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# Solving for the Wigner functions of the Morse potential in deformation quantization

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## Abstract

We consider the time-independent Wigner functions of phase-space quantum mechanics (also known as deformation quantization) for a Morse potential. First, we find them by solving the  $*$ -eigenvalue equations, using a method that can be applied to potentials that are polynomial in an exponential. A Mellin transform converts the  $*$ -eigenvalue equations to difference equations, and factorized solutions are found directly for all values of the parameters. The symbols found this way are of both diagonal and off-diagonal density operator elements in the energy basis. The Wigner transforms of the density matrices built from the known wavefunctions are then shown to confirm the solutions.

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## 1. Introduction

Phase-space quantum mechanics (see e.g. [1, 2]) is also known as deformation quantization (see [3]), where the density operator is replaced by its symbol, the Wigner function (or distribution) on phase space, and its equations of motion involve the Moyal  $*$ -product. Although a completely autonomous formulation of quantum mechanics results, the  $*$ -eigenvalue equations obtained are difficult to solve. Few closed-form solutions have been found; see [1, 4] and references therein. Here we derive a new, explicit solution of the  $*$ -eigenvalue equations of phase-space quantum mechanics by treating the Morse potential.

The Morse potential is used in a wide variety of physical applications<sup>1</sup>. The original work [5] discussed the vibrational states of diatomic molecules. Other seminal uses of the Morse potential include the description of the rotating vibrational states of diatomic molecules [6], the interatomic potential of cubic metals [7] and the potential for the adsorption of a molecule

<sup>1</sup> No review of these applications seems to have been published, however.

or atom by a solid surface [8]. This list is far from comprehensive and new applications continue to be found as well.

Our motivation, however, came from the deformation quantization of contact interactions. In particular, [9] uses the Morse potential to produce Robin boundary conditions at an infinite potential wall, one of the simplest contact interactions, as a limit of a smooth potential.

In this paper, we present the mathematical aspects leading to a ‘pure’ deformation quantization of the Morse potential (see equation (12) below) with general coefficients.

The exponentials in the Morse potential allow the pseudo-differential form of the  $*$ -eigenvalue equations to be replaced by a difference-differential equation. The difference-differential equations are then transformed into difference equations that can be solved for all values of the parameters. The properties of the Mellin and the inverse Mellin transform to relate derivatives with finite differences are extensively used. The details are given in the next section, where we also re-derive the known solution for the special case of a Liouville potential [4].

Finding exact solutions to the dynamical equations of deformation quantization is challenging. Since, as an alternative, Wigner functions can be found from wavefunctions, only a limited number of simple systems have been solved directly. These include the free particle, the simple harmonic oscillator, the linear potential, the Liouville potential and the Kepler system. Some of these solutions have also been found only recently when interest in deformation quantization was renewed (see [1, 3, 4, 10]). This work adds to that effort, by adding the Morse potential to the list.

We should mention that for a Morse potential with a simple choice of the parameter values, a solution was found in [4]. We generalize that deformation quantization to Morse potentials for arbitrary parameter values, so that the properties of the potential can be varied.

Our method should be applicable whenever difference-differential equations emerge, as in the case of potentials that are linear combinations of exponential functions of the position.

In the third section we provide an explicit check to show that the solution provided is indeed consistent with the Wigner transform of the density matrix of the Morse wavefunctions. Our final section is a short conclusion.

## 2. Deformation quantization with a Morse potential

Let us start with a brief review of Wigner functions and the Wigner–Weyl correspondence (see e.g. [1, 2]). For simplicity, we will restrict to one coordinate  $x$  and one conjugate momentum  $p$ , describing a flat two-dimensional phase space  $\mathbb{R}^2$ . The generalization to  $\mathbb{R}^{2N}$  is straightforward.

The Wigner function is related to the density operator of canonical quantization. More generally, every operator  $\hat{Q}$  has a Weyl symbol  $Q(x, p)$  defined by

$$\begin{aligned} Q(x, p) &= \mathcal{W}\hat{Q} = \frac{1}{(2\pi)^2} \int_{-\infty}^{\infty} d\xi d\eta \text{Tr}[\hat{Q} e^{-i(\xi\hat{x}+\eta\hat{p})}] e^{i\xi x+i\eta p} \\ &= \frac{1}{2\pi} \int_{-\infty}^{\infty} dy e^{-iyp} \langle x + \hbar y/2 | \hat{Q} | x - \hbar y/2 \rangle. \end{aligned} \tag{1}$$

The map  $\mathcal{W} : \hat{Q} \mapsto Q(x, p)$ , from operators to phase-space functions (and distributions), is called the Wigner transform. It is a homomorphic map from the algebra of operators to the  $*$ -algebra of symbols:

$$\mathcal{W}(\hat{Q}\hat{R}) = \mathcal{W}(\hat{Q}) * \mathcal{W}(\hat{R}). \tag{2}$$

Here the symbols are multiplied using the Moyal  $*$ -product,

$$* = \exp \left\{ \frac{i\hbar}{2} (\overleftarrow{\partial}_x \overrightarrow{\partial}_p - \overrightarrow{\partial}_p \overleftarrow{\partial}_x) \right\}, \quad (3)$$

for consistency with the Wigner transform (1). An inverse  $\mathcal{W}^{-1}$  also exists—it is commonly referred to as the Weyl map:

$$\hat{Q} =: \mathcal{W}^{-1} Q(x, p) = \frac{1}{(2\pi)^2} \int_{-\infty}^{\infty} d\xi d\eta dx dp Q(x, p) e^{i\xi(\hat{x}-x)+i\eta(\hat{p}-p)}. \quad (4)$$

Up to normalization, the Wigner function  $\rho(x, p)$  is defined as the Wigner transform of the density operator  $\hat{\rho}$ :

$$\rho(x, p) := \frac{1}{2\pi\hbar} \mathcal{W}(\hat{\rho}). \quad (5)$$

The Wigner function is a quasi-probability distribution. Expectation values are calculated as

$$\langle Q \rangle = \int dx dp \rho(x, p) Q(x, p). \quad (6)$$

However, even with a pure state density operator  $\hat{\rho} = |\psi\rangle\langle\psi|$ ,

$$\rho(x, p) = \frac{1}{(2\pi)^2\hbar} \int_{-\infty}^{\infty} dy e^{-iyp} \psi(x + \hbar y/2) \psi^*(x - \hbar y/2) \quad (7)$$

is negative somewhere (except for the special case of Gaussian wavefunctions).

The Wigner function satisfies the equation of motion

$$i\hbar \partial_t \rho(x, p, t) = [H, \rho(x, p, t)]_*, \quad (8)$$

where  $[H, \rho]_* = H * \rho - \rho * H$ . It can be expressed as a linear combination of stationary Wigner functions with time-dependent coefficients:

$$\rho(x, p, t) = \sum_{E_L, E_R} C_{E_L E_R} e^{-i(E_L - E_R)t/\hbar} \rho_{E_L E_R}(x, p). \quad (9)$$

Here  $\rho_{E_L E_R} = \mathcal{W}(|E_L\rangle\langle E_R|)/2\pi\hbar$  denotes the Wigner transform of a matrix element of the density operator in the energy basis. As  $*$ -eigenfunctions, they can be found by solving the system of equations

$$\begin{aligned} H * \rho_{E_L E_R}(x, p) &= E_L \rho_{E_L E_R}(x, p), \\ \rho_{E_L E_R}(x, p) * H &= E_R \rho_{E_L E_R}(x, p). \end{aligned} \quad (10)$$

These are known as the  $*$ -eigenvalue (or sometimes ‘stargenvalue’) equations.

Alternatively, the Wigner transform

$$\rho_{E_L E_R}(x, p) = \int_{-\infty}^{\infty} dy e^{iyp} \langle x + \hbar y/2 | E_L \rangle \langle E_R | x - \hbar y/2 \rangle \quad (11)$$

allows them to be determined from the wavefunctions, if known. In the case of smooth potentials, the resulting Wigner functions are known to agree<sup>2</sup>.

The goal here is to perform a ‘pure’ deformation quantization by solving the  $*$ -eigenvalue equations directly, without reference to operators or wavefunctions. This will be done for the Morse potential

$$V(x) = \frac{\hbar^2 \kappa^2}{2m} (e^{-2\alpha x} - \beta e^{-\alpha x}). \quad (12)$$

<sup>2</sup> For discontinuous potentials, however, that is not necessarily the case [9, 11–13]. In [9] the results reported here are applied to study the example of the infinite wall or, equivalently, a particle confined to the half-line.

With its short-range repulsion and longer range attraction, this smooth potential has been useful in many physical applications. In particular, the Morse potential can be used to recover infinite wall with Robin boundary conditions in deformation quantization [9]. We will use the Mellin transform to convert the  $*$ -eigenvalue equations to difference equations.

We use a new method that produces difference equations for potentials that are polynomials of an exponential in  $x$ . This is significant since solutions to the  $*$ -eigenvalue equations are generally difficult to find (see e.g. [4]). To see why, let us start with a more general Hamiltonian and then specialize to the Morse potential. Writing

$$E_L =: \frac{\hbar^2 k_L^2}{2m}, \quad E_R =: \frac{\hbar^2 k_R^2}{2m}; \quad (13)$$

the  $*$ -eigenvalue equations (10) are of infinite order in momentum derivatives for a generic Hamiltonian  $H = p^2/2m + V(x)$ :

$$\left(\frac{p^2 - \hbar^2 k_L^2}{2m}\right)\rho - \frac{\hbar^2}{8m}\partial_x^2\rho - \frac{i\hbar p}{2m}\partial_x\rho + \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{i\hbar}{2}\right)^n \partial_x^n V \partial_p^n \rho = 0, \quad (14)$$

and similarly for the ‘right’ equation. However, the exponential form of the Morse potential (12) allows them to be written as differential-difference equations—the exponentials generate translations in the momentum. Their explicit form becomes

$$\begin{aligned} \frac{\hbar^2}{8m}\partial_x^2\rho + \frac{i\hbar p}{2m}\partial_x\rho &= \frac{\hbar^2\kappa^2}{2m} e^{-2\alpha x}\rho(x, p - i\hbar\alpha) \\ &- \frac{\beta\hbar^2\kappa^2}{2m} e^{-\alpha x}\rho\left(x, p - \frac{i\hbar\alpha}{2}\right) + \left(\frac{p^2 - \hbar^2 k_L^2}{2m}\right)\rho \end{aligned} \quad (15)$$

and

$$\begin{aligned} \frac{\hbar^2}{8m}\partial_x^2\rho - \frac{i\hbar p}{2m}\partial_x\rho &= \frac{\hbar^2\kappa^2}{2m} e^{-2\alpha x}\rho(x, p + i\hbar\alpha) \\ &- \frac{\beta\hbar^2\kappa^2}{2m} e^{-\alpha x}\rho\left(x, p + \frac{i\hbar\alpha}{2}\right) + \left(\frac{p^2 - \hbar^2 k_R^2}{2m}\right)\rho. \end{aligned} \quad (16)$$

The integral transform technique leads to further simplifications. Suppose the Wigner function can be written as

$$\rho(x, p) = R(u, p), \quad u := 16 e^{4\alpha x} \alpha^4 / \kappa^4. \quad (17)$$

The Mellin transform of the Wigner function is

$$W(s, p) := \mathcal{M}\{R\}(s, p) = \int_0^\infty u^{s-1} R(u, p) du. \quad (18)$$

To transform (15) and (16) into difference equations for  $W(s, p)$ , we consider the inverse Mellin transform

$$R(u, p) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} u^{-s} W(s, p) ds, \quad (19)$$

where the constant  $c$  can be any constant for which the transform converges according to the Mellin inversion theorem.

### 2.1. Solution for the Liouville potential

We will first apply the method to the Liouville potential

$$V_L(x) = \frac{\hbar^2\kappa^2}{2m} e^{-2\alpha x}. \quad (20)$$

It is the simplest case as it can be viewed as a Morse potential for  $b = 0$ . Also, we can check our results since the Wigner functions for this potential have already been found in [4].

The  $*$ -eigenvalue equations (10) imply the difference equations

$$\begin{aligned} (p/\hbar + 2i\alpha s)^2 W_0(s, p) + (2\alpha)^2 W_0(s - 1/2, p - i\alpha\hbar) &= k_L^2 W_0(s, p), \\ (p/\hbar - 2i\alpha s)^2 W_0(s, p) + (2\alpha)^2 W_0(s - 1/2, p + i\alpha\hbar) &= k_R^2 W_0(s, p). \end{aligned} \quad (21)$$

Let us now assume that the solution is factorized into two parts—‘left’ and ‘right’ factors—each depending on  $k_L$  or  $k_R$  only:

$$W(s, p) = N w_L \left( s - \frac{ip}{2\alpha\hbar}, k_L \right) w_R \left( s + \frac{ip}{2\alpha\hbar}, k_R \right), \quad (22)$$

with  $N$  a normalization constant. The factorization (22) is motivated by solutions found for specific values of the parameter  $b$ . In [4] the Wigner functions are found for  $b = 0$  and  $b = 1$ . They can be written as Meijer  $G$ -functions or, alternatively, as contour integrals. In addition, using the Darboux method outlined in [4], we found the solution for  $b = 2$ . In all three cases we observed the factorization (22), which was then assumed for  $b \in \mathbb{R}$ . While possibly omitting some solutions of the  $*$ -eigenvalue equations, this ansatz allows us to find those describing the physical states, as we confirm in section 3.

For the left factor, we find

$$(p/\hbar + 2i\alpha s)^2 w_L(s - ip/2\alpha\hbar) + (2\alpha)^2 w_L(s - ip/2\alpha\hbar - 1) = k_L^2 w_L(s - ip/2\alpha\hbar), \quad (23)$$

and for the right factor,

$$(p/\hbar - 2i\alpha s)^2 w_R(s + ip/2\alpha\hbar) + (2\alpha)^2 w_R(s + ip/2\alpha\hbar - 1) = k_R^2 w_R(s + ip/2\alpha\hbar). \quad (24)$$

Using the substitution  $t = s - ip/2\alpha\hbar$ , we arrive at

$$w(t - 1, k_L) = \left[ t^2 + \frac{k_L^2}{(2\alpha)^2} \right] w(t, k_L). \quad (25)$$

Equation (24) also leads to the above equation if we use  $t = s + ip/2\alpha\hbar$  and  $k_R$  instead. Therefore we need to work only with (25) and the solutions will just differ in their arguments and labels of  $k$ .

The solution of (25) is

$$w(t, k_L) = \Gamma(-t + ik_L/2\alpha) \Gamma(-t - ik_L/2\alpha), \quad (26)$$

by the defining property  $\Gamma(z + 1) = z\Gamma(z)$  of the gamma function. Tracing back to equations (22)–(23), (19) and (17), we can write the Wigner function in terms of the inverse Mellin transform:

$$\rho_{k_L k_R}(x, p) \propto \int_{c-i\infty}^{c+i\infty} ds u^{-s} \prod_{\pm, \pm'} \Gamma \left( -s + \frac{i(p/\hbar \pm k_L)}{2\alpha} \right) \Gamma \left( -s - \frac{i(p/\hbar \pm' k_R)}{2\alpha} \right). \quad (27)$$

This last is an integral representation of the Meijer  $G$ -function. Using equation (43) on p 353 in [14], the Wigner function becomes

$$\rho_{k_L k_R}(x, p) \propto G_{04}^{40} \left( \frac{1}{u} \middle| \frac{i(p/\hbar + k_L)}{2\alpha}, \frac{i(p/\hbar - k_L)}{2\alpha}, -\frac{i(p/\hbar - k_L)}{2\alpha}, -\frac{i(p/\hbar + k_L)}{2\alpha} \right), \quad (28)$$

where we used the identity

$$G_{04}^{40}(u|1 - a_1, 1 - a_2, 1 - a_3, 1 - a_4) = G_{04}^{40}(1/u|a_1, a_2, a_3, a_4). \quad (29)$$

As it should, the formula for the Wigner function (29) coincides with the one obtained using different methods in [4]. It describes the phase-space quasi-distribution for a particle in a Liouville potential. The advantage of the method proposed here is that it can be generalized to the Morse potential.

## 2.2. Solution for the Morse potential

Now let us go back to the original problem of finding the Wigner function for the potential (12). The left  $*$ -eigenvalue equation has the form

$$(p/\hbar + 2i\alpha s)^2 W_b(s, p) + (2\alpha)^2 W_b(s - 1/2, p - i\alpha\hbar) - \frac{b}{2}(2\alpha)^2 W_b(s - 1/4, p - i\alpha\hbar/2) = k_L^2 W_b(s, p), \quad (30)$$

where we set  $b = \beta\kappa/\alpha$ . We also have the complex conjugate (right) equation, with  $k_L$  replaced by  $k_R$ . To solve the new left difference equation (30), we substitute the ansatz (22) to obtain

$$(p/\hbar + 2i\alpha s)^2 w_L(s - ip/2\alpha\hbar, k_L) + (2\alpha)^2 w_L(s - ip/2\alpha\hbar - 1, k_L) - \frac{b}{2}(2\alpha)^2 w_L(s - ip/2\alpha\hbar - 1/2, k_L) = k_L^2 w_L(s - ip/2\alpha\hbar, k_L). \quad (31)$$

Using the same substitution  $t = s - ip/2\alpha\hbar$  as in (24) and switching to  $w_b = w_L$  to account for the parameter dependence, we arrive at the difference equation relevant to the Morse potential:

$$w_b(t - 1, k_L) - \frac{b}{2} w_b(t - 1/2, k_L) = \left[ t^2 + \frac{k_L^2}{(2\alpha)^2} \right] w_b(t, k_L). \quad (32)$$

This equation has a trivial solution for  $b = 0$ , the Liouville case. The right factor satisfies an identical equation with  $k_L$  replaced by  $k_R$  and  $t = s + ip/2\alpha\hbar$ .

For  $b = 1$ , the solution can be written in terms of gamma functions, as in the  $b = 0$  case:

$$w_1(t, k) \propto \Gamma\left(-t + \frac{ik}{2\alpha}\right) \Gamma\left(-t + \frac{1}{2} - \frac{ik}{2\alpha}\right) + \Gamma\left(-t + \frac{1}{2} + \frac{ik}{2\alpha}\right) \Gamma\left(-t - \frac{ik}{2\alpha}\right). \quad (33)$$

The inverse Mellin transform then gives us the Wigner function:

$$\begin{aligned} \rho_{k_L k_R}(x, p) \propto & G_{04}^{40} \left( \frac{1}{u} \left| \frac{ip}{2\alpha\hbar} + \frac{ik_L}{2\alpha}, \frac{1}{2} + \frac{ip}{2\alpha\hbar} - \frac{ik_L}{2\alpha}, -\frac{ip}{2\alpha\hbar} + \frac{ik_R}{2\alpha}, \frac{1}{2} - \frac{ip}{2\alpha\hbar} - \frac{ik_R}{2\alpha} \right. \right) \\ & + G_{04}^{40} \left( \frac{1}{u} \left| \frac{ip}{2\alpha\hbar} + \frac{ik_L}{2\alpha}, \frac{1}{2} + \frac{ip}{2\alpha\hbar} + \frac{ik_L}{2\alpha}, \frac{1}{2} - \frac{ip}{2\alpha\hbar} + \frac{ik_R}{2\alpha}, -\frac{ip}{2\alpha\hbar} - \frac{ik_R}{2\alpha} \right. \right) \\ & + G_{04}^{40} \left( \frac{1}{u} \left| \frac{1}{2} + \frac{ip}{2\alpha\hbar} + \frac{ik_L}{2\alpha}, \frac{ip}{2\alpha\hbar} - \frac{ik_L}{2\alpha}, -\frac{ip}{2\alpha\hbar} + \frac{ik_R}{2\alpha}, \frac{1}{2} - \frac{ip}{2\alpha\hbar} - \frac{ik_R}{2\alpha} \right. \right) \\ & + G_{04}^{40} \left( \frac{1}{u} \left| \frac{1}{2} + \frac{ip}{2\alpha\hbar} + \frac{ik_L}{2\alpha}, \frac{ip}{2\alpha\hbar} - \frac{ik_L}{2\alpha}, \frac{1}{2} - \frac{ip}{2\alpha\hbar} + \frac{ik_R}{2\alpha}, -\frac{ip}{2\alpha\hbar} - \frac{ik_R}{2\alpha} \right. \right). \end{aligned} \quad (34)$$

Another solution that is easy to find is for  $b = 2$ :<sup>3</sup>

$$w_2(t, k) \propto (t + 1/4) \prod_{\pm} \Gamma\left(-t \pm \frac{ik}{2\alpha}\right) - \prod_{\pm} \Gamma\left(-t + \frac{1}{2} \pm \frac{ik}{2\alpha}\right). \quad (35)$$

It can be written in a different form which shows a pattern shared with the case  $b = 1$ :

$$\begin{aligned} w_2(t, k) \propto & (2ik/\alpha + 1) \Gamma(-t + ik/2\alpha) \Gamma(-t + 1 - ik/2\alpha) \\ & + \frac{4ik}{\alpha} \Gamma(-t + 1/2 + ik/2\alpha) \Gamma(-t + 1/2 - ik/2\alpha) \\ & + (2ik/\alpha - 1) \Gamma(-t + 1 + ik/2\alpha) \Gamma(-t - ik/2\alpha). \end{aligned} \quad (36)$$

<sup>3</sup> The  $b = 2$  Wigner function can also be found from the Liouville case using supersymmetric quantum mechanics. In deformation quantization, the ladder operators of supersymmetric quantum mechanics are replaced by functions and a star product is used; however, the transition is fairly straightforward [4].

The Wigner function can be found with a trivial but lengthy calculation that is essentially identical to the  $b = 0$  and  $b = 1$  cases. The exact combination of Meijer  $G$ -functions is not of interest to us; we will derive a general expression that includes this later.

A useful observation is that the left factors (for different  $b$ ) can be written as

$$w_1 = C_1 w_0(t - 1/4, k + i\alpha/2) + C_2 w_0(t - 1/4, k - i\alpha/2) \tag{37}$$

and

$$w_2 = C_1 w_0(t - 1/2, k + i\alpha) + C_2 w_0(t - 1/2, k) + C_3 w_0(t - 1/2, k - i\alpha). \tag{38}$$

This suggests that by choosing the constants correctly, we can write the solution for any integer  $b$  as

$$w_b(t, k) \propto \sum_{n=-\frac{b}{2}, -\frac{b}{2}+1, \dots, \frac{b}{2}} C_n^b w_0(t - b/4, k - in\alpha). \tag{39}$$

We can substitute this ansatz into equation (32) using undetermined coefficients. In principle, a comparison of the coefficients of independent terms can determine  $C_n^b$  for any  $b$ . This seems to fail, however, in the case of non-integer  $b$ . Furthermore, even for the simplest cases, this program is very difficult to carry out<sup>4</sup>. Clearly we need an algorithm that reproduces the constants directly and allows a generalization to include all Morse potentials of the form (12).

### 2.3. Systematic solution of the difference equations

We now show how to find the relevant solutions of the  $*$ -eigenvalue equations for the Morse potential, for all  $b \in \mathbb{R}$ . We exploit once again the property of the Mellin transform to relate differential equations and their solutions to difference equations and their solutions.

To convert our difference equation (32) into a differential equation, we use the following two properties of the Mellin transform:

$$\mathcal{M}\{\tau^2 f''(\tau) + \tau f(\tau)\}(s) = s^2 \mathcal{M}\{f(\tau)\}(s), \tag{40}$$

$$\mathcal{M}\{\tau^a f(\tau)\}(s) = \mathcal{M}\{f(\tau)\}(s + a). \tag{41}$$

If we apply the inverse Mellin transform directly to (32), we end up with an equation that we cannot solve. This is because the Mellin transform converts argument translations into powers of the argument via (41). To eliminate fractional powers, we use the substitution  $s = 2t$ . The new equation for  $\tilde{w}_b(s) = w(t(s))$ ,

$$\tilde{w}_b(s - 2) - \frac{b}{2} \tilde{w}_b(s - 1) = \left[ \left(\frac{s}{2}\right)^2 + \frac{k^2}{(2\alpha)^2} \right] \tilde{w}_b(s), \tag{42}$$

results in a simpler, integrable equation

$$\tau^2 f''(\tau) + \tau f'(\tau) + [(k/\alpha)^2 - 4/\tau^2 + 2b/\tau] f(\tau), \tag{43}$$

where  $\tilde{w}(s) = \mathcal{M}\{f(\tau)\}(s)$ .

The solution  $f(\tau)$  of this equation can be found if we make the substitution  $f(\tau) = \tau^{-1/2} g(\tau)$  and then  $u(z) = g(t(z))$ , where  $z = 1/\tau$ . The new function  $u(z)$  satisfies the so-called Whittaker equation, treated in [15], chapter XVI, and also in the appendix. Its two linearly independent solutions are defined in [16], p 755. They are called Whittaker functions

<sup>4</sup> For integer  $b$ , see equation (52) below, however.



and can be expressed in terms of the Tricomi confluent hypergeometric function  $U(\mu, \nu, z)$  and the Kummer confluent hypergeometric function  $M(\mu, \nu, z)$ :<sup>5</sup>

$$M_{lm}(z) = z^{m+1/2} e^{-z/2} M(1/2 + m - l, 1 + 2m; z), \tag{44}$$

$$W_{lm}(z) = z^{m+1/2} e^{-z/2} U(1/2 + m - l, 1 + 2m; z). \tag{45}$$

For our purposes, we only need the definitions of those functions:

$$M(\mu, \nu; z) = \sum_{n=0}^{\infty} \frac{(\mu)_n y^n}{(\nu)_n n!}, \tag{46}$$

$$U(\mu, \nu; z) = \frac{\Gamma(\nu - 1)}{\Gamma(\mu)} z^{1-\nu} M(1 + \mu - \nu, 2 - \nu; z) + \frac{\Gamma(1 - \nu)}{\Gamma(\mu - \nu + 1)} M(\mu, \nu; z). \tag{47}$$

Here we use the Pochhammer symbol  $(\mu)_n := \mu(\mu + 1) \cdots (\mu + n - 1)$ ,  $(\mu)_0 := 1$ .

The solution is

$$f(\tau) = \tilde{C}_1 \tau^{1/2} M_{\frac{b}{2}, \frac{ik}{\alpha}}(4/\tau) + \tilde{C}_2 \tau^{1/2} W_{\frac{b}{2}, \frac{ik}{\alpha}}(4/\tau). \tag{48}$$

This is the general solution and therefore depends on two arbitrary constants,  $\tilde{C}_1, \tilde{C}_2$ . We must set  $\tilde{C}_1 = 0$  to describe the physical states, however. To see that, we have to transform this back to the solutions of the difference equations and compare with the known solutions, re-derived in the previous sections. Alternatively, one can impose the properties of the  $*$ -eigen Wigner functions:  $\rho_{ij} = \rho_{ji}^*$  and  $\rho_i = \rho_i^*$ . For example, in the case of diagonal elements one finds that the reality of the Wigner function implies that the right and left factors are also real. Since the Whittaker  $M$ -function in (48) transforms into a complex function one must set  $\tilde{C}_1$  to zero.

Let us first confirm that (48), with  $\tilde{C}_1 = 0$ , indeed recovers the known solutions (26), (33), (36) for  $b = 0, 1, 2$ , respectively, and that it also justifies ansatz (39) for all non-negative integer  $b$ . For  $b \in \mathbb{N}_0$ , we can write the Whittaker  $W$ -function in terms of the modified Bessel functions

$$W_{\frac{n}{2}, \mu}(y) = \frac{y^{\frac{n+1}{2}}}{\sqrt{\pi}} \left( \frac{1-n}{2} + \mu \right) \sum_{k=0}^n \frac{(-1)^{n+k} (2k - n + 2\mu) (-n)_{n-k}}{\Gamma(n-k)(k - n + 2\mu)_{n+1}} K_{-k + \frac{n}{2} - \mu} \left( \frac{y}{2} \right). \tag{49}$$

With the help of the integral representation of the Bessel functions (effectively finding the inverse Mellin transform),

$$K_\nu(z) = \frac{1}{4\pi i} \int_{c-i\infty}^{c+i\infty} \Gamma(s) \Gamma(s - \nu) \left( \frac{z}{2} \right)^{\nu - 2s} ds, \tag{50}$$

we can find the solution of (42) for integer  $b$ :

$$w_b(t, k) \propto \sum_{n=0}^b C_n^b \Gamma(-t + n/2 + ik/2\alpha) \Gamma(-t - n/2 + b/2 - ik/2\alpha). \tag{51}$$

This is precisely (39), but with a shifted summation index. The coefficients are now explicit:

$$C_n^b = \frac{(-1)^n (2n - b + 2ik/\alpha) (-b)_{b-n}}{(b-n)! (n - b + 2ik/\alpha)_{b+1}}. \tag{52}$$

<sup>5</sup> The Whittaker function  $M_{lm}(z)$  should not be confused with the Kummer function  $M(\mu, \nu, z)$  in the above equation. Subscripts are used to denote the parameters of the Whittaker functions in the literature, and the explicit bracket notation is used for confluent hypergeometric functions. For further information involving the hypergeometric functions, see [16], p 753, and [17], pp 503–6.

The Wigner function for  $b \in \mathbb{N}_0$  can be found from (51) as in the preceding two subsections, with the result

$$\rho_{k_L k_R}(x, p) = \sum_{m,n=0}^b C_m^b C_n^b G_{04}^{40} \left( \frac{1}{u} \left| \frac{n}{2} + \frac{i(p/\hbar + k_L)}{2\alpha}, \frac{b}{2} - \frac{n}{2} + \frac{i(p/\hbar - k_L)}{2\alpha}, \right. \right. \\ \left. \left. \frac{m}{2} - \frac{i(p/\hbar - k_R)}{2\alpha}, \frac{b}{2} - \frac{m}{2} - \frac{i(p/\hbar + k_R)}{2\alpha} \right) \right). \quad (53)$$

Bound states can also be treated this way; one only needs to consider imaginary  $k$ , for energies  $E < 0$ . The resulting form of the Wigner function differs, however, from the expression found by the Wigner transform:

$$\rho(z, p) \propto z^{2\nu-b+1} \sum_{l_1, l_2=0}^{\nu} \binom{b-\nu-1}{\nu-l_1} \binom{b-\nu-1}{\nu-l_2} \frac{(-z)^{l_1+l_2}}{l_1! l_2!} K_{l_1-l_2-2ip/\alpha}(z). \quad (54)$$

To write it in this form, we use the properties of the Whittaker functions. Recall that the energies are given by (A.9), and we can write

$$f(\tau) \propto \tau^{1/2} W_{\frac{b}{2}, \frac{ik}{\alpha}}(4/\tau) = \tau^{1/2} W_{\frac{b}{2}, \frac{b}{2}-\nu-\frac{1}{2}}(4/\tau). \quad (55)$$

The relationship

$$W_{a, a-\nu-\frac{1}{2}}(z) = (-1)^\nu \nu! z^{a-\nu} e^{-z/2} L_\nu^{2a-2\nu-1} \quad (56)$$

(for integer  $\nu$ ) and (A.8) allow us to write the solution as

$$f(\tau) \propto e^{-2/\tau} \sum_{l=0}^{\nu} \frac{(-1)^l}{l!} \binom{b-\nu-1}{\nu-l} \left( \frac{4}{\tau} \right)^{l+b/2-\nu-1/2}. \quad (57)$$

Transforming the above, we find the corresponding factor

$$w(t) \propto \sum_{l=0}^{\nu} \frac{(-2)^l 2^{2t}}{l!} \binom{b-\nu-1}{\nu-l} \Gamma(-2t+l+b/2-\nu-1/2). \quad (58)$$

With the help of the inverse Mellin transform, we find (54) as in the unbound case, using (50) and (19).

Let us proceed to the case of non-integer  $b$ . For  $b \in \mathbb{R}$ , we find an explicit and closed expression for the solution of the difference equation. We start by rewriting the solution of the differential equation (43) in terms of hypergeometric functions:

$$f(\tau) = e^{-2/\tau} \tau^{-ik/\alpha} U \left( \frac{1}{2} - \frac{b}{2} + \frac{ik}{\alpha}, 1 + \frac{2ik}{\alpha}; \frac{4}{\tau} \right). \quad (59)$$

This is necessary in order to perform the inverse Mellin transform of  $f(\tau)$  in closed terms, which presents a technical problem if we use the Whittaker function.

We use relationship (47) between the Kummer and Tricomi hypergeometric function and the integral expression

$$e^{-\sigma x} M(\beta, \gamma; \lambda x) = \int_{c-i\infty}^{c+i\infty} ds x^{-s} \sigma^{-s} \Gamma(s) {}_2F_1(\beta, s; \gamma; \lambda \sigma^{-1}) \quad (60)$$

to make it possible to find the inverse Mellin transform of (59). It is given in terms of the Gauss hypergeometric function  ${}_2F_1$ . Switching back to our original variable  $t$ , and indicating the  $k$ -dependence explicitly, we can write

$$\begin{aligned}
 w_b(t, k) \propto & \frac{4^{t+ik/2\alpha} \Gamma(-2ik/\alpha)}{\Gamma(1/2 - b/2 - ik/\alpha)} \Gamma(-2t + ik/\alpha) \\
 & \times {}_2F_1(1/2 - b/2 + ik/\alpha, -2t + ik/\alpha; 1 + 2ik/\alpha; 2) \\
 & + \frac{4^{t-ik/2\alpha} \Gamma(2ik/\alpha)}{\Gamma(1/2 - b/2 + ik/\alpha)} \Gamma(-2t - ik/\alpha) \\
 & \times {}_2F_1(1/2 - b/2 - ik/\alpha, -2t - ik/\alpha; 1 - 2ik/\alpha; 2). \tag{61}
 \end{aligned}$$

This is the solution of the difference equation (32) for any real  $b$ , including the ones we already found. After substitution in (17), (19), (22), it yields our main result:

$$\rho_{E_L E_R}(x, p) \propto \int_{c-i\infty}^{c+i\infty} ds u^{-s} w_b\left(s - \frac{ip}{2\alpha\hbar}, k_L\right) w_b\left(s + \frac{ip}{2\alpha\hbar}, k_R\right). \tag{62}$$

### 3. Wigner functions from wavefunctions for a Morse potential

For completeness, let us confirm that our solutions of the  $*$ -eigenvalue equations (10) are the same as the Wigner functions derived from the wavefunctions (see the appendix) using (11).

Consider the unbound states first:

$$\begin{aligned}
 \psi(y) = & C e^{-y/2} \tilde{A} y^{ik/\alpha} M\left(\frac{1}{2} - \frac{b}{2} + \frac{ik}{\alpha}, 1 + \frac{2ik}{\alpha}; y\right) \\
 & + C e^{-y/2} \tilde{A}^* y^{-ik/\alpha} M\left(\frac{1}{2} - \frac{b}{2} - \frac{ik}{\alpha}, 1 - \frac{2ik}{\alpha}; y\right). \tag{63}
 \end{aligned}$$

Using the substitutions  $w = e^{-\alpha\hbar y/2}$  and  $v = 2\kappa e^{-\alpha x}/\alpha$ , we can rewrite the integral transform (11). The result involves integration over  $w$  of the products of the type

$$\exp[-v(w + w^{-1})/2] w^m v^n M(a_1, b_1; vw) M(a_2, b_2; v/w), \tag{64}$$

which (to the best of our knowledge) are not integrable in a closed form. However, we can expand the Kummer  $M$ -function as in (46). Then all the integrations can be performed explicitly using the integral representation of the Bessel  $K$ -function

$$K_\nu(z) = \frac{1}{2} \int_0^\infty dw w^{-(\nu+1)} e^{-\frac{1}{2}z(w+1/w)}. \tag{65}$$

This procedure leads to an infinite sum:

$$\begin{aligned}
 \rho(v, p) \propto & \sum_{m,n=0}^\infty \frac{v^{m+n}}{m!n!} \left[ \tilde{A}^2 v^{2ik/\alpha} \frac{(\chi)_m (\chi)_n}{(\zeta)_m (\zeta)_n} K_{n-m-2ip/\hbar\alpha}(v) \right. \\
 & + |\tilde{A}|^2 \frac{(\chi)_m (\bar{\chi})_n}{(\zeta)_m (\bar{\zeta})_n} K_{m-n+2i(k-p/\hbar)/\alpha}(v) \\
 & + |\tilde{A}|^2 \frac{(\bar{\chi})_m (\chi)_n}{(\bar{\zeta})_m (\zeta)_n} K_{m-n-2i(k+p/\hbar)/\alpha}(v) \\
 & \left. + (\tilde{A}^*)^2 v^{-2ik/\alpha} \frac{(\bar{\chi})_m (\bar{\chi})_n}{(\bar{\zeta})_m (\bar{\zeta})_n} K_{n-m-2ip/\hbar\alpha}(v) \right], \tag{66}
 \end{aligned}$$

with  $\chi := 1/2 - b/2 + ik/\alpha$  and  $\zeta := 1 + 2ik/\alpha$ . This expression can now be used to compare with (61), (62).

To do that we need to calculate explicitly the contour integral (62). We are facing a similar problem—the integrand is too complicated and we need to rewrite the Gauss hypergeometric function as

$${}_2F_1(a, b; c; z) = \sum_{n=0}^\infty \frac{(a)_n (b)_n}{(c)_n} \frac{z^n}{n!} \tag{67}$$

in order to integrate in a closed form. With the use of the contour representation of the Bessel  $K$ -function (50) and some simple algebra, we recover the infinite sum (66). This confirms that the Wigner function (62) indeed coincides with the Wigner transform of the density matrix for the Morse potential from the Schrödinger treatment.

The Wigner functions of the bound states can be obtained from the known wavefunctions (A.7) using the integral transform (11).<sup>6</sup> Equation (A.8) allows us to evaluate the integral in a closed form using the modified Bessel functions  $K_\nu(x)$ . The substitutions  $v = 2\kappa e^{-\alpha x}/\alpha$  and  $w = \exp(-\alpha\hbar y/2)$  in (11) and the integral representation (65) are used.

#### 4. Conclusion

Our main result is the solution (62), (61) of the  $*$ -eigenvalue equations (10) for the Morse potential (12) with arbitrary real  $b$ . It subsumes the simpler formula (62), (39), (52) valid for all  $b \in \mathbb{N}_0$ .

The solutions obtained have already been applied to a study of Robin boundary conditions in phase-space quantum mechanics [9].

It should also be possible to use our method to solve the  $*$ -eigenvalue equations for other potentials that are polynomial in an exponential (say  $\exp(-\alpha x)$ ).

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#### Appendix. The Morse potential in Schrödinger quantum mechanics

Following Matsumoto [18], we can solve the stationary Schrödinger equation for the unbound wavefunctions of the Morse potential (12). The substitution  $\psi(x) = \phi(z)$ ,  $z = \exp(-\alpha x)$ , changes the Schrödinger equation into

$$z^2 \phi'' + z \phi' + \frac{1}{\alpha^2} \left[ \frac{2mE}{\hbar^2} - \kappa^2 z^2 + \kappa^2 \beta z \right] \phi = 0. \quad (\text{A.1})$$

This can be further transformed into a canonical form (without a first derivative term) using the substitution  $\phi(z) = z^{-1/2} F(z)$ . Changing the variables to  $y := 2\kappa z/\alpha$  leads to the Whittaker equation, treated in [15], chapter XVI:

$$f'' + \left\{ -\frac{1}{4} + \frac{b}{2} \frac{1}{y} + \frac{1}{y^2} \left[ \frac{1}{4} - \left( \frac{ik}{\alpha} \right)^2 \right] \right\} f = 0, \quad (\text{A.2})$$

where  $f(y) := F(\alpha y/2\kappa)$  and, as before,  $k = \sqrt{2mE}/\hbar$  and  $b = \beta\kappa/\alpha$ .

<sup>6</sup> For  $b = 2$ , the bound-state Wigner functions for the Morse potential (12) have already been treated this way in [19]. However, they are not obtained there by solving their dynamical equations, as we have done. In addition, while we find the unbound-state Wigner functions in the same way, the unbound states are not considered in [19].

Now the wavefunction can be written as

$$\psi_k(x) = e^{\alpha x/2} [\tilde{C}_1 M_{\frac{b}{2}, \frac{ik}{\alpha}}(y(x)) + \tilde{C}_2 W_{\frac{b}{2}, \frac{ik}{\alpha}}(y(x))]. \quad (\text{A.3})$$

Imposing reality yields  $\tilde{C}_1 = 0$ . The second term has physical asymptotic behaviour: for large positive  $x$ , it is sinusoidal with a phase depending on the potential parameters; for negative  $x$  far from the origin, there is the expected rapid exponential decay of a classically forbidden region. The wavefunction is therefore

$$\psi_k(x) = C e^{\alpha x/2} W_{\frac{b}{2}, \frac{ik}{\alpha}}\left(\frac{2\kappa}{\alpha} e^{-\alpha x}\right). \quad (\text{A.4})$$

With the help of equation (47), we can rewrite this result in a form similar to that given by Matsumoto in [18] for a Morse potential with  $b = 2$ . The wavefunction is manifestly real in this form:

$$\begin{aligned} \psi(y) = & C e^{-y/2} \tilde{A} y^{ik/\alpha} M\left(\frac{1}{2} - \frac{b}{2} + \frac{ik}{\alpha}, 1 + \frac{2ik}{\alpha}; y\right) \\ & + C e^{-y/2} \tilde{A}^* y^{-ik/\alpha} M\left(\frac{1}{2} - \frac{b}{2} - \frac{ik}{\alpha}, 1 - \frac{2ik}{\alpha}; y\right), \end{aligned} \quad (\text{A.5})$$

with  $C$  a real normalization constant, and

$$\tilde{A} = \frac{\Gamma(-\frac{2ik}{\alpha})}{\Gamma(\frac{1}{2} - \frac{b}{2} - \frac{ik}{\alpha})}. \quad (\text{A.6})$$

Let us now consider the bound states. Their wavefunctions are given in [19] as

$$\psi(x) \propto \exp(-\kappa e^{-\alpha x}/\alpha) e^{-\alpha(v-b/2+1/2)x} L_v^{b-2v-1}(2\kappa e^{-\alpha x}/\alpha), \quad (\text{A.7})$$

where

$$L_n^\lambda(x) = \sum_{m=0}^n (-1)^m \binom{n+\lambda}{n-m} \frac{x^m}{m!} \quad (\text{A.8})$$

are the associated Laguerre polynomials  $L_n^\lambda(x)$ . The energies are

$$E_v = -\frac{\hbar^2 \alpha^2}{2m} (v - b/2 + 1/2)^2, \quad (\text{A.9})$$

for integer  $v \in [0, \lfloor b/2 \rfloor]$ , where  $\lfloor a \rfloor$  is the smallest integer less than  $a$ .

## References

- [1] Zachos C, Fairlie D and Curtright T 2005 *Quantum Mechanics in Phase Space* (Singapore: World Scientific)
- [2] Hancock J, Walton M A and Wynder B 2004 *Eur. J. Phys.* **25** 525 (arXiv:physics/0405029)
- [3] Bayen F, Flato M, Fronsdal C, Lichnerowicz A and Sternheimer D 1978 *Ann. Phys.* **111** 61  
Bayen F, Flato M, Fronsdal C, Lichnerowicz A and Sternheimer D 1978 *Ann. Phys.* **111** 111
- [4] Curtright T, Fairlie D and Zachos C 1998 *Phys. Rev. D* **58** 025002 (arXiv:hep-th/9711183)
- [5] Morse P M 1929 *Phys. Rev.* **34** 57
- [6] Dunham J L 1932 *Phys. Rev.* **41** 721
- [7] Girifalco L A and Weirzer V G 1959 *Phys. Rev.* **114** 687
- [8] Lennard-Jones J E and Strachan C 1935 *Proc. R. Soc. A* **150** 442
- [9] Belchev B and Walton M A 2010 *J. Phys. A: Math. Theor.* **43** 085301 (arXiv:quant-ph/1002.2139)
- [10] Curtright T, Uematsu T and Zachos C 2001 *J. Math. Phys.* **42** 2396 (arXiv:hep-th/0011137v2)
- [11] Dias N C and Prata J N 2002 *J. Math. Phys.* **43** 4602 (arXiv:quant-ph/0012140)  
Dias N C and Prata J N 2006 *Ann. Phys.* **321** 495 (arXiv:quant-ph/0012140)
- [12] Kryukov S and Walton M A 2005 *Ann. Phys.* **317** 474 (arXiv:quant-ph/0412007)  
Kryukov S and Walton M A 2006 *Can. J. Phys.* **84** 557 (arXiv:quant-ph/0508005)

- [13] Walton M A 2007 *Ann. Phys.* **322** 2233 (arXiv:quant-ph/0609213)
- [14] Erdelyi A, Magnus W, Oberhettinger F and Tricomi F G 1954 *Tables of Integral Transforms* vol 1 (New York: McGraw-Hill)
- [15] Whittaker E T and Watson G N 1962 *A Course of Modern Analysis* 4th edn (Cambridge: Cambridge University Press)
- [16] Polyanin A P and Zaitsev V F 2003 *Handbook of Exact Solutions for Ordinary Differential Equations* 2nd edn (London: Chapman & Hall)
- [17] Abramowitz M and Stegun I A 1972 *Handbook of Mathematical Functions* (Washington, DC: National Bureau of Standards)
- [18] Matsumoto A 1988 *J. Phys. B: At. Mol. Opt. Phys.* **21** 2863
- [19] Frank A, Rivera A L and Wolf K B 2000 *Phys. Rev. A* **61** 054102