} \equiv (\omega_s q_s - ip_s) / \sqrt{2\hbar \omega_s} \) and \( p_s = -i\hbar \partial / \partial q_s \). The interpretation of \( b_s^{\dagger} \) is that it creates a quantum of energy \( \hbar \omega_s \) on the vibrational mode \( s \). This vibrational mode \( s \) comprises a collective motion of several particles described by the coordinates \( u_i \), which can be verified by solving the coordinates \( q_s \) from equation (4). This collective motion is due to the non-diagonal interaction terms in the Hamiltonian and the strength of the interaction is determined by the parameters \( \Phi_{ij} \). If \( \Phi_{ij} = 0 \) for all \( i \neq j \), the Hamiltonian given by equation (1) describes independent harmonic oscillators with the frequencies \( \omega^2_i = \Phi_{ii} / m_i \). We refer to the frequency \( \omega_i \) as the frequency of the \( i \)th independent harmonic oscillator.

With the non-diagonal terms vanishing, each of the particle coordinates \( u_i \) are independent and the total wave function is of the product form. These functions for each \( u_i \) are of a simple harmonic oscillator form.

Another commonly used approach to diagonalize \( H \) is the use of phonon coordinates [2, 38]. The procedure comprises establishing the transformation to mass scaled coordinates, Fourier transforming the mass scaled coordinates (periodic boundary conditions used) and finally transforming to the phonon coordinates by using the eigenvectors of the dynamical matrix. The dynamical matrix is the Fourier transform of the interatomic force constant matrix (\( D_{ij} \) in our notation). After this procedure, the Hamiltonian is again diagonal and can be written in terms of creation and annihilation operators as in equation (6), but this time the collective coordinates are different. However, the principle and the physical picture remains similar and in the excitation of a phonon mode, a collective excitation of the original particle coordinates occurs.

The approach [31, 32] used in the field of entanglement [22, 33, 34] does not differ from the aforementioned approaches in that the diagonal form of the Hamiltonian is obtained in the transformed coordinates. The transformed coordinates, in turn, involve two or more of the original position observables.
3. New diagonalization procedure

Here we introduce a new transformation to diagonalize $H$. The starting point is the time-independent Schrödinger equation

$$H\chi = E\chi.$$  \hfill (7)

We assume that $U\tilde{\chi} = \chi$, where $U$ is some suitable transformation, an explicit form of which will be given later. We write the corresponding Schrödinger equation for the transformed system as

$$\tilde{H}\tilde{\chi} = E\tilde{\chi}, \quad \tilde{H} = U^{-1}HU.$$  \hfill (8)

We seek a transformation $U$ such that $\tilde{H}$ is diagonal. Consider a transformation of the form

$$U \equiv e^{\alpha u_1 \frac{\partial}{\partial u_2}}, \quad U^{-1} = e^{-\alpha u_1 \frac{\partial}{\partial u_2}},$$  \hfill (9)

where $\alpha$ is some real parameter. We see that the operator $u_1 \partial / \partial u_2 = iu_1 p_2 / \hbar$ is Hermitian and therefore $U$ is unitary, $U^{-1} = U^\dagger$. The transformation $U$ is a translation operator such that when we act on a function $f(u_1,u_2)$ it follows that

$$Uf(u_1,u_2) = f(u_1,u_2 + \alpha u_1),$$

$$U^\dagger f(u_1,u_2) = f(u_1,u_2 - \alpha u_1).$$  \hfill (10)

With equations (9) and (10) we can show that

$$U^\dagger u_1 U = u_1, \quad U^\dagger u_2 U = u_2 - \alpha u_1,$$

$$U^\dagger p_2 U = p_2, \quad U^\dagger p_1 U = \alpha p_2 + p_1.$$  \hfill (11)

Given these results we see that the quadratic Hamiltonian $H$ is still quadratic after the transformation. That is, $\tilde{H}$ is quadratic after using $U$ given by equation (9). However, the Hamiltonian is not necessary diagonal and in general non-diagonal terms appear also in the kinetic energy. We claim that we can find a suitable form of $U$ and parameters like $\alpha$ such that the resulting quadratic Hamiltonian $\tilde{H}$ is diagonal. With these results in mind, we formulate our new diagonalization procedure in the general case as follows.

We re-write the Hamiltonian of equation (1) as

$$H = \sum_{i} \frac{p_i^2}{2m_i} + \sum_{i} d_i u_i^2 + \sum_{i<j} d_{ij} u_i u_j,$$  \hfill (12)

where

$$d_i \equiv \frac{1}{2} \Phi_{ii}, \quad d_{ij} \equiv \frac{1}{2} (\Phi_{ij} + \Phi_{ji}).$$  \hfill (13)

We would like to find a transformation which acts on all the cross terms with the parameters $d_{ij}$ separately and thus the number of these transformations is $1/2 \left( \frac{n(n-1)}{2} \right) \equiv N$. We choose
the total transformation as
\[ U \equiv U_1 \ldots U_N, \]
\[ U_1 = \exp \left[ \alpha_1 u_2 \frac{\partial}{\partial u_1} \right] \exp \left[ \beta_1 u_1 \frac{\partial}{\partial u_2} \right], \]
\[ U_2 = \exp \left[ \alpha_2 u_3 \frac{\partial}{\partial u_1} \right] \exp \left[ \beta_2 u_1 \frac{\partial}{\partial u_3} \right], \]
\[ \vdots \]
\[ U_N = \exp \left[ \alpha_N u_{N+1} \frac{\partial}{\partial u_1} \right] \exp \left[ \beta_{N-1} u_{N-1} \frac{\partial}{\partial u_N} \right], \]
where
\[ \beta_1 = -\frac{\alpha_1}{\alpha_1 + \frac{m_1}{m}}, \]
\[ \beta_2 = -\frac{\alpha_2}{\alpha_2 + \frac{m_1}{m}}, \]
\[ \vdots \]
\[ \beta_N = -\frac{\alpha_N}{\alpha_N + \frac{m_{N-1}}{m_{N-1}}}. \]

After each of the transformations, \( U_k \), the Hamiltonian \( \tilde{H} \) remains quadratic. After the transformation, the Hamiltonian can be written as
\[ \tilde{H} = \sum_i \frac{p_i'^2}{2m_i} + \sum_i d_i u_i'^2 + \sum_{i<j} \tilde{d}_{ij} u_i' u_j, \]
where \( u_i' \equiv U^\dagger u_i U \) and \( p_i' \equiv U^\dagger p_i U \). The original and transformed observables satisfy the canonical commutation relations \([u_i, p_j] = [u_i', p_j'] = i\hbar \delta_{ij}\). We can write the transformed observables \( u_i', p_i' \) in terms of the original ones \( u_i, p_i \) and thus we write equation (16) as
\[ \tilde{H} = \sum_i \frac{p_i'^2}{2m_i} + \sum_{i,j} T_{ij} p_i p_j + \sum_i d_i u_i'^2 + \sum_{i<j} \tilde{d}_{ij} u_i u_j. \]

The aim is to find the parameters \( \alpha_k, \beta_k \) such that
\[ T_{ij} = 0, \quad \tilde{d}_{ij} = 0, \]
for all \( i,j \). It turns out that \( T_{ij} = 0 \) is automatically satisfied when we use \( \beta_k \) given by equation (15), we see this when we go through the two-body case explicitly in section 4.1. What is left is to solve the \( N \) equations \( \tilde{d}_{ij} = 0 \) such that each \( \alpha_k \) can be written as a function of the original parameters \( m_i, d_i \) and \( d_{ij} \). If equation (18) holds, the transformed Hamiltonian reads
\[ \tilde{H} = \sum_{i=1}^{n} \left( \frac{p_i^2}{2\tilde{m}_i} + \tilde{d}_i u_i^2 \right), \]  
(19)

and we have reached our goal. We can further write equation (19) in terms of creation and annihilation operators as

\[ \tilde{H} = \sum_{i=1}^{n} \hbar \omega_i \left( \frac{1}{2} + a_i^\dagger a_i \right), \]  
(20)

where \( \omega_i \equiv 2\tilde{d}_i/\tilde{m}_i \) and the creation operator is defined as \( a_i^\dagger \equiv (\bar{\tilde{m}}_i \bar{\omega}_i u_i - ip_i) / \sqrt{2\tilde{m}_i \hbar \bar{\omega}_i} \). These operators satisfy

\[ [a_i, a_j^\dagger] = \delta_{ij}, \quad [a_i, a_j] = [a_i^\dagger, a_j^\dagger] = 0, \]  
(21)

and the physical interpretation of these operators is the usual one [39]. The resulting Hamiltonian \( \tilde{H} \) is diagonal and all the original interactions are hidden in the masses \( \tilde{m}_i \) and coefficients \( \tilde{d}_i \), which we call the effective masses and the effective force constants. Therefore a general quadratic Hamiltonian \( H \) can be transformed to a diagonal form such that the resulting Hamiltonian \( \tilde{H} \) seems to be the one of \( n \) independent harmonic oscillators. We note that the position \( u_i \) and momentum operators \( p_i \) in \( \tilde{H} \) are still the original observables, not the collective ones as in the case of conventional techniques in diagonalizing the quadratic Hamiltonian. The system seems to have only the non-interacting independent harmonic oscillators in terms of the original position observables, even though we are still working with the exact Hamiltonian. The independent harmonic oscillators are, however, different from those we obtain from the original Hamiltonian due to the effective masses \( \tilde{m}_i \) and coefficients \( \tilde{d}_i \) leading to the effective frequencies \( \bar{\omega}_i \). We have only assumed that the \( \Phi_{ij} \) are real constants and our method is valid for all such cases. With some values of \( \Phi_{ij} \) and masses, the transformed coefficients \( \tilde{d}_i \) could be negative. In such cases the frequencies \( \bar{\omega}_i \) are purely imaginary and the Hamiltonian is called the inverted oscillator Hamiltonian. The inverted Hamiltonian has also significance in describing physical systems [40–42]. In the molecular vibration and lattice dynamical application, the imaginary frequencies imply that the system is unstable [2] and such systems are not usually physically relevant. We provide the stability conditions for a particular two-body case in appendix B.

The solution of the corresponding Schrödinger equation is known and for instance the ground state wave function \( \tilde{\chi}_0 \) satisfying \( \tilde{H}\tilde{\chi}_0 = E_0\tilde{\chi}_0 \) (equation (8) for the ground state) can be written in terms of the functions

\[ \tilde{\chi}_0 (u) = \left( \frac{\tilde{m}_i \bar{\omega}_i}{\pi \hbar} \right)^{1/4} \exp \left[ -\frac{\tilde{m}_i \bar{\omega}_i}{2\hbar} u_i^2 \right], \]  
(22)

such that \( \tilde{\chi}_0 (u) = \tilde{\chi}_0 (u_1) \ldots \tilde{\chi}_0 (u_n) \), where we use \( u \) for all the position observables. The total wave function is thus a product of the single particle functions since \( \tilde{H} \) is diagonal. This means, by definition, that the wave function \( \tilde{\chi} \) satisfying equation (8) is not entangled [43]. On the other hand, the wave function for the Hamiltonian \( H \) with cross terms is entangled from which we deduce that the transformation \( U^\dagger \) disentangles the entangled wave function \( \chi \) when it acts on it, namely \( \tilde{\chi} = U^\dagger \chi \). Therefore, \( U^\dagger \) is a disentangling transformation of the quadratic Hamiltonian wave functions satisfying equation (7). The explicit form of such disentangling transformation can be seen by looking equations (14) and (15).

Here we described our new and general procedure to diagonalize quadratic Hamiltonians. Whether or not we are able to diagonalize the Hamiltonian with \( U \) given by equation (14)
depends on the fact, whether or not we are able to solve equation (18). To answer this question, we discuss the two-body special case in section 4.1 and the special $n$-body case with the nearest neighbour interactions in section 4.2. We consider the three-body case in appendix A.

3.1. Physical interpretation

In order to give a physical interpretation of our method we first consider the following situation. For now, let the unitary transformation $T$ connecting one particle wave functions $\tilde{\chi} = \chi$ be a translation by a constant $a$ in one dimension, namely $T\tilde{\chi}(u_1) = \tilde{\chi}(u_1 + a)$ for one-body case. We have $T^\dagger u_1 T = u_1 - a = u'_1$, by following the convention of equation (16) for the position operator. We have for the expectation value of the position operator

$$\langle \chi | \hat{u}_1 | \chi \rangle = \langle \tilde{\chi} | \hat{T}^\dagger \hat{u}_1 \hat{T} | \tilde{\chi} \rangle = \langle \tilde{\chi} | \hat{u}'_1 | \tilde{\chi} \rangle.$$  

(23)

The result obtained implies that the expected value of position for the original position observable, taken with respect to the original states, is the same as the expected value of translated position operator $\hat{u}'_1 = \hat{u}_1 - a$, taken with respect to the translated states. However, from equation (23) it follows that $\langle \chi | \hat{u}_1 | \chi \rangle = \langle \tilde{\chi} | \hat{u}_1 | \tilde{\chi} \rangle - a$ and thus, when one measures the original position observable with respect to the translated states $\langle \tilde{\chi} | \hat{u}_1 | \tilde{\chi} \rangle = \langle \chi | \hat{u}_1 | \chi \rangle + a$. The result therefore depends on the states with respect to which we measure the observables. One observer measures for the original observable the value $\langle \chi | \hat{u}_1 | \chi \rangle$, while other observer, translated from the original observer by a constant $a$, measures for the original position observable the value $\langle \chi | \hat{u}_1 | \chi \rangle + a$. In other words, we have changed the original reference frame to another one, translated by a constant $a$ from the original one. The unitary transformation $T$ connects the states and observables in different frames of reference.

This discussion is analogous to our method to diagonalize a quadratic Hamiltonian. The transformation $U$ in equation (14) maps the original observables to observables of relative position and momenta and can be interpreted as a change of reference frame [35, 36], to a frame of relative observables. After fixing the functional form of the unitary transformation by equation (14), the choice of the reference frame depends only on the masses and interactions of the particles in the original frame of reference $F$ through the parameters $\alpha_i$. The Hamiltonian of equation (17) satisfies the Schrödinger equation in the new frame of reference $\tilde{F}$ described by the states $\tilde{\chi}$. As in our example, the observer in $\tilde{F}$ sees the system from a different point of view and consequently the states $\tilde{\chi}$ are disentangled meaning that the entanglement is a frame-dependent feature [36]. The change of the frame of reference causes some peculiar consequences. For instance, the conduction of heat in semiconducting materials is mostly transmitted by the lattice vibrations described by the Hamiltonian of equation (1) [13, 14]. The propagation of energy from one oscillator to another naturally requires interactions between the individual oscillators which are present in $F$. However, the observer in $\tilde{F}$ sees only the non-interacting effective oscillators and the propagation of energy by the observables $u$ and $p$ in $\tilde{F}$ is absent.

To summarize, in our method we change the reference frame from $F$ to $\tilde{F}$ and the system is non-interacting in $\tilde{F}$ with respect to the original observables while it is interacting and entangled in $F$. In the conventional collective coordinate approach, the collective modes of vibration appear to be non-interacting in $F$. Both methods give the same results when we consider the original observables in $F$. 


4. Special cases

4.1. Two-body case

Here we consider the two-body case by setting \( n = 2 \) in equation (12). We diagonalize \( H \) by transformation of the form (see equation (14))

\[
U = e^{\alpha u_1 \frac{\partial}{m_1}} e^{\beta u_2 \frac{\partial}{m_2}}.
\] (24)

We find that with this choice of \( U \), the position operators \( u_i \) and the corresponding momentum operators \( p_i \) transform as

\[
\begin{align*}
U^\dagger u_1 U &= u_1 (1 + \alpha \beta) - \alpha u_2, \\
U^\dagger u_2 U &= u_2 - \beta u_1, \\
U^\dagger p_1 U &= \beta p_2 + p_1, \\
U^\dagger p_2 U &= (1 + \alpha \beta) p_2 + \alpha p_1,
\end{align*}
\] (25)

and the remaining relations can be found, for instance, by using \( U^\dagger u_i U = U^\dagger u_i U U^\dagger u_j U \) and then equation (25). By using these results, we find that the condition \( T_{ij} = 0 \) (equation (18)) in the present case reads

\[
0 = \frac{\beta}{m_1} + \frac{(1 + \alpha \beta) \alpha}{m_2} \Leftrightarrow \beta = -\frac{\alpha (m_2 - m_1)}{m_1 + \alpha^2},
\] (26)

and therefore, with this choice of \( \beta \), the kinetic energy is diagonal. Since the general transformation 14 is product of transformations 24, the kinetic energy is diagonal after transforming the Hamiltonian of equation (12) by \( U \) given by equation (14). The condition \( \tilde{d}_{ij} = 0 \) of equation (18) can be written in the present case as

\[
0 = d_{12} (1 + 2 \alpha \beta) - 2d_1 \alpha (1 + \alpha \beta) - 2d_2 \beta \Leftrightarrow 0 = a \alpha^2 + b \alpha + c,
\] (27)

where (we use \( k_{ij} \equiv m_i/m_j \))

\[
a \equiv -d_{12}, \quad b \equiv -2(d_{k_21} - d_{22}), \quad c \equiv d_{12} k_{21}.
\] (28)

We solve equation (27) for \( \alpha \) and thus

\[
\alpha = -\frac{d_{12} k_{21} - d_2 \pm \sqrt{(d_{12} k_{21} - d_2)^2 + d_{12}^2 k_{21}^2}}{d_{12}}.
\] (29)

Either of the solutions of equation (29) with \( \pm \) for \( \alpha \) is acceptable. We have now obtained the diagonal form of the Hamiltonian \( \tilde{H} \) given by equation (19) with \( n = 2 \) and the corresponding
effective masses and coefficients can be written as
\[
\bar{m}_1 \equiv \frac{m_1 m_2}{m_2 + m_1 \alpha^2}, \quad \bar{m}_2 \equiv m_2 + m_1 \alpha^2, \quad \bar{d}_1 \equiv \frac{d_1 + d_{12} k_{12} \alpha + d_2 k_{12}^2 \alpha^2}{(1 + k_{12}^2 \alpha^2)^2}, \quad \bar{d}_2 \equiv d_1 \alpha^2 + d_2 - d_{12} \alpha.
\] (30)

We found that the system of two coupled harmonic oscillators can be considered as two independent \((n = 2)\) harmonic oscillators still written in terms of the original operators of position and momentum, but with the effective masses \(\bar{m}\) and force constants \(\bar{d}\). The stability conditions, relevant for example in the molecular vibration and lattice dynamical case, are considered in appendix B.

We write down the explicit form of the entangled wave function as an example. For simplicity, we assume that the particles are identical and therefore
\[
\alpha = \mp \left| \frac{d_{12}}{d_{12}} \right|, \quad \bar{m}_1 = m/2, \quad \bar{m}_2 = 4 \bar{m}_1,
\]
\[
\bar{\omega}_1^2 = \frac{2 d_1 + d_{12} \alpha}{m} = \frac{\Phi_{11} - \Phi_{12}}{m}, \quad \bar{\omega}_2^2 = \frac{2 d_1 - d_{12} \alpha}{m} = \frac{\Phi_{11} + \Phi_{12}}{m},
\] (31)

where we have chosen the solution \(\alpha = -1\) in all cases, what ever the value of \(\left| \frac{d_{12}}{d_{12}} \right|\) is and we denoted \(m_1 \equiv m\). Here the stability condition simplifies to \(0 < \Phi_{11} - |\Phi_{12}|\) and is the same as in the normal coordinate approach. We can find the exact wave function satisfying the corresponding Schrödinger equation written for the Hamiltonian \(H\) by using \(\tilde{\chi} = U\chi\). Any two-body eigenfunction of \(H\) can be written as \(\chi(u) = \tilde{\chi}(\tilde{u}_1) \tilde{\chi}(\tilde{u}_2)\), where \(\tilde{u}_1 = u_1 + \alpha u_2\) and \(\tilde{u}_2 = u_2 + \beta (u_1 + \alpha u_2)\). The explicit form of the entangled \(\chi_0(u)\) can be therefore found by using these results together with equation (22) and in the present case
\[
\chi_0(u) = \left(\frac{m \bar{\omega}_1}{\pi \hbar}\right)^{1/4} \exp \left[ -\frac{m}{4\hbar} (\bar{\omega}_1 + \bar{\omega}_2) u_1^2 \right] \times \left(\frac{m \bar{\omega}_2}{\pi \hbar}\right)^{1/4} \exp \left[ -\frac{m}{4\hbar} (\bar{\omega}_1 + \bar{\omega}_2) u_2^2 \right] \times \exp \left[ \alpha \frac{m}{2\hbar} (\bar{\omega}_2 - \bar{\omega}_1) u_1 u_2 \right].
\] (32)
The last term of equation (32) is the entangled part while the first two terms are the independent harmonic oscillator ground state functions. We see that the entanglement is only dependent on the force constants \(\Phi_{ij}\) and the mass of the particles.

The eigenfunctions \(\chi(u)\) will be the same when obtained by the normal coordinate approach. In the present case the eigenvector components can be written as \(e_{11} = e_{12} = e_{22} = 1/\sqrt{2}\) and \(e_{21} = -1/\sqrt{2}\). The eigenvalues from equation (2) are \(\bar{\omega}_1^2 = (\Phi_{11} - \Phi_{12})/m = \bar{\omega}_1^2\) and \(\bar{\omega}_2^2 = (\Phi_{11} + \Phi_{12})/m = \bar{\omega}_2^2\). The eigenvalues and the stability conditions are therefore the same with both methods. The ground state eigenfunction of equation (5) is of the form \(\psi_0(q) = \psi_0(q_1) \psi_0(q_2)\) such that \(\psi_0(q_j) = (\omega_j/\pi \hbar)^{1/4} \exp[-\omega_j q_j^2/2\hbar]\), which are normalized as \(1 = \int dq_1 dq_2 |\psi_0(q_j)|^2\). The final step is to write \(q\) as a function of \(u\) and establish integration by substitution in the latter normalizing condition and we finally find that \(\chi_0(u) = \sqrt{m} \psi_0(q)\), which is given by equation (32).
4.2. Chain with nearest neighbour interaction

In this section we consider a special case of the $n$-body Hamiltonian given by equation (12) with the nearest neighbour interactions. We can think of the situation as follows. Consider a linear chain of $n$ particles with one spatial dimension only. Suppose that the particles are arranged such that the observable $u_i$ is for the particle which is in the vicinity of the left most site, $u_2$ to the right-hand side of this site and so on. The right most particle site is described with the observable $u_n$. If some periodic boundary conditions are imposed, then $u_1$ and $u_n$ could be observables of neighbouring sites. We further assume that only the nearest neighbours interact with each other, that is, in equation (12) we set $d_{ij} = 0$ if $|i - j| > 1$. With this assumption we write equation (12) as

$$H = \sum_{i=1}^{n} \frac{p_i^2}{2m_i} + \sum_{i=1}^{n} d_i u_i^2 + \sum_{i}^{n-1} d_{i(i+1)} u_i u_{i+1}. \quad (33)$$

In order to make use of our earlier results obtained for the two-body case we rearrange the Hamiltonian and write

$$H = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} + d_1 u_1^2 + d_2 u_2^2 + d_{12} u_1 u_2 + \cdots$$

$$+ \frac{p_{n-1}^2}{2m_{n-1}} + \frac{p_n^2}{2m_n} + d_{n-1} u_{n-1}^2 + d_n u_n^2 + d_{(n-1)n} u_{n-1} u_n. \quad (34)$$

We assume that $n$ is an even number. By doing so we do not miss any relevant properties of the system provided $n$ is sufficiently large. It can be seen that in the present case, the $n$-body Hamiltonian can be written as a sum of two-body Hamiltonians which we have already diagonalized in section 4.1. That is, we need $n/2$ transformations to diagonalize this particular $n$-body Hamiltonian and we already know the resulting Hamiltonian and the quantities related from our previous results. Namely, the resulting Hamiltonian is given by equation (19) and it can be obtained with the following transformations and the other quantities involved

$$U_i \equiv \exp \left[ \alpha_i u_i \frac{\partial}{\partial u_i} \right] \exp \left[ -\frac{\alpha_i}{\alpha_i^2 + \frac{\beta_{i-1}}{m_{i-1}}} u_i \frac{\partial}{\partial u_i} \right],$$

$$\alpha_i = -\frac{d_{i-1} k_{i(i-1)} - d_i \pm \sqrt{\left[d_{i-1} k_{i(i-1)} - d_i\right]^2 + d_{j(i-1)}^2 k_{i(i-1)}^2}}{d_{(i-1)n}},$$

$$\tilde{m}_{i-1} = \frac{m_{i-1} m_i}{m_i + m_{i-1} \alpha_i^2}, \quad \tilde{m}_i = m_i + m_{i-1} \alpha_i^2, \quad \tilde{d}_{i-1} = \frac{d_{i-1} + d_{i-1} k_{i(i-1)} \alpha_i + d_{j(i-1)}^2 k_{i(i-1)}^2}{\left[1 + k_{(i-1)\alpha_i^2}^2\right]^2},$$

$$\tilde{d}_i = d_{i-1} \alpha_i^2 + d_i - d_{(i-1)\alpha_i}, \quad (35)$$

where $i = 2, 4, \ldots, n$. We have therefore diagonalized the $n$-body Hamiltonian completely with all the quantities given in closed form as functions of the original parameters of the Hamiltonian, $m_i, d_i, d_{ij}$. Here the stability conditions can be derived in a similar way as in the two-body case considered in appendix B.

In the case of Bravais chains all the masses $m_i$ and the force constants $d_i$ are the same. We therefore denote these quantities as $m_1 \equiv m$ and $d_1 = d_i$ for all $i$. Moreover, the coefficients $d_{ij}$
have the following symmetry \( d_{i(k+k+1)} \) for any suitable integer \( k \). From this it follows that we can denote \( d_{i-1} = d_{i+1} = d_{12} \) for all \( i \). With these identifications, we write in the Bravais chain case for the quantities in equation (35)

\[
\begin{align*}
\tilde{m}_{i-1} &= \frac{m}{2}, & \tilde{m}_i &= 2m, \\
\tilde{d}_{i-1} &= \frac{2d_1 \mp |d_{12}|}{4}, & \tilde{d}_i &= 2d_1 \pm |d_{12}|, \\
\alpha_i &= \mp |d_{12}| / d_{12}, & i &= 2, 4, \ldots, n.
\end{align*}
\]

(36)

From these results we obtain the frequencies

\[
\omega^2_i = \frac{\Phi_{11} + \Phi_{12}}{m}, \quad \tilde{\omega}^2_i = \frac{\Phi_{11} - \Phi_{12}}{m}, \quad i = 2, 4, \ldots, n.
\]

(37)

Here we used equation (13), assumed that \( \Phi_{ij} = \Phi_{ji} \) and we have chosen the solution \( \alpha_i = -1 \) in all cases, whatever the value of \( |d_{12}| / d_{12} \) is. We have \( n \) frequencies in total, but only two possible values for them.

The Hamiltonian given by equation (33) can be also diagonalized by using other methods like the normal coordinate transformation discussed in section 2. In the following, the Bravais chain is considered. We write the Hamiltonian in terms of the quantities \( \Phi_{ij} \), apply the scale transformation \( w_i = \sqrt{m_i} u_i \) and then write an eigenvalue equation for the matrix \( D_{ij} = \Phi_{ij} / \sqrt{m_i m_j} \). The matrix \( D \) is a tridiagonal Toeplitz matrix with the following eigenvalues and eigenvectors

\[
\omega^2_j = \frac{\Phi_{11}}{m} + 2 \frac{\Phi_{12}}{m} \cos \left( \frac{3\pi}{n+1} \right), \quad \epsilon_j = \sin \left( \frac{j\pi}{n+1} \right),
\]

(38)

where \( j, s = 1, \ldots, n \). We note that for \( n = 2 \), equations (37) and (38) give exactly the same frequencies. The diagonal Hamiltonian is written in terms of the collective normal coordinates \( q_s \) and is of the form given by equation (5) or equivalently by equation (6). At zero temperature the total energy \( E \) is the sum of zero point energies and we obtain the same result by both diagonalization methods, namely

\[
\sum_s \frac{\hbar \omega_s}{2} = \sum_i \frac{\hbar \tilde{\omega}_i}{2} = E.
\]

(39)

5. Conclusions

We used a unitary transformation to diagonalize a generic quadratic Hamiltonian appearing in many relevant areas of physics and chemistry. As a result we obtain a diagonal Hamiltonian in the original observables, but with the effective masses and force constants replacing the original ones. The transformation works as a disentangling transformation in a sense that it connects the entangled and disentangled wave functions, both written in terms of the original position observables, but in different frames of reference.
Our general methodology to diagonalize a quadratic Hamiltonian supplements the already extensive variety of approaches to establish the same task. All the approaches developed earlier for this purpose have found their place in building understanding of the wide area of physics described by the quadratic Hamiltonian. We see many potential uses for the approach presented here in these systems, including the lattice dynamics related fields of research and the study of entanglement.

**Data availability statement**

No new data were created or analysed in this study.

**Appendix A. Three-body case**

Here we consider the special case of equation (12) with \( n = 3 \). The number of transformations needed in the diagonalization process is \( N = 3 \). We establish the transformations given by equation (14) in three stages. We denote the intermediate Hamiltonians as \( H' \equiv U_1^\dagger H U_1 \), \( H'' \equiv U_2^\dagger H' U_2 \), explicitly

\[
H' = \sum_i \frac{p_i^2}{2m'_i} + \sum_i d'_i u_i^2 + \sum_{i<j} d'_{ij} u_i u_j, \\
H'' = \sum_i \frac{p_i^2}{2m''_i} + \sum_i d''_i u_i^2 + \sum_{i<j} d''_{ij} u_i u_j.
\]  

(A.1)

The final Hamiltonian is

\[
\tilde{H} = \sum_i \frac{p_i^2}{2\tilde{m}_i} + \sum_i d_i u_i^2 + \sum_{i<j} d_{ij} u_i u_j. \\
\]  

(A.2)

After the first transformation, we obtain for the quantities appearing in \( H' \)

\[
m'_i = \frac{m_1 m_2}{m_2 + m_1 \alpha^2}, \quad m''_2 = m_2 \left(1 + k_{12} \alpha^2 \right), \quad m'_3 = m_3,
\]

\[
d'_1 = \frac{d_1 - d_{12} k_{12} \alpha_1}{1 + k_{12} \alpha^2}, \quad d''_1 = \frac{d_1 \alpha_1^2 + d_2 - d_{12} \alpha_1}{\alpha_1}, \quad d''_3 = d_3,
\]

\[
d''_{12} = \frac{d_{12} - 2 (d_1 + d_{12} \alpha_1)}{1 + k_{12} \alpha^2},
\]

\[
d''_{13} = \frac{d_{13} - d_{23} k_{12} \alpha_1}{1 + k_{12} \alpha^2}, \quad d''_{23} = d_{23} - d_{13} \alpha_1.
\]

(A.3)
The quantities included to $H''$ are
\[
m_1'' = m_1', \quad m_2'' = \frac{m_2'm_3'}{m_1' + m_3'\alpha_3'^2}, \quad m_3'' = m_3' \left(1 + \kappa_{23}\alpha_2'^2\right),
\]
\[
d_1'' = d_1', \quad d_2'' = \frac{d_2' - d_3'k_{32}\alpha_2 + d_3'k_{32}'\alpha_2'}{(1 + k_{23}'\alpha_2'^2)},
\]
\[
d_3'' = d_3'\alpha_2^2 + d_3' - d_{32}'\alpha_2,
\]
\[
d_{12}'' = \frac{d_{12}' - d_{13}'k_{23}'\alpha_2}{1 + k_{23}'\alpha_2'^2}, \quad d_{13}'' = d_{13}' - d_{12}'\alpha_2,
\]
\[
d_{23}'' = d_{23}' - \frac{2 \left(d_2' + d_3'k_{32}'\right)\alpha_3}{1 + k_{31}'\alpha_3'^2}.
\]

Finally, we transform $H''$ and obtain equation (A.2) with the quantities of the following form
\[
\tilde{m}_1 = m_1'' \left(1 + \kappa_{31}'\alpha_3'^2\right), \quad \tilde{m}_2 = m_2'', \quad \tilde{m}_3 = \frac{m_3''m_1''}{m_1'' + m_3''\alpha_3'^2},
\]
\[
\tilde{d}_1 = d_2'\alpha_3^2 + d_1' - d_13'\alpha_3, \quad \tilde{d}_2 = d_2'',
\]
\[
\tilde{d}_3 = \frac{d_3' - d_{13}'k_{31}'\alpha_3 + d_{13}'k_{31}'\alpha_3'}{(1 + k_{31}'\alpha_3')^2},
\]
\[
\tilde{d}_{12} = d_{12}' - d_{23}'\alpha_3, \quad \tilde{d}_{13} = d_{13}' - \frac{2 \left(d_2' + d_3'k_{32}'\right)\alpha_3}{1 + k_{31}'\alpha_3'^2},
\]
\[
\tilde{d}_{23} = d_{23}' - \frac{d_{12}'k_{13}'\alpha_3}{1 + k_{31}'\alpha_3'^2}.
\]

The Hamiltonian $\tilde{H}$ is diagonal if
\[
0 = d_{12}' - d_{23}'\alpha_3,
\]
\[
0 = \frac{d_{13}'}{\alpha_3^2} - \frac{2 \left(d_2' + d_3'k_{32}'\right)\alpha_3}{1 + k_{31}'\alpha_3'^2},
\]
\[
0 = \frac{d_{23}'}{1 + k_{31}'\alpha_3'^2}.
\]

We can solve the quantities $\alpha_i (i = 1, 2, 3)$ from this set of three equations as a function of the original masses $m_i$ and coupling constants $d_i, d_ij$. Given equation (A.6) holds, we have obtained a diagonal Hamiltonian $\tilde{H}$ given by equation (19) such that the quantities $\tilde{m}_i$ and $\tilde{d}_i$ are given by equation (A.5). These results can be used, for instance, to solve the $n$-body case with the second nearest neighbour interactions. The exact eigenfunction of the three-body Hamiltonian satisfying equation (7) can be written as
\[
\chi(u_1, u_2, u_3) = \tilde{\chi}(u_1 + \alpha_1u_2 + \alpha_2u_3) \tilde{\chi}(u_2 + \beta_1\tilde{u}_{21} + \alpha_3\tilde{u}_{23})
\]
\[
\times \tilde{\chi}(u_3 + \beta_2\tilde{u}_{32} + \beta_3\tilde{u}_{33}),
\]
where
\[
\tilde{u}_{21} \equiv u_1 + \alpha_1 u_2, \quad \tilde{u}_{23} \equiv u_3 + \beta_2 \left( (u_1 + \alpha_1 u_2) + \alpha_2 u_3 \right), \\
\tilde{u}_{32} \equiv (u_1 + \alpha_1 u_2) + \alpha_2 u_3, \quad \tilde{u}_{33} \equiv u_2 + \beta_1 (u_1 + \alpha_1 u_2) + \alpha_3 \left( u_3 + \beta_2 \left( (u_1 + \alpha_1 u_2) + \alpha_2 u_3 \right) \right).
\]
\[\text{(A.8)}\]

We leave the more detailed analysis of the three-body case to future work.

**Appendix B. Stability conditions**

By equation (30), the general stability conditions for two-body systems can be written as
\[
\begin{align*}
0 & \leq d_1 + d_{12} k_{12} \alpha + d_2 k_2^2 \alpha^2, \\
0 & \leq d_1 \alpha^2 + d_2 - d_{12} \alpha.
\end{align*}
\]
\[\text{(B.1)}\]

In some cases a simpler form of these conditions can be written. For example, when the coupling constants $\Phi_{ij}$ are the interatomic force constants, they are symmetric and satisfy [2]
\[
\sum_j \Phi_{ij} = 0.
\]
\[\text{(B.2)}\]

By equation (B.2) we have for the two-body case $d_1 = d_2 = -d_{12}/2$. These coefficients are also positive by the positive definiteness of the interatomic force constant matrix $\Phi_{ij}$, required for the stability of the oscillator system. From equation (29)
\[
\alpha_{\pm} = \frac{k_{21} - 1 \pm (1 + k_{21})}{2},
\]
\[\text{(B.3)}\]

where we differentiate the different solutions by the subscript. We see that $\alpha_+ = k_{21} > 0$ and $\alpha_- = -1 < 0$ and thus one of the relations in equation (B.1) always holds. We choose $\alpha = \alpha_-$ and thus the first relation of equation (B.1) holds automatically and the second relation leads to
\[
1 \leq \alpha_2^2,
\]
\[\text{(B.4)}\]

which holds by equation (B.3). We have therefore shown that one can always find a transformation $U$ for the two-body oscillator case such that the resulting Hamiltonian $\tilde{H}$ describes a stable system.

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