

**Supersymmetry and coherent
states of the Morse oscillator;
application to molecular
photodissociation**

A thesis presented by

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Introduction

The one-dimensional Morse oscillator is a useful model in the physics of non-linear oscillations. By its help one can describe a number of real physical problems in an analytic manner. Perhaps the best known application of the Morse potential is in atomic and molecular physics. In the pioneering paper [1] P. M. Morse pointed out that the inter-atomic interaction in a non-rotating diatomic molecule can be satisfactorily approximated by his potential-energy function – called as Morse potential since then – allowing to treat the problem analytically. It was also shown that the influence of rotation on vibration can be taken into account by suitably adjusting the parameters of the Morse potential [2]. The Morse oscillator model was also used to study the interaction of atoms and molecules with solid surfaces [3].

Since the 1970's, when the possibility of dissociating molecules by multi-photon absorption processes [4] using infrared lasers was discovered, the Morse oscillator has been attracting some renewed interest. Focusing on the excitation and dissociation of diatomic molecules induced by infrared lasers, several authors have been studying the problem of the Morse oscillator coupled to an external classical electromagnetic field in the dipole approximation [5, 6, 7]. In the Bohr-Oppenheimer approximation for infrared exciting fields, when the electron transitions can be neglected, this driven Morse oscillator serves adequate description for diatomic molecules. If one wishes to deal also with electron transitions, one has to consider several vibronic potentials corresponding to the different electronic levels. It should be mentioned here that the local mode concept employing also the Morse oscillator has been used extensively in the study of overtone vibrational spectra of polyatomic molecules [8].

It has been recently shown that the anharmonicity of the Morse oscillator naturally leads to an interesting collapse-revival phenomenon in the vibronic

dynamics of diatomic molecules [9]. In [10] similar character in the time evolution of the populations of two electronic levels subject to resonant laser excitation was pointed out due to the quantization of molecular vibration.

The object of this work is to give a detailed mathematical analysis of the Morse oscillator and to present the underlying algebraic structures relevant to the model. Moreover, on the basis of these algebraic results we propose a new approach for the study of the infrared absorption processes in diatomic molecules. Our method allows one to proceed analytically much further, than it was possible earlier.

The outline of the present work is the following. In Chapter 1 we give a short overview of supersymmetric quantum mechanics (SUSY QM). This method, that is similar to the ladder operator treatment of the harmonic oscillator, provides an elegant and useful algebraic tool to find the bound states of Hamiltonians corresponding to the class of the one-dimensional shape invariant potentials including the Morse potential, as well [11]-[18]. This method is the starting point of our algebraic ladder operator technique throughout this work.

In Chapter 2 we start the analysis of the quantum mechanics of the Morse oscillator. Using the method of supersymmetric quantum mechanics, we rederive the bound states and the corresponding wave functions of the Morse oscillator. For the sake of completeness we also solve the second order ordinary differential equation corresponding to the eigenvalue equation of the Hamiltonian in the traditional way and write down the scattering states of the Morse oscillator, as well. Until that point we present earlier results which are necessary for further study of the problem.

In Section 2.3 we begin to present our own results. In order to avoid the problem caused by the incompleteness of the Morse bound states we introduce a new class of complete orthonormal bases, each of them allowing one to give the full quantum mechanical description of the system. In Section 2.4 using the SUSY ladder operators we give the algebraic construction of the Morse coherent states [19]. This construction is similar to the one given by Glauber and Klauder for the coherent states of the harmonic oscillator [20, 21].

In Chapter 3 we prove that the Morse coherent states are strongly connected to the affine group of the real line and some of its extensions. They

are generated by the affine group from the ground states, being itself coherent, and in addition they minimize the strong uncertainty relation associated to the affine algebra generators [22]. We also show how one can describe certain quantum states of the Morse oscillator in phase space [22] by the help of a quasi-probability density function (affine Wigner function).

In Chapter 4 we apply these mathematical results to a real physical situation of a diatomic molecule. We consider the problem of the dynamics of infrared absorption processes for the NO (nitrogen-oxide) molecule. First we determine analytically the matrix elements of a realistic dipole moment operator in the basis of quasi-number states spanning not only the bound subspace but the whole dissociated region, too. Then we transform the Schrödinger equation into a set of coupled ordinary differential equations which can already be solved by straightforward numerical methods [23]. We follow the dynamics of photodissociation of the NO molecule and show that by using appropriate chirped infrared laser pulses a significant dissociation can be achieved under the ionization threshold of the molecule [24].

Chapter 1

Overview of Supersymmetric Quantum Mechanics

The notion of supersymmetry (SUSY) was originally introduced in the context of field theory in the early 1970's [25, 26, 27]. The concept of SUSY predicts a new symmetry of nature unifying the description of bosonic and fermionic types of particles into the same algebraic structure. The corresponding infinitesimal supersymmetry transformations constitute an extended version of a Lie algebra containing both commutators and anticommutators. These so-called graded Lie algebras [28] have been successfully applied in particle physics and field theory [29], and nowadays it is widely assumed that supersymmetry will be a necessary ingredient in any unification approach of the electromagnetic, weak, strong and gravitational interactions.

On the other hand, supersymmetry has been penetrating into other areas of mathematical physics. The model that is now called supersymmetric quantum mechanics (SUSY QM) was introduced by Witten [30] in 1981 in order to investigate the mechanism of the spontaneous breaking of SUSY non-perturbatively. Soon after, it turned out that SUSY QM is interesting not only for testing field theoretical methods but in its own right, as a method for solving traditional quantum mechanical problems. With the additional concept of shape invariance discovered by Gendenstein in 1983 [13], SUSY QM gives a nice algebraic insight into why the eigenvalue problems connected to a certain class of potentials are analytically solvable [11]-[18]. It should be

mentioned here that similar ideas to those involved behind the SUSY property and shape invariance were formulated earlier by Infeld and Hull in 1951 [31]. They developed their 'factorization method' in order to treat the eigenvalue problems of certain Hamiltonians corresponding to one-dimensional quantum systems. In fact, the factorization method was first used by Schrödinger [32] to solve the hydrogen atom problem analytically. Subsequently, Infeld and Hull generalized this method for a wide class of potentials. It also turned out that the factorization method as well as the methods of SUSY QM including the concept of shape invariance are both reformulations [33] of Riccati's idea of using the equivalence between the solution of Riccati's equation and a related second order linear differential equation.¹

In this chapter we give a brief overview of supersymmetric quantum mechanics. We show how the SUSY ladder operator factorization of Hamiltonian can be used for solving one-dimensional quantum mechanical problems. We also present the integrability condition of shape invariance. For further and more detailed survey of SUSY QM we refer to the comprehensive review paper of Cooper et al [11].

1.1 Factorization

Let us start with a Hamiltonian $H^{(-)}$ of the form:

$$H^{(-)} = \frac{P^2}{2m} + V^-(X), \quad (1.1)$$

where X denotes the coordinate variable and P is the momentum operator obeying the usual canonical commutation relation $[X, P] = i\hbar$. Let us assume that there exists a single ground state $|\Psi_0^{(-)}\rangle$, i.e.: the Hamiltonian is bounded from below, and the ground state energy $E_0^{(-)}$ is known which – without loss of generality – is set to be exactly zero:

$$H^{(-)} |\Psi_0^{(-)}\rangle = E_0^{(-)} |\Psi_0^{(-)}\rangle = 0 \quad (1.2)$$

¹This method was supposedly used for the first time by the Bernoulli family and the history is discussed in detail in Ref. [34].

Because $H^{(-)}$ is a positive semi-definite self-adjoint operator, it can be factorized as

$$H^{(-)} = A^\dagger A, \quad (1.3)$$

where the yet unknown operator A and its adjoint A^\dagger are called as SUSY annihilation and creation operators, respectively [11]. The terminology of annihilation operator reflects the crucial fact that the operator A annihilates the ground state:

$$A \left| \Psi_0^{(-)} \right\rangle = 0. \quad (1.4)$$

This relation can be immediately seen by recognizing that the norm $\|A \left| \Psi_0 \right>\|$, that equals $\sqrt{\langle \Psi_0 | H^{(-)} | \Psi_0 \rangle}$, vanishes. Introducing the operator $W(X)$, that is generally referred to superpotential in SUSY QM, one tries to find the SUSY ladder operators A and A^\dagger in the form [11]:

$$A = \frac{i\hbar}{\sqrt{2m}}P + W(X) \quad \text{and} \quad A^\dagger = \frac{-i\hbar}{\sqrt{2m}}P + W(X), \quad (1.5)$$

respectively. Substituting these latter expressions into (1.3) one obtains the following relationship between the potential $V^{(-)}(X)$ and the superpotential $W(X)$:

$$W^2(X) - \frac{\hbar}{\sqrt{2m}}W'(X) = V^{(-)}(X). \quad (1.6)$$

By solving the differential equation² above, the superpotential $W(X)$ can be determined. The ground state wave function $\Psi_0^{(-)}(x)$ can be easily obtained by solving the coordinate representation of (1.4), which is according to (1.5) a first order differential equation:

$$\frac{\hbar}{\sqrt{2m}} \frac{\partial \Psi_0^{(-)}(x)}{\partial x} = -W(X) \Psi_0^{(-)}(x). \quad (1.7)$$

Apart from a multiplicative factor this latter equation has the following unique solution:

$$\Psi_0^{(-)}(x) \propto e^{-\int dx' W(x')}. \quad (1.8)$$

²This first order ordinary differential equation is the previously mentioned Riccati equation [33].

One can see that the asymptotic behaviour of the superpotential determines the normalizability of $\Psi_0^{(-)}(x)$. In the present case, when by assumption the normalizable ground state does exist, the superpotential $W(x)$ has to take on positive (negative) values if x tends to the positive (negative) infinity. It is important to note here that for a superpotential behaving asymptotically as above, there is no such normalizable state which is annihilated by A^\dagger . This latter state would be written in the form

$$\Psi_0^{(+)}(x) \propto e^{\int dx' W(x')}, \quad (1.9)$$

which can not be normalized if once $\Psi_0^{(-)}(x)$ is normalizable. In other words, there is no Hilbert state element, other than the zero ket, which would be annihilated by A and A^\dagger at the same time [11].

The key object of SUSY QM is the supersymmetric partner Hamiltonian $H^{(+)}$ defined by reversing of the order of the annihilation and creation operators in $H^{(-)}$ [11]:

$$H^{(+)} := AA^\dagger = \frac{P^2}{2m} + V^{(+)}(X). \quad (1.10)$$

This new Hamiltonian $H^{(+)}$ is strictly positive and corresponds to a new potential $V^{(+)}(X)$ which differs according to (1.5) and (1.6) from the original one as

$$V^{(+)}(X) = W^2(X) + \frac{\hbar}{\sqrt{2m}}W'(X) = V^{(-)}(X) + 2\frac{\hbar}{\sqrt{2m}}W'(X). \quad (1.11)$$

As we shall see below, the energy eigenvalues and the eigenstates of $H^{(-)}$ and $H^{(+)}$ are related. It will turn out that the two spectra are identical except for the ground state energy of $H^{(-)}$ [11]. First, the eigenvalue equation of Hamiltonian $H^{(-)}$

$$H^{(-)}|\Psi_n^{(-)}\rangle = E_n^{(-)}|\Psi_n^{(-)}\rangle \quad (1.12)$$

implies for $n > 0$ that $A|\Psi_n^{(-)}\rangle$ is the eigenstate of $H^{(+)}$:

$$H^{(+)}A|\Psi_n^{(-)}\rangle = AH^{(-)}|\Psi_n^{(-)}\rangle = E_n^{(-)}A|\Psi_n^{(-)}\rangle. \quad (1.13)$$

For $n = 0$ the ground state is annihilated by A , hence $A |\Psi_n^{(-)}\rangle$ is only a trivial zero vector eigenstate of $H^{(+)}$. Similarly, the eigenvalue equation for the SUSY partner Hamiltonian $H^{(+)}$ written as

$$H^{(+)} |\Psi_n^{(+)}\rangle = E_n^{(+)} |\Psi_n^{(+)}\rangle \quad (1.14)$$

implies that

$$H^{(-)} A^\dagger |\Psi_n^{(+)}\rangle = A^\dagger H^{(+)} |\Psi_n^{(+)}\rangle = E_n^{(+)} A^\dagger |\Psi_n^{(+)}\rangle. \quad (1.15)$$

Let us remember that the energy $E_n^{(+)}$ is always positive and there is no non-zero normalizable state annihilated by A^\dagger . These relations all together indicate that the two spectra are identical except for the ground energy of $H^{(-)}$:

$$E_0^{(-)} = 0 \quad \text{and} \quad E_n^{(-)} = E_{n-1}^{(+)} \quad (n > 0), \quad (1.16)$$

and the eigenstates are intertwined by the following relations:

$$|\Psi_n^{(+)}\rangle = \frac{1}{\sqrt{E_{n+1}}} A |\Psi_{n+1}^{(-)}\rangle \quad (n > 0), \quad (1.17)$$

$$|\Psi_{n+1}^{(-)}\rangle = \frac{1}{\sqrt{E_{n+1}}} A^\dagger |\Psi_n^{(+)}\rangle. \quad (1.18)$$

One can see that for $n > 0$ the operator A (A^\dagger) not only converts an eigenfunction of $H^{(-)}$ ($H^{(+)}$) into $H^{(+)}$ ($H^{(-)}$) with the same energy eigenvalues but also decreases (increases) the value of the index n with 1. Since the ground state of $H^{(-)}$ is annihilated by A , this has no SUSY partner. Thus, the picture we obtained is that once knowing all the eigenvectors and eigenvalues of $H^{(+)}$ one can reconstruct all the eigenvectors of $H^{(-)}$ except for the ground state using the operator A^\dagger , and vice versa using A one can determine all the eigenvectors of $H^{(+)}$ from those of $H^{(-)}$. This is illustrated in Figure 1.1.

1.2 Superalgebra

As we have seen, except for the ground state of $H^{(-)}$ the energies of the partner Hamiltonians are the same. This can be considered as a “degeneracy” in the spectrum of the following matrix SUSY Hamiltonian built up by the partners

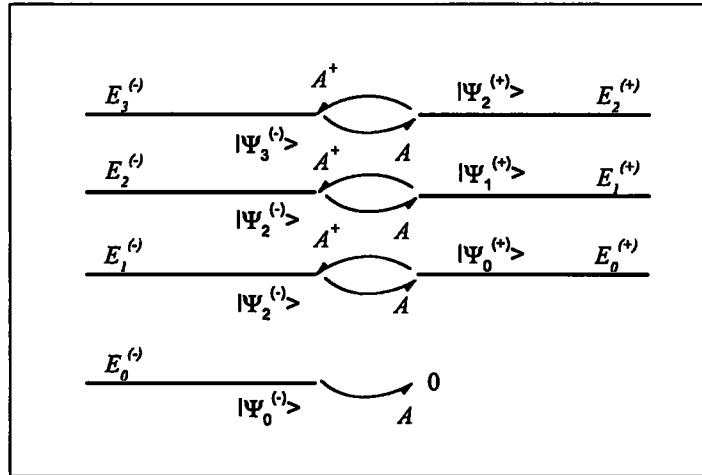


Figure 1.1: The energy spectrum of the SUSY partner Hamiltonians.

[11]:

$$H = \begin{bmatrix} H^{(-)} & 0 \\ 0 & H^{(+)} \end{bmatrix}. \quad (1.19)$$

This Hamiltonian acts on the direct sum Hilbert space spanned by states $\begin{bmatrix} |\Psi_n^{(-)}\rangle \\ 0 \end{bmatrix}$ and $\begin{bmatrix} 0 \\ |\Psi_m^{(+)}\rangle \end{bmatrix}$, where n, m are positive integers or zeros. Let us introduce the operator Q which is built up with the annihilation operator A as

$$Q = \begin{bmatrix} 0 & 0 \\ A & 0 \end{bmatrix}, \quad (1.20)$$

and its adjoint operator Q^\dagger which is given by

$$Q^\dagger = \begin{bmatrix} 0 & A^\dagger \\ 0 & 0 \end{bmatrix}. \quad (1.21)$$

The operator Q and its adjoint Q^\dagger are called supercharges. These latter operators with the matrix Hamiltonian H of (1.19) span the $sl(1/1)$ superalgebra which closes under the following commutation and anti-commutation relations [11, 35]:

$$[H, Q] = 0 \quad \text{and} \quad [H, Q^\dagger] = 0, \quad (1.22)$$

$$\{Q, Q^\dagger\} = H, \quad \{Q, Q\} = 0 \quad \text{and} \quad \{Q^\dagger, Q^\dagger\} = 0. \quad (1.23)$$

The fact that the supercharges Q and Q^\dagger commute with H is responsible for the degeneracy. We note that often instead of Q and Q^\dagger one uses an other but equivalent Hermitian version of supercharges: $Q_1 = \frac{1}{\sqrt{2}}(Q + Q^\dagger)$ and $Q_2 = \frac{1}{\sqrt{2}i}(Q - Q^\dagger)$.

The eigenstates of the SUSY matrix Hamiltonian can be written as the following two-dimensional column vectors:

$$|0\rangle = \begin{bmatrix} |\Psi_0^{(-)}\rangle \\ 0 \end{bmatrix}, \quad \text{and} \quad |n\rangle = \begin{bmatrix} c_n^- |\Psi_n^{(-)}\rangle \\ c_n^+ |\Psi_{n-1}^{(+)}\rangle \end{bmatrix} \quad \text{for } n > 0, \quad (1.24)$$

where c_n^- and c_n^+ are complex numbers satisfying the normalizability condition $|c_n^-|^2 + |c_n^+|^2 = 1$. The corresponding energy spectrum is exactly that of $H^{(-)}$ including the eigenvalue $E_n^{(-)} = 0$, too. While the ground state energy is non-degenerate, the excited energy eigenvalues are 2-fold degenerate.

A finite SUSY transformation has the form [36]

$$U(\alpha) = e^{\alpha Q^\dagger - \alpha^* Q}, \quad (1.25)$$

where the complex number α parameterizes the transformation. The action of $U(\alpha)$ on the states $|n\rangle$ is

$$U(\alpha) |n\rangle = e^{\alpha Q^\dagger - \alpha^* Q} |n\rangle = \begin{bmatrix} e^{\alpha \sqrt{E_n}} c_- |\Psi_n^{(-)}\rangle \\ e^{-\alpha^* \sqrt{E_n}} c_+ |\Psi_{n-1}^{(+)}\rangle \end{bmatrix}. \quad (1.26)$$

First, one can immediately see that the ground state is left invariant by any $U(\alpha)$. This is the consequence of that the ground state energy is zero and thus the supercharges annihilate the ground state:

$$Q |0\rangle = Q^\dagger |0\rangle = 0. \quad (1.27)$$

Since the ground state has the same symmetry as the Hamiltonian H does ($U^\dagger(\alpha) H U(\alpha) = H$), thus the supersymmetry is unbroken, or in other words, complete [11].

Here we note briefly that sometimes there is no ground state destroyed by either Q or Q^\dagger , the ground state subspace gets 2-dimensional and the supersymmetry is broken. The problem can be connected with a slightly different form of SUSY factorization of $H^{(-)}$ to that used in (1.3):

$$H^{(-)} = A^\dagger A + \varepsilon \quad (1.28)$$

where the parameter $\varepsilon < 0$ is smaller than the ground state energy³ $E_0^{(-)} = 0$. One can realize that in this case no state is destroyed by either A or A^\dagger corresponding to this new factorization and the energy spectra of SUSY partners are entirely identical including the ground state energies, as well. In consequence, the ket $\frac{1}{\sqrt{E_0 - \varepsilon}} A \left| \Psi_0^{(-)} \right\rangle$ is the ground state $\left| \Psi_0^{(+)} \right\rangle$ of Hamiltonian $H^{(+)}$, and vice versa $\frac{1}{\sqrt{E_0 - \varepsilon}} A^\dagger \left| \Psi_0^{(+)} \right\rangle$ is the ground state $\left| \Psi_0^{(-)} \right\rangle$ of Hamiltonian $H^{(-)}$. The effect of the supersymmetry transformation $U(\alpha)$ on any arbitrary vector $|0\rangle = \begin{bmatrix} c_- \left| \Psi_0^{(-)} \right\rangle \\ c_+ \left| \Psi_0^{(+)} \right\rangle \end{bmatrix}$ of the now 2-dimensional eigensubspace corresponding to ground state energy $E_0 = E_0^{(-)} = E_0^{(+)} = 0$ is

$$U(\alpha) |0\rangle = e^{\alpha Q^\dagger - \alpha^* Q} \begin{bmatrix} c_- \left| \Psi_0^{(-)} \right\rangle \\ c_+ \left| \Psi_0^{(+)} \right\rangle \end{bmatrix} = \begin{bmatrix} e^{\alpha \sqrt{-\varepsilon}} c_- \left| \Psi_0^{(-)} \right\rangle \\ e^{-\alpha^* \sqrt{-\varepsilon}} c_+ \left| \Psi_0^{(+)} \right\rangle \end{bmatrix}. \quad (1.29)$$

Since $\varepsilon < 0$, an arbitrary ket $|0\rangle$ of the ground state subspace is transformed into another state in the same eigensubspace but as a vector it does not remain invariant. Thus the supersymmetry gets spontaneously broken [11].

1.3 Shape invariance

Let us suppose that in addition to the coordinate X the potential $V^{(-)}(X) \equiv V^{(-)}(X, a)$ depends also on a set of parameters a . We would like to emphasize that the parameter set a consists of just real numbers and not operators. The potential $V^{(-)}(X)$ is said to be shape invariant [13] if its partner has the same functional dependence on the coordinate X as the original potential but with a possibly altered parameter. More precisely, the potential $V^{(-)}(X; a)$ and its partner $V^{(+)}(X; a)$ are shape invariant if there exist the functions $f(a)$ and $R(a)$ of the parameter set a so that the following identity is fulfilled [11]-[18]:

$$V^{(+)}(X; a) = V^{(-)}(X; f(a)) + R(f(a)) \quad (1.30)$$

³Let us recognize that until now the factorization energy shift ε has been chosen to be the ground state energy $E_0^{(-)} = 0$.

This relation can be equivalently written in terms of the partner Hamiltonians or the ladder operators:

$$\begin{aligned} H^{(+)}(a) &= H^{(-)}(f(a)) + R(f(a)), \\ A(a)A^\dagger(a) &= A^\dagger(f(a))A(f(a)) + R(f(a)). \end{aligned} \quad (1.31)$$

As it was pointed out by Gendenstein [13] the shape invariance property above is an integrability condition, and enables one to solve the eigenvalue problems of the partners. In order to see this, let us consider the eigenvalue equations

$$H^{(-)}(a) |\Psi_n^{(-)}(a)\rangle = E_n^{(-)}(a) |\Psi_n^{(-)}(a)\rangle, \quad (1.32)$$

$$H^{(+)}(a) |\Psi_n^{(+)}(a)\rangle = E_n^{(+)}(a) |\Psi_n^{(+)}(a)\rangle. \quad (1.33)$$

The obvious consequence of (1.30) is that

$$E_n^{(+)}(a) = E_n^{(-)}(f(a)) + R(f(a)). \quad (1.34)$$

Combining this latter formula⁴ with (1.16) leads to

$$E_n^{(-)}(a) = \sum_{i=1}^n R(f^i(a)) \quad (n > 0). \quad (1.35)$$

Further, from equations (1.17) and (1.18) one obtains ($n \geq 0$)

$$|\Psi_n^{(-)}(a)\rangle = \frac{1}{\sqrt{E_n^{(-)}(a)}} A(f^{-1}(a)) |\Psi_{n+1}^{(-)}(f^{-1}(a))\rangle, \quad (1.36)$$

$$|\Psi_{n+1}^{(-)}(a)\rangle = \frac{1}{\sqrt{E_{n+1}^{(-)}(a)}} A^\dagger(a) |\Psi_n^{(-)}(f(a))\rangle. \quad (1.37)$$

In summary, if one knows one of the eigenvectors and eigenvalues of a shape invariant potential $V^{(-)}(X, a)$ for arbitrary a , then the whole eigenvalue problem (all eigenvalues and eigenstates) can be found. The eigenvectors corresponding to neighboring eigenvalues are connected by the SUSY annihilation and creation operators in a pleasant, algebraic manner similar to the well-known ladder operator method of the harmonic oscillator. The list of the known shape invariant potentials which can be treated in this way is rather large containing all the commonly used 'textbook' potentials: harmonic oscillator, 3-dimensional harmonic oscillator, Coulomb, Morse, Rosen-Morse, Eckart and Pöschl-Teller I and II potentials [13]-[18].

⁴Throughout the construction it has been supposed that the ground state energy of $H^{(-)}(a)$ is $E_n^{(-)}(a) = 0$ for any a .

Chapter 2

Morse oscillator

The Morse or anharmonic oscillator is a frequently used model in physics, especially in molecular physics [1, 37]. The Morse potential provides a simplified but satisfactory potential curve for vibrations of a diatomic molecule. While the harmonic oscillator is acceptable only for vibrations with small displacements from the equilibrium, the Morse oscillator describes larger, non-harmonic excitations and dissociation, as well. Figure 2.1 shows the interatomic Morse potential-energy function for the NO (nitrogen-oxide) molecule:

$$V(x) = D_0[e^{-2\alpha x} - 2e^{-\alpha x}], \quad (2.1)$$

where $D_0 = -6.5\text{eV}$ is the dissociation energy, and $\alpha = 1/3.61\text{\AA}$ is the range of the interatomic potential [37].

In this chapter we present the mathematical apparatus which is needed to treat the quantum problem of the anharmonic Morse oscillator in an algebraic manner. First we consider the eigenvalue problem of the Morse Hamiltonian. Applying the method of SUSY QM discussed in the previous chapter, one can determine the bound states and the corresponding energies of the system. As it is known, part of the spectrum lies in the continuum, and therefore the Morse Hamiltonian cannot be diagonalized – in a strict sense – in the entire Hilbert space of square integrable wave functions. The diagonalization can be performed only by restricting the Hamiltonian to the finite dimensional subspace which is spanned by the bound states. In other words the bound states do not form a complete set of states in the Hilbert space. For a full quantum description of the Morse oscillator we introduce a class of sets of

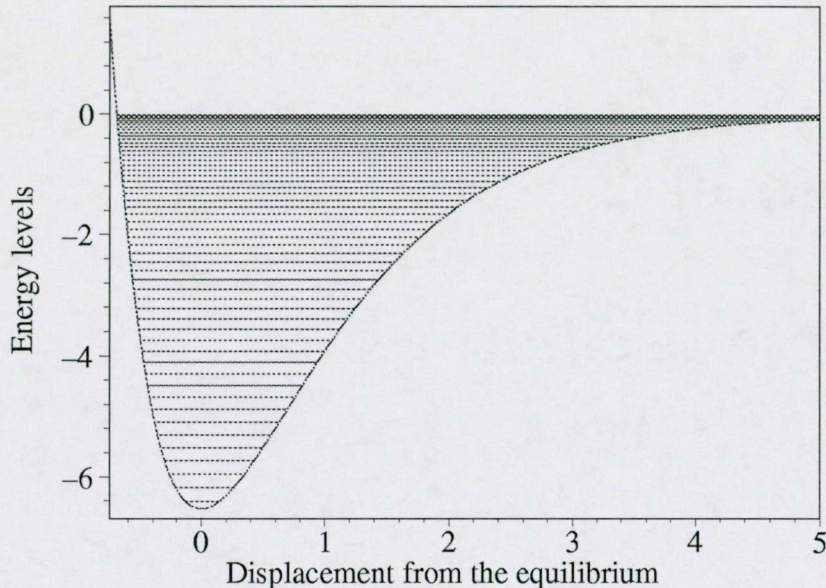


Figure 2.1: The Morse potential and the vibration energy levels for NO molecule. The energy and the position values are given in units 1eV and $1/\alpha = 3.61\text{\AA}$, respectively.

normalizable states where each set provides a complete orthonormal basis in the Hilbert space. These bases will be constructed by consecutive application of SUSY creation operators to ground states of Morse potentials with different shape parameters. The advantage of using these sets of states, to be called as Morse-Laguerre bases, is that the Hamiltonian has a tridiagonal form in them. In certain special cases the Hamiltonian can be further decomposed into two tridiagonal blocks that simplifies a series of problems.

2.1 Bound states

The Hamiltonian of the Morse oscillator is given by [1, 38]

$$\hat{H}_0 = \frac{\hat{P}^2}{2m} + D_0(1 - e^{-\alpha\hat{X}})^2 - D_0 = \frac{\hat{P}^2}{2m} + D_0(e^{-2\alpha\hat{X}} - 2e^{-\alpha\hat{X}}). \quad (2.2)$$

The operators \widehat{X} and \widehat{P} have the commutator $[\widehat{X}, \widehat{P}] = i\hbar$. It is worth to introduce dimensionless operators. To that purpose, first let us start with the notations:

$$\omega_0 = \alpha \sqrt{\frac{2D_0}{m}} \quad (2.3)$$

and the dimensionless number

$$s = \frac{\sqrt{2mD_0}}{\alpha\hbar} - 1/2. \quad (2.4)$$

The frequency ω_0 is the so-called Morse frequency that is the circular frequency of the harmonic oscillator which approximates the Morse potential for small vibrations. The parameter s is by assumption a positive number connected with the number of the bound (normalizable) energy eigenstates. As we shall see, the number of normalizable bound states is $[s]$: the largest integer which is smaller than s . Now let us define the dimensionless operators

$$X = \alpha\widehat{X}, \quad Y = (2s + 1)e^{-X} \quad \text{and} \quad P = \frac{1}{\alpha\hbar}\widehat{P}. \quad (2.5)$$

These satisfy the following commutation relations:

$$[X, P] = i \quad \text{and} \quad [Y, P] = -iY. \quad (2.6)$$

Throughout this work we prefer to use the exponentially scaled coordinate Y operator rather than X . The reason for this is that the potential has a simple quadratic form in P and Y . We introduce the dimensionless Hamiltonian $H_0(s)$:

$$H_0(s) = \frac{2s + 1}{\hbar\omega_0} \widehat{H}_0 = P^2 + \frac{Y^2}{4} - (s + 1/2)Y. \quad (2.7)$$

This Hamiltonian is not positive semi-definite. However, it is bounded from below as one expects that from physical reasons (see Figure 2.1). In order to apply the SUSY technique presented in the previous chapter we need to identify the lowest energy eigenvalue and then to shift the energy scale so that the ground state energy will be exactly zero. To that purpose, let us use the following modified SUSY factorization with the energy shift parameter ε as

$$H_0(s) = A^\dagger(s)A(s) + \varepsilon, \quad (2.8)$$

The annihilation operator has the form

$$A(s) = iP + W(Y; s) \quad (2.9)$$

with the superpotential $W(Y; s)$ which is the solution of the differential equation (1.6):

$$W^2(Y; s) + YW'(Y; s) + \varepsilon = \frac{Y^2}{4} - (s + 1/2)Y. \quad (2.10)$$

One can seek the solution in a linear functional form:

$$W(Y; s) = aY + bI, \quad (2.11)$$

As the kernel of A should contain a normalizable state (see Section 1.1) the superpotential has to take on definitely positive (negative) values if $Y \rightarrow 0$ ($Y \rightarrow \infty$). This requirement restricts the range of the parameters a and b to be negative real and positive real numbers, respectively. Substituting (2.11) in (2.10) one obtains

$$(a^2 + a)Y^2 + 2a(b + 1)Y + b^2 + \varepsilon = \frac{Y^2}{4} - (s + 1/2)Y, \quad (2.12)$$

which leads to the following equations for the parameters a, b and ε :

$$(a^2 + a) = 1/4, \quad a(2b + 1) = -(s + 1/2) \quad \text{and} \quad b^2 = -\varepsilon. \quad (2.13)$$

The solution fulfilling the requirements of the appropriate asymptotic behavior of $W(Y; s)$ is

$$a = -1/2, \quad b = s \quad \text{and} \quad \varepsilon = -s^2. \quad (2.14)$$

With these values the superpotential and the ladder operators are written as

$$W(Y; s) = sI - \frac{Y}{2}, \quad A(s) = iP + sI - \frac{Y}{2} \quad \text{and} \quad A^\dagger(s) = -iP + sI - \frac{Y}{2}, \quad (2.15)$$

respectively. For the Hamiltonian one obtains

$$H_0(s) = A^\dagger(s)A(s) - s^2. \quad (2.16)$$

Using coordinate representation, it can be seen that the wave function $\Psi_0(y; s)$ corresponding to the vector $|\Psi_0(s)\rangle$ annihilated by A is the solution of the differential equation

$$-y \frac{\partial \Psi_0(y; s)}{\partial y} + W(y; s) \Psi_0(y; s) = 0. \quad (2.17)$$

Hence the normalized ground state can be found in the form:

$$\Psi_0(y; s) = \frac{1}{\sqrt{\Gamma(2s)}} y^s e^{-y/2} \quad (2.18)$$

This wave function is normalizable for any $s > 0$. For $s \leq 0$ the potential has no bound states. Because the superpotential $W(Y; s)$ does not have any singularity, the wave function $\Psi_0(y; s)$ above has no zeros. This means that $|\Psi_0(s)\rangle$ must be the ground state of $H_0(s)$ with the energy $E_0(s) = -s^2$.

Now we are in the position to apply the results of Chapter 1 to the shifted Hamiltonian $H_0 - s^2 \equiv H^{(-)}$. It can be verified that the SUSY ladder operators A and A^\dagger depending on the parameter s obey the shape invariance condition (1.31):

$$A(s)A^\dagger(s) = A^\dagger(f(s))A(f(s)) + R(f(s)) \quad (2.19)$$

with:

$$f(s) = s - 1 \quad \text{and} \quad R(s) = 2s + 1, \quad (2.20)$$

Then according to (1.35) and (1.37) the energy eigenvalues $E_n(s)$ are

$$E_n(s) = E_0(s) + \sum_{i=1}^n R(s - i) = -(n - s)^2, \quad (2.21)$$

and the eigenvectors $|\Psi_n(s)\rangle$ of $H_0(s)$ can be written

$$|\Psi_{n+1}(s)\rangle = [\varepsilon_n(s)]^{-1/2} A^\dagger(s - 1) |\Psi_n(s - 1)\rangle, \quad (2.22)$$

$$|\Psi_n(s)\rangle = [\varepsilon_n(s)]^{-1/2} A(s + 1) |\Psi_{n+1}(s + 1)\rangle, \quad (2.23)$$

where the normalization factor $\varepsilon_n(s)$ is

$$\varepsilon_n(s) = \sqrt{E_n(s) - E_0(s)} = \sqrt{n(2s - n)}. \quad (2.24)$$

Using the relations above repeatedly, one obtains that the n -th bound state can be generated from the ground state as:

$$|\Psi_n(s)\rangle = \sqrt{\frac{(2s-2n)!}{n!(2s-n)!}} A^\dagger(s) \dots A^\dagger(s-n+1) |\Psi_0(s-n)\rangle. \quad (2.25)$$

Starting from (2.18) in coordinate representation by the help of the Rodrigues' formula for the generalized Laguerre polynomials $L_n^\alpha(y)$ [39, 40] one can translate the abstract generation (2.25) of the energy eigenstates into wave function language and obtain the following form for the bound states [38]

$$\Psi_n(y; s) = \sqrt{\frac{n!(2s-2n)}{(2s-n)!}} y^{s-n} L_n^{2s-2n}(y) e^{-y/2}. \quad (2.26)$$

This wave function is normalizable with respect to the measure dy/y on the positive half line if and only if $s > n$. With the original coordinate variable x (note: $y = (2s+1)e^{-x}$) one can see that only for $s > n \geq 0$ the corresponding wave functions $\Psi_n(x; s)$ are the elements of the function space $L^2(dx, \mathbb{R})$, therefore the number of bound states is $[s] + 1$ where $[s]$ denotes the largest integer that is smaller than s . Consequently the states $|\Psi_n(s)\rangle$ do not constitute a complete set in the (infinite dimensional) Hilbert space of the problem.¹ The latter is the direct sum:

$$\mathcal{H} = \mathcal{H}^- \oplus \mathcal{H}^+ \quad (2.27)$$

where \mathcal{H}^- is the finite ($[s] + 1$) dimensional subspace spanned by the bound states, while its orthogonal complement \mathcal{H}^+ is an infinite dimensional subspace with normalizable elements producing positive energy mean values. These latter states can be interpreted therefore as normalizable dissociated states of the Morse oscillator. We would like to emphasize here that the positive energy (scattering) eigenfunctions of H_0 are not normalizable (they do not belong to the Hilbert space) but they can be interpreted as well-defined kernels of linear functionals over \mathcal{H} . Moreover, appropriate continuous sums (integrals) of these functionals can be identified as Hilbert space elements in the subspace \mathcal{H}^+ .

¹For instance, the wave function $\psi(y) = \sqrt{\frac{1}{\Gamma(2(s+1))}} y^{s+1} e^{-y/2}$, which is obviously the element of the function space above, cannot be decomposed into the terms of only the energy eigenfunctions (2.26).

2.2 The continuous part of the spectrum

For the sake of completeness we also give the wave functions of the non-normalizable energy eigenstates. Let us start with the second order differential equation corresponding to the eigenvalue problem of the Morse Hamiltonian (2.7):

$$\frac{d^2\Psi}{dx^2} + \left(s + \frac{1}{2}\right)^2 (2e^{-x} - e^{-2x})\Psi = -E\Psi. \quad (2.28)$$

By the help of the rescaled coordinate $y = (2s+1)e^{-x}$ and the notation $k^2 = E$ this equation can be transformed into the form of Whittaker's equation [38, 39]:

$$\frac{d^2\Psi(y)}{dy^2} + \frac{1}{y} \frac{d\Psi(y)}{dy} + \left(\frac{k^2}{y^2} + \frac{s+1/2}{y} - \frac{1}{4}\right) \Psi(y) = 0. \quad (2.29)$$

One can verify that each positive energy solution $\Psi(x)$ must tend to $e^{\pm ikx} \sim (2s+1)^{\mp ik} y^{\pm ik}$ if $x \rightarrow \infty$ ($y \rightarrow 0$) and to $\exp\{-(s+1/2)e^{-x}\} \sim e^{y/2}$ if $x \rightarrow -\infty$ ($y \rightarrow 0$). Taking into account this asymptotic behaviour and substituting $\Psi(y) = e^{-y/2} y^{ik} w(y)$ into (2.29) one arrives at the equation [39]

$$yw''(y) + (b-y)w'(y) - aw(y) = 0 \quad (2.30)$$

with parameters $b = 2ik + 1$ and $a = -s + ik$. This latter equation has two linearly independent solutions and the general solution can be written as

$$w(y) = C_M M(a, b, y) + C_U U(a, b, y) \quad (2.31)$$

where the so-called Kummer's functions² $M(a, b, y)$ and $U(a, b, y)$ are given by

$$M(a, b, y) = \sum_{n=0}^{\infty} \frac{(a)_n}{(b)_n} \frac{1}{n!} y^n, \quad (2.32)$$

where the notation $(z)_n$ denotes the Pochhammer's symbol $\frac{\Gamma(z+n)}{\Gamma(z)}$, and

$$U(a, b, y) = \frac{\pi}{\sin(\pi b)} \left\{ \frac{M(a, b, y)}{\Gamma(1+a-b)\Gamma(b)} - y^{1-b} \frac{M(1+a-b, 2-b, y)}{\Gamma(a)\Gamma(2-b)} \right\}, \quad (2.33)$$

² $M(a, b, y)$ is denoted sometimes by $\Phi(a, b, y)$ or ${}_1F_1(a, b, y)$ and called confluent hypergeometric function.

respectively [39]. One can verify that $\lim_{y \rightarrow \infty} U(y) = 0$ and $\lim_{y \rightarrow \infty} M(y) \neq 0$. Keeping in mind that for large y the wave function $\Psi(y)$ has to tend to 0, one finds that the solution of (2.29) is:

$$\Psi(y) = C e^{-y/2} \left\{ y^{ik} \frac{M(-s + ik, 2ik + 1, y)}{\Gamma(-s - ik)\Gamma(2ik + 1)} - y^{-ik} \frac{M(-s - ik, 1 - 2ik, y)}{\Gamma(-s + ik)\Gamma(1 - 2ik)} \right\}. \quad (2.34)$$

For small y (or alternatively $x \rightarrow \infty$) the asymptotic form of this latter wave function is

$$\Psi^{as}(x) \sim \left\{ e^{-ikx} - (s + 1/2)^{+i2k} \frac{\Gamma(-s + ik)\Gamma(1 - 2ik)}{\Gamma(-s - ik)\Gamma(2ik + 1)} e^{+ikx} \right\}, \quad (2.35)$$

where $k = \sqrt{E}$. Therefore one can read off the reflection coefficient R which is

$$R = -e^{i2 \ln(s+1/2)k} \frac{\Gamma(-s + ik)\Gamma(1 - 2ik)}{\Gamma(-s - ik)\Gamma(1 + 2ik)} \quad (2.36)$$

As it can be expected on physical grounds (see Figure 2.1), one obtains that $|R|^2 = 1$, i.e. the particle incoming from the positive infinity ($x \rightarrow \infty$) is totally reflected by the Morse potential.

2.3 Morse-Laguerre basis, quasi-number and pseudo-number states

From the present section we begin to present our own results concerning the quantum problem of the Morse oscillator. As we have seen, the Morse Hamiltonian $H_0(s)$ has only a finite number (precisely $[s] + 1$) of bound states which cannot form a complete set of states in the Hilbert space \mathcal{H} . Hence the full quantum description of the Morse potential is impossible by restricting oneself only to these bound states. One could of course use the continuous part of the spectrum of $H_0(s)$, but – in a strict sense – they are not the elements of the Hilbert space. Therefore we consider here the following infinite series of states $|\varphi_n(q)\rangle$ given by the recurrence relations [19, 22]:

$$|\varphi_0(q)\rangle \equiv |\Psi_0(q)\rangle \quad \text{and} \quad |\varphi_n(q)\rangle \equiv C_n^{-1} A^\dagger(q + n - 1) |\varphi_{n-1}(q)\rangle, \quad (2.37)$$

where n is a positive integer and $C_n = \sqrt{n(2q + n - 1)}$ is a normalization coefficient. The first state $|\varphi_0(q)\rangle \equiv |\Psi_0(q)\rangle$ in the series above is the ground state of a Morse Hamiltonian $H_0(q)$ with the positive shape parameter value q which is not necessarily equal to s . From now on we consider that the value of the parameter s of the Hamiltonian has been fixed but q in $A(q)$ can be changed arbitrarily. Let us note the difference between the sign of the parameter shifts in (2.20) and (2.37).

A key observation from our point of view is that the SUSY ladder operators

$$A(q) = iP + qI - \frac{Y}{2} \quad \text{and} \quad A^\dagger(q') = -iP + q'I - \frac{Y}{2}, \quad (2.38)$$

(with arbitrary real q and q') and the identity I span a three-dimensional Lie algebra. Since for any reals q and q' we have:

$$A(q') = A(q) + (q' - q)I \quad (2.39)$$

the Lie algebra is invariant with respect of a shift of the parameter q , and an easy calculation shows that the SUSY ladder operators satisfy the following commutation relations:

$$[A(q), A(q')] = 0, \quad [A^\dagger(q), A^\dagger(q')] = 0, \quad (2.40)$$

$$[A(q), A^\dagger(q')] = (q + q')I - (A(q) + A^\dagger(q')). \quad (2.41)$$

In Chapter 3 we shall give a detailed discussion of this algebra and shall show that it is the central extension of the affine Lie algebra of the real line [41].

Now, using only the commutation relations (2.40)-(2.41) and the fact that for $q > 0$ the operator $A(q)$ annihilates the state $|\varphi_0(q)\rangle$

$$A(q) |\varphi_0(q)\rangle = 0, \quad (2.42)$$

we verify that the states defined in (2.37) are mutually orthogonal:

$$\langle \varphi_n(q) | \varphi_m(q) \rangle = \delta_{nm}. \quad (2.43)$$

First let us realize that the operator product $A(q + n + 1)A^\dagger(q + n)$ can be rearranged as

$$A(q + n + 1)A^\dagger(q + n) = 2(q + n) + A^\dagger(q + n - 1)A(q + n). \quad (2.44)$$

To see this one has to use only the property (2.39) and the commutation relations (2.40)-(2.41). Because the first state in the series (2.37) is annihilated by $A(q)$ according to (2.42) the expression above implies that

$$C_{n+1}^{-1}A(q+n+1)|\varphi_{n+1}(q)\rangle = |\varphi_n(q)\rangle \quad (n \geq 0). \quad (2.45)$$

Equations (2.45) are the inversion of the defining formulae (2.37). Using them with (2.39) one finds the following recurrence relation for the scalar product $\langle\varphi_n(q)|\varphi_m(q)\rangle$:

$$\langle\varphi_n(q)|\varphi_m(q)\rangle = \frac{C_m}{C_n} \langle\varphi_{n-1}(q)|\varphi_{m-1}(q)\rangle + \frac{(n-m-1)}{C_n} \langle\varphi_{n-1}(q)|\varphi_m(q)\rangle. \quad (2.46)$$

Taking also into the account that

$$\langle\varphi_0(q)|\varphi_m(q)\rangle = \begin{cases} 1 & (m=0) \\ \frac{m!}{\prod_{i=0}^m C_i} \langle A(q)\varphi_0(q)|\varphi_0(q)\rangle = 0 & (m>0), \end{cases} \quad (2.47)$$

ie.: the state $|\varphi_0(q)\rangle$ is orthogonal to all the other states, one arrives at the orthogonality relation (2.43).

We are going to call these states as the Morse-Laguerre basis of the anharmonic oscillator and we give here the corresponding wave functions in terms of the variable $y = (2q+1)\exp(-x)$. By the help of (2.15) and (2.37) we find that the wave functions in question obey the following recursion relations ($n > 0$):

$$\varphi_0(y; q) \equiv \langle y | \varphi_0(q) \rangle = \frac{1}{\sqrt{\Gamma(2q)}} y^q \exp(-y/2), \quad (2.48)$$

$$\varphi_n(y; q) \equiv \langle y | \varphi_n(q) \rangle = C_n^{-1} \left(y \frac{\partial}{\partial y} + (q+n-1) - \frac{y}{2} \right) \varphi_{n-1}(y; q). \quad (2.49)$$

Comparing (2.48) and (2.49) and with the Rodrigues' formula for the generalized Laguerre polynomials $L_n^\alpha(y)$ [40] one finds that the normalized wave functions of the Morse-Laguerre states are:

$$\varphi_n(y; q) = \left(\Gamma(2q) \binom{n+2q-1}{n} \right)^{-\frac{1}{2}} y^q \exp(-y/2) L_n^{2q-1}(y). \quad (2.50)$$

Due to the completeness of the Laguerre polynomials $L_n^{2q-1}(y)$ with respect of the weight function $\exp(-y)y^{2q-1}$ [40], the functions (2.50) form a complete orthonormal set in the space $L^2\left((0, \infty), \frac{dy}{y}\right)$, (the square integrable functions on the $(0, \infty)$ interval, with respect to the measure dy/y), and therefore the set of Morse Laguerre states is a complete, orthonormal basis in the Hilbert space for any $q > 0$.

We would like to note here that for the problem of the Morse potential these latter basis plays analogous role as the Coulomb-Sturmian basis does for the Coulomb potential [42]. Though the Coulomb potential has infinite number of bound states, they do not constitute a true basis either. But one can achieve a full quantum treatment by employing the Coulomb-Sturmian basis which is a complete set of states and includes vectors representing states also from the ionized region. The prize one has to pay for completeness is also similar to the current case: the elements of the basis are not eigenstates of the Hamiltonian any more [42, 43].

We now calculate the matrices of the SUSY ladder operators in the $|\phi_n(q)\rangle$ basis. Using (2.37) and (2.39) one obtains the following matrix elements:

$$\langle \varphi_m(q) | A(s) | \varphi_n(q) \rangle = \sqrt{n(2q+m)}\delta_{m+1,n} - (m+q-s)\delta_{m,n}, \quad (2.51)$$

$$\langle \varphi_m(q) | A^\dagger(s) | \varphi_n(q) \rangle = \sqrt{m(2q+n)}\delta_{m,n+1} - (n+q-s)\delta_{m,n}. \quad (2.52)$$

In a similar manner the matrix of the Hamiltonian $H_0(s)$ can be determined, too:

$$\begin{aligned} \langle \varphi_m(q) | H_0(s) | \varphi_n(q) \rangle &= [n(2q+n-1) + (q-s+m) + E_0(s)] \delta_{m,n} \\ &\quad - (q-s+m)\sqrt{n(2q+n-1)}\delta_{m+1,n} \\ &\quad - (q-s+n)\sqrt{m(2q+m-1)}\delta_{m,n+1}. \end{aligned} \quad (2.53)$$

We see that the Hamiltonian is not diagonal in the $|\varphi_n(q)\rangle$ basis but it is quite close to a diagonal matrix. It has non-vanishing elements only in, above and below the main diagonal, ie: the Hamiltonian is tridiagonal. If $r = s - q$ is a positive integer or zero, then the matrix of the Hamiltonian splits into a more simple form of two tridiagonal blocks. The first block is $s - q + 1$ dimensional

while the other one is infinite. This indicates that the first $s - q + 1$ Morse-Laguerre states $|\varphi_n(q)\rangle$ constitute a finite invariant subspace for $H_0(s)$ while – of course – the states with $n > s - q$ span the orthogonal complement.

To obtain more insight into the structure of the invariant subspaces of $H_0(s)$, and also to present the advantage of the SUSY operator technique, let us calculate the scalar product of $|\varphi_n(q)\rangle$ with the bound states $|\Psi_m(s)\rangle$. Using equation (2.39) we have:

$$A(q)\dots A(n+q-1) = \sum_{j=0}^n A^{(j)}(s) \binom{n}{j} \frac{(n-r-1)!}{(j-r-1)!}, \quad (2.54)$$

where the notation

$$A^{(j)}(s) := A(s-j+1)\dots A(s) \quad \text{and} \quad A^{(0)}(s) := I \quad (2.55)$$

has been introduced. By (2.54) and with the defining formula (2.37) of the Morse-Laguerre states one obtains that the scalar product is the sum

$$\langle \Psi_m(s) | \varphi_n(q) \rangle = \frac{1}{\prod_{i=1}^n C_i(q)} \sum_{j=0}^n \binom{n}{j} \frac{(n-r-1)!}{(j-r-1)!} \langle A^{(j)}(s) \Psi_m(s) | \varphi_0(q) \rangle. \quad (2.56)$$

Here we have used $C_i(q) = \sqrt{i(2q+i-1)}$ in accordance with our previous notation $C_i \equiv C_i(q=s)$. Let us recognize that for an integer r the term $\frac{(n-r-1)!}{(j-r-1)!} = (n-r-1)\dots(j-r)$ gives non-zero contribution to the sum only if either $n-r > 1$ and $j > r$ or if $n-r < 1$ and $j < r$. The action of the operator product $A^{(j)}(s) = A(s-j+1)\dots A(s)$ on the state $|\Psi_m(s)\rangle$ can be determined by (2.23) which leads to

$$A(s-j+1)\dots A(s) |\Psi_m(s)\rangle = \sqrt{\frac{m!\Gamma(2s-m+1)}{(m-j)!\Gamma(2s-m-j+1)}} |\Psi_{m-j}(s-j)\rangle. \quad (2.57)$$

For $j > m$ this latter state is necessarily zero, otherwise the scalar product in question is

$$\begin{aligned} \langle \Psi_m(s) | \varphi_n(q) \rangle &= \sqrt{\frac{m!\Gamma(2s-m+1)\Gamma(2q)}{n!\Gamma(2q+n)}} \times \\ &\sum_{j=0}^{\min(n,m)} \binom{n}{j} \frac{(n-r-1)! \langle \Psi_{m-j}(s-j) | \varphi_0(q) \rangle}{\sqrt{\Gamma(2s-m-j+1)(m-j)!(j-r-1)!}}, \end{aligned} \quad (2.58)$$

where we have used that $\prod_{i=1}^n C_i(q) = \sqrt{\frac{\Gamma(2q)}{n!\Gamma(2q+n)}}$. To calculate the terms $\langle \Psi_{m-j}(s-j) | \varphi_0(q) \rangle$ one has first to realize that

$$\langle \Psi_{m-j}(s-j) | \varphi_0(q) \rangle = \frac{r-j}{\varepsilon_{m-j}(s-j)} \langle \Psi_{m-j-1}(s-j-1) | \varphi_0(q) \rangle. \quad (2.59)$$

Using this formula repeatedly one obtains

$$\langle \Psi_{m-j}(s-j) | \varphi_0(q) \rangle = \frac{(r-j)! \sqrt{\Gamma(2s-2j-2m+1)}}{(r-m)! \sqrt{(m-j)! \Gamma(2s-m-j+1)}} \langle \Psi_0(s-m) | \varphi_0(q) \rangle \quad (2.60)$$

The scalar product $\langle \Psi_{m-j}(s-j) | \varphi_0(q) \rangle$ can be determined by taking into account that

$$\begin{aligned} \langle \Psi_0(s-m) | \varphi_0(q) \rangle &= \frac{1}{\sqrt{\Gamma(2s-2m)\Gamma(2q)}} \int_0^\infty dy e^{y^2} y^{s-m+q-1} \quad (2.61) \\ &= \frac{\Gamma(s-m+q)}{\sqrt{\Gamma(2s-2m)\Gamma(2q)}} \end{aligned}$$

Finally one arrives at the formula:

$$\begin{aligned} \langle \Psi_m(s) | \varphi_n(q) \rangle &= \sqrt{\frac{m!\Gamma(2s-m+1)}{n!\Gamma(2q+n)\Gamma(2s-2m)}} \frac{\Gamma(s-m+q)}{(r-m)!} \times \quad (2.62) \\ &\sum_{j=0}^{\min(n,m)} \binom{n}{j} \frac{(n-r-1)! (r-j)! \sqrt{\Gamma(2s-2j-2m+1)}}{(j-r-1)! (m-j)! \Gamma(2s-m-j+1)} \end{aligned}$$

Summing up the non-vanishing terms in (2.62) one can verify that the scalar product has values

$$\langle \Psi_m(s) | \varphi_n(q) \rangle = \begin{cases} 0 & n > r, m \leq r \\ 0 & n \leq r, m > r \\ \text{non-zero} & n \leq r, m \leq r \\ \text{non-zero} & n > r, m > r \end{cases} \quad (2.63)$$

According to (2.63) we can see that in the case of the parameter setting $r = 0$, ie.: $s = q$, the ground state coincides with the first Morse-Laguerre state $|\varphi_0(q = s)\rangle$ and is orthogonal to the other ($n > 0$) Morse-Laguerre basis elements. On the other hand, the first Morse-Laguerre state has zero overlap

with each of the bound states other than the ground state. These could be already seen from construction (2.37). In the present case, when $s = q$ and therefore $r = 0$, we call these Morse-Laguerre states $|\varphi_n(s)\rangle$ as *pseudo-number states* [19, 22, 23]. We shall see in the next chapter that although the pseudo-number states are not the energy eigenstates, they play similar role for the construction of coherent states for the Morse oscillator as the number-states do in the case of the harmonic oscillator [19, 22, 23].

Another important and useful case can be obtained by setting $r = [s]$ or equivalently $q = s - [s]$. With this parameter choice we call these Morse-Laguerre basis elements *quasi-number states* [24]. In this basis the matrix of the Hamiltonian $H_0(s)$ consists of two tridiagonal blocks. The first one is $[s] + 1$ dimensional and the second one is infinite dimensional. The origin of this decomposition is that the first $[s] + 1$ quasi-number states span the same subspace \mathcal{H}^- as the bound states do, and the quasi-number states with $n > [s]$ belong to the orthogonal complement \mathcal{H}^+ consisting of dissociated states with positive energy mean value. Therefore the quasi-number states provide useful tools to investigate the dynamics of dissociation or other processes leading out of the bound subspace \mathcal{H}^- [23, 24].

2.4 Morse coherent states

Coherent states for systems other than the harmonic oscillator have attracted much attention for several years [44]-[47]. There are a number of different approaches to this problem and the one presented here is based on the methods of SUSY QM [19]. Since it is the generalization of the ladder operator method of the harmonic oscillator it seems straightforward to use the SUSY ladder operators to construct coherent states for other, non-harmonic potentials, too. Based on this idea, an algebraic construction of coherent states was proposed by Fukui and Aizawa [47] for the class of shape invariant potentials having an infinite number of bound-energy eigenstates. Their definition, however, does not work for potentials, where the number of normalizable energy eigenstates is finite, thus not for the Morse potential either.

In what follows, using the pseudo-number states which was introduced

earlier we give the algebraic construction of an *overcomplete* set of *continuously* labeled states called as *Morse coherent states*. Let us use the SUSY operator analogy with the harmonic oscillator, and define the coherent states of the Morse potential as follows [19]

$$|\beta\rangle = g(\beta) \left\{ I + \sum_{n=1}^{\infty} \frac{\beta^n}{n!} A^\dagger(s+n-1) \cdots A^\dagger(s) \right\} |\Psi_0(s)\rangle, \quad (2.64)$$

where β is a complex number and $g(\beta)$ is a normalization function to be determined below. The expression of C_n in the defining formulae of the pseudo-number states (2.37) implies the introduction of a generalized factorial $\{n\}!$ with the definition:

$$\{0\}! = 1, \quad \{n\}! = \frac{n!}{2s \cdots (2s+n-1)} = \binom{n+2s-1}{n}^{-1} \quad (n > 0) \quad (2.65)$$

Then the coherent states in (2.64) can be written by the help of (2.37) as:

$$|\beta\rangle = g(\beta) \sum_{n=0}^{\infty} \frac{\beta^n}{\sqrt{\{n\}!}} |\varphi_n(s)\rangle. \quad (2.66)$$

To obtain the explicit form of $g(\beta)$, and to find the label space (the set of allowed β -s) we set:

$$1 = \langle\beta|\beta\rangle = |g(\beta)|^2 \sum_{n=0}^{\infty} \frac{|\beta|^{2n}}{\{n\}!} = |g(\beta)|^2 \left\{ 1 + \sum_{n=1}^{\infty} \frac{2s \cdots (2s+n-1)}{n!} |\beta|^{2n} \right\}. \quad (2.67)$$

The sum in the above expression is convergent if and only if $|\beta| < 1$, i.e. the label space is the complex open unit disk, and then the sum in the braces in equation (2.67) yields $(1 - |\beta|^2)^{-2s}$. So we have finally for the coherent states of the Morse potential³:

$$|\beta\rangle = e^{-i\phi} (1 - |\beta|^2)^s \sum_{n=0}^{\infty} \sqrt{\binom{n+2s-1}{n}} \beta^n |\varphi_n(s)\rangle \quad (\beta \in \mathbf{C}, |\beta| < 1)$$

where ϕ is a phase term to be fixed later.

³This expansion of the Morse coherent states on the *pseudo-number states* is essentially the same that was found by Y. Aharonov et al in [48] for the regular phase states of a mode of the radiation field in terms of the *number states* of the mode [49].

The various sets of coherent states that have been introduced in the past for an arbitrary system, have two fundamental common properties established in [21]: continuity in the label space and completeness in the sense that there exists a positive measure on the label space such that the identity operator admits the resolution of unity. The first property follows from the definition: if $\beta \rightarrow \beta'$, ($|\beta|, |\beta'| < 1$), then $\| |\beta\rangle - |\beta'\rangle \|^2 \rightarrow 0$. To verify the second property, valid for $s > 1/2$, we consider the measure $\delta\beta = (2s - 1)/(1 - |\beta|^2)^2 d\text{Re } \beta d\text{Im } \beta$ ($|\beta| < 1$) and find:

$$\int_{|\beta|<1} |\beta\rangle \langle\beta| \delta\beta = (2s - 1) \sum_{n,m=0}^{\infty} \frac{|\varphi_n(s)\rangle \langle\varphi_m(s)|}{\sqrt{\{n\}! \{m\}!}} \times \int_{|\beta|<1} (\beta^*)^m \beta^n (1 - |\beta|^2)^{2s-2} d\text{Re } \beta d\text{Im } \beta. \quad (2.68)$$

Introducing polar coordinates in the label space, the integral above can be calculated easily, and we find the resolution of unity as:

$$\int_{|\beta|<1} |\beta\rangle \langle\beta| \delta\beta = \pi \sum_{n=0}^{\infty} |\varphi_n(s)\rangle \langle\varphi_n(s)| = \pi I. \quad (2.69)$$

Here we have used the fact proven previously in Section 2.3 that the pseudo-number states constitute a complete set of states in the Hilbert space.

We also present here the wave functions $\varphi_\beta(y)$ corresponding to the states $|\beta\rangle$. From (2.50) and (2.66) we have:

$$\begin{aligned} \varphi_\beta(y) &= (1 - |\beta|^2)^s \sum_{n=0}^{\infty} \frac{\beta^n}{\sqrt{\{n\}!}} \varphi_n(y; s) \\ &= \frac{e^{-i\phi} (1 - |\beta|^2)^s}{\sqrt{\Gamma(2s)}} y^s \exp(-y/2) \sum_{n=0}^{\infty} \beta^n L_n^{2s-1}(y). \end{aligned} \quad (2.70)$$

Using the generating function formula for the Laguerre polynomials [40]:

$$\sum_{n=0}^{\infty} \beta^n L_n^\alpha(z) = (1 - \beta)^{1-\alpha} \exp\left(-\frac{z}{1 - \beta}\right) \quad (2.71)$$

one obtains that the corresponding wave functions in the y coordinate are [19]:

$$\varphi_\beta(y) = \frac{e^{-i\phi} (1 - |\beta|^2)^s}{\sqrt{\Gamma(2s)} (1 - \beta)^{2s}} y^s \exp\left(-\frac{y}{2} \frac{1 + \beta}{1 - \beta}\right). \quad (2.72)$$

These wave functions are essentially the same which have been discovered in another way by Nieto et al [44], who called them as generalized minimal uncertainty coherent states (MUCS) of the Morse potential. They introduced certain special coordinates in the classical phase space transforming the trajectories of the bound motions into ellipses. According to [44], the MUCS type coherent states are those which minimize the uncertainty relation of the quantum operators corresponding to these new classical coordinates called “natural classical variables” in [44].

Here we also present another interpretation for the states $|\beta\rangle$ by giving the *physical meaning* of its parameter β [19]. We recast the wave function (2.72) in the original coordinate variable x . Substituting $y = 2(s + \frac{1}{2}) \exp(-x)$, one has for $\varphi_\beta(x) := \langle x | \beta \rangle$

$$\varphi_\beta(x) = \frac{2^s}{\sqrt{\Gamma(2s)}} e^{-s(x-\tilde{x}+\ln(s+\frac{1}{2}))} \exp\left\{-e^{-(x-\tilde{x}+\ln(s+\frac{1}{2}))}\right\} \times \exp\left\{\frac{-i}{s}\tilde{p}e^{-(x-\tilde{x}+\ln(s+\frac{1}{2}))}\right\}, \quad (2.73)$$

where \tilde{x} and \tilde{p} are real numbers depending on β :

$$\tilde{x} := \ln\left(\operatorname{Re} \frac{1+\beta}{1-\beta}\right), \quad \tilde{p} := s \frac{\operatorname{Im} \frac{1+\beta}{1-\beta}}{\operatorname{Re} \frac{1+\beta}{1-\beta}}. \quad (2.74)$$

and the phase term $e^{-i\phi}$ has been chosen so that $e^{-i\phi} = \left(\frac{1-\beta}{|1-\beta|}\right)^{2s}$. Calculating the expectation values of the operators X and P in the state $|\beta\rangle$ one obtains:

$$\langle \beta | X | \beta \rangle = \tilde{x} + \langle X \rangle_0, \quad \langle \beta | P | \beta \rangle = \tilde{p}. \quad (2.75)$$

We see that apart from an additive constant $\langle X \rangle_0$ the parameters \tilde{x} and \tilde{p} are just the position and momentum operator expectation values, respectively. The constant $\langle X \rangle_0 = \ln(2) - \tilde{\psi}(2s)$ is the position mean value in the ground state. (Here $\tilde{\psi}(x)$ denotes Euler's digamma function [39].) Hence we can introduce a new labeling for the coherent states by the help of the real numbers \tilde{x} and \tilde{p} instead of the original complex β . In these coordinates $|\beta\rangle$ can be written as $|\tilde{x}, \tilde{p}\rangle$ and the appropriate label space is \mathbb{R}^2 with the measure $d\tilde{x}d\tilde{p}$ on it. Then the resolution of unity (2.69) has a similar form as in the case of

the harmonic oscillator [19]:

$$\frac{2s-1}{4\pi s} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} |\tilde{x}, \tilde{p}\rangle \langle \tilde{x}, \tilde{p}| d\tilde{x}d\tilde{p} = I \quad (2.76)$$

It is not hard to see that the square of the modulus of the wave function in (2.73) is equal to that of the ground state function shifted along the x -axis. Equation (2.73) also implies that our coherent states can be written as [19]:

$$|\tilde{x}, \tilde{p}\rangle = e^{-i\tilde{x}P} e^{-\frac{i}{s}\tilde{p}e^{-X}} |0\rangle = D(\tilde{x}, \tilde{p}) |0\rangle \quad (2.77)$$

where $|0\rangle := |\beta = 0\rangle = |\tilde{x} = 0, \tilde{p} = 0\rangle$ is identical to the ground state, being itself a coherent state, and $D(\tilde{x}, \tilde{p})$ is a displacement operator. Using equation (2.15) for $A(s)$ and $A^\dagger(s)$, the latter can be rewritten as [19]:

$$D(\tilde{x}, \tilde{p}) = e^{\frac{i}{2s}\tilde{p}(A(s)+A^\dagger(s))} e^{\frac{\tilde{x}}{2}(A^\dagger(s)-A(s))}. \quad (2.78)$$

We see that $D(\tilde{x}, \tilde{p})$ is unitary for arbitrary \tilde{x} , and \tilde{p} , and it also proves that our states belong to the category of displacement operator coherent states (DOCS) according to [44]. The displacement operator is the element of the unitary irreducible representation of the Lie group which can be obtained by the exponentiation of the affine group [19, 22]. The precise connection between the Morse coherent states and the affine group and other consequences will be discussed in the next chapter.

Chapter 3

The affine group and the Morse oscillator

In the previous chapter the coherent states of the Morse potential were constructed using the ladder operator technique of supersymmetric quantum mechanics. The aim of the present chapter is to show the group theoretical background of this construction and to elucidate the relation between the Morse Hamiltonian and the affine group of the real line and some of its extensions [22, 50]. We are going to show that the affine group plays similar role for the Morse oscillator as does the Heisenberg-Weyl algebra, and the corresponding group is the Heisenberg-Weyl group for the harmonic oscillator. This is not a symmetry group of the harmonic oscillator, because the group translations, in general do not commute with the Hamiltonian. The relevance of this algebra for the harmonic oscillator lies in the following facts:

- (a) The specific set of generators of the algebra, namely a and a^\dagger are spectrum-generating (ladder) operators, in the sense that they connect eigenstates belonging to neighboring eigenvalues.
- (b) The elements of the irreducible representation of the corresponding group, known as the displacement operators of the harmonic oscillator, create the coherent states from the ground state [20].

We now turn to the case of the Morse potential, and the affine group. The operators in which the Hamiltonian (2.7) is quadratic are $P = iy \frac{\partial}{\partial y}$ and $Y = y$,

and they obey the commutation relation

$$[P, Y] = iY. \quad (3.1)$$

Equation (3.1) shows that the operators Y and P form a closed Lie algebra. It is known and will be demonstrated briefly below, that this is just the algebra corresponding to the affine group of the real line [51]. The ladder operators in the equation (2.15) are linear combinations of Y and P plus the identity operator I . Therefore, we need to extend the algebra spanned by Y and P with the identity operator, which commutes with all the other generators. This standard procedure is known as a central extension in group theory. The operators P , Y , and I , or alternatively, A , A^\dagger , I form the basis of an extended Lie algebra, to be denoted here by \mathcal{G}_0 .

In what follows we shall need to use an even larger group, denoted by \tilde{G}_0 which is a further extension of G_0 . Later we will also show that \tilde{G}_0 is closely connected to the minimal states of the strong uncertainty relation of the operators Y and P . Now we are going to characterize the groups in question: the affine group, G_0 and \tilde{G}_0 , and the corresponding algebras in some more detail:

(a) *The affine group.* The elements of the two-parameter affine group (a, b) , $a > 0$, $b \in \mathbb{R}$ act on the points x of the real line as $(a, b)x = ax + b$, and satisfy the group multiplication property: $(a, b)(a', b') = (aa', ab' + b)$.

(b) *The group G_0 .* This group is a direct product of the affine group and the real line \mathbb{R} and it can be realized in the following way. G_0 has elements $(a, b, c)(a', b', c') = (aa', ab' + b, c + c')$

(c) *The group \tilde{G}_0 .* This four-parameter group has the following composition rule: $(a, b, c, d)(a', b', c', d') = (aa', ab' + b, c + c' + \rho d' \ln a, d + d')$, where $a > 0$, $b, c, d \in \mathbb{R}$, and ρ is a fixed real number.

The simplest faithful representation of the group \tilde{G}_0 is given by the four-dimensional matrices

$$g(a, b, c, d) = \begin{pmatrix} a & b & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & c & 1 & \rho \ln a \\ 0 & d & 0 & 1 \end{pmatrix} \quad (3.2)$$

obeying the required multiplication rule. Disregarding the last row and column, or alternatively setting $d = 0$ one gets back the group G_0 . Disregarding the last two rows and columns, or alternatively setting $c = d = 0$, one arrives back at the affine group. The group G_0 can also be recovered as a quotient of \tilde{G}_0 by the subgroup T consisting of the elements $(1, 0, c, 0)$, $c \in \mathbb{R}$. The elements of the quotient \tilde{G}_0/T are the equivalence classes $[a, b, d] = \{(a, b, c, d), \forall c \in \mathbb{R}\}$. As can be seen from the composition law of \tilde{G}_0 , the set of elements $[a, b, d]$ transforms as G_0 , and is thus isomorphic to it. The group \tilde{G}_0 is, in fact, can be constructed as the extension of the group G_0 by the group T [50].

A representation of the generators of the Lie algebra $\tilde{\mathcal{G}}_0$ corresponding to the group \tilde{G}_0 is obtained by taking the derivatives of $g(a, b, c, d)$ at the unit element. We are going to use here the self-adjoint generators as

$$X_a = i \left. \frac{\partial g}{\partial a} \right|_{a=1, b=c=d=0} \quad (3.3)$$

and similarly for X_b , X_c and X_d . Calculating these derivatives of the matrix above, and evaluating their commutators, one obtains

$$[X_a, X_b] = iX_b, \quad [X_a, X_d] = i\rho X_c, \quad [X_b, X_d] = 0. \quad (3.4)$$

while X_c commutes with all the others. Setting the correspondence:

$$X_a \implies P, \quad X_b \implies Y, \quad X_c \implies I, \quad X_d \implies Z = \rho \ln Y = -\rho X + \ln(2s + 1)\rho I \quad (3.5)$$

one arrives at the following commutation relations:

(a)

$$[X_a, X_b] = iX_b \implies [P, Y] = iY \quad (3.6)$$

(b)

$$[X_k, X_c] = 0 \implies [X_k, I] = 0 \quad k = a, b, c \quad (3.7)$$

(c)

$$\begin{aligned} [X_a, X_d] &= i\rho X_c \implies [P, Z] = i\rho I \\ [X_b, X_d] &= 0 \implies [Y, Z] = 0 \end{aligned} \quad (3.8)$$

Considering only (a), one sees that the commutation relation (3.1) is really that of the algebra of the affine group, having only these two generators.

The relations (a) and (b) together yield the Lie algebra of the group G_0 . In view of equation (2.15) the ladder operators for the Morse potential can be considered as elements of the extended affine Lie algebra \mathcal{G}_0 , and according to equation (2.25) the eigenstates are generated by the consecutive applications of A^\dagger . We note that this Lie algebra corresponds to case III in the Bianchi classification of the three-dimensional Lie algebras [52].

We turn now to the unitary irreducible representation of the above groups on the space of the functions $\psi \in L^2(0, \infty; dy/y)$ with inner product

$$(\psi, \psi') = \int \frac{dy}{y} \psi^*(y) \psi'(y). \quad (3.9)$$

The widest group \tilde{G}_0 can be represented unitarily and irreducibly on the function space above:

$$U(a, b, c, d)\psi(y) = e^{-i(by+c+\rho d \ln y)}\psi(ay) \quad (a, b, c, d) \in \tilde{G}_0 \quad (3.10)$$

where ρ is a real parameter [41, 50]. Keeping in mind that G_0 and the affine group are subgroups of \tilde{G}_0 , one sees that the unitary irreducible representations of G_0 and that of the affine group can be obtained by setting $d = 0$ and $c = d = 0$, respectively. Alternatively, the whole transformation (3.10) yields a projective representation for the group \tilde{G}_0/T consisting of elements $[a, b, d]$.

The generators of the representation (3.10) of G_0 are:

$$P\psi(y) \equiv i \frac{\partial U\psi(y)}{\partial a} = iy \partial_y \psi(y), \quad (3.11)$$

$$Y\psi(y) \equiv i \frac{\partial U\psi(y)}{\partial b} = y\psi(y), \quad (3.12)$$

$$I\psi(y) = i \frac{\partial U\psi(y)}{\partial c} = \psi(y), \quad (3.13)$$

$$Z\psi(y) = i \frac{\partial U\psi(y)}{\partial d} = \rho \ln y \psi(y), \quad (3.14)$$

where the derivatives were taken at $a = 1$ and $b = c = d = 0$.

It can be also shown that the exponentiation of the Lie algebra elements $X = uP + vY + wI + tZ$, yields the following Baker-Capbell-Hausdorff-type relation between the parameters $u, v, w, t \in \mathbb{R}$ and the group parameters a, b, c, d

of (3.2):

$$e^{-i(uP+vY+wI+tZ)} = U(a = e^u, b = \frac{v}{u}(e^u - 1), c = w + \frac{\rho}{2}tu, d = t). \quad (3.15)$$

In order to obtain this relation let us recall the four dimensional matrix representation given by equation (3.2). We will prove that the identifications of parameters

$$a = e^u, \quad b = \frac{v}{u}(e^u - 1), \quad c = w + \frac{\rho}{2}ut, \quad d = t \quad (3.16)$$

yield the equality

$$e^{-i(uX_a+vX_b+wX_c+tX_d)} = g(a, b, c, d), \quad (a, b, c, d) \in \tilde{G}_0, \quad (3.17)$$

where the Lie algebra generators X_a, X_b, X_c and X_d are defined by (3.3) and parameters u, v, w and t are arbitrary real numbers.

To prove the identity above let us first set $d = 0$ and calculate the left hand side of equation (3.17). A straightforward calculation gives:

$$e^{-i(uX_a+vX_b+wX_c)} = \begin{pmatrix} e^u & v\frac{e^u-1}{u} & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & w & 1 & \rho u \\ 0 & 0 & 0 & 1 \end{pmatrix} = g(e^u, v\frac{e^u-1}{u}, w, 0) \quad (3.18)$$

In the case of arbitrary d we can use the commutators (3.4)-(3.8). With the notation $B \equiv -itX_d$ and $C \equiv -i(uX_a+vX_b+wX_c)$ one has $[B, C] = -iut\rho X_d$ and $[[B, C], B] = [[B, C], C] = 0$. Then $e^{\{B+C\}} = e^{-\frac{1}{2}[B,C]}e^Ae^B$ and one can write:

$$e^{-i(uX_a+vX_b+wX_c+tX_d)} = e^{-itX_d}e^{-i(uX_a+vX_b+(w+\frac{1}{2}ut\rho)X_c)}, \quad (3.19)$$

By (3.18) and the multiplication rule of the group \tilde{G}_0 :

$$e^{-i(uX_a+vX_b+wX_c+tX_d)} = g(1, 0, 0, t)g(e^u, v\frac{e^u-1}{u}, w + \frac{\rho}{2}ut, 0) = g(a, b, c, d), \quad (3.20)$$

where $a = e^u$, $b = \frac{v}{u}(e^u - 1)$, $c = w + \frac{\rho}{2}ut$ and $d = t$. Finally taking into account that $(a, b, c, d) = (1, 0, 0, d)(1, 0, c, 0)(1, b, 0, 0)(a, 0, 0, 0)$ one arrives at equation (3.17).

3.1 The affine group and the Morse coherent states

Let us use the following notation:

$$U(a, b) = U(a, b, 0, 0), \quad (3.21)$$

where (a, b) is an element of the affine group. This with (3.10) defines an unitary irreducible representation for the affine group on $L^2(0, \infty; dy/y)$. Since

$$A^\dagger(s) - A(s) = -2iP, \quad A^\dagger(s) + A(s) = 2sI - Y \quad (3.22)$$

the unitary displacement operator $D(\tilde{x}, \tilde{p})$ given by equation (2.78) can be written as:

$$D(\tilde{x}, \tilde{p}) = e^{-i\tilde{x}P} e^{-\frac{i}{2s}\tilde{p}Y}. \quad (3.23)$$

This operator acts on wave functions that are defined on the half-line and square integrable for the measure dy/y . According to the Baker-Cambell-Hausdorff relation (3.15) and (3.21) we have:

$$e^{-i\tilde{x}P} e^{-\frac{i}{2s}\tilde{p}Y} = U(e^{\tilde{x}}, 0)U(1, \frac{\tilde{p}}{2s}). \quad (3.24)$$

Using the fact that

$$U(a, b) = U(1, b)U(a, 0) = U(a, 0)U(1, \frac{b}{a}) \quad (3.25)$$

we obtain that the coherent states are generated from the ground state as:

$$|\tilde{x}, \tilde{p}\rangle = D(\tilde{x}, \tilde{p})\Psi_0(y) = U(a, b)\Psi_0(y), \quad (3.26)$$

where the parameters a and b of the affine group are related to \tilde{x} and \tilde{p} according to:

$$a = \exp(\tilde{x}), \quad b = \frac{\tilde{p} \exp(\tilde{x})}{2s}. \quad (3.27)$$

3.2 Minimal states and the group \tilde{G}_0

The coherent states will be shown here to be the states minimizing the strong uncertainty relation [53, 54, 55] with respect of the non-commuting operators P and Y . The derivation of this relation will now be recalled. Given two Hermitian operators B_1, B_2 , the norm of the vector $(B_1 + i\lambda B_2)|\Phi\rangle$ is nonnegative for any complex number λ :

$$\langle\Phi, (B_1 - i\lambda^* B_2)(B_1 + i\lambda B_2)\Phi\rangle \geq 0. \quad (3.28)$$

Using the notation: $\langle B_i B_j \rangle \equiv \langle\Phi, B_i B_j \Phi\rangle$ and setting $\lambda = i \frac{\langle B_2 B_1 \rangle}{\langle B_2^2 \rangle}$ we obtain by linearity and hermicity:

$$\langle B_1^2 \rangle \langle B_2^2 \rangle \geq |\langle B_1 B_2 \rangle|^2 = (1/4) (\langle B_1 B_2 + B_2 B_1 \rangle^2 - \langle [B_1, B_2] \rangle^2). \quad (3.29)$$

The latter equality¹ is obtained by splitting $\langle B_1 B_2 \rangle$ into its symmetric (real) and antisymmetric (imaginary) parts. Applying this result to:

$$B_1 = P - p_0, \quad B_2 = Y - y_0 \quad (3.30)$$

with $\langle P \rangle \equiv p_0$ and $\langle Y \rangle \equiv y_0$ leads to the strong uncertainty relation:

$$\sigma_{yy} \sigma_{pp} - \sigma_{py}^2 \geq \langle Y \rangle^2 / 4 \quad (3.31)$$

where:

$$\begin{aligned} \sigma_{yy} &= \langle (Y - y_0)^2 \rangle & \sigma_{pp} &= \langle (P - p_0)^2 \rangle \\ \sigma_{py} &= \frac{\langle PY + YP \rangle}{2} - \langle Y \rangle \langle P \rangle \end{aligned} \quad (3.32)$$

According to relations (3.28) and (3.30), the minimal uncertainty states for which equation (3.31) turns into equality obey the equation

$$[(P - p_0) + i\lambda(Y - y_0)]|\Phi\rangle = 0, \quad (3.33)$$

where p_0 and y_0 are real and λ is a (generally) complex parameter. In the space of functions $L^2(0, \infty, dy/y)$ one has to solve the corresponding differential equation:

$$\left[iy \frac{\partial}{\partial y} - p_0 + i\lambda(y - y_0) \right] \Phi(y) = 0. \quad (3.34)$$

¹In fact, the relation $\langle B_1^2 \rangle \langle B_2^2 \rangle \geq |\langle B_1 B_2 \rangle|^2$ is the Cauchy-Schwarz inequality for the pair of vectors $B_1|\Phi\rangle$ and $B_2|\Phi\rangle$.

The solution is

$$\Phi(y; \lambda, p_0, y_0, \phi) = C e^{-i\phi} y^{\lambda y_0 - i p_0} e^{-\lambda y}. \quad (3.35)$$

where $C = (2\text{Re}\lambda)^{(y_0\text{Re}\lambda)} / \sqrt{\Gamma(y_0 2\text{Re}\lambda)}$ is fixed by the normalization.

The special case of the Morse coherent states $\varphi_\beta(y)$, defined in equation (2.72), is obtained for:

$$p_0 = y_0 \text{Im}\lambda, \quad \phi = 0$$

The relation of parameters β , and s to λ and y_0 is written as:

$$\beta = \frac{2\lambda - 1}{2\lambda + 1}, \quad s = y_0 \text{Re}\lambda \quad (3.36)$$

The normalizability condition, $\text{Re}\lambda > 0$ implies $|\beta| < 1$, while the condition $\text{Re}\lambda > 1/2y_0$, required for completeness of the set of coherent states, leads to $s > 1/2$. Moreover, the Morse coherent states can be obtained by applying the group element $U(a, b)$ to the ground state with the appropriate shape parameter.

On the other hand, the states for which $\sigma_{py} = 0$ are exactly the ones for which λ is set to be real in equation (3.33), see [53, 54, 55]. These are the states which minimize the more customary and weaker form of the uncertainty relation: $\Delta P \Delta Y \geq \langle Y \rangle / 2$. In the family of Morse coherent states, only those with $\text{Im}\lambda = 0$ and hence $p_0 = 0$ are minimal in the usual sense. They coincide with the minimal states introduced by Klauder [56] and proved useful as basic analyzing wavelets in signal theory [57].

Now let us turn our attention to the problem, how the whole set of minimal states can be generated from the ground state. Considering the representation of \tilde{G}_0 in equation (3.10) an easy calculation shows that the group elements $U(a, b, c, d)$ generate the minimal states with parameter s which satisfy the constraint $y_0 \text{Re}\lambda = s$:

$$U(a, b, c, d) \Psi_0(y, s) = \Phi(y; \lambda = \frac{a}{2} + ib, p_0 = \rho d + \frac{2sb}{a}, y_0 = \frac{2s}{a}, \phi = c), \quad (3.37)$$

where $(a, b, c, d) \in \tilde{G}_0$. Using the analogy with the harmonic oscillator case the above states minimizing the uncertainty relation of (3.31) and including the

coherent states can be regarded as the intelligent states of the Morse potential characterized by the shape parameter s . It is obvious that by changing the shape parameter one obtains disjoint sets of intelligent states which exhaust the entire set of minimal states of the affine algebra.

We would like to note here that in the case of the harmonic oscillator the set of intelligent states is identical to the whole set of minimal states of the uncertainty relation. This is in accordance with the fact that the frequency playing the shape parameter for the harmonic oscillator [11, 12] does not change by constructing the SUSY partner Hamiltonian. This is in contrast with the case of Morse partner-Hamiltonians where the shape parameter s is shifted. We have also shown that each of these sets of intelligent states are generated from the corresponding ground state with the appropriate shape parameter s by the elements of the unitary irreducible representation of the group \tilde{G}_0 .

3.3 Affine Wigner function

The introduction of Wigner functions in quantum mechanical problems leads to a description in phase space that is equivalent to the operator description but that is more pertinent in some respects. In particular, the usual coherent and squeezed coherent states of the harmonic oscillator are represented by positive functions and their squeezing is clearly exhibited in the (x, p) phase space.

It is known that the coherent states of (2.72) will not be represented by a positive Wigner function, (for ordinary Wigner functions of Morse eigenstates, see [58, 59, 60]). More basically, the usual Wigner function is constructed on the Heisenberg group and has a larger covariance by the metaplectic group [61, 62]. As it has been shown above, it is the group \tilde{G}_0 which plays a fundamental role in the Morse problem, and hence it seems more desirable to use a phase space representation constructed on this latter group. This will be the affine Wigner function. We will now recall its construction and exhibit some of its properties that are relevant to the present problem.

The natural phase space is spanned here by coordinates p and y . It can be defined as an orbit of the group \tilde{G}_0 under its coadjoint representation deter-

mined as follows. Consider the adjoint representation of \tilde{G}_0 defined by

$$ad(a, b, c, d)X = U(a, b, c, d)XU^{-1}(a, b, c, d) \quad (3.38)$$

where $X = x_P P + x_Y Y + x_I I + x_Z Z$ denote the elements of the corresponding Lie algebra. Using the commutation relations (3.4)-(3.8) one obtains:

$$ad(a, b, c, d) \begin{pmatrix} x_P \\ x_Y \\ x_I \\ x_Z \end{pmatrix} = \begin{bmatrix} 1 & -b & -\rho d & 0 \\ 0 & a & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & \rho \ln a & 1 \end{bmatrix} \begin{pmatrix} x_P \\ x_Y \\ x_I \\ x_Z \end{pmatrix} \quad (3.39)$$

The coadjoint representation [63] acting on the dual space element $(p, y, \iota, z)^\top$ is given by

$$coad(a, b, c, d) \begin{pmatrix} p \\ y \\ \iota \\ z \end{pmatrix} = \begin{bmatrix} 1 & a^{-1}b & \rho d & 0 \\ 0 & a^{-1} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & -\rho \ln a & 1 \end{bmatrix} \begin{pmatrix} p \\ y \\ \iota \\ z \end{pmatrix} \quad (3.40)$$

This representation has four different types of orbits in the dual space of \tilde{G}_0 :

$$\begin{aligned} O^0(\eta_1, \eta_2) &= \{(\eta_1, 0, 0, \eta_2)\}, \\ O^H(\xi) &= \{(p, 0, \xi, z), \quad p, z \in \mathbb{R}\}, \\ O^\pm(\xi_1, \xi_2) &= \{(p, \pm y, \xi_1, \rho \xi_1 \ln y - \xi_2), \quad y > 0, p \in \mathbb{R}\}. \end{aligned} \quad (3.41)$$

where the real parameters $\eta_1, \eta_2, \xi, \xi_1$, and ξ_2 are constants characterizing the individual orbits [22].

Theoretically the above classes of orbits serve four different possibilities to define phase space but not each of them has physical relevance in the present problem. The first class O^0 is singular, because it includes only one-point orbits which are invariant under the action of group \tilde{G}_0 in the coadjoint representation space. It is obvious that these zero dimensional orbits do not meet the requirements of phase space. The orbits of the second one, O^H give the usual phase space spanned by coordinates (p, x) , because the fourth parameter, z originates from the operator $Z = \rho \ln Y = -\rho X + (\ln(2s + 1))\rho I$, which is essentially identical to X . Additionally, on these orbits the coadjoint

representation above acts as the Heisenberg-Weyl group. This is the consequence of that the subgroup with elements $U(u, v = 0, w, t)$ is identical to the Heisenberg-Weyl group. We have shown, however, that the operators P and Y are the relevant operators in the Morse problem and it is obvious that by choosing the class O^H , the affine subgroup of \tilde{G}_0 would be lost. Hence it is seen that the appropriate choice of the phase space is an orbit from the class O^+ or O^- parameterized by (p, y) . Among them only the class O^+ with positive valued coordinate y is well adapted to the current problem [22]. The action of the group \tilde{G}_0 on the phase space corresponding to the orbit $O^+(\xi_1, \xi_2)$ can be written:

$$\begin{pmatrix} p' \\ y' \end{pmatrix} = \begin{pmatrix} p + a^{-1}by + \rho\xi_1 d \\ a^{-1}y \end{pmatrix} \quad (3.42)$$

This gives the action of \tilde{G}_0 on the phase space parameterized by coordinates (p, y) and consequently on any function $F(p, y)$:

$$(a, b, c, d) : F(p, y) \longrightarrow F'(p, y) \equiv F(p - by - \rho\xi_1 d, ay) \quad (3.43)$$

In the following, we will set $\xi_1 = 1$ as this does not restrict generality.

Now the affine Wigner function is defined as a real quadratic functional of the wave function written as:

$$W(p, y; \psi) = \int_{\mathbb{R}^+ \times \mathbb{R}^+} K(p, y; y_1, y_2) \psi(y_1) \psi^*(y_2) dy_1 dy_2 \quad (3.44)$$

where the kernel K is such that:

$$K^*(p, y; y_1, y_2) = K(p, y; y_2, y_1) \quad (3.45)$$

Now, the correspondence $\psi(y) \rightarrow W(p, y; \psi)$ has to fulfill the following requirements:

1. *Covariance by the group \tilde{G}_0*

When the wave function $\psi(y)$ is transformed by the representation $U(a, b, c, d)$ according to (3.10), the corresponding phase space function $W(p, y; \psi)$ undergoes a point-like transformation of the form (3.43). In other words, the following diagram is commutative:

$$\begin{array}{ccc} \psi(y) & \longrightarrow & U(a, b, c, d)\psi(y) = e^{-i(by+c+\rho d \ln y)} \psi(ay) \\ \downarrow & & \downarrow \\ W(p, y) & \longrightarrow & W'(p, y) \equiv W(p - by - \rho d, ay) \end{array} \quad (3.46)$$

Writing explicitly this condition with the functional $W(p, y; \psi)$ defined in (3.44) leads necessarily to a phase space function of the form [57]:

$$W(p, y; \psi) = \int_{-\infty}^{\infty} e^{ivp} \psi \left(\frac{yve^{v/2}}{2 \sinh(v/2)} \right) \psi^* \left(\frac{yve^{-v/2}}{2 \sinh(v/2)} \right) \mu(v) dv \quad (3.47)$$

where the function $\mu(v)$ is such that:

$$\mu^*(v) = \mu(-v) \quad (3.48)$$

and otherwise arbitrary.

2. Unitarity

This is also called Moyal property in the case of the usual Wigner function. Here it is written as:

$$\int_{\mathbb{R} \times \mathbb{R}^+} W(p, y; \psi_1) W(p, y; \psi_2) dp(dy/y) = |(\psi_1, \psi_2)|^2 \quad (3.49)$$

with the scalar product of wave functions given by equation (3.9). The constraint (3.49) leads to the determination of $\mu(v)$: $\mu(v) = \frac{1}{2\pi}$.

Finally the affine Wigner function is given by:

$$W(p, y; \psi) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ivp} \psi \left(\frac{yve^{v/2}}{2 \sinh(v/2)} \right) \psi^* \left(\frac{yve^{-v/2}}{2 \sinh(v/2)} \right) dv \quad (3.50)$$

This function is not positive everywhere for an arbitrary state, and is thus only a pseudo-distribution. However it provides a phase space interpretation for the properties relative to the minimal states and for the action of the group \tilde{G}_0 .

Due to the non-commutativity of the affine algebra, there is no state having a phase space representation $W(p, y)$ exactly localized in one point. The optimal concentration of the affine Wigner function will occur for the minimal states. Consider first the Morse ground state, which is identical to the coherent state with $\beta = 0$:

$$\Psi_0(y) = \frac{1}{\sqrt{\Gamma(2s)}} y^s e^{-(y/2)}. \quad (3.51)$$

Substitution into expression (3.50) gives:

$$\begin{aligned} W(p, y; \Psi_0(s)) &= \frac{y^{2s}}{2\pi\Gamma(2s)} \int_{-\infty}^{\infty} e^{ivp} \left(\frac{v}{2 \sinh(v/2)} \right)^{2s} e^{-y(v/2) \coth(v/2)} dv \\ &\equiv W_0(p, y; s) \end{aligned} \quad (3.52)$$

This expression can be shown to be positive, as the Fourier transform of a function of positive type [64], and it is localized around the point $p = 0$, $y = 2s$. The use of the covariance property (3.46) shows that the phase space representation of a general minimal state, as defined by equation (3.37), is obtained from W_0 by a point transformation and is thus positive as well. In particular, the affine Wigner representation of any Morse coherent state (2.72) written as:

$$\varphi_\beta(y) = U(a, b)\Psi_0(y) = \frac{a^s}{\sqrt{\Gamma(2s)}} y^s e^{-(a/2+ib)y}, \quad a/2 + ib = \frac{1}{2} \frac{1 + \beta}{1 - \beta}. \quad (3.53)$$

is equal to:

$$W(p, y; \varphi_\beta) = W_0(p - by, ay; s) \quad (3.54)$$

Thus, for a given s , there is a Morse coherent state attached to any point of the phase space and the extension of its (positive) affine Wigner function depends only on that point.

More generally, any intelligent state (3.35) is represented by:

$$W(p, y; \Phi(\lambda, p_0, y_0, \phi)) = W_0(p - p_0 - (y - y_0) \operatorname{Im}\lambda, 2\operatorname{Re}\lambda y; y_0 \operatorname{Re}\lambda). \quad (3.55)$$

The parameter λ , which appeared in equation (3.33), can thus be interpreted as a factor determining the shape of the function $W(p, y)$. In the limit $\lambda = 0$, the functions $\Phi(y)$ collapse into eigenstates of the operator P :

$$\psi_P(y) = y^{-ip_0}, \quad (3.56)$$

and sharp localization is obtained in phase space:

$$W(p, y; \psi_P) = \delta(p - p_0) \quad (3.57)$$

The group \tilde{G}_0 has been seen to perform point transformations in the affine Wigner function. In fact, it is the largest group with this property which can be represented unitarily on the wave function. It thus plays a role analogous as does the metaplectic group [61] in the harmonic oscillator case.

To make a comparison of the present phase space representation (3.50) with what would be obtained from Wigner's, it is useful to go back to the original variable x and to define:

$$\bar{\psi}(x) \equiv \psi((2s+1)e^{-x}), \quad \bar{W}(p, x; \tilde{\psi}) \equiv W(p, (2s+1)e^{-x}; \psi) \quad (3.58)$$

The expression (3.50) leads to:

$$\bar{W}(p, x; \bar{\psi}) = \int_{-\infty}^{\infty} e^{ivp} \bar{\psi}\left(x - \frac{v}{2} - r(v)\right) \bar{\psi}^*\left(x + \frac{v}{2} - r(v)\right) dv, \quad (3.59)$$

where $r(v)$ is given by

$$r(v) = \ln \frac{v + (2s+1) \sinh(v/2)}{2 \sinh(v/2)}. \quad (3.60)$$

It can be seen that, in the vicinity of $v = 0$, the argument of ψ (resp ψ^*) is approximated by $x - v/2$ (resp $x + v/2$). Hence the function $\bar{W}(p, x; \bar{\psi})$ will be close to the original Wigner function only for states $\psi(x)$ which have support on a narrow interval. In particular, the usual Wigner function cannot localize exactly states of the form (3.56).

Chapter 4

Dissociation in the Morse oscillator

Since the first observation of infrared multiphoton absorption in molecules in the 1970's, these processes have been attracting much attention because of their potential applicability in the laser control of molecular reactions [5, 6, 65, 66, 67]. The focus of the current chapter is on the dynamics of multiphoton absorption for diatomic molecules. These processes have been investigated theoretically by solving the time dependent Schrödinger equation of the molecule in external fields. In the present work we will describe a new method for treating the case when the molecule is in its ground electronic state and the potential energy curve between the atoms is of the realistic Morse form. We will give an almost completely analytical description of the Morse oscillator subject to an external classical electromagnetic field, where the interaction is treated in the dipole approximation. In other words we shall give the solution of the time dependent Schrödinger equation:

$$i\hbar \frac{d|\Phi\rangle}{dt} = (\hat{H}_0 - \hat{\mu}E(t))|\Phi\rangle \quad (4.1)$$

where \hat{H}_0 is the Morse Hamiltonian, $\hat{\mu}$ is the dipole moment operator of the molecule, and $E(t)$ is the classical electric field strength of the excitation.

Time dependent problems can be treated in principle in quantum mechanics by an expansion in terms of stationary states of the unperturbed Hamiltonian, but if a part of the spectrum falls into the continuum, then this method is not

very convenient. Therefore other methods have been worked out, an overview of which can be found in the review paper of Kosloff [68]. They are using mainly the coordinate representation and the so-called split operator method, that solves the time dependent Schrödinger equation by using coordinate and momentum representations alternating, and have a precision of the order $(\Delta t)^2$ in the time variable increment. The method we propose for the Morse oscillator leads to a system of ordinary differential equations, with given constant coefficients where the precision can be of much higher order.

Our method uses the ladder operator technique of supersymmetric quantum mechanics (SUSY QM) and the complete orthogonal and normalizable set of quasi-number states which is defined as special case of Morse-Laguerre states $|\varphi_n(\sigma)\rangle$ with the parameter choice $\sigma = s - [s]$ (see section 2.3). The formalism introduced by us in [19]-[24], and its mathematical background has already been discussed in previous chapters. Besides of its higher precision another advantage of our treatment is that we use essentially an algebraic operator method. This technique is widely exploited if the molecular vibrations are treated in the harmonic approximation because of its clarity. The Morse problem is however essentially anharmonic and its classical dynamics is not linear either, therefore we think that the algebraic approach to the corresponding quantum problem will be of interest on its own. Besides working out this method we shall demonstrate the power of our formalism in a concrete application, we shall calculate the dissociation probability of the NO molecule under the action of a short chirped laser pulse.

4.1 Matrix elements of the interaction term

We consider now the time evolution of the molecular vibration subject to an external classical field with the field strength $E(t)$. In the dipole approximation the interaction term is given by

$$\hat{H}_{int} = -E(t)\hat{\mu}(\hat{X}), \quad (4.2)$$

where $\hat{\mu}(\hat{X})$ is the molecular dipole moment depending on the interatomic separation. Using the units introduced in Section 2.1 given by the equation (2.5) we define $\mu = \frac{\alpha}{q_e}\hat{\mu}$, the dimensionless dipole moment operator, where

$q_e = \frac{d\tilde{\mu}(x)}{dx}|_{x=0}$ is an effective charge and α is the range parameter of the Morse potential. Then for the dimensionless interaction Hamiltonian one obtains that

$$H_{int} = -\mu(X)\mathcal{E}(t), \quad (4.3)$$

where $\mathcal{E}(t) = \frac{(2s+1)q_e}{\hbar\omega_0\alpha} E(t)$ denotes the electric field strength in our units. If one wishes to solve the Schrödinger equation (4.1) in the quasi-number state basis, one also need to know the matrix of the dipole moment in this basis. Due to the algebraic properties of the quasi-number states $|\varphi_n(\sigma)\rangle$, the matrix of $\mu(X)$ can also be determined analytically for certain simple cases. Let us suppose first that the dipole moment can be approximated by an operator of the form:

$$\mu(X) = X \exp(-\gamma X). \quad (4.4)$$

Using equation (2.37) and the fact that $[f(X), A^\dagger(k)] = [f(X), -iP] = \frac{df(X)}{dX}$ for an arbitrary operator function $f(X)$ of X , the following recurrence relation is obtained:

$$\langle\varphi_m|\mu(X)|\varphi_{n+1}\rangle = \frac{1}{C_{n+1}}((n-m-\gamma)\langle\varphi_m|\mu(X)|\varphi_n\rangle + C_m\langle\varphi_{m-1}|\mu(X)|\varphi_n\rangle + \langle\varphi_m|\exp(-\gamma X)|\varphi_n\rangle). \quad (4.5)$$

Here we have introduced the obvious abbreviations $|\varphi_n\rangle \equiv |\varphi_n(\sigma)\rangle$, $C_m = C_m(\sigma) = \sqrt{m(m+2\sigma-1)}$. By the same procedure a similar recurrence relation can be derived for the matrix elements $\langle\varphi_m|\exp(-\gamma X)|\varphi_n\rangle$:

$$\langle\varphi_m|\exp(-\gamma X)|\varphi_{n+1}\rangle = \frac{1}{C_{n+1}}((n-m-\gamma)\langle\varphi_m|\exp(-\gamma X)|\varphi_n\rangle + C_m\langle\varphi_{m-1}|\exp(-\gamma X)|\varphi_n\rangle). \quad (4.6)$$

Then all matrix elements can be calculated, if one has the first of these series: $\langle\varphi_0|\mu(X)|\varphi_0\rangle$ and $\langle\varphi_0|\exp(-\gamma X)|\varphi_0\rangle$. These latter can be calculated via integration in coordinate representation:

$$\langle\varphi_0|\mu(X)|\varphi_0\rangle = \frac{\Gamma(2\sigma+\gamma)}{\Gamma(2\sigma)(2s+1)^{-\gamma}} \left[\ln(2s+1) - \tilde{\psi}(2\sigma+\gamma) \right] \quad (4.7)$$

$$\langle\varphi_0|\exp(-\gamma X)|\varphi_0\rangle = \frac{\Gamma(2\sigma+\gamma)}{\Gamma(2\sigma)(2s+1)^{-\gamma}}, \quad (4.8)$$

where $\tilde{\psi}$ denotes the digamma (Euler's $\tilde{\psi}$) function [39]. Using the recurrence relations (4.5)-(4.6) above, one can determine the symmetric matrix $\langle \varphi_m | \mu(X) | \varphi_n \rangle$ for arbitrary indices m and n .

This result can be trivially extended to the case when the dipole moment is a sum of terms like the one in equation (4.4):

$$\mu(X) = \sum_j d_j X \exp(-\gamma_j X), \quad (4.9)$$

which is a rather general form. The values of the parameters d_j and γ_j can be obtained by fitting this function to experimental dipole curves, or to those obtained from molecular calculations. Taking only a single term with $\gamma = 0$ would mean the simplest linear dipole moment borrowed from atomic calculations and used sometimes for molecules, as well. This latter approach, however, overestimates the strength of the interaction at large atomic separations and leads to an unrealistic dissociation probability.

4.2 Time evolution and dissociation

The quasi-number states constitute a complete orthonormal basis, hence one can expand any state $|\Phi(t)\rangle$ in the form: $|\Phi(t)\rangle = \sum_{n=0}^{\infty} c_n(t) |\varphi_n\rangle$. Measuring the time t in units of $2\pi/\omega_0$, the Schrödinger equation can be written as the following infinite system of ordinary differential equations:

$$\frac{dc_n(t)}{dt} = -i \frac{2\pi}{(2s+1)} \sum_{m=0}^{\infty} \{ \langle \varphi_n | H_0 | \varphi_m \rangle - \mathcal{E}(t) \langle \varphi_n | \mu | \varphi_m \rangle \} c_m(t). \quad (4.10)$$

where $\langle \varphi_n | H_0 | \varphi_m \rangle$ and $\langle \varphi_n | \mu | \varphi_m \rangle$ are given by analytical expressions as detailed in the previous sections.

We will apply our method to determine the dissociation probability of a molecule. This probability is a time dependent quantity defined as the projection probability of $|\Phi(t)\rangle$ on the continuum, or identically as the part of its norm that has already flown out of the bound subspace \mathcal{H}^- , and is given exactly by:

$$\mathcal{P}(t) = 1 - \sum_{m=0}^{[s]} |\langle \Phi(t) | \Psi_m \rangle|^2 = 1 - \sum_{m=0}^{[s]} c_m^*(t) c_m(t). \quad (4.11)$$

(Here we have used the abbreviation $|\Psi_m\rangle$ for the bound state $|\Psi_m(s)\rangle$.) To calculate the dissociation probability above, we have to solve the set of the dynamical equations (4.10) and to determine the coefficients $c_m(t)$ for $0 \leq m \leq [s]$. The coefficients we are looking for are, however, coupled to those with $m > [s]$ by the dipole interaction, thus the set of equation one has to solve is infinite dimensional. Therefore in practice we have to truncate the system (4.10), and we have to use a numerical method to find the solution.

The restriction of the number of the dynamical equations to a finite number is done here in two steps. First we consider the problem in a very large subspace of dimension $N \gg [s]$, and neglect the contribution of those states $|\varphi_n\rangle$ for which $n > N$. Essentially, this truncation means that the infinite dimensional subspace of dissociated states, \mathcal{H}^+ is approximated by a large, but finite dimensional subspace. We note that the dimension of the subspace of the bound states $[s]+1$ is typically of the order of a few tens, therefore the subspace of the scattering states is approximated by an $N - [s] - 1$ dimensional space, where N is of the order of 10^3 . Then the Hamiltonian is represented by an operator that is restricted to the finite N dimensional subspace spanned by the orthonormal system $\{|\Psi_m\rangle, |\varphi_n\rangle\}$ with $n = [s] + 1, \dots, N$ and $m = 0, 1, \dots, [s]$:

$$H^{(N)} = H_0^{(N)} - \mathcal{E}(t)\mu^{(N)}, \quad (4.12)$$

where $H_0^{(N)}$ and $\mathcal{E}(t)\mu^{(N)}$ are the truncated operators, so that their matrices are of dimension N . The matrix of $H_0^{(N)}$ is built up by an $[s] + 1$ dimensional diagonal (see equation (2.21)) and an $N - [s] - 1$ dimensional tridiagonal block matrix (2.53) corresponding to the bound state subspace and to the approximated positive energy subspace, respectively. Before solving the already finite number of ordinary differential equations we perform a unitary transformation on our truncated basis to bring this restricted free Hamiltonian into diagonal form. Due to the fact that the matrix of $H_0^{(N)}$ is finite tridiagonal, this can be done by the help of a very fast algorithm. This yields positive energy eigenvalues $E_n^{(N)}$ ($1 + [s] \leq n \leq N$) and the corresponding eigenstates $|\Psi_n^N\rangle$ which we can use for the description of the dissociated part of the spectrum. If N is large enough, then the lowermost positive energies $E_n^{(N)}$ follow densely each other, and approximate satisfactorily the continuous energy spectrum above the dissociation threshold.

In the second step of the approximation, we restrict the calculation to the bound subspace and to those $|\Psi_n^N\rangle$ states with $n > [s]$, for which the dipole couplings with the bound states are non-negligible. In the application to be discussed below, it will turn out that these matrix elements are significant only for those $|\Psi_n^N\rangle$ states that correspond to the lowest positive energy eigenvalues $E_n^{(N)}$ with $n = [s]+1, \dots, M$, so that $M \ll N$. Therefore, in order to follow the dissociation process, it is enough to solve (4.10) in the basis $|\Psi_m\rangle, |\Psi_n^N\rangle$, which means that we expand the time dependent states as $|\Phi(t)\rangle = \sum_{n=0}^M b_n(t) |\psi_n\rangle$, where now the notation

$$|\psi_n\rangle \equiv \begin{cases} |\Psi_n\rangle & \text{if } 0 \leq n \leq [s] \\ |\Psi_n^N\rangle & \text{if } [s] < n \leq N \end{cases} \quad (4.13)$$

has been introduced. Then we solve the system of M ordinary differential equations

$$\frac{db_n(t)}{dt} = -i \frac{2\pi}{(2s+1)} \sum_{m=0}^M \{ \langle \psi_n | H_0 | \psi_m \rangle - \mathcal{E}(t) \langle \psi_n | \mu | \psi_m \rangle \} b_m(t). \quad (4.14)$$

that describes the time evolution of the coefficients b_n and calculate the dissociation probability via equation (4.11) with the obvious $c_m(t) \rightarrow b_m(t)$ replacement:

$$\mathcal{P}(t) = 1 - \sum_{m=0}^{[s]} b_m^*(t) b_m(t). \quad (4.15)$$

4.3 An example: the NO molecule

In what follows we are going to illustrate our method through a calculation for a concrete molecule. We are going to determine the dissociation probability starting from the ground state for the nitrogen-oxide (NO) molecule, excited by an appropriate laser field. The dissociation of this molecule has attracted a certain interest in the last few years. We have used a Morse potential with the molecular data in the electronic ground state which are summarized in Table 4.1. These values of parameters m , α and D are taken from [37].

The potential and the dependence of the dipole moment on the interatomic separation are depicted in Figure 4.1. The circles show the dipole moments

parameter	symbol	value
reduced mass	m	7.46 a.u.
range parameter	α	27.68 nm ⁻¹
dissociation energy	D	6.497 eV
Morse frequency	$\omega_0 = \sqrt{2D\alpha^2/m}$	1904, 2cm ⁻¹
s parameter	$s = \sqrt{2mD}/\hbar\alpha - 1/2$	54.54

Table 4.1: Typical parameters for NO

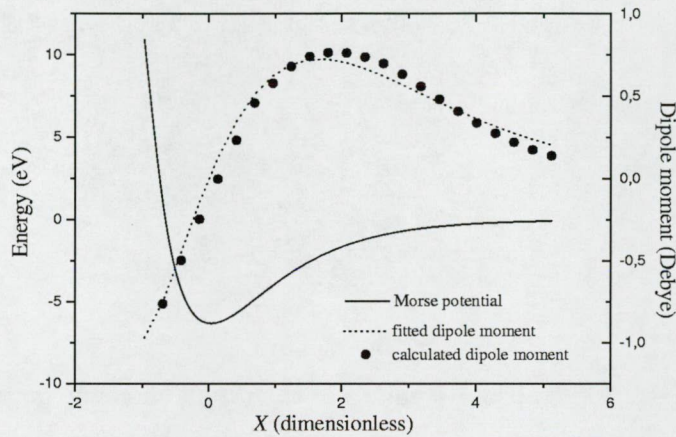


Figure 4.1: The dipole moment function of NO

of NO at various interatomic separations that have been calculated by an unrestricted density functional method [69]. The dotted line is a fitted function of the form (4.9)

$$\mu(X) = d_1 X \exp(-\gamma_1 X) + d_2 X \exp(-\gamma_2 X), \quad (4.16)$$

with the parameter values: $d_1 = -9.66$, $d_2 = 10.64$, $\gamma_1 = 0.927$ and $\gamma_2 = 0.870$. The matrix elements corresponding to these operators have been determined analytically by using the recurrence relations of (4.5) and (4.6).

In order to carry out concrete calculations we have chosen the truncation indices to be $N = 3000$, and $M = 200$, as increasing these values had no effect on the result. (Note that the number of bound states is now $[s] + 1 = 55$.) The

dipole moment matrix corresponding to the set of states $|\psi_n\rangle$ is shown in Figure 4.2. One can see that it has negligible elements far away from the diagonal, that

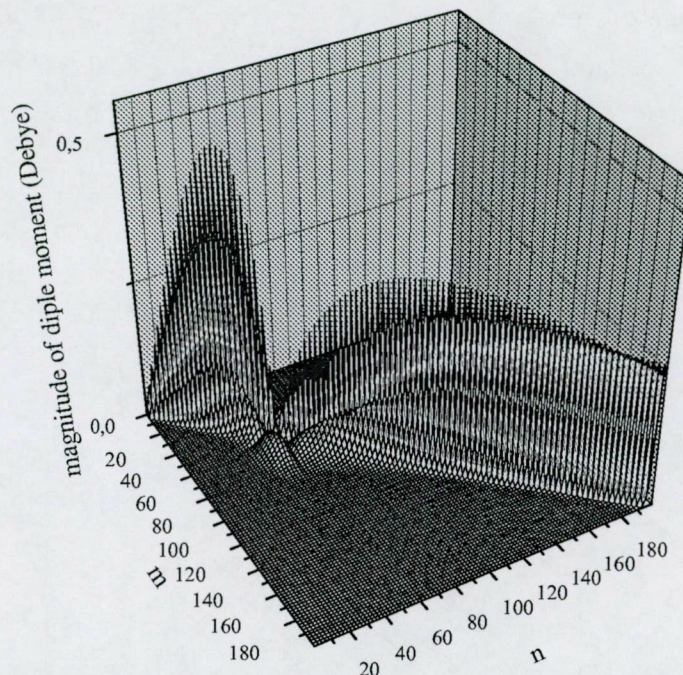


Figure 4.2: The absolute values of the dipole moment matrix elements

justifies the truncation procedure, in calculating the dissociation probability. The initial state was taken to be the vibrational ground state, and we devised the excitation with the aim to achieve a significant dissociation probability.

According to [7] one can think of the desired time evolution as a sequence of two-level transitions. In the ideal case the electric field is resonant with every single transition and its pulse area is π . In order to maintain the resonance condition during the whole process, it is appropriate to use continuously chirped pulses. If the frequency of the pulses decreases slowly enough, then it is possible to consider its effect as a sequence of approximately resonant two-level transitions. For low vibrational quantum numbers the coupling is the largest between the nearest neighbors, therefore at the beginning the excitation has to drive the system through the ladder of neighboring eigenstates towards the continuum. However, as it is seen in Figure 4.3, there is a minimum in the $m \rightarrow m+1$ couplings at $m = 42$, therefore this vibrational quantum number

corresponds to a trapping state.

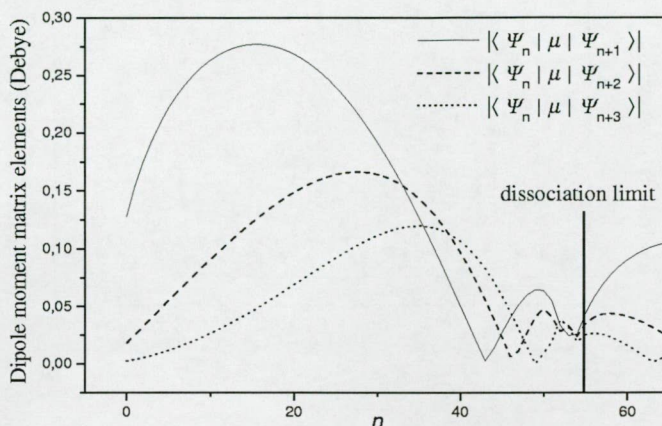


Figure 4.3: The neighbouring matrix elements

This is a consequence of the shape of the dipole moment curve (Figure 4.1) and it would be absent in the linear approximation $\mu(X) \sim X$. One can circumvent the problem by lengthening the pulse time, but we present a different route here with the three pulses shown in Figure 4.4, exploiting other than first neighbor transitions, as well. The area condition could be met for all three pulses with the distorted secant-hyperbolic envelopes:

$$\mathcal{E} = \mathcal{E}_a / [\exp(t_0 - t)/\tau_f + \exp(t - t_0)/\tau_t] \quad (4.17)$$

with different exponentials in their fronts τ_f and tails τ_t . The chirping rates can be seen in Figure 4.4 while the other data of the pulses are given by (a) pulse 1: $\tau_f = 10.27$, $\tau_t = 246.4$, $t_0 = 41.0$, (b) pulse 2: $\tau_f = 71.87$, $\tau_t = 61.61$, $t_0 = 1297.5$ and (c) pulse 3: $\tau_f = 71.87$, $\tau_t = 61.61$, $t_0 = 2087.6$. Further the peak values for all three pulses are $1.05 \times 10^8 \text{V/cm}$. Using these parameters, the first pulse drives the molecule into a superposition of a few states $|\psi_m\rangle$ around $m = 42$. This implies that a second laser pulse with an initial carrier frequency being in approximate resonance with the corresponding $m \rightarrow m+2$ transition will continue this dissociation process and let the molecular state jump over the trap state. After this second pulse, the distribution of the

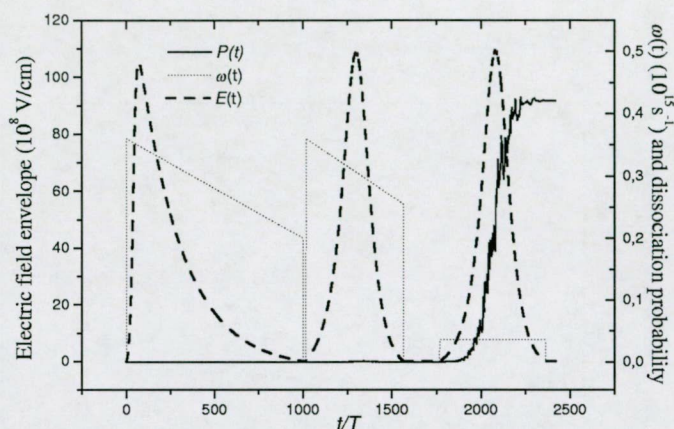


Figure 4.4: The sequence of three chirped laser pulses and corresponding dissociation rates

populated states is not so narrow as it was before, which is a consequence of the presence of second neighbor transitions. The most probably populated states are now so close to the continuum limit that a final pulse - even without chirping - leads to a dissociation probability that is more than 40%. As shown in Figure 4.4, this probability is practically zero before the third pulse.

In this chapter, we have presented a method based on SUSY QM that leads to a system of ordinary differential equations describing molecular time evolution. The key object of our approach was the complete and orthonormal basis of the pseudo-number states serving full description of the Hilbert space and allowing to evaluate the matrices of both the free Hamiltonian and the perturbation term, too. We have applied this method for devising laser pulses leading to a significant dissociation probability of the NO (nitrogen-oxide) molecule with a realistic dipole moment.

Summary

In the present work we have pursued the detailed algebraic analysis of the anharmonic Morse oscillator. Our approach is essentially based on the ladder operator technique which was originally introduced in the context of supersymmetric quantum mechanics. Using the supersymmetric creation operator of the Morse oscillator we have generated a class of complete sets of normalizable states which enabled us to formulate the problem of the Morse oscillator entirely in Hilbert space even above the dissociation threshold. We have also introduced coherent states for the Morse potential in an algebraic manner and have proven their connection to the affine group of the real line. We have also shown that from certain points of view in the case of the Morse potential the affine group and its further extensions play similar roles as the Heisenberg-Weyl group and the metaplectic group do for the harmonic oscillator. To emphasize also the practical applicability of our algebraic results we have applied them to the study of a concrete physical problem: the dissociation of the NO (nitrogen-oxide) molecule induced by external electromagnetic pulses.

Chapter 1: Overview of SUSY QM. In this chapter we introduced those objects which are necessary to treat the quantum problem of the Morse oscillator by an algebraic method. We reviewed the concepts of SUSY QM and shape invariance. We presented how SUSY QM can be used to solve eigenvalue problems corresponding to shape invariant Hamiltonians in an algebraic way similarly to the commonly used ladder operator method of the harmonic oscillator.

Chapter 2: Morse oscillator. In this chapter we first started with known results. In the first two sections we recalled the bound states and non-normalizable scattered states of the Morse potential where these latter ones do not belong to the Hilbert space of normalizable vectors. There exists only a finite

number of bound states and the dimension of the subspace spanned by them is given by the expression $[s] + 1$, depending on the shape parameter s characterizing the depth of the potential well. (Notation: $[s]$ denotes the largest integer less than parameter s .) For sake of completeness we also recalled the scattering wave functions of the Morse oscillator which obey other boundary conditions than the bound states, and they do not belong to the Hilbert space of square integrable function. However, these wave functions can be interpreted as the kernels of non-bounded linear functionals over the Hilbert space and certain appropriate continuous sums (integrals) of them lead to normalizable states in the orthogonal complement of the bound state subspace.

Obviously, it is impossible to have a full quantum description restricting the system only to this finite bound state subspace. In order to avoid the problem of the incompleteness and to describe the dissociated part of the Hilbert space we have introduced a new complete set of mutually orthogonal and normalizable states depending on a positive parameter q . In general we referred to these basis states as *Morse-Laguerre states*. An additional advantage of these bases is that for certain appropriate choice of the parameter q the Morse Hamiltonian takes on the form of a simple tridiagonal matrix consisting of two blocks which correspond to a finite and an infinite dimensional invariant subspaces, respectively.

It is worth to distinguish two particular cases. In one of these q coincides exactly with the positive shape parameter s of the Morse potential. Then the first Morse-Laguerre state is the ground state, while the excited bound eigenstates are infinite linear combination of the Morse-Laguerre states other than this first one. We call this special case of the Morse-Laguerre states as the *pseudo-number state* basis. By the help of these pseudo-number states we constructed the coherent states for the anharmonic Morse potential analogously to the way one expands the coherent states of the harmonic oscillator in terms of its eigenstates.

In the second particular case, we set $q = s - [s]$. Then each of the first $[s] + 1$ Morse-Laguerre states becomes exactly the linear combinations of the bound states. In other words, the bound subspace is spanned by the first $[s] + 1$ Morse-Laguerre states while its orthogonal complement subspace corresponding to the dissociated part of the Hilbert space is spanned by the rest

of the Morse-Laguerre states. In this case, i.e., when $q = s - [s]$, we call the Morse-Laguerre states as *quasi-number states*. They serve useful tools to study the state evolution when an external field forces the system to flow out of the bound subspace.

Chapter 3: The affine group and the Morse oscillator. In Chapter 2 we had introduced the *coherent states* of the Morse oscillator as the superpositions of pseudo-number states in complete analogy to the case of harmonic oscillator. In this chapter we elucidated the connection of the Morse coherent states with the affine group of the real line and some of its extensions. In the case of the Morse oscillator the central extension of the affine Lie algebra plays a similar spectrum generating role as the Heisenberg-Weyl algebra does for the harmonic oscillator. We also pointed out that the elements of the unitary irreducible representation of the affine group are *displacement operators* for the Morse coherent states in the sense that they create them from the ground state being itself coherent. We showed that the Morse coherent states minimize the strong version of the *uncertainty relation* associated to the affine group. Therefore they can also be interpreted as minimal uncertainty states of the affine group. We proved how the whole set of minimal states - which is larger than the coherent state set - is connected to a certain further non-trivial extension of the affine group (the extension by the torus group).

We also presented a *phase space* picture for the Morse coherent states and minimal states via a quasi-distribution density function called the affine Wigner function introduced originally in signal processing theory.

Chapter 4: Dissociation in the Morse oscillator. The multiphoton absorption processes in diatomic molecules have been attracting continuous attention for a long while. The driven Morse oscillator is a widely used model to study such molecular processes especially the photodissociation. In this chapter by applying the basis of the quasi-number states we transformed the time-dependent Schrödinger equation corresponding to the Morse oscillator that is driven by an external classical laser field into a set of *ordinary* differential equations. The parameters of the Morse potential were chosen to be of the real nitrogen-oxide molecule. We approximated the dipole moment values calculated by an ab-initio method with a special dipole moment function. The functional form of these latter function allowed us to determine the corre-

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sponding dipole matrix elements algebraically. By straightforward numerical methods we solved the dynamical equations and found significant dissociation induced by a sequence of appropriately tailored chirped laser pulses.

Összefoglalás

A dolgozatban elvégeztük a kvantummechanikai anharmonikus Morse oszcillátor részletes algebrai analízisét. Módszerünk lényegében a szuperszimmetrikus kvantummechanika léptető operátoros technikáján alapul. A Morse oszcillátor szuperszimmetrikus keltő operátorán keresztül normálható, ortogonális állapotok teljes rendszereinek egy osztályát állítottuk elő, amely lehetővé teszi a Morse potenciál teljes, Hilbert-térbeli leírását még a disszociációs küszöb felett is. Algebrai módon koherens állapotokat vezettünk be a Morse potenciál esetére, és bizonyítottuk azok kapcsolatát a valós számegyenes affin csoportjával. Megmutattuk, hogy az affin csoport és annak további kiterjesztettjei a Morse potenciál esetében hasonló szerepet játszik, mint a Heisenberg-Weyl csoport és a metaplektikus csoport a harmonikus oszcillátor estén. Gyakorlati jelentőségét hangsúlyozandó, algebrai eredményeinket egy konkrét fizikai probléma, a NO (nitrogén-monoxid) molekula külső elektromágneses tér indukálta disszociációjának tanulmányozására alkalmaztuk.

1. Fejezet: A szuperszimmetrikus kvantummechanika áttekintése. A fejezetben az irodalom alapján bevezettük mindazokat az objektumokat, amelyek a Morse oszcillátor kvantummechanikai problémájának algebrai leírásához szükségesek. Röviden áttekintettük mind a szuperszimmetrikus kvantummechanika, mind az alakinvarianca koncepcióját. Bemutattuk hogyan oldható meg egy alakinvariáns potenciál Hamilton operátorának sajátérték problémája algebrai úton, hasonlóan a harmonikus oszcillátornál már megszokott léptető operátoros tárgyalásához.

2. Fejezet: Morse oszcillátor. A fejezet első két szakaszában korábbról ismert tényekkel foglalkoztunk. Felidéztük a Morse potenciál kötött illetve nem normálható szórt állapotait. Amennyiben létezik, akkor mindig véges számú normálható kötött állapot írható fel, és az ezek által kifeszített altér di-

menzióját pontosan a Morse potenciál mélységét jellemző s paramétertől függő $[s] + 1$ kifejezés adja meg. (A jelölés: $[s]$ azt a legnagyobb egész számot jelenti, amely szigorúan kisebb s -nél.) A szórt állapotok a Hamilton operátor pozitív sajátértékeihez tartozó, nem Hilbert-térbeli sajátfüggvények, amelyek a megfelelő határfeltételeknek tesznek eleget. A szórt állapotok, mint nem korlátos lineáris funkcionálok már jól értelmezhetőek a Hilbert-tér felett, és a velük képzett megfelelő integrálok a kötött állapotok ortogonális komplementerének elemei. Ezen az utóbbi végtelen dimenziós ortogonális komplementer altéren (disszociált altéren) a Hamilton operátor azonban szigorú értelemben már nem diagonalizálható.

Nyilvánvalóan, csupán a véges kötött állapotok altérré szorítkozva a rendszer teljes kvantummechanikai leírása, illetve a fizikailag lényeges disszociációs folyamat vizsgálata nem valósítható meg, mivel ekkor a Hilbert-tér disszociált altérét figyelmen kívül hagyjuk. Ezt a problémát megoldandó a 2.3 pontban, ahonnét a saját eredményeink ismertetését kezdtük el, bevezettünk ortonormált bázisok egy új családját, amelynek mindegyike ténylegesen kifeszíti a teljes Hilbert teret. Ezeket a bázisokat, amelyeket egy pozitív q paraméter különböztet meg egymástól, közös néven *Morse-Laguerre bázisoknak* nevezzük. A teljességen túl a Morse-Laguerre bázisok további előnye, hogy a Hamilton operátor mátrixa bennük tridiagonális. A q paraméter bizonyos jól meghatározott értékeinél a Hamilton operátor mátrixa egy véges és egy végtelen dimenziós tridiagonális blokkra bomlik szét.

Itt két különösen hasznos esetet vizsgáltunk meg részletesen. Az első esetben, amikor a q paraméter pontosan megegyezik a Morse potenciál s pozitív alakparaméterével, az első Morse-Laguerre állapot éppen az alapállapot, míg a gerjesztett állapotok a további Morse-Laguerre állapotok végtelen lineáris kombinációi. Ebben a speciális esetben a Morse-Laguerre állapotokat *pszeudo-számállapotoknak* nevezzük. A pszeudo-számállapotokon keresztül az anharmonikus Morse oszcillátor koherens állapotai ahhoz az eljáráshoz hasonlóan konstruálhatók meg, ahogyan a harmonikus oszcillátor esetén a koherens állapotok a számállapotokon keresztül fejthetők ki. A Morse koherens állapotok illetően való konstrukcióját szintén ebben a fejezetben tárgyaltuk.

A második esetben, a $q = s - [s]$ paraméter választással az első $[s] + 1$ Morse-Laguerre állapot a kötött állapotok egymástól lineárisan független

kombinációi. Más szavakkal, a kötött állapotú alteret az első $[s] + 1$ Morse-Laguerre báziselem, míg a disszociált állapotú alteret (a kötött állapotú alter ortogonális komplementerét) a további Morse-Laguerre bázisvektorok feszítik ki. Az ilyen paraméterválasztással adódó Morse-Laguerre állapotokat *kvázi-számállapotoknak* hívjuk. Ez utóbbi állapotok hasznos eszközül szolgálnak állapotok időfejlődésének nyomonkövetésére, még abban az összetett esetben is, amikor egy külső gerjesztő tér hatására a rendszer "kifolyik" a kötött altérből.

3. Fejezet: Az affin csoport és a Morse oszcillátor. Az előző fejezetben – a harmonikus oszcillátor esetével analóg módon – bevezettük a Morse *koherens állapotok* túlteljes rendszerét, mint pszeudo-számállapotok megfelelő szuperpozícióit. Ebben a fejezetben kifejtettük a Morse koherens állapotok kapcsolatát a valós számegyenes affin csoportjával, illetve annak néhány további kiterjesztésével. Először megmutattuk, hogy a Morse oszcillátor esetén az affin algebra centrális kiterjesztése játssza ugyanazt a spektrumgeneráló szerepet, amit a Heisenberg-Weyl algebra a harmonikus oszcillátor számára. Azt is bizonyítottuk, hogy az affin csoport megfelelő unitér irreducibilis reprezentációjának elemei a Morse koherens állapotok *eltolási operátorai*. A koherens állapotokat ezek az eltolási operátorok állítják elő az alapállapotból, amely maga is koherens állapot. Megmutattuk továbbá, hogy a Morse koherens állapotok minimalizálják az affin csoport generátoraihoz társított *határozatlansági reláció* "erősebb" vátozatát. Ezért azokat az affin csoport minimális állapotaként is értelmezhetjük. Beláttuk azt is, hogy a minimális állapotok egész halmaza, amely bővebb, mint csak a koherens állapotoké, az affin csoport egy nem triviális, a tórusz csoporttal tötendő, kiterjesztésével kapcsolatos.

Megadjuk a Morse koherens és minimális állapotok fázistérbeli reprezentációját az ún. affin Wigner függvények segítségével, amelyek máshol, eredetileg a jelfeldolgozás elméletében kerültek bevezetésre.

4. Fejezet: Disszociáció Morse oszcillátorban: Kéttomos molekulák többfotonos abszorpciós folyamatait már hosszú ideje jelentős érdeklődés övezi. A kényszerített Morse oszcillátor gyakran használt modell ilyen molekuláris folyamatok, különösen a fotodisszociáció, tanulmányozására. Ebben a fejezetben a kvázi-számállapotok bázisán a külső klasszikus lézer tér által gerjesztett Morse oszcillátor időfüggő Schrödinger egyenletét egy közönséges dif-

ferenciálegyenlet-rendszer formájában írtuk fel. A Morse oszcillátor paramétereit egy valódi molekuláénak, a nitrogén-monoxidénak (NO), választottuk. A molekula dipól momentumát, amelynek értékei különböző magtávolságokon egy mások által végrehajtott kvantumkémiai módszerrel adódtak, mi egy konkrét függvénnyel közelítettük. E függvény funkcionális alakja lehetővé teszi, hogy a megfelelő dipól mátrix elemeket analitikusan, algebrai úton határozzuk meg. Ezután numerikus módszerekkel megoldjuk a dinamikai egyenleteket és megmutatjuk, hogy megfelelően tervezett infravörös lézerimpulzusok hatására a molekula jelentős mértékben disszociál.

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