Localization and Other Common Features of Degenerate Perturbations

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Diverse problems lead to groups of states with wave functions localized into different regions of space. This result is shown to be characteristic of a large number of problems in physics (atomic and nuclear examples are given) where states of highly degenerate manifolds are mixed by an interaction, which may be one or two particle in nature. Common analytical structures are derived and their origin traced. Random distributions and statistical arguments have often been used for the form of the localizations which we derive, however, as a consequence of specific structures in the interaction Hamiltonians.

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Drawing upon examples from atomic and nuclear physics, this paper points out universal features shared by a large number of problems in physics in which states group into different classes, distinguished by wave-function localization into different regions of space. Novel spectroscopic features have been seen when an atom is placed in a static electric or magnetic field.[1] A full explanation is unavailable, notably for the effect of a magnetic field on highly excited states. But, it has become clear that two classes of states play a crucial role, with wave functions concentrated along, and perpendicular to, the direction of the magnetic field.[1,2] Likewise, in an electric field, wave-function concentrations in the up- and down-field directions characterize what is observed.[1,3] Wave-function localization has also been emphasized in recent studies of the motion of a particle in random potentials used for modeling disordered systems.[4] Studies of chaos, that is, of the quantal spectrum for nonseparable potentials in two or more variables whose corresponding classical motion is irregular, also involve wave functions localized in different regions of space.[5] Finally, in a two-particle example in atomic physics, namely states of two highly excited electrons, localization of the wave function into a small portion of the total space available is known to be a key feature.[6,7] We will consider the following problems. (i) The electron (charge $e=1$, mass $m=1$) in combined Coulomb and diamagnetic potentials: $V=1/r+\frac{1}{2}B^2\rho^2$, where $\rho^2=x^2+y^2=r^2-z^2$, and B is the magnetic field in units of 4.7×10^9 G. (ii) The electron in combined Coulomb and electric fields: $V=-1/r+Fz$, with F the electric field in units of 5.14×10^9 V/cm. (iii) The particle ($m=1$) in the potential $V=\frac{1}{2}(x^2+y^2)+\alpha x^2y^2$. (iv) Two electrons and a fixed positive charge Z: $V=Z/r_1-Z/r_1+1/r_{12}$. (v) Two nucleons interacting through the quadrupole coupling: $V=\frac{1}{2}(r_1^2+r_2^2)+\alpha r_1^2Y_1^{(2)}\cdot r_2^2Y_2^{(2)}$, where $Y_i^{(2)}$ are rank-two tensor operators.

For the high-energy region of the spectrum that will be of interest, all these problems involve the mixing of a very large number of basis states. Often, this number diverges. Also, they all involve nonseparable potentials except for (ii). In each case, upon dropping the last "interaction" term, the Coulomb or harmonic-oscillator bases which are the natural starting points of the analysis show a high degeneracy with increasing principal quantum number n. Although states with different n are also mixed by the interaction the dominant mixing can be expected to be of intra-n states, given their degeneracy. A recent study[8] of (i) showed that the subdivision of states into two classes, parallel and perpendicular to the magnetic field direction, sets in already upon a diagonalization of the interaction within a degenerate n manifold. The tridiagonal matrix eigenvalue problem was transformed into a second-order linear differential equation for angular prolate spheroidal functions.[9] Two such equations, related by a "conjugation" transformation,[8] together describe the eigenvalues which span a finite range and which are equally spaced from the bottom up and from the top down (with different spacings). The former, called vibrator states, and the latter, called rotor states, show localization of the eigenvectors. Only a small fraction ($\sim n^{-1/2}$) of the degenerate angular momentum states ($l=0,1,2,\ldots,n-1$) are appreciably present in them. Correspondingly, in real space, the states are confined to lie, respectively, parallel or perpendicular to the magnetic field. Only a few eigenstates in the middle extend over the full available range of l.

The above results for the specific problem (i) are valid also for all the others listed above. The same form of the differential equation, namely an angular spheroidal equation, the same conjugation transformation linking a pair of these equations, and the same algebraic expression for the localization in l of the eigenvectors is obtained for each of the problems. We will now consider each of them in turn.

Coulomb plus diamagnetic.—In a degenerate hydrogenic manifold n, the only nonzero matrix elements of $\frac{1}{2}\rho^2$ are diagonal in m (we set $m=0$ below) and parity, and are restricted to $\Delta l=0,2$. The angular part of the matrix elements, $\langle lm|\sin^2\theta|l+\Delta l,m\rangle$, is easily rendered in terms of Wigner $3j$ symbols.[10] Already at very low l, they attain (for low m) the asymptotic values of $\frac{1}{2}$ and $-\frac{1}{4}$, respectively, for $\Delta l=0$ and 2.[8] The radial factor in the matrix element, $\langle n,l-\frac{1}{2}\Delta l|\frac{1}{2}r^2|n,l+\frac{1}{2}\Delta l\rangle$, is adequately described[8] at large n and $l/n\ll1$ (a condition

that will be satisfied by the states of interest) by $(n^4/4)(5-3u^2)$ and $(5n^4/4)(1-u^2)$ for $\Delta l=0$ and 2, respectively, where we have introduced $u=(l+\frac{1}{2})/n$. As a result, diagonalization involves solution of the three-term recurrence relation $W_{l-1}a_{l-2}+V_l a_l+W_{l+1}\times a_{l+2}=\epsilon a_l$, where ϵ is the eigenvalue of $\frac{1}{2}\rho^2/n^4$ and $\{a_l\}$ is the eigenvector, with $V_l=(5-3u^2)/8$, $W_l=-5\times(1-u^2)/16$.

Regarding u as a continuous variable from 0 to 1, we pass[8] to the angular spheroidal differential equation[9] through the simple replacements $a_{l\pm2}=a\pm(2/n)a'+(2/n^2)a''$,

$$[(1-u^2)a'(u)]'+n^2[b\epsilon+d-cu^2]a(u)=0, \quad (1)$$

with $b=\frac{4}{5}$, $d=0$, and $c=\frac{1}{5}$. The positive value of c makes $a(u)$ a prolate spheroidal function. Further, the large-n^2 factor for the coefficient of u^2 allows the use of an asymptotic formula[9] to get

$$d+b\epsilon=2\sqrt{c}\,(K+\tfrac{1}{2})/n, \quad (2)$$

where K is akin to a one-dimensional oscillator quantum number. Its values are fixed by boundary conditions on the difference equation at small l.[8] The spectrum of eigenvalues is equally spaced. The above expression for ϵ records only the leading term in powers of $1/n$ of the asymptotic formula (21.7.6 of Ref. 9); further terms can be easily written down if desired.

In the diamagnetic problem, Eq. (2) describes the vibrator spectrum. K takes values in the sequence $\frac{1}{2}(4v+1)$, where $v=0,1,2,\ldots$. The (doubly degenerate) eigenvalues are, therefore, given by $\epsilon=(\sqrt{5}/n)(v+\frac{1}{2})$. The lowest eigenvector has the form[9] $\sqrt{u}\exp(-n\times\sqrt{c}\,u^2/2)$, the initial $\sqrt{u}$ factor stemming from $K=\frac{1}{2}$. In the normalized form, we have[8]

$$a_l=(4c)^{1/4}[(2l+1)/n]^{1/2}\exp[-\sqrt{c}\,l(l+1)/2n]. \quad (3)$$

Note the initial rise of $|a_l|^2\propto 2l+1$ and the rapid fall-off at higher l in the form of a Gaussian in u. In the complementary real-space coordinate θ, the squared wave function is Gaussian peaked around $\theta=0°$ and 180° with the form $\exp(-n\gamma^2/\sqrt{c})$, where γ is the departure from the longitudinal direction.

A conjugation transformation,[8] which is a local gauge transformation that multiplies a_l in each eigenvector by alternating $\pm$ signs to give $\tilde{a}_l$, changes only the sign of W. The resulting conjugate differential equation satisfied by $\tilde{a}(u)$ is again a prolate spheroidal equation (1) but with $b=-\frac{4}{5}$, $d=1$, and $c=\frac{4}{5}$. The new eigenvalues are also equally spaced but with twice the spacing as before, descending from a maximum value $-d/b=5/4$: $\epsilon=\frac{5}{4}-(\sqrt{5}/n)(K+\frac{1}{2})$. The values of K now run over the even (odd) integers for even (odd) parity. The extreme eigenvector is given by[8]

$$a_l=(\pi\sqrt{c})^{1/4}[(2l+1)/\sqrt{n}]^{1/2}P_l(0)\times\exp[-\sqrt{c}\,l(l+1)/2n]. \quad (4)$$

As with (3), we again have a localization in l, with $l\le l_{\max}\approx\sqrt{n}$. In real space, (4) describes a wave function that is Gaussian concentrated around $\theta=90°$, that is, perpendicular to the magnetic field direction.

Coulomb plus electric.—This is the only separable problem in our list, the Schrödinger equation separating in parabolic coordinates.[11] In a degenerate hydrogenic n manifold, the interaction Fz mixes all the l states (with m again set equal to zero). This linear-Stark-effect problem is exactly solvable, giving rise to equally spaced eigenvalues with spacing $3Fn$ lying between the two extremes $\pm 3Fn(n-1)/2$. The extreme eigenvectors are given exactly[11] by the angular momentum coupling coefficient $\langle jjl0\,|\,jj,\pm j,\mp j\rangle$, with $j=\frac{1}{2}(n-1)$, and have wave-function concentration in the $\pm z$ directions. For large n and $l\ll n$, these coefficients are[12]

$$a_l=(\pm1)^l[(2l+1)/n]^{1/2}\exp[-l(l+1)/2n].$$

These exact results can also be recovered through our formalism[8] in this paper, the only nonzero matrix element of z being for $\Delta l=1$. The angular part $\langle l\,|\times\cos\theta\,|\,l\pm1\rangle$ is described to a very good approximation for all l by the asymptotic value of $\frac{1}{2}$.[10] The radial factor $\langle nl\,|\,r\,|\,nl\pm1\rangle$ equals $(3n^2/2)(1-u^2)^{1/2}$ so that in the difference equation $W_{l-1}a_{l-1}+W_{l+1}a_{l+1}=\epsilon a_l$ for the eigenvalues ϵ of Z/n^2, $W_l=\frac{3}{4}(1-u^2)^{1/2}$. The resulting differential equation is again (1) as before, with coefficients $b=\pm\frac{4}{3}$, $d=2$, and $c=1$. The conjugate pair [now $\tilde{a}_l=(-1)^l a_l$] differ only in the sign of b and are again prolate spheroidal equations. The eigenvalues and eigenvectors that follow from (2) and (3) coincide with the well-known exact results recorded in the previous paragraph. Here again $K=\frac{1}{2}(4v+1)$ and $\epsilon=\pm\frac{3}{2}[1-(2v+1)/n]$.

The potential $V(x,y)=\frac{1}{2}(x^2+y^2)+\alpha x^2y^2$.—Model potentials such as $x^4+y^4+\alpha x^2y^2$, irregular classical motion in them, and the corresponding quantal spectrum are being studied as examples of chaos.[13] Plots of eigenvalues as a function of α display sharply avoided crossings suggestive of two classes of states. This is both reminiscent of the previous two problems and immediately plausible in terms of wave-function concentrations, one along the x and y axes and, another along the 45° lines, $y=\pm x$.

To see the incipient formation of two classes of states within a degenerate manifold, we examine an allied model with harmonic x and y potentials, $\frac{1}{2}(x^2+y^2)+\alpha x^2\times y^2$, which has similar features. An n manifold with unperturbed energy $n+1$ has an $(n+1)$-fold degeneracy, either the oscillator quantum number in x or in y taking on the sequence of values $l=0,1,\ldots,n$, with the other running down the complementary sequence such that the sum is n. Diagonalization of x^2y^2 in such a basis leads to a tridiagonal matrix[14] with $V_l=\tilde{u}(1-\tilde{u})$, $W_l=\tilde{u}(1-\tilde{u})/4$, where $\tilde{u}=l/n$. Once again, only even l or odd l are coupled by the interaction. The resulting

differential equation for the eigenvalues ϵ of x^2y^2/n^2 is now (1) with $u=1-2\tilde{u}$ and $b=-1$, $d=\frac{3}{8}$, $c=\frac{3}{8}$. The general result in (2) gives $\epsilon=\frac{3}{8}-(\frac{3}{2})^{1/2}(K+\frac{1}{2})/n$, with $K=0,1,2,\ldots$, to describe the upper end of the spectrum as equally spaced levels descending from $\frac{3}{8}$. The highest eigenvector is

$$a_l=2(\sqrt{6}/\pi n)^{1/4}\exp[-(\tfrac{3}{2})^{1/2}(l-n/2)^2].$$

This Gaussian function is appreciable only for l values clustered in the middle of their range around $n/2$, reflecting the structure $\langle x^2\rangle\simeq\langle y^2\rangle$ for these states.

The conjugate equation for $\tilde{a}_l$ is, on the other hand, (1) with $b=1$, $d=-\frac{1}{8}$, and $c=-\frac{1}{8}$. For the first time in the discussion, so far, c is negative. This means we have an angular oblate spheroidal equation[9] with the coefficient of u^2 in (1) positive. This coefficient still involves the large multiplicative n^2 so that from an asymptotic formula now for oblate functions (21.8.2 of Ref. 9), we have $d+b\epsilon=c+2\sqrt{-c}K/n$, each of these occurring twice. With the coefficients in this paragraph, the eigenvalues are $\epsilon=K/\sqrt{2}n$ and ascend from zero in equally spaced steps, with $K=1,3,\ldots$, for the odd l and $K=0,2,\ldots$, for the even l states. The lowest eigenvector is given by $a_l=2^{1/4}\{\exp[-(l+\frac{1}{2}/\sqrt{2}]+\exp[-(n-l+\frac{1}{2}/\sqrt{2}]\}$. The appreciable values are, therefore, clustered around $l\simeq 0$ and $l\simeq n$ as anticipated, with $\langle x\rangle$ or $\langle y\rangle$ near zero. These analytical expressions agree very well with the results of numerical diagonalization of x^2y^2 in a large-n manifold.[15]

Two excited electrons.—Doubly excited states in atoms also group into two classes, with either r_1/r_2 very different from unity or $r_1\simeq r_2$.[7] The total orbital angular momentum L is conserved and $1/r_{12}$ diagonal in it. It suffices to examine any one L and we will consider $L=0$, that is, $(nl)^2S$ states. Unlike in our previous examples, the matrix $\langle(nl)^2S\,|\,1/r_{12}\,|\,(nl')^2S\rangle$ is neither tridiagonal nor is there a simple analytical expression available. For this reason, we will first consider a model based on the orthogonal group O(4) which has often been used to describe the electron-electron interaction in an n manifold.[16,17]

In the O(4) model, one considers the operator r_{12}^2, with the reciprocal square root of its eigenvalues taken to represent $1/r_{12}$. The operator $r_{12}^2=r_1^2+r_2^2-2\mathbf{r}_1\cdot\mathbf{r}_2$ can be expressed in terms of the generators of O(4) through the replacement $\mathbf{r}\rightarrow en\mathbf{a}/2$, where $\mathbf{a}$ is the Runge-Lenz vector.[11] The only nonzero matrix elements of $\Lambda=9a_{12}^2/4$ are for $l'-l=0,\pm 1$. The angular part of the off-diagonal matrix element $\langle l^2S\,|\cos\theta_{12}|\,(l\pm 1)^2S\rangle$ can be adequately approximated by the asymptotic value $-\frac{1}{2}$. The tridiagonal problem[18] $W_{l-1/2}a_{l-1}+V_la_l+W_{l+1/2}\times a_{l+1}=\epsilon a_l$ has $V_l=9(1-u^2)/2$, $W_l=-9(1-u^2)/4$, with $u=(l+\frac{1}{2})/n$. The differential equation (1), therefore, has $b=\frac{4}{9}$, $d=0$, and $c=0$. With c vanishing, (1) reduces to the Legendre equation so that the eigenvalues are given by a rotor spectrum $\epsilon=9\nu(\nu+1)/n^2$, $\nu=0,1,2,\ldots,n-1$.

The conjugate equation for $\tilde{a}_l=(-1)^la_l$ is, on the other hand, of prolate spheroidal form with $b=-\frac{4}{9}$, $d=4$, and $c=4$. From (2), the spectrum descends from 9 in equal steps: $\epsilon=9-9(2\nu+1)/n$ which is identical to the above result to order $1/n$. Therefore, a rotor spectrum with a maximum cutoff can be viewed as a vibrator spectrum descending from a maximum value. The highest eigenvector (maximum r_{12}^2 and, therefore, minimum $1/r_{12}$ repulsion) is given as in (3) by

$$a_l=(-1)^l[2(2l+1)/n]^{1/2}\exp[-l(l+1)/n].$$

This expression for the localization in l and its relation to the Gaussian peaking of the two-electron wave function around $\theta_{12}=180°$ have been explored elsewhere.[17]

We have also been able to case $1/r_{12}$ directly in tridiagonal form. Retaining only the first two terms in its multipole expansion,

$$V_l=(3+u^2)/5,\quad W_l=-(1-u^2)^{1/2}/5,$$

fit the numerical values fairly well. With these, we again get (1) with $b=10$, $d=-2$, $c=8$, and $b=-10$, $d=10$, $c=0$, for the conjugate pair. The occurrence of $c=0$ in one of the pairs leads again to an exact rotor spectrum as in the O(4) model.

Two nucleons interacting through quadrupole-quadrupole coupling.—This problem with two nucleons in a major shell is a standard model in nuclear physics.[19] It is also the two-particle analog of our problem (iii). With both nucleons in the same major shell n, different l values are degenerate. We will again work with S states. The angular part of the matrix element, $\langle l^2S\,|\,Y_2^{(2)}\cdot Y_2^{(2)}\,|\,l^2S\rangle$, is nonzero only for $\Delta l=0,2$ and, as in our previous examples, essentially constant at the asymptotic value of $\frac{1}{4}$ and $\frac{3}{8}$, respectively.[10] For the harmonic-oscillator potential, the radial matrix elements of r^2 are $n+\frac{3}{2}$ and $-[(n-l)(n+l+3)]^{1/2}$, respectively. The difference equation $W_{l+1}a_{l+2}+V_la_l+W_{l-1}a_{l-2}=\epsilon a_l$ is specified by $V_l=\frac{1}{4}(1+3/n)$, $W_l=3(1-u^2)/8$, giving rise to (1) with $b=-\frac{2}{3}$, $d=\frac{2}{3}$, and $c=\frac{1}{2}$. For the conjugate equation, we get $b=\frac{2}{3}$, $d=\frac{1}{3}$, and $c=\frac{1}{2}$. The eigenvalue spectrum follows from (2) and is again equally spaced at either end, and extreme eigenvectors are localized in l according to (3) with $c=\frac{1}{2}$. Details will be published elsewhere.

Discussion.—Diverse problems, both one and two particle, from atomic and nuclear physics are seen then to have a common structure. The emergence of two classes of states sets in already upon considering manifolds of degenerate states with principle quantum number n, even before the full mixing involving a different n is accounted for. A conjugate pair of spheroidal differential equations describes the upper and lower ends of the spectrum of eigenvalues, each associated with one of the classes. Except when one of the conjugate pair reduces to a Legendre equation with the spectrum then that of a pure rotor,

the spectrum at either end has equal spacing. The eigenvectors are localized in the quantum number l that labels the degenerate states. This distribution has the characteristic structure in (3). Correspondingly, in real space, the states are confined to different regions of the configuration space in the form of Gaussians with a width proportional to $1/\sqrt{n}$. Remarkably, the distribution in (3) is of the same form as the one argued for in nuclear and many-body physics based on a statistical distribution of angular momentum values.[20] It has features characteristic of a random walk or diffusion in l, namely $\exp[-(l+\frac{1}{2})^2/n]$, and $l_{\max}$ growing proportional to $\sqrt{n}$. But, we have obtained it with no recourse to any underlying statistical or stochastic cause. Rather its origin in all these problems rests on the vanishing of W_l in the $u \rightarrow 1$ or $l \rightarrow n$ limit.

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