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1987 J. Phys. A: Math. Gen. 20 L965

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LETTER TO THE EDITOR

**Efficient quantisation scheme for the anisotropic Kepler problem**

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Received 17 July 1987

**Abstract.** We have developed an efficient quantisation scheme for highly excited states of the anisotropic Kepler problem. This applies to the level spectrum of a donor impurity in semiconductors. Results for silicon and germanium are presented.

In this letter we report on an efficient calculation scheme for highly excited states of the anisotropic Kepler problem. This applies to level spectra of donor impurities in semiconductors. These systems are very accurately described by the Hamiltonian [1-3]

$$H_0 = -\frac{\hbar^2}{2m_{\perp}} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) - \frac{\hbar^2}{2m_{\parallel}} \frac{\partial^2}{\partial z^2} - \frac{e^2}{Kr} \tag{1}$$

Here  $K$  is the dielectric constant. Measuring length in units of the Bohr radius  $a_0 = \hbar^2 K / m_{\perp} e^2$  and energies in units of the Rydberg energy  $E_R = m_{\perp} e^4 / 2 \hbar^2 K^2$  we arrive at the dimensionless Hamiltonian

$$H = -\left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \gamma \frac{\partial^2}{\partial z^2} \right) - \frac{2}{r} \tag{2}$$

where  $\gamma = m_{\perp} / m_{\parallel}$  is the mass ratio. Experimental information on  $\gamma$  was derived from cyclotron resonances [4, 5] and typical values are  $\gamma = 0.2079$  for silicon and  $\gamma = 0.05134$  for germanium. Good quantum numbers are the azimuthal quantum number  $m$  and parity  $\pi$ , but no further reduction of variables is possible and the resulting Schrödinger equation is two dimensional and non-separable. The eigenvalue problem for the lowest nine states in a given  $m^{\pi}$ -subspace has been tackled by Faulkner [1] with a hydrogen-like basis expansion. Here we will use a scaling property of the Hamiltonian and an expansion in a complete set of Sturmian functions.

The Sturmian functions are defined as

$$\langle r | nlm \rangle = \frac{1}{r} \phi_n^l(r; \lambda) Y_{lm}(\theta, \varphi) \tag{3a}$$

with

$$\phi_n^l(r; \lambda) = \left( \frac{n!}{(2l+n+1)!} \right)^{1/2} \exp(-\lambda r/2) (\lambda r)^{l+1} L_n^{2l+1}(\lambda r) \tag{3b}$$

where  $Y_{lm}(\theta, \varphi)$  are the usual spherical harmonics and  $L_n^{2l+1}$  are Laguerre polynomials [6].  $\lambda$  represents a free parameter and can be chosen arbitrarily. The Sturmians are

eigenfunctions of the Kepler Hamiltonian (hydrogen atom) if  $2\lambda$  equals an orbital quantum number  $n$ . Note that the Sturmians are orthonormal with respect to the weight function  $1/r$

$$\langle n'l'm' | 1/r | nlm \rangle = \delta_{nn'} \delta_{ll'} \delta_{mm'}. \quad (4)$$

Matrix elements of the unit (Id) and of the Laplace operator are easy to derive, whereas the calculation for  $\partial^2/\partial z^2$  is tedious. They are given by

$$\langle n'l'm' | \text{Id} | nlm \rangle = \delta_{ll'} \delta_{mm'} \frac{1}{\lambda} \begin{cases} 2(n+l+1) & n' = n \\ -[(n+1)(2l+m+2)]^{1/2} & n' = n+1 \end{cases} \quad (5)$$

$$\langle n'l'm' | \Delta | nlm \rangle = (-1)^{n+m'+1} \frac{1}{4} \lambda^2 \langle n'l'm' | \text{Id} | nlm \rangle \quad (6)$$

$$\langle n'l'm' | \partial^2/\partial z^2 | nlm \rangle = \frac{1}{3} \langle n'l'm' | \Delta | nlm \rangle$$

$$-\sqrt{\frac{2}{3}} (-1)^{l'-m'} \begin{pmatrix} l' & 2 & l \\ -m' & 0 & m \end{pmatrix} \langle n'l' | \| [\nabla \nabla]^{(2)} \| nl \rangle. \quad (7a)$$

For the reduced matrix elements  $\langle n'l' | \| [\nabla \nabla]^{(2)} \| nl \rangle$  we need the radial integrals

$$J_p(n'l'; nl) = \int_0^\infty dr \phi_n^{l'} r^{-p} \phi_n^l \quad p = 0, 1, 2; l' = l, l+2. \quad (7b)$$

They are given by the numerically convenient expressions

$$J_2(n'l'; nl) = \lambda(2l)! \left( \frac{n'!n!}{(2l+n'+1)!(2l+n+1)!} \right)^{1/2} \frac{(2l+1+\min(n, n'))!}{(\min(n, n'))!} \quad (7c)$$

$$J_p(n'l+2; nl) = \lambda^{p-1} \left( \frac{n'!}{n!(2l+n'+5)!(2l+n+1)!} \right)^{1/2} (2l+n+4-p)! \binom{n'-n+3}{n'-n+3-p} \\ \times \sum_{\nu=\max(0, n-n')}^{\min(n, 3-p)} (-1)^\nu \frac{(n'-n+\nu+1)_{3-p-\nu}}{(n'-n+p+\nu+1)_{3-p-\nu}} \\ \times \binom{3-p}{\nu} \frac{(n-\nu+1)_\nu}{(2l+n+5-p-\nu)_\nu} \quad (7d)$$

the remaining ones being given by (4) and (5). Thus we arrive at the following matrix equation:

$$[-\lambda(\overrightarrow{\Delta}) + (1-\gamma)\lambda(\overrightarrow{\partial^2/\partial z^2}) - 2(\overrightarrow{1/r})] \psi = (E/\lambda)(\overrightarrow{1d}) \psi \quad (8)$$

where the matrices are real symmetric. They can be ordered to be banded and sparse. Because the dependences on  $\gamma$  and  $\lambda$  factor out, the matrices have to be computed, in principle, only once and can then be used for diagonalisations with arbitrary  $\gamma$  and  $\lambda$ . Equation (8) represents a generalised eigenvalue problem, but it can be reduced to a standard one. Therefore we divide (8) by  $\lambda$  and put the Coulomb potential matrix into the right-hand side, which yields

$$[-(\overrightarrow{\Delta}) + (1-\gamma)(\overrightarrow{\partial^2/\partial z^2}) - (E/\lambda^2)(\overrightarrow{1d})] \psi = (2/\lambda)(\overrightarrow{1/r}) \psi = (2/\lambda) \psi. \quad (9)$$

Because of (4), the  $(\overrightarrow{1/r})$  matrix is the identity matrix. We can now choose a particular value  $\varepsilon$  of  $E/\lambda^2$  and diagonalise the resulting matrix of the left-hand side which gives the eigenvalues  $\lambda$ . The energies are then given by  $E = \varepsilon \lambda^2$ . For calculations in a restricted Hilbert space (truncated basis) the quantity  $\varepsilon$  plays the role of a variational parameter. However, if the basis size is chosen large enough, the calculated energy

spectra become independent of the particular choice of  $\epsilon$  because the (untruncated) basis set is always complete. Compared to (8), (9) represents a much more powerful computational scheme. Note that for  $\epsilon = -\frac{1}{4}$  each basis state included is already a first-order eigenstate (in  $\gamma - 1$ ) of the anisotropic Kepler problem in contrast to the case where we fix the Sturmian parameter  $\lambda$  and diagonalise the matrix equation (8), as is usually done in the literature. However we still diagonalise in a *complete* basis, in contrast to the case where we diagonalise the Hamiltonian in the bound-state hydrogen basis! Note that the use of such scaling methods is always applicable if the Hamiltonian consists of a sum of homogenous parts only (the homogeneity may, however, differ). Recently, a breakthrough in the theoretical treatment of the diamagnetic Kepler problem (hydrogen atom in a uniform magnetic field) has been made possible [7–11] by the use of similar scaling techniques.

Including all states with  $n + 1 < 10$  gives rise to small matrices of order 30. Choosing the free parameter  $\epsilon$  appropriately we are able to improve the results of Faulkner [1] in that our eigenvalues are consistently lower. We then diagonalised the Hamiltonian in a very large basis, where all states with  $n + 1 < 75$  were included ( $\epsilon = -0.01$  used). The matrix size was 1406 with a bandwidth of 78. Such calculations need only a few minutes on a Sperry 1182. Tables 1 and 2 give the results for silicon and germanium,

**Table 1.** Effective-mass binding energies of donor levels in silicon ( $\gamma = 0.2079$ ). Energies are given in units of  $E_R$ . Convergence is obtained in all digits quoted. Column 3 gives the quantum mechanical result of Faulkner [1], column 4 the semiclassical results of Gutzwiller [3]. The notation of the states is taken from [1].

1S	1.567 51	1.568	1.457	2P <sub>0</sub>	0.576 20	0.577	0.526	2P <sub>±</sub>	0.321 00	0.321
2S	0.444 13	0.443	0.419	3P <sub>0</sub>	0.275 06	0.275	0.256	3P <sub>±</sub>	0.156 44	0.156
3S	0.239 55	0.238	0.232	4P <sub>0</sub>	0.165 95	0.167	0.156	4P <sub>±</sub>	0.109 66	0.110
3D <sub>0</sub>	0.188 08	0.188	0.183	4F <sub>0</sub>	0.117 29	0.117	0.115	4F <sub>±</sub>	0.094 99	0.095
4S	0.146 07	0.143	0.141	5P <sub>0</sub>	0.112 07	0.112	0.108	5P <sub>±</sub>	0.072 68	0.072
4D <sub>0</sub>	0.107 43	0.106	0.106	5F <sub>0</sub>	0.081 79	0.081	0.082	5F <sub>±</sub>	0.063 16	0.064
5S	0.096 77	0.094	0.094	6P <sub>0</sub>	0.075 71	0.076	0.075	6P <sub>±</sub>	0.053 69	0.052
5D <sub>0</sub>	0.077 62	0.076	0.077	6F <sub>0</sub>	0.062 33	0.060	0.066	6F <sub>±</sub>	0.050 26	0.049
5G <sub>0</sub>	0.073 20	0.069	0.072	6H <sub>0</sub>	0.055 26	0.055	0.055	6H <sub>±</sub>	0.044 45	0.044
6S <sub>0</sub>	0.064 22		0.063	7P <sub>0</sub>	0.050 32		0.050	7P <sub>±</sub>	0.041 28	
6D <sub>0</sub>	0.058 37		0.057	7F <sub>0</sub>	0.049 21			7F <sub>±</sub>	0.037 61	
6G	0.052 45		0.052	7H <sub>0</sub>	0.042 23			7H <sub>±</sub>	0.033 98	

**Table 2.** Same as table 1, but for germanium ( $\gamma = 0.051 34$ ). Column 3 gives the results of Faulkner [1].

1S	2.092 64	2.087		2P <sub>0</sub>	1.015 87	1.008		2P <sub>±</sub>	0.367 81	0.368
2S	0.765 61	0.749		3P <sub>0</sub>	0.550 37	0.545		3P <sub>±</sub>	0.221 79	0.219
3S	0.458 08	0.428		4P <sub>0</sub>	0.361 27	0.355		4P <sub>±</sub>	0.160 55	0.155
3D <sub>0</sub>	0.316 29	0.285		4F <sub>0</sub>	0.260 30	0.247		4F <sub>±</sub>	0.129 81	0.130
4S	0.257 85	0.249		5P <sub>0</sub>	0.198 55	0.179		5P <sub>±</sub>	0.122 72	0.113
4D <sub>0</sub>	0.228 82	0.185		5F <sub>0</sub>	0.171 17	0.170		5F <sub>±</sub>	0.100 05	0.087
5S	0.179 91	0.153		6P <sub>0</sub>	0.157 29	0.130		6P <sub>±</sub>	0.085 37	0.081
5D <sub>0</sub>	0.148 80	0.130		6F <sub>0</sub>	0.128 40	0.117		6F <sub>±</sub>	0.082 39	0.068
5G <sub>0</sub>	0.141 72	0.113		6H <sub>0</sub>	0.119 01	0.085		6H <sub>±</sub>	0.076 04	0.062
6S <sub>0</sub>	0.119 34			7P <sub>0</sub>	0.106 99			7P <sub>±</sub>	0.067 20	
6D <sub>0</sub>	0.109 04			7F <sub>0</sub>	0.091 84			7F <sub>±</sub>	0.062 09	
6G <sub>0</sub>	0.099 52			7H <sub>0</sub>	0.090 57			7H <sub>±</sub>	0.060 54	

respectively, together with the results obtained by Faulkner [1] and Gutzwiller [3]. The agreement of Gutzwiller's results, which were derived with classical periodic orbit theory [2], with our converged quantum calculations for excited states is remarkable.

Although it seems that the results shown in the tables are obtained by 'brute force' methods they can in fact be calculated quite accurately with small basis expansions. We point out that the great advantage of the method is not only the high accuracy of the low-lying levels, but the convergence of many hundreds of excited states not listed in the tables. This will allow us to make a statistical analysis of the spectra. This seems to be interesting because the classical motion is ergodic, independent of how small the deviation of  $\gamma$  from the integrable case  $\gamma = 1$  is [2, 3]. However, trajectory calculations, not presented in this letter, show that the classical motion is confined to partly destroyed tori, so-called vague tori [12] or cantori [13], most of the time. The quantum behaviour of such systems is a topical subject of recent research studies [14]. Work in this direction is in progress.

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