The quartic anharmonic oscillator and its associated nonconstant magnetic field

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Quantum mechanical anharmonic oscillators and Hamiltonians for particles in external magnetic fields are related to representations of nilpotent groups. Using this connection the eigenfunctions of the quartic anharmonic oscillator with potential $V_\alpha(x)=(\alpha+(x^2/2))^2$ can be used to determine the eigenfunctions of a charged particle in a nonconstant magnetic field, of the form $B_z=\beta_2+\beta_3 x$. The quartic anharmonic oscillator eigenvalues for low-lying states are obtained numerically and a function which interpolates between $\alpha \ll 0$ (a double harmonic oscillator) and $\alpha \gg 0$ (a harmonic oscillator) is shown to give a good fit to the numerical data. Approximate expressions for the quartic anharmonic oscillator eigenfunctions are then used to get the eigenfunctions for the magnetic field Hamiltonian. © *1997 American Institute of Physics.* [S0022-2488(97)03010-7]

I. INTRODUCTION

It is well known that there are many completely integrable systems in classical mechanics that are not soluble in quantum mechanics. The class of one-dimensional anharmonic oscillators provide one such example. Another is a charged, spinless particle in an external magnetic field with a vector potential of the form $A_x=A_z=0$, $A_y=A_y(x)$. Such a vector potential generates a magnetic field in the z direction that in general varies in x. Classically, for motion confined to the $x-y$ plane, such a system is completely integrable because two integrals of the motion exist: the Hamiltonian H and the generalized momentum p_y. However, the only known quantum mechanical solution for such systems is for a constant magnetic field, $A_y(x)=B_0 x$. In that case, as shown by Landau,[1] the eigenfunctions and eigenvalues are closely related to those of the harmonic oscillator.

In fact, this quantum mechanical relationship between two different classically completely integrable systems, namely, the harmonic oscillator and the constant magnetic field, can be generalized. If the function $A_y(x)$ is a polynomial in x, then there exists a nilpotent group with representations on the Hilbert space $L^2(\mathbb{R}^2)$ (the Hilbert space for a particle in the $x-y$ plane) whose generators give the Hamiltonian for the charged particle. Furthermore, if the representation for the nilpotent group on $L^2(\mathbb{R}^2)$ is reducible, then the space of irreducible representations of the nilpotent group is $L^2(\mathbb{R})$, in which case the Hamiltonian is that of an anharmonic oscillator. One of the goals of this paper is to obtain numerical solutions of quartic anharmonic oscillators which can then be used to obtain solutions for particles in a nonconstant magnetic field.

As an illustration, consider the case of a constant magnetic field.[2] Then the nilpotent group is the Heisenberg group, which can be written as the set of matrices

$$G_H:=\left\{\begin{pmatrix}1 & a & c\\ & 1 & b\\ & & 1\end{pmatrix}\right\}\equiv\{(a,b,c)\},\quad a,b,c\in\mathbb{R}. \tag{1}$$

To get a unitary representation on $L^2(\mathbb{R}^2)$, we induce with the subgroup $(0,0,c)\rightarrow e^{i\gamma}$, γ real. This representation is given by

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$$(U^{\gamma}_{(a,b,c)}\Psi)(x,y)=e^{i\gamma(bx+c)}\Psi(x+a,y+b),\quad \Psi\in L^2(\mathbb{R}^2). \tag{2}$$

Lie algebra representations are given by the (anti-Hermitian) operators

$$(a,0,0)\rightarrow A=\frac{\partial}{\partial x},\quad (0,b,0)\rightarrow B=\frac{\partial}{\partial y}+i\gamma x,\quad (0,0,c)\rightarrow C=i\gamma,\quad [A,B]=C. \tag{3}$$

The Hamiltonian for the particle in a constant magnetic field is quadratic in the generators A and B

$$-2H^{\gamma}=A^2+B^2=\frac{\partial^2}{\partial x^2}+\left(\frac{\partial}{\partial y}+i\gamma x\right)^2, \tag{4}$$

where γ is the (dimensionless) strength of the magnetic field. If H^{γ} is Fourier transformed in y, the Hamiltonian for the harmonic oscillator results. Group theoretically, this corresponds to decomposing a reducible representation on $L^2(\mathbb{R}^2)$ to irreducible ones on $L^2(\mathbb{R})$.

The irreducible representations of the Heisenberg group are induced by the subgroup $(0,b,c)\rightarrow e^{i(b\beta+c\gamma)}$, β, γ real. These representations are given by

$$(U^{\beta\gamma}_{(a,b,c)}\varphi)(x)=e^{i(\beta b+\gamma xb+\gamma c)}\varphi(x+a),\quad \varphi\in L^2(\mathbb{R}). \tag{5}$$

The infinitesimal generators are

$$(a,0,0)\rightarrow A=\frac{\partial}{\partial x},\quad (0,b,0)\rightarrow B=i(\beta+\gamma x),\quad (0,0,c)\rightarrow C=i\gamma, \tag{6}$$

and the Hamiltonian is

$$-2H=A^2+B^2=\frac{\partial^2}{\partial x^2}-(\beta+\gamma x)^2, \tag{7}$$

the harmonic oscillator Hamiltonian.

It is also possible to analyze the Hamiltonian for the regular representation on $L^2(\mathbb{R}^3)$, where

$$(R_gF)(x)=F(xg),\quad F\in L^2(\mathbb{R}^3),$$

$$(R_{(a,b,c)}F)(x,y,z)=F(x+a,y+b,z+c+xb), \tag{8}$$

with the Lie algebra representation

$$A=\frac{\partial}{\partial x},\quad B=\frac{\partial}{\partial y}+x\,\frac{\partial}{\partial z},\quad C=\frac{\partial}{\partial z}. \tag{9}$$

In this case the Hamiltonian is called a sub-Laplacian and is written as

$$\Delta:=A^2+B^2=\frac{\partial^2}{\partial x^2}+\left(\frac{\partial}{\partial y}+x\,\frac{\partial}{\partial z}\right)^2. \tag{10}$$

The sub-Laplacian plays an important role in dealing with the generalized heat equation,

$$\Delta p_t=\frac{\partial p_t}{\partial t},\quad p_{t=0}=\delta^3(\mathbf{x}), \tag{11}$$

the solution of which is given in Refs. 3 and 4.

More generally if $\mathbf{A}(\mathbf{x})$ is any polynomial in $\mathbf{x}$, there exists a nilpotent group with representations on $L^2(\mathbb{R}^3)$ whose generators give the charged-particle Hamiltonian. This can be shown in the following way.

Let $\mathbf{A}(\mathbf{x})$ be the vector potential associated with a magnetic field $\mathbf{B}(\mathbf{x})$ that couples to a charged particle. Then the commutator of the generalized momentum will be

$$\left[\frac{1}{i}\frac{\partial}{\partial x_j}-A_j(\mathbf{x}),\quad \frac{1}{i}\frac{\partial}{\partial x_k}-A_k(\mathbf{x})\right]=i\epsilon_{jkl}B_l(\mathbf{x}),$$
$$\left[\frac{1}{i}\frac{\partial}{\partial x_j}-A_j(\mathbf{x}),\quad B_k(\mathbf{x})\right]=\frac{1}{i}\frac{\partial B_k}{\partial x_j},$$
$$\vdots \tag{12}$$

If the vector potential $\mathbf{A}(\mathbf{x})$ is a polynomial in $\mathbf{x}$, then these commutation relations will close to give a nilpotent Lie algebra. A quadratic sum of the generators gives the charged-particle Hamiltonian

$$2H=\sum_{j=1,2,3}\left[\frac{1}{i}\frac{\partial}{\partial x_j}-A_j(\mathbf{x})\right]^2. \tag{13}$$

Thus any vector potential that is polynomial in its spatial variables generates a representation of some nilpotent Lie algebra acting on $L^2(\mathbb{R}^3)$.

On $L^2(\mathbb{R})$, on the other hand, consider the nilpotent Lie algebra generated by $1/i(\partial/\partial x)$ and a polynomial $p(x)$; again commutators starting with

$$\left[\frac{1}{i}\frac{\partial}{\partial x},p(x)\right]=\frac{1}{i}\frac{\partial p}{\partial x}$$
$$\vdots \tag{14}$$

will eventually close, giving a representation of some nilpotent Lie algebra. The Hamiltonian in this case is again a quadratic sum of generators, of the form

$$2H=-\frac{\partial^2}{\partial x^2}+[p(x)]^2, \tag{15}$$

which is the Hamiltonian for an anharmonic oscillator.

In Sec. II we will work out these connections for a nilpotent group called the quartic group Q, and show that representations of Q link the quartic anharmonic oscillator to a particle in a nonconstant magnetic field of the form $B_z=\beta_2+\beta_3 x$, $A_x=A_z=0$. In Sec. III we analyze the quartic anharmonic oscillator using a combination of numerical methods and analytic approximations. In Sec. IV we relate these oscillator solutions to the charged particle problem.

II. THE QUARTIC GROUP Q

In this paper we will look at the simplest nilpotent group generalization of the Heisenberg group, a group denoted by Q because it generates the quartic anharmonic oscillator (as well as a nonconstant magnetic field Hamiltonian).

Define the quartic nilpotent group Q by

$$Q:=\left\{\begin{pmatrix}1 & b & b^2/2 & b_3\\ & 1 & b & b_2\\ & & 1 & b_1\\ & & & 1\end{pmatrix}\right\}\equiv\{(b,\mathbf{b})\},\quad b,b_i\in\mathbb{R}. \tag{16}$$

Then Q forms a group under ordinary matrix multiplication, with group multiplication given by

$$\begin{gathered}(b,\mathbf{b})(b',\mathbf{b}')=\left(b+b',b_1+b_1',b_2+b_2'+bb_1',b_3+b_3'+bb_2'+\frac{b^2}{2}\,b_1'\right),\\ (b,\mathbf{b})^{-1}=\left(-b,-b_1,-b_2+bb_1,-b_3+bb_2-\frac{b^2}{2}\,b_1\right).\end{gathered} \tag{17}$$

Important subgroups of Q include the Heisenberg group $G_H=\{(b,0,b_2,b_3)\}$ and the invariant Abelian subgroup $\{(0,b_1,b_2,b_3)\}$.

The irreducible representations of Q are obtained by inducing from the invariant Abelian subgroup

$$(0,\mathbf{b})\rightarrow e^{i\boldsymbol{\beta}\cdot\mathbf{b}},\quad \boldsymbol{\beta}\in\mathbb{R}^3; \tag{18}$$

then

$$\begin{gathered}(U^{\boldsymbol{\beta}}_{(b,\mathbf{b})}\varphi)(x)=e^{i[\beta_1b_1+\beta_2(b_2+xb_1)+\beta_3(b_3+xb_2+(x^2/2)b_1)]}\varphi(x+b),\\ (b,\mathbf{b})\in Q,\quad \varphi\in L^2(\mathbb{R}).\end{gathered} \tag{19}$$

From these irreducible representations on $L^2(\mathbb{R})$, it is possible to compute the (anti-Hermitian) infinitesimal operators corresponding to one-parameter subgroups of Q

$$\begin{gathered}(b,0,0,0)\rightarrow X_0=\frac{\partial}{\partial x},\quad (0,b_1,0,0)\rightarrow X_1=i\left(\beta_1+\beta_2x+\beta_3\,\frac{x^2}{2}\right),\\ (0,0,b_2,0)\rightarrow X_2=i(\beta_2+\beta_3x),\quad (0,0,0,b_3)\rightarrow X_3=i(\beta_3).\end{gathered} \tag{20}$$

The commutation relations are

$$[X_0,X_1]=X_2,\quad [X_0,X_2]=X_3, \tag{21}$$

with all other commutators zero; these commutation relations agree with those coming from the Lie algebra of Q, as is easily checked by making use of the matrix realization of Q, Eq. (16). The relationship between Q and quartic anharmonic oscillators is given by writing the Hamiltonian as a quadratic sum of generators

$$-2H^{\boldsymbol{\beta}}=X_0^2+X_1^2=\frac{\partial^2}{\partial x^2}-\left(\beta_1+\beta_2x+\frac{\beta_3}{2}\,x^2\right)^2. \tag{22}$$

The nonconstant magnetic field related to Q is obtained from the reducible representation induced from the subgroup $(0,0,b_2,b_3)\rightarrow e^{i(\beta_2b_2+\beta_3b_3)}$

$$(U^{\beta_2\beta_3}_{(b,\mathbf{b})}\psi)(x,y)=e^{i[\beta_2(b_2+xb_1)+\beta_3(b_3+xb_2+(x^2/2)/b_1)]}\times\psi(x+b,y+b_1),\quad \psi\in L^2(\mathbb{R}^2),$$

$$X_0=\frac{\partial}{\partial x},\quad X_1=i\left(\beta_2 x+\beta_3\frac{x^2}{2}\right)+\frac{\partial}{\partial y},$$

$$X_2=i(\beta_2+\beta_3 x),\quad X_3=i\beta_3; \tag{23}$$

$$-2H^{\beta_2\beta_3}=X_0^2+X_1^2=\frac{\partial^2}{\partial x^2}+\left[i\left(\beta_2 x+\beta_3\frac{x^2}{2}\right)+\frac{\partial}{\partial y}\right]^2,$$

which is the Hamiltonian for a particle in a nonconstant magnetic field given by $A_x=A_z=0$, $A_y=\beta_2 x+\beta_3 x^2/2$, $B_z=\beta_2+\beta_3 x$.

Though the Hamiltonian in Eq. (23) appears to be the usual Hamiltonian for a particle in an external magnetic field, all the quantities, including the representation labels $\beta_2\beta_3$, are dimensionless. To connect the Hamiltonian Eq. (23) with a Hamiltonian that has the dimensions of energy the following transformations must be made.

Let $H=hH'$, h carrying units of energy and H' a dimensionless operator. Likewise let $\mathbf{A}=a\mathbf{A}'$, $\boldsymbol{\mu}=M\boldsymbol{\mu}'$, and $\mathbf{B}=b\mathbf{B}'$. Suppose we write $\boldsymbol{\nabla}$ as $(\partial/\partial w_1,\partial/\partial w_2,\partial/\partial w_3)$, where w_i are Cartesian coordinates. Let L be a constant with units of length, and let $w_1=Lx$, $w_2=Ly$, $w_3=Lz$, where x, y, and z are now dimensionless variables. Then we have

$$hH'=\frac{1}{2m}\left(-\frac{\hbar i}{L}\boldsymbol{\nabla}_{x,y,z}-\frac{ea}{c}\mathbf{A}'\right)^2-\frac{1}{2}Mb\boldsymbol{\mu}'\cdot\mathbf{B}'. \tag{24}$$

Note that the combinations $h_0\equiv(hmL^2/\hbar^2)$, $a_0\equiv(aLe/\hbar c)$ and $M_0b_0\equiv(MbmL^2/\hbar^2)$ are dimensionless parameters. If we now define new, dimensionless operators $H_0=h_0H'$, $\mathbf{A}_0=a_0\mathbf{A}'$, $\boldsymbol{\mu}_0=M_0\boldsymbol{\mu}'$ and $\mathbf{B}_0=b_0\mathbf{B}'$; then the operator

$$H_0=\tfrac{1}{2}(-i\boldsymbol{\nabla}-\mathbf{A}_0)^2-\tfrac{1}{2}\boldsymbol{\mu}_0\cdot\mathbf{B}_0 \tag{25}$$

is completely dimensionless as well.

As before, we will now restrict the class of vector potentials to $\mathbf{A}_0=(0,\beta_2 x+\beta_3(x^2/2)+\cdots,0)\equiv(0,A_y(x),0)$, which produces an inhomogeneous, x-dependent magnetic field in the z-direction. In this case the Hamiltonian becomes

$$H_0=-\frac{1}{2}\frac{\partial^2}{\partial x^2}+\frac{1}{2}\left(-i\frac{\partial}{\partial y}-A_y(x)\right)^2-\frac{1}{2}\frac{\partial}{\partial z^2}. \tag{26}$$

If the eigenfunctions of this Hamiltonian are written as $\Psi(x,y,z)=e^{-i\beta_1 y-ip_z z}\times\Phi(x)$, then we have (ignoring the constant p_z^2 term)

$$H=-\frac{1}{2}\frac{\partial^2}{\partial x^2}+\frac{1}{2}(\beta_1+A_y(x))^2. \tag{27}$$

In particular, if we choose $A_y=\beta_2 x+\beta_3(x^2/2)$ the Hamiltonian becomes

$$-2H=\frac{\partial^2}{\partial x^2}-\left(\beta_1+\beta_2 x+\beta_3\frac{x^2}{2}\right)^2, \tag{28}$$

which is identical to Eq. (22).

Introducing the linear transformation $x'=\beta_3^{1/3}(x+\beta_2/\beta_3)$ and defining

$$\alpha \equiv \frac{\beta_1\beta_3 - (1/2)\beta_2^2}{\beta_3^{4/3}}, \tag{29}$$

$$e_n(\alpha) \equiv 2\beta_3^{-2/3}E, \tag{30}$$

we find that the Schrödinger equation $H\Phi_n = E\Phi_n$ reduces to

$$\frac{\partial^2\Phi_n}{\partial x'^2} - \left(\alpha + \frac{x'^2}{2}\right)^2 \Phi_n = -e_n(\alpha)\Phi_n . \tag{31}$$

From Eq. (29), we see that α depends on β_1, the momentum along the y direction which can take any value. So for a given magnetic field (i.e., a given β_2 and β_3) H has a continuous spectrum. Physically this means that particles can drift along the y axis to infinity, corresponding classically to a grad-B drift.

Finally, before considering particular solutions, we note that the quartic potential [Eq. (31)] is equivalent to the problem of a general quartic potential $V_c = c_0 + c_1x' + c_2x'^2 + c_3x'^3 + c_4x'^4$, where $c_4 > 0$ and $-2H\Phi(x') = -e_c\Phi(x')$. Because we will frequently use this equivalence to translate results from other studies into the variables used in this paper, we list the equations here:

$$\begin{gathered} \alpha = (4c_4)^{-2/3}\left(c_2 - \frac{3c_3^2}{8c_4}\right), \quad \mu_z = -(4c_4)^{-1/2}\left(c_1 - \frac{c_2c_3}{2c_4} + \frac{c_3^3}{8c_4^2}\right), \\ e(\alpha) = \alpha^2 + (4c_4)^{-1/3}\left(e_c - c_0 + \frac{c_1c_3}{4c_4} - \frac{c_2c_3^2}{16c_4^2} + \frac{3c_3^4}{256c_4^3}\right), \end{gathered} \tag{32}$$

where $\mu_z X_2$ can be added to the magnetic field Hamiltonian, Eq. (23), to allow for external electric fields.

III. NUMERICAL ANALYSIS

Much of the previous work on the quartic Hamiltonian has centered on finding precise methods of determining its eigenvalues for specific values of α. Success is often measured by how many decimals one can produce after N iterations of one's procedure. We take a somewhat different approach. Instead of seeking very precise energies for particular values of α, we wish to find functions that approximate $e_n(\alpha)$ for all $\alpha \in \mathbb{R}$, as these $e_n(\alpha)$ and their associated eigenfunctions are needed to obtain the magnetic field eigenfunctions.

We have used a Runge–Kutta numerical integration program to calculate the eigenvalues for a wide range of α. The results agree with those of other researchers.[5–8] These data are shown in Fig. 1 (solid lines) and compared with the eigenvalues for a simple harmonic oscillator (dotted lines). Furthermore, the integration technique can provide the values of the zeros of the eigenfunctions. These data are shown in Fig. 2 for $n = 2,3$, as a function of α.

We now wish to construct functions $e_n(\alpha)$ and $z_n(\alpha)$ that interpolate the energy and zero data. The asymptotic behavior of $e_n(\alpha)$ is already known. In the case $\alpha \gg 0$, the potential $V_\alpha = \alpha^2 + \alpha x^2 + x^4/4$ may be approximated by ignoring the x^4 term. This leaves a simple harmonic potential plus a constant potential. The asymptotic solutions become

$$e_n(\alpha) = \alpha^2 + (2n+1)\sqrt{\alpha}, \quad \alpha \gg 0, \tag{33}$$

$$\Phi_n = h_n\left(\frac{x}{\alpha^{1/4}}\right)e^{(-\sqrt{\alpha}x^2/2)}, \quad \alpha \gg 0. \tag{34}$$

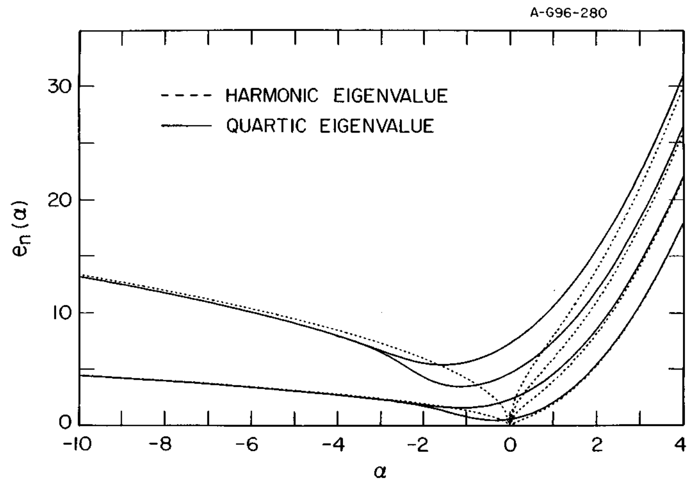

FIG. 1. Eigenvalues of the quartic potential as a function of α.

The numerical results confirm this behavior. For example, for the ground state, the difference between the quartic eigenvalue and the harmonic asymptote at $\alpha=4$ is already as small as 0.04.

Describing the asymptotic behavior in the case $\alpha \leqslant 0$ requires a different approach. For any $\alpha<0$, V_α becomes a double-well potential, each well centered about $x=\pm\sqrt{-2\alpha}$. Rewriting the potential around either of these points, we obtain

$$V_\alpha=\tfrac{1}{4}(x\pm\sqrt{-2\alpha})^4\mp\sqrt{-2\alpha}(x\pm\sqrt{-2\alpha})^3-2\alpha(x\pm\sqrt{-2\alpha})^2. \tag{35}$$

For α large and negative, the main contribution will come from the final, quadratic term. Eigenfunctions will approach the sum or difference of two independently displaced harmonic oscillator wave functions. Consequently, eigenvalues will pair up at each harmonic energy level, which we can write as $e_n(\alpha)=(n+[1+(-1)^n]/2)\sqrt{-2\alpha}$. Numerically, the pairing occurs as early as $\alpha=-2.90$ for the ground and first excited states, and $\alpha=-4.30$ for the second and third.

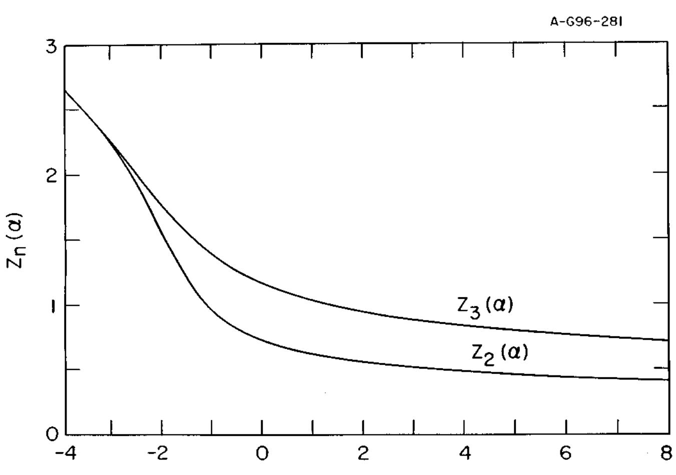

FIG. 2. Zeros of the quartic eigenfunctions as a function of α.

TABLE I. Best fit eigenvalue coefficients.

	s_-	t_1	t_2	s_1	p_0	p_1	p_2	q_1	q_2
e_0	2	0.817 5	1.2052	0.713	0.3398	0.6170	0.0622	−0.669	0.1934
e_1	2	0.256 3	1.862	1.2245	13.79	14.50	1.553	−0.5775	0.2407
e_2	18	0.000 436	6.448	0.953	105.5	113.1	2.34	−0.208	0.133
e_3	18	3.983 7	6.2445	0.8612	408.9	197.4	7.93	−0.335	0.0927

The numerical results shown in Fig. 1 provide yet another guide to the functional form of $e_n(\alpha)$. When the harmonic eigenvalues are subtracted from the total anharmonic eigenvalues, the difference falls off as $1/\alpha$ for large magnitudes of α.

For these reasons, we have tried to fit the numerical data to a function of the form

$$e_n(\alpha)=\alpha^2\theta(\alpha)+\left((\alpha s(\alpha))^{3/2}+\frac{p}{q}\right)^{1/3}, \tag{36}$$

where $\theta(\alpha)$ is an analytic approximation to the step function; s is a similar, step-like function describing the asymptotic behavior and p/q is a ratio (of order unity) of polynomials that correctly approximates the numerical behavior for $\alpha\approx 0$.

Specifically, we have chosen the forms

$$\theta(\alpha)=\frac{1}{1+t_1e^{-t_2\alpha}},\quad s(\alpha)=s_-s_+\frac{(1-e^{-s_1\alpha})}{s_-+s_+e^{-s_1\alpha}},$$
$$p(\alpha)=p_0+p_1\alpha+p_2\alpha^2,\quad q(\alpha)=1+q_1\alpha+q_2\alpha^2, \tag{37}$$

where $s_+=(2n+1)^2$, and it and s_- are predetermined by the required asymptotic slopes, but the rest of the coefficients are found using some fitting method.

Our current best fit, in terms of $\langle|e_n-e_{\text{num}}|^2\rangle$, uses the coefficients in Table I. Note that for e_n, $n\geqslant 1$, $p_0\approx 0.17(2n+1)^4$, so that for $\alpha\approx 0$, $e_n\propto(2n+1)^{4/3}$ as predicted by WKB methods.[6] The fit is sufficiently good that it cannot be distinguished from the solid line in Fig. 1.

We also wish to construct a function $z_n(\alpha)$ describing the zeros of the eigenfunctions. In doing so, we need to incorporate the following asymptotic behavior:

$$\alpha\gg 0:\quad z_n\to\frac{\xi_n}{\alpha^{1/4}},$$
$$\alpha\ll 0:\quad z_2,z_3\to\sqrt{-2\alpha}, \tag{38}$$

where ξ_n is a zero of the corresponding nth Hermite polynomial. For example, $\xi_2=\sqrt{1/2}$ and $\xi_3=\sqrt{3/2}$.

We have chosen to try to fit the data for $z_2(\alpha)$ and $z_3(\alpha)$ using a function of the form

$$z_n(\alpha)=\frac{(2\alpha\tanh\alpha)^{1/2}e^{-d_z\alpha}+\xi_ne^{d_z\alpha}+(p'/q')}{e^{-d_z\alpha}+(\alpha\tanh\alpha)^{1/4}e^{d_z\alpha}}, \tag{39}$$

where d_z and the coefficients in the ratio of polynomials p'/q' are found using some fitting method. (The tanh α term acts as a continuously differentiable approximation to the absolute value function.) Our current best fit, in terms of $\langle|z_n-z_{\text{num}}|^2\rangle$, uses the coefficients in Table II.

The same Runge–Kutta program that provided us with the data for the eigenvalues and zeros also calculated values of the unnormalized eigenfunction $\Phi_n(x,\alpha)$ at various points $x\in\mathbb{R}$. We

TABLE II. Best fit zero coefficients.

	d_z	p'_0	p'_1	p'_2	q'_1	q'_2
z_2	0.564	0.068	−0.766	−1.460	1.370	1.826
z_3	0.469	0.142	−0.896	−0.622	0.599	0.989

wish to use these data, along with our knowledge of the eigenvalues and zeros, to formulate analytic approximations to $\Phi_n(x,\alpha)$, which we will do here for $n=0-3$.

Different researchers have used various Ansätze as the approximate forms of quartic oscillator eigenfunctions. One common approach, useful for $\alpha>0$, is to assume an eigenfunction of the form

$$\Phi_n = e^{-(x^2/2)} \sum_{i=0}^{\infty} c_n x^{2n}, \tag{40}$$

and to substitute that into the differential equation. A three-term difference equation results, which may then be solved approximately using determinant methods.[5,9] Alternatively, one can use the zeroth-order WKB approximation and make appropriate simplifications for large or small α.[9]

Mindful of the WKB results, one could also choose some specific form for the eigenfunction that obeys the correct asymptotic behavior, such as

$$\Phi_0 = e^{-[\alpha E_0^2 x^4 + (1/36)x^6]^{1/2}}, \quad E_0^3 - \frac{1}{4} E_0 - \frac{1}{24\alpha^{3/2}} = 0, \tag{41}$$

as was done by Ginsburg and Montroll.[10]

For $\alpha<0$, Balsa *et al.* suggest using harmonic oscillator eigenfunctions and a variational method wherein not only the variational parameter but also the excited state number n are varied.[11] Arias de Saavedra and Buendía, on the other hand, propose that a basis set of sums of displaced harmonic oscillators be used as the Ansatz in a variational procedure.[12]

In all these cases, however, the Ansatz is decided upon first, then used to approximate the quartic eigenvalues. Such methods can produce extremely precise results. For example, Bacus, Meurice, and Soemadi have recently devised a method giving 30-digit accuracy for the first ten excited states,[13] and Vinette and Čížek have produced a 62-digit result for the ground-state, $\alpha=0$ case.[8]

However, because we wish to translate the quartic eigenfunctions into eigenfunctions of the corresponding magnetic field problem, which requires solutions for all values of α, we do not seek precise determination of the eigenvalues by variational or other methods. Instead, we assume that the eigenvalues, the zeros of the eigenfunctions, and other pertinent features of the problem have been determined numerically and strive to find approximate, analytic functions that mimic an exact solution for all α. In other words, instead of approximating the eigenvalues by assuming a form for the eigenfunction, we attempt the inverse: approximate the eigenfunction by assuming a form for the eigenvalues.

Toward this end, we desire a general form for the eigenfunction that incorporates the cases of α both positive and negative, its magnitude both large and small. For $\alpha \geqslant 0$ (the single-well potential), the eigenfunction will be centered on the origin. For $\alpha<0$ (the double-well potential), it will resemble the sum or difference of two oscillator eigenfunctions displaced a distance $\pm\sqrt{-2\alpha}$ from the origin. Further, we know that asymptotically, the eigenfunctions approach a single harmonic oscillator eigenfunction when $\alpha \gg 0$ and two displaced harmonic oscillator eigenfunctions when $\alpha \ll 0$.

We will make an assumption similar to that of Aharonov and Au,[14] that the exponent of the eigenfunctions may be expressed as an infinite series. We use powers of x^2 rather than a series of orthogonal functions because the potential itself is a polynomial in x^2. A form for the even parity eigenfunctions that has the correct asymptotic limits is

$$\begin{aligned}\Phi_0^\alpha(x)&=A_0(\alpha)\cosh(b_0(\alpha)x)e^{-(a_{02}x^2+a_{04}x^4+\cdots)},\\ \Phi_2^\alpha(x)&=A_2(\alpha)(x^2-z_2^2(\alpha))\cosh(b_2(\alpha)x)e^{-(a_{22}x^2+a_{24}x^4+\cdots)},\end{aligned}\tag{42}$$

and so on. For the odd parity eigenfunctions we write

$$\begin{aligned}\Phi_1^\alpha(x)&=A_1(\alpha)\sinh(b_1(\alpha)x)e^{-(a_{12}x^2+a_{14}x^4+\cdots)},\\ \Phi_3^\alpha(x)&=A_3(\alpha)(x^2-z_3^2(\alpha))\sinh(b_3(\alpha)x)e^{-(a_{32}x^2+a_{34}x^4+\cdots)},\end{aligned}\tag{43}$$

and so on. Here, $A_n(\alpha)$ are normalizations depending on α and the $a_{nk}(\alpha)$ are as yet unspecified functions of α. The $\cosh(b_n(\alpha)x)$ and $\sinh(b_n(\alpha)x)$ terms have been introduced so that as $\alpha\to-\infty$, two independent harmonic oscillators with the same energy result. This means that as $\alpha\to-\infty$, $b_n(\alpha)=2\sqrt{-2\alpha}a_{n2}(\alpha)$. Further, for $\alpha\geqslant 0$, $b_n(\alpha)\to 0$. The quantities $z_n(\alpha)$ occurring in Eqs. (42) and (43) are the zeros of the eigenfunctions and are given in Eq. (39).

By substituting each eigenfunction, Eqs. (42), (43) into the Schrödinger equation, and expanding about $x=0$, we obtain recursion relations for each eigenfunction. For example, for the ground state

$$\begin{aligned}a_{02}&=\tfrac{1}{2}(e_0'+b_0^2),\\ a_{04}&=\tfrac{1}{12}((e_0'^2-\alpha)-b_0^4),\\ a_{06}&=\tfrac{1}{45}(e_0'(e_0'^2-\alpha)+b_0^6-\tfrac{3}{8}),\\ &\vdots\end{aligned}\tag{44}$$

where $e_0'=e_0-\alpha^2$.

There are a number of ways of obtaining $b_n(\alpha)$. We have chosen to determine $b_n(\alpha)$ by minimizing the integral

$$\|\Phi_n^{\alpha_i}-\Phi_{n,\mathrm{num}}^{\alpha_i}\|^2=\int_{-\infty}^{+\infty}dx|\Phi_n^{\alpha_i}-\Phi_{n,\mathrm{num}}^{\alpha_i}(x)|^2,\tag{45}$$

where $\Phi_{n,\mathrm{num}}^{\alpha_i}(x)$ are the numerically determined values of the eigenfunctions for the potential $(\alpha_i+(x^2/2)^2)$; and $\Phi_n^\alpha(x)$ are the functions in Eqs. (42) and (43) along with the corresponding recursion relations. The results for $b_0(\alpha)$ and $b_1(\alpha)$ are shown in Fig. 3 for $\alpha>-2$. A function that roughly approximates $b_1(\alpha)$ is

$$b_1(\alpha)=\frac{-2\alpha e^{-0.0242\alpha}+\dfrac{2.423+2.033\alpha+0.394\alpha^2}{1+0.190\alpha+0.00869\alpha^2}}{1+e^{-0.0242\alpha}}.\tag{46}$$

The difficulty we have with determining the $b_n(\alpha)$ is that when the eigenvalues become nearly degenerate for $\alpha<0$, it is very difficult to get reliable eigenfunctions numerically and hence, to obtain the $b_n(\alpha)$ for those values of α. For that reason $b_0(\alpha)$ and $b_1(\alpha)$ are not given for $\alpha<-2$ in Fig. 3. However, for $\alpha\geqslant 0$, when $b_n(\alpha)\sim 0$, we are able to obtain very good fits for $\Phi_n^{\alpha>0}(x)$. In this case using three terms in the recursion relations, the quantity $\|\Phi_n^\alpha-\Phi_{n,\mathrm{num}}^\alpha\|^2$ is less than 10^{-7} for $n=0,1,2,3$. For $-2\leqslant\alpha<0$ the fits are not as good. In Figs.

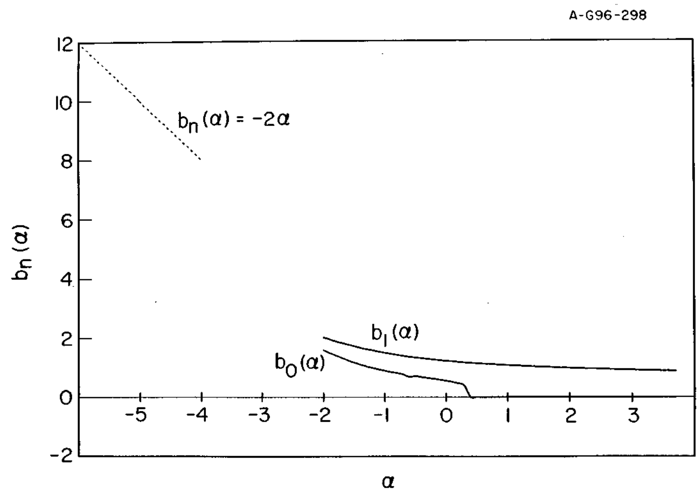

FIG. 3. Numerical results for $b_0(\alpha)$ and $b_1(\alpha)$.

4 and 5 we show the results for $\alpha = -1.5$ for Φ_0 and Φ_1. Clearly more work is needed in obtaining reliable numerical data for the eigenfunctions in the region $\alpha < 0$, where the eigenvalues are nearly degenerate.

IV. CONCLUSION

Using group theoretical methods, we have shown that eigenfunctions for a particle in a nonconstant magnetic field given by the vector potential $A_y(x) = \beta_2 x + \beta_3(x^2/2)$, $A_x = A_z = 0$, are related to the eigenfunctions of a quartic anharmonic oscillator with a potential $V(x) = (\alpha$

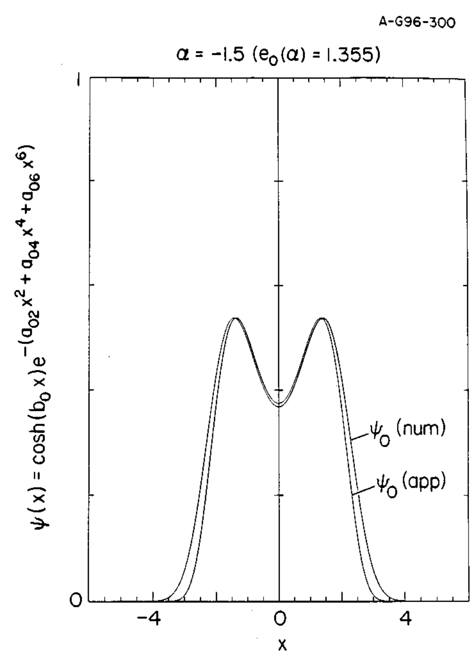

FIG. 4. $\psi_0(x)$ for $\alpha = -1.5$.

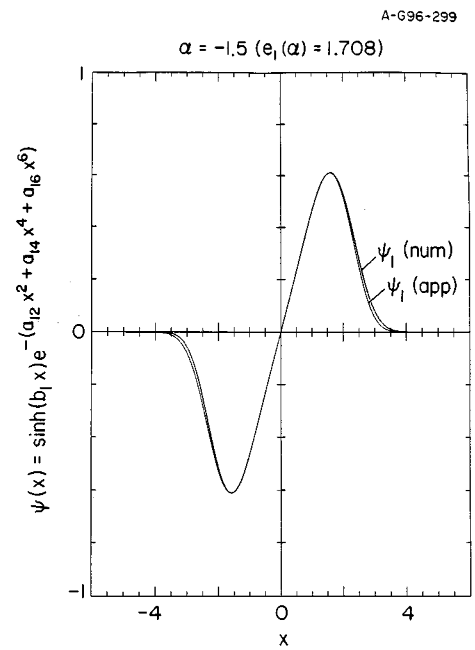

FIG. 5. $\psi_1(x)$ for $\alpha=-1.5$.

$+(x^2/2)^2)$. No exact solutions to this potential are known. However, with suitable approximate eigenfunctions and eigenvalues for the quartic anharmonic oscillator, we can construct the eigenfunctions for a particle in a nonconstant magnetic field.

Given $\Phi_n^\alpha(x)$, Eqs. (42), (43) the magnetic field eigenfunctions are

$$\psi_{E,\beta_1,p_z}^{\beta_2\beta_3}(\mathbf{x})=e^{-i\beta_1 y}e^{-ip_z z}\Phi_n^\alpha(x), \quad E=\tfrac{1}{2}\beta_3^{2/3}e_n(\alpha), \quad \alpha=\frac{(\beta_1\beta_3-\frac{1}{2}\beta_2^2)}{\beta_3^{4/3}}, \tag{47}$$

where β_2 and β_3 give the (dimensionless) field strength, and β_1 is the (conserved) momentum in the y direction.

Though the Hamiltonian for the quartic anharmonic oscillator has a discrete spectrum, the Hamiltonian for the particle in a nonconstant magnetic field has a continuous spectrum, in contrast to a particle in a constant magnetic field (confined to a plane). And, since the $\Phi_n^\alpha(x)$ are anharmonic oscillator solutions, they die off as $|x|$ gets large, which means the motion of the particle is bounded in the x direction. It is not, however, bounded in the y direction. Physically, these results correspond to a quantized grad-B drift, in which particles in a nonconstant magnetic field do not execute circular motion, but rather drift in the y direction to infinity.

To obtain approximations for the magnetic field eigenfunctions, we require the eigenfunctions and eigenvalues of the quartic anharmonic oscillator for all values of $\alpha\in\mathbb{R}$. As discussed in Sec. III, for large magnitudes of α, the potential $V_\alpha(x)$ approaches harmonic oscillator potentials. Thus the asymptotic forms of the quartic anharmonic oscillator eigenfunctions and eigenvalues are constrained to approach known harmonic oscillator values.

In contrast to what is done in many numerical studies of the anharmonic oscillator (where α is fixed and very precise values of the eigenfunctions and eigenvalues are sought), we have instead used the numerical data to approximate the eigenfunctions and eigenvalues of the quartic anharmonic oscillator for all values of α. We have chosen functions that have the correct asymptotic behavior and which contain parameters that can be adjusted to give a best fit to numerical data.

From the functional forms we have chosen for the energy eigenvalues $e_n(\alpha)$, given in Eqs. (36) and (37), and for the zeros of the eigenfunctions, given in Eq. (39), the parameters have been chosen to give a best fit for each value of $n=0-3$.

Similarly, a functional form for the eigenfunctions $\Phi_n^\alpha(x)$, given in Eq. (42), provides the means for approximating the eigenfunctions for $n=0-3$. Here, however, the procedure is somewhat more complicated than for the eigenvalues and zeros, for it is necessary to know the parameter $b_n(\alpha)$ before the coefficients appearing in the eigenfunctions can be determined; we have chosen to determine the $b_n(\alpha)$ by minimizing $\|\Phi_n - \Phi_{n,\mathrm{num}}\|$ for all α. A more effective procedure might describe the b_n using Ansatz-indepedent parameters such as wave function extrema. Alternatively, an Ansatz that did not require this extra parameter b_n might be sought. Indeed, if α is restricted to nonnegative values, the parameter b_n can be set equal to zero (see Fig. 3). In this case, our approximation method successfully and efficiently describes the eigenfunctions.

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