Two electrons in a magnetic field[*]

The problem of two electrons interacting via their $1/r_{12}$ Coulomb potential in a constant magnetic field may be solved by a simple transformation of coordinates [Taut 1994]. Following Burke, the Hamiltonian for two electrons in a magnetic field is given by,

$$H = \sum_{i=1,2} \left\{ \frac{1}{2} \left(\vec{p}_i + \frac{1}{c} \vec{A}(\vec{r}_i) \right)^2 \right\} + \frac{1}{|\vec{r}_2 - \vec{r}_1|} \tag{1}$$

Using $\vec{A}(\vec{r}_i) = \frac{1}{2}(\vec{B} \times \vec{r}_i)$ with $\vec{B}$ constant and perpendicular to the $(\vec{r}_1, \vec{r}_2)$ plane, one obtains,

$$H = \sum_{i=1,2} \left\{ -\frac{1}{2}\nabla^2_{r_i} + \frac{1}{2} k r_i^2 \right\} + \frac{1}{|\vec{r}_2 - \vec{r}_1|} \tag{2}$$

where $k = B^2/4c^2$. This is of the form of a Hamiltonian for two interacting electrons connected to an infinite mass by springs with the same spring constant k.

Analytic solutions may be found by using the simple transformation $\vec{R} = (\vec{r}_1 + \vec{r}_2)/2$ and $\vec{u} = \vec{r}_2 - \vec{r}_1$, whence,

$$\begin{aligned} H &= -\frac{1}{4}\nabla^2_R + kR^2 - \nabla^2_u + \frac{1}{4}ku^2 + \frac{1}{u} \\ &= H_R + H_u \end{aligned} \tag{3}$$

The wavefunction separates into a product of a three-dimensional oscillator in $\vec{R}$ (of mass 2 and spring constant $2k$) and a simple equation in $\vec{u}$:

$$\Psi(\vec{r}_1, \vec{r}_2) = \left(\frac{2\omega}{\pi}\right)^{3/4} \exp\left(-\omega R^2\right)\, \phi_0(\vec{u}) \tag{4}$$

where $\omega = \sqrt{k}$ is the Larmor frequency. Now $\phi_0(\vec{u})$ satisfies,

$$\left(-\nabla^2_u + \frac{1}{4}ku^2 + 1/u \right)\phi_0(\vec{u}) = \epsilon\phi_0(\vec{u}), \tag{5}$$

where the total energy $E = 3\omega/2 + \epsilon$. Equation (5) can easily be solved numerically [Laufer and Kreiger, 1986; Burke, 1996], but can also be solved analytically for certain discrete values of k.

To obtain an analytic solution, expand $\phi_0(\vec{u})$ as a power series in u times the gaussian decay due to the oscillator potential:

$$\phi_0(\vec{u}) = Y_{lm}(\Omega_u) \sum_{j=1}^{N} c_j u^j \exp(-u^2/2u_o^2), \tag{6}$$

where $u_o = \sqrt{2/\omega}$ is the length scale of the oscillator in the absence of the Coulomb repulsion, and Ω_u denotes the direction of $\vec{u}$. Insertion of this form into Eq. (5) yields a double recursive series for the coefficients c_j which terminates at finite j only for certain values of k [Taut, 1994]. For $l = 0$, the first few values are $k = \infty$ (the independent electron limit), $k = 1/4$, and $k = 1/100$, with energies $\epsilon = 3\omega/2, 5/4, 7/20$, for $N = 0, 1, 2$, respectively. For these values of k, the wavefunction may be written analytically e.g., for $k = 1/4$ [Kais et al., 1989],

$$\phi_0(u) = \frac{(1 + u/2)\exp(-u^2/8)}{\sqrt{4\pi(5\sqrt{\pi} + 8)}}. \tag{7}$$

This 'Hooke's law atom' has been used to study the Coulomb cusp condition on the ground state two electron wavefunction at $\vec{r}_1 = \vec{r}_2$ [Burke et al., 1994], the "pair" Wigner crystal in solid state physics [Taut, 1994a], as a test of density functional approximations to the ground-state energy of electronic systems [Filippi et al., 1994] and as a pedagogic tool for illustrating concepts of conditional probability densities [Burke et al., 1995].

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