Physics 362k, Spring 2015

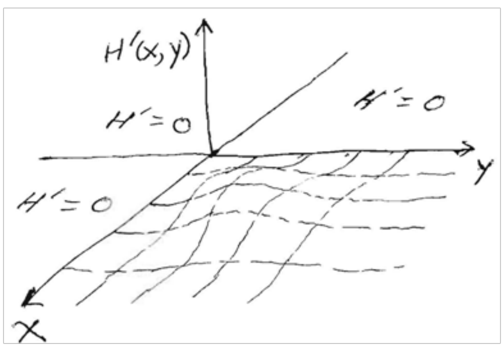
Degenerate Perturbation Theory Example Problem

<u>Perturbed 2-D harmonic oscillator</u>.

A particle of mass *m* moves in a two-dimensional harmonic oscillator potential $V(x,y)=\frac{1}{2}m\omega^2x^2+\frac{1}{2}m\omega^2y^2$. This potential is perturbed by the added potential

$$H'(x,y)=\begin{cases} V_0\dfrac{xy}{x_0^2}e^{-\frac{x^2+y^2}{x_0^2}}, \text{ if } (x>0 \text{ and } y>0) \\ 0, \text{ otherwise} \end{cases}$$

where $V_0=\frac{1}{4}\hbar\omega$ and $x_0=\sqrt{\frac{\hbar}{m\omega}}$, as sketched below.



a) Find the energy of the ground state of this system, correct to first order in H'.

b) The first excited energy state of the unperturbed 2-D harmonic oscillator is doubly degenerate. This degeneracy is removed by the perturbation H'. Use degenerate perturbation theory to find the eigenfunctions of these states (correct eigenfunctions in the limit of small but non-zero H') and their energies correct to first order in H'. (To do this calculation, use products of one dimensional oscillator functions $\psi_{nm}(x,y)=\psi_n(x)\psi_m(y)$ as your unperturbed basis functions for the calculation of the matrix of H'.)

c) Make a level diagram that shows the energies of the few lowest unperturbed states, and also shows how the energies of those states are shifted by the perturbation H'. Make a qualitative sketch that shows the perturbed wavefunctions from part (b), and explain why the energy of one of them is higher than the other.

<u>Solution</u>

a) For this problem solution, we are going to need the following integrals:

$$I_1 = \int_0^\infty z e^{-2z^2} dz = \frac{1}{4} \qquad I_2 = \int_0^\infty z^2 e^{-2z^2} dz = \frac{1}{8}\sqrt{\frac{\pi}{2}} \qquad I_3 = \int_0^\infty z^3 e^{-2z^2} dz = \frac{1}{8} \tag{1}$$

I obtained the value for I_1 with the Mathematica instruction

`Integrate[z Exp[-2 z^2],{z,0, Infinity}],` and similarly for I_2 and I_3.

The Hamiltonian is $H = H_0 + H'$ (2)

$$\text{where } H_0 = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) + V(x,y) \tag{3}$$

$$\text{with } V(x,y) = \frac{1}{2}m\omega^2 x^2 + \frac{1}{2}m\omega^2 y^2 \tag{4}$$

H_0 is the unperturbed Hamiltonian for an isotropic two-dimensional harmonic oscillator, and

$$H'(x,y) = \begin{cases} V_0 \dfrac{xy}{x_0^2} e^{-\frac{x^2+y^2}{x_0^2}}, & \text{if } (x>0 \text{ and } y>0) \\ 0, & \text{otherwise} \end{cases} \tag{5}$$

with $x_0 = \sqrt{\dfrac{\hbar}{m\omega}}$ and $V_0 = \dfrac{1}{4}\hbar\omega$

the perturbing potential. The unperturbed two-dimensional harmonic oscillator problem is separable into two one-dimensional harmonic oscillator problems, and has solutions

$$H_0 \left|\psi_{k\ell}^{(0)}\right\rangle = E_{k\ell}^{(0)} \left|\psi_{k\ell}^{(0)}\right\rangle, \quad k = 0,1,2,\ldots \quad \ell = 0,1,2,\ldots \tag{6}$$

$$\text{where } \psi_{k\ell}^{(0)}(x,y) = \left\langle x,y \middle| \psi_{k\ell}^{(0)}\right\rangle = \psi_k^{(0)}(x)\psi_\ell^{(0)}(y) \tag{7}$$

$$\text{with } \psi_k(x) = \left(\frac{1}{\pi x_0^2}\right)^{1/4} \frac{1}{\sqrt{2^k k!}} H_k\left(\frac{x}{x_0}\right) e^{-\frac{x^2}{2x_0^2}} \tag{8}$$

and $H_k = k$th Hermite polynomial, $H_0(\xi) = 1, \quad H_1(\xi) = 2\xi$ (9)

and $E_{k\ell}^{(0)} = (k + \ell + 1)\hbar\omega$ (10)

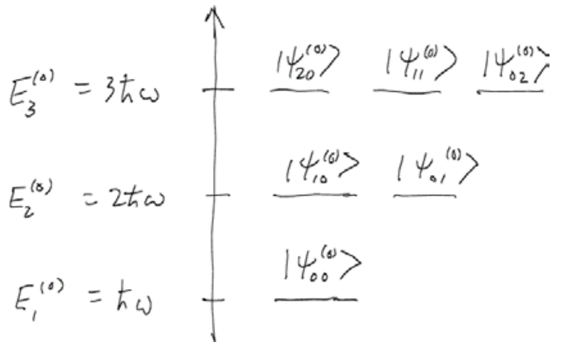


Fig. 1. Lowest energy levels of the isotropic two-dimensional harmonic oscillator.

we can also write $$\psi_0(x) = \left(\frac{1}{\pi x_0^2}\right)^{1/4} e^{-\frac{x^2}{2x_0^2}}, \qquad \psi_1(x) = \left(\frac{1}{\pi x_0^2}\right)^{1/4} \sqrt{2}\,\frac{x}{x_0} e^{-\frac{x^2}{2x_0^2}} \tag{11}$$

The lowest few energy levels are illustrated in Fig. 1. The level energies are $E_n^{(0)} = n\hbar\omega$, where $n = k + \ell + 1 = 1, 2, 3, \ldots$ The ground state is non-degenerate, has $k = \ell = 0 \Rightarrow n = 1$, and energy

$$E_1^{(0)} = E_{00}^{(0)} = \hbar\omega. \tag{12}$$

The unperturbed state vector for the ground state is $\left|\psi_{00}^{(0)}\right\rangle$ and its wavefunction is

$$\psi_{00}^{(0)}(x,y) = \psi_0^{(0)}(x)\psi_0^{(0)}(y) = \left(\frac{1}{\pi x_0^2}\right)^{1/2} e^{-\frac{x^2}{2x_0^2}} e^{-\frac{y^2}{2x_0^2}} \tag{13}$$

Since the ground state is non-degenerate, we can calculate its energy with non-degenerate perturbation theory. The first-order correction to the energy is

$$\begin{aligned} E_1^{(1)} &= \left\langle \psi_{00}^{(0)} \middle| H' \middle| \psi_{00}^{(0)} \right\rangle = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \psi_{00}^{(0)*}(x,y) H'(x,y) \psi_{00}^{(0)}(x,y)\,dx\,dy = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \left|\psi_{00}^{(0)}(x,y)\right|^2 H'(x,y)\,dx\,dy \\ &= \int_0^{\infty}\int_0^{\infty} \left(\frac{1}{\pi x_0^2}\right) e^{-\frac{x^2}{x_0^2}} e^{-\frac{y^2}{x_0^2}} V_0 \frac{xy}{x_0^2} e^{-\frac{x^2+y^2}{x_0^2}}\,dx\,dy = \frac{V_0}{\pi}\int_0^{\infty}\frac{x}{x_0} e^{-2\frac{x^2}{x_0^2}}\frac{dx}{x_0}\int_0^{\infty}\frac{y}{x_0} e^{-2\frac{y^2}{x_0^2}}\frac{dy}{x_0} = \frac{V_0}{\pi}\left[\int_0^{\infty}\frac{x}{x_0} e^{-2\frac{x^2}{x_0^2}}\frac{dx}{x_0}\right]^2 \\ &= \frac{V_0}{\pi}\left[\int_0^{\infty} z e^{-2z^2}\,dz\right]^2 = \frac{V_0}{\pi} I_1^2 = \frac{V_0}{16\pi} \qquad (z = x/x_0) \end{aligned} \tag{14}$$

The integrals over x and y in eq. (14) extend only from 0 to ∞ because the perturbation H' is zero if x or y is negative. To first order, the ground state energy is

$$E_1 \approx E_1^{(0)} + E_1^{(1)} = \hbar\omega + \frac{V_0}{16\pi} = \hbar\omega + \frac{1}{16\pi}\frac{1}{4}\hbar\omega = \left(1 + \frac{1}{64\pi}\right)\hbar\omega = 1.00497\hbar\omega \tag{15}$$

b) The first excited levels have energy $E_2^{(0)} = 2\hbar\omega$. These are the levels with state vectors $\left|\psi_{kl}^{(0)}\right\rangle = \left|\psi_{01}^{(0)}\right\rangle$ and $\left|\psi_{kl}^{(0)}\right\rangle = \left|\psi_{10}^{(0)}\right\rangle$; *i.e.* the level is doubly degenerate. We'll adopt this new labeling of these states:

$$\left|\tilde{\psi}_{21}^{(0)}\right\rangle = \left|\psi_{01}^{(0)}\right\rangle \qquad\qquad \left|\tilde{\psi}_{22}^{(0)}\right\rangle = \left|\psi_{10}^{(0)}\right\rangle \tag{16}$$

The notation $\left|\psi_{10}^{(0)}\right\rangle$ indicates that the subscripts give the values of k and ℓ in our set of unperturbted wavefunctions given in eq. (7); for example $\left\langle x, y\middle|\psi_{10}^{(0)}\right\rangle = \psi_1^{(0)}(x)\psi_0^{(0)}(y)$. The notation $\left|\tilde{\psi}_{21}^{(0)}\right\rangle$ indicates that the subscripts given the value of n and i, where n is the energy level ($n = 2$ for this level), and $i = 1, ..., g_n$ indicates which of the degenerate zero-order levels we are referring to. For this level $g_n = 2$, and the identification of $\left|\tilde{\psi}_{ni}^{(0)}\right\rangle$ with specific $\left|\psi_{k\ell}^{(0)}\right\rangle$ is given by eqs. (16). To find the correct eigenfunctions and energies, we must first calculate all the matrix elements $H'_{ij} = \left\langle\tilde{\psi}_{2i}^{(0)}\middle|H'\middle|\tilde{\psi}_{2j}^{(0)}\right\rangle$ of the perturbation in the degenerate subspace. These are

$$\begin{aligned}
H'_{11} &= \left\langle\tilde{\psi}_{21}^{(0)}\middle|H'\middle|\tilde{\psi}_{21}^{(0)}\right\rangle = \left\langle\psi_{01}^{(0)}\middle|H'\middle|\psi_{01}^{(0)}\right\rangle = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\left|\psi_{01}^{(0)}(x,y)\right|^2 H'(x,y)\,dx\,dy \\
&= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\left|\psi_0(x)\right|^2\left|\psi_1(y)\right|^2 H'(x,y)\,dx\,dy = \int_0^{\infty}\int_0^{\infty}\left(\frac{1}{\pi x_0^2}\right)e^{-\frac{x^2}{x_0^2}}\,2\frac{y^2}{x_0^2}e^{-\frac{y^2}{x_0^2}}V_0\frac{xy}{x_0^2}e^{-\frac{x^2+y^2}{x_0^2}}\,dx\,dy \\
&= \frac{2V_0}{\pi}\int_0^{\infty}\frac{x}{x_0}e^{-2\frac{x^2}{x_0^2}}\frac{dx}{x_0}\int_0^{\infty}\frac{y^3}{x_0^3}e^{-2\frac{y^2}{x_0^2}}\frac{dy}{x_0} = \frac{2V_0}{\pi}I_1 I_3 = \frac{2V_0}{\pi}\cdot\frac{1}{4}\cdot\frac{1}{8} = \frac{V_0}{16\pi}
\end{aligned} \tag{17}$$

$$\begin{aligned}
H'_{12} &= \left\langle\tilde{\psi}_{21}^{(0)}\middle|H'\middle|\tilde{\psi}_{22}^{(0)}\right\rangle = \left\langle\psi_{01}^{(0)}\middle|H'\middle|\psi_{10}^{(0)}\right\rangle = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\psi_{01}^{(0)*}(x,y)H'(x,y)\psi_{10}^{(0)}(x,y)\,dx\,dy \\
&= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\psi_0^*(x)\psi_1^*(y)H'(x,y)\psi_1(x)\psi_0(y)\,dx\,dy \\
&= \int_0^{\infty}\int_0^{\infty}\left(\frac{1}{\pi x_0^2}\right)e^{-\frac{x^2}{2x_0^2}}\sqrt{2}\frac{y}{x_0}e^{-\frac{y^2}{2x_0^2}}V_0\frac{xy}{x_0^2}e^{-\frac{x^2+y^2}{x_0^2}}\sqrt{2}\frac{x}{x_0}e^{-\frac{x^2}{2x_0^2}}e^{-\frac{y^2}{2x_0^2}}\,dx\,dy \\
&= \frac{2V_0}{\pi}\int_0^{\infty}\frac{x^2}{x_0^2}e^{-2\frac{x^2}{x_0^2}}\frac{dx}{x_0}\int_0^{\infty}\frac{y^2}{x_0^2}e^{-2\frac{y^2}{x_0^2}}\frac{dy}{x_0} = \frac{2V_0}{\pi}I_2^2 = \frac{2V_0}{\pi}\frac{\pi}{128} = \frac{V_0}{64}
\end{aligned} \tag{18}$$

$$H'_{21} = \left\langle\tilde{\psi}_{22}^{(0)}\middle|H'\middle|\tilde{\psi}_{21}^{(0)}\right\rangle = H_{21}'^{\,*} = \frac{V_0}{64} \qquad \text{(since } H' \text{ is Hermitian)} \tag{19}$$

$$H'_{22} = \left\langle \tilde{\psi}_{22}^{(0)} \middle| H' \middle| \tilde{\psi}_{22}^{(0)} \right\rangle = \left\langle \psi_{10}^{(0)} \middle| H' \middle| \psi_{10}^{(0)} \right\rangle = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \left|\psi_{10}^{(0)}(x,y)\right|^2 H'(x,y)\,dx\,dy$$
$$= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \left|\psi_1(x)\right|^2 \left|\psi_0(y)\right|^2 H'(x,y)\,dx\,dy = H'_{11} = \frac{V_0}{16\pi} \tag{20}$$

$$\Rightarrow \quad H' = \begin{bmatrix} \frac{V_0}{16\pi} & \frac{V_0}{64} \\ \frac{V_0}{64} & \frac{V_0}{16\pi} \end{bmatrix} \tag{21}$$

Keep in mind that this is the matrix of H' *in the degenerate subspace only*. The ordered basis in this subspace is $\left\{ \left|\tilde{\psi}_{21}^{(0)}\right\rangle, \left|\tilde{\psi}_{21}^{(0)}\right\rangle \right\} = \left\{ \left|\psi_{01}^{(0)}\right\rangle, \left|\psi_{10}^{(0)}\right\rangle \right\}$. Next, we need to solve the eigenvalue problem

$$H' \left|\varphi_{2i}^{(0)}\right\rangle = E_{2i}^{(1)} \left|\varphi_{2i}^{(0)}\right\rangle \tag{22}$$

in the 2-dimensional degenerate subspace with n = 2. The eigenvalues are given by the solutions of the characteristic equation

$$\det\left(H' - IE_{2i}^{(1)}\right) = 0 \tag{23}$$

$$\begin{vmatrix} H'_{11} - E_{2i}^{(1)} & H'_{12} \\ H'_{21} & H'_{22} - E_{2i}^{(0)} \end{vmatrix} = 0$$
$$\left(H'_{11} - E_{2i}^{(1)}\right)\left(H'_{22} - E_{2i}^{(1)}\right) - \left|H'_{12}\right|^2 = 0 \tag{24}$$
$$\left(H'_{11} - E_{2i}^{(1)}\right)^2 = \left|H'_{12}\right|^2 \quad \text{(since here } H'_{11} = H'_{22}; \text{ not always true)}$$

$$E_{2i}^{(1)} = H'_{11} \pm \left|H'_{12}\right| = \frac{V_0}{16\pi} \pm \frac{V_0}{64} = \frac{V_0}{16\pi}\left(1 \pm \frac{\pi}{4}\right) \tag{25}$$

We have two solutions for the eigenvalues, which we label in an arbitrary way as $i = 1, 2$:

$$E_{21}^{(1)} = \frac{V_0}{16\pi}\left(1 - \frac{\pi}{4}\right) = 0.00427\ V_0 = 0.00427\frac{1}{4}\hbar\omega = 0.00107\hbar\omega \tag{26}$$

$$E_{22}^{(1)} = \frac{V_0}{16\pi}\left(1 + \frac{\pi}{4}\right) = 0.03552\ V_0 = 0.03552\frac{1}{4}\hbar\omega = 0.00888\hbar\omega \tag{27}$$

Therefore we have found the energies to first order:

$$E_{21} \simeq E_2^{(0)} + E_{21}^{(1)} = 2\hbar\omega + 0.00107\hbar\omega = 2.00107\hbar\omega \tag{28}$$

$$E_{22} \simeq E_2^{(0)} + E_{22}^{(1)} = 2\hbar\omega + 0.00888\hbar\omega = 2.0888\hbar\omega \tag{29}$$

The zeroth-order eigenvectors are found by substituting the two eigenvalues from eqs. (26) and (27) back into the eigenvalue equation (22). We do this first for eigenvalue $i = 1$:

$$H'\left|\varphi_{21}^{(0)}\right\rangle = E_{21}^{(1)}\left|\varphi_{21}^{(0)}\right\rangle \qquad \Rightarrow \qquad \frac{V_0}{16\pi}\begin{bmatrix} 1 & \frac{\pi}{4} \\ \frac{\pi}{4} & 1 \end{bmatrix}\begin{bmatrix} c_{11} \\ c_{12} \end{bmatrix} = \frac{V_0}{16\pi}\left(1-\frac{\pi}{4}\right)\begin{bmatrix} c_{11} \\ c_{12} \end{bmatrix}$$
$$\Rightarrow \quad c_{11} + \frac{\pi}{4}c_{12} = \left(1-\frac{\pi}{4}\right)c_{11} \quad \Rightarrow \qquad c_{12} = -c_{11} \tag{30}$$

The last line just gives the first row of the matrix equation. The second row gives a redundant equation to the first row. A satisfactory normalized choice is $c_{11} = -c_{12} = \frac{1}{\sqrt{2}}$. So the zeroth order eigenvector with energy E_{21} is

$$\left|\varphi_{21}^{(0)}\right\rangle = c_{11}\left|\tilde{\psi}_{21}^{(0)}\right\rangle + c_{12}\left|\tilde{\psi}_{22}^{(0)}\right\rangle = \frac{1}{\sqrt{2}}\left|\psi_{01}^{(0)}\right\rangle - \frac{1}{\sqrt{2}}\left|\psi_{10}^{(0)}\right\rangle \tag{31}$$

The normalized wavefunction for this state is

$$\varphi_{21}^{(0)}(x,y)\frac{1}{\sqrt{2}}\left(\psi_{01}^{(0)}(x,y) - \psi_{10}^{(0)}(x,y)\right) = \left(\frac{1}{\pi x_0^2}\right)^{1/2} e^{-\frac{x^2}{2x_0^2}} e^{-\frac{y^2}{2x_0^2}} \left(\frac{y}{x_0} - \frac{x}{x_0}\right) \tag{32}$$

We can repeat this for $i = 2$:

$$H'\left|\varphi_{22}^{(0)}\right\rangle = E_{22}^{(1)}\left|\varphi_{22}^{(0)}\right\rangle \qquad \Rightarrow \qquad \frac{V_0}{16\pi}\begin{bmatrix} 1 & \frac{\pi}{4} \\ \frac{\pi}{4} & 1 \end{bmatrix}\begin{bmatrix} c_{21} \\ c_{22} \end{bmatrix} = \frac{V_0}{16\pi}\left(1+\frac{\pi}{4}\right)\begin{bmatrix} c_{21} \\ c_{22} \end{bmatrix}$$
$$\Rightarrow c_{21} + \frac{\pi}{4}c_{22} = \left(1+\frac{\pi}{4}\right)c_{21} \quad \Rightarrow \qquad c_{22} = c_{21} \tag{33}$$

(Ditto about the first and second row of this matrix equation.) A satisfactory normalized choice is $c_{21} = c_{22} = \frac{1}{\sqrt{2}}$. So the zeroth order eigenvector with energy E_{21} is

$$\left|\varphi_{22}^{(0)}\right\rangle = c_{21}\left|\tilde{\psi}_{21}^{(0)}\right\rangle + c_{22}\left|\tilde{\psi}_{22}^{(0)}\right\rangle = \frac{1}{\sqrt{2}}\left|\psi_{01}^{(0)}\right\rangle + \frac{1}{\sqrt{2}}\left|\psi_{10}^{(0)}\right\rangle \tag{34}$$

and the wavefunction for this state is

$$\varphi_{22}^{(0)}(x,y)\frac{1}{\sqrt{2}}\left(\psi_{01}^{(0)}(x,y) + \psi_{10}^{(0)}(x,y)\right) = \left(\frac{1}{\pi x_0^2}\right)^{1/2} e^{-\frac{x^2}{2x_0^2}} e^{-\frac{y^2}{2x_0^2}} \left(\frac{y}{x_0} + \frac{x}{x_0}\right) \tag{35}$$

These results are illustrated in Fig. 2.

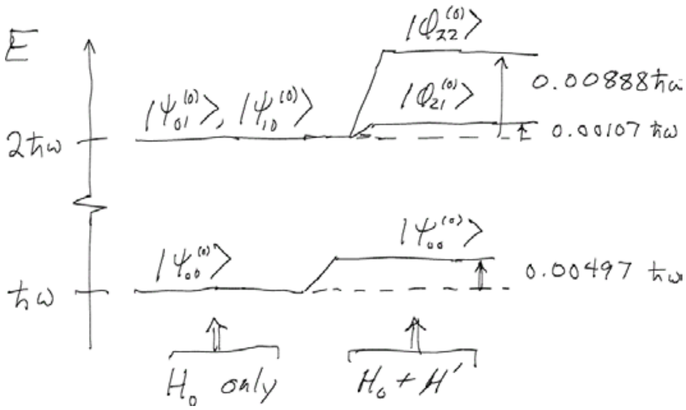


Fig. 2. Energy level diagram for the unperturbed (H_0 only) and perturbed $(H_0 + H')$ $n = 1$ and $n = 2$ levels.

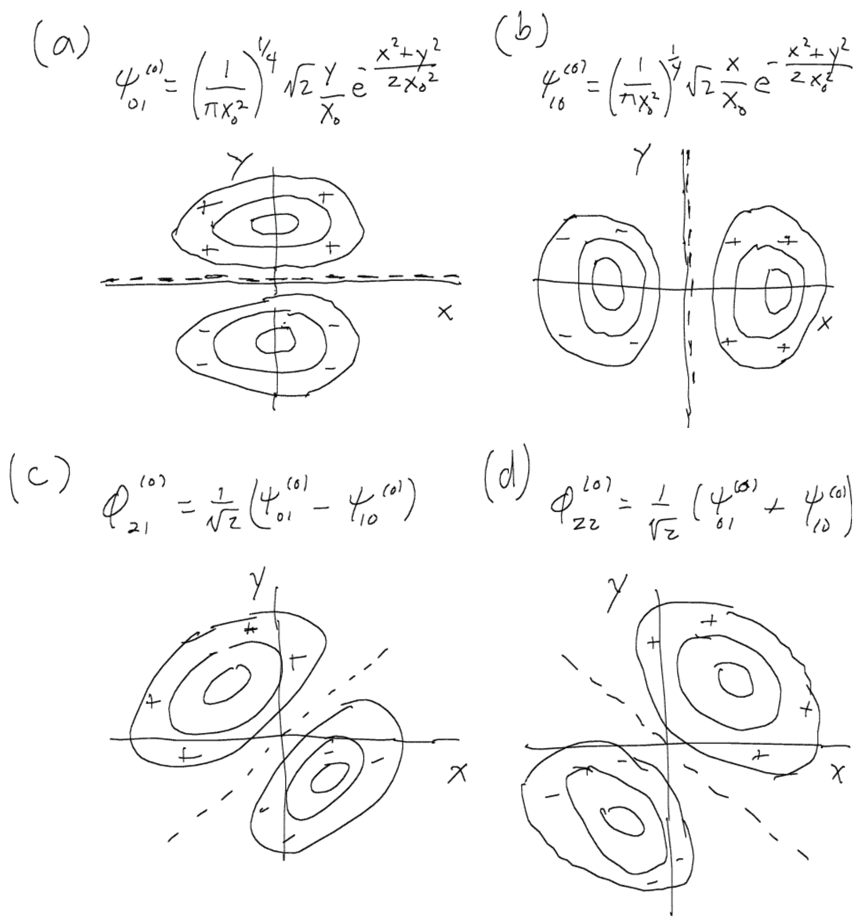


Fig. 3. (a), (b): Basis set wavefunctions in the $n = 2$ degenerate subspace.

(c), (d): zeroth-order $n = 2$ eigenfunctions of *H.*

The dashed lines represent nodal lines in the wavefunctions, and the signs denote signs of the wavefunction. The curves represent contours of constant probability amplitude.

c) Fig. 3 (a) and (b) show contour plots of the basis functions $\psi_{01}^{(0)}$ and $\psi_{10}^{(0)}$. Fig. 3 (c) and (d) show contour plots of the eigenfunctions $\varphi_{21}^{(0)}$ and $\varphi_{22}^{(0)}$. The lower energy state is $\varphi_{21}^{(0)} = \psi_{12}^{(0)} - \psi_{21}^{(0)}$. If we look at the plots, we see that the difference $\psi_{12}^{(0)} - \psi_{21}^{(0)}$ has destructive interference in upper right and lower left quadrants of the space, and constructive interference in the other two quadrants. This substantially lowers the probability density in the upper right quadrant. The perturbation to the energy is $H'(x,y)$, weighted by the probability density $\left|\varphi_{21}^{(0)}(x,y)\right|^2$. The only place where $H'(x,y)$ is non-zero is the upper right quadrant. Since $\left|\varphi_{21}^{(0)}(x,y)\right|^2$ is suppressed in this quadrant, the first-order perturbation to its energy is small.

The higher energy state is $\varphi_{22}^{(0)} = \psi_{12}^{(0)} + \psi_{21}^{(0)}$. For this state, the interference is constructive in the upper right and lower left quadrants, and destructive in the other two quadrants. This tends to substantially increase the probability density in the upper right quadrant where H' is non-zero, and to raise the energy.