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,

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

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,

$$H = \sum_{i=1,2} \left\{ -\frac{1}{2} \nabla^2_{\vec{r}_i} + \frac{1}{2} kr_i^2 \right\} + \frac{1}{|\vec{r}_2 - \vec{r}_1|} \quad (2)$$

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,

$$H = -\frac{1}{4} \nabla^2_{\vec{R}} + kR^2 - \nabla^2_{\vec{u}} + \frac{1}{4} ku^2 + \frac{1}{u} = H_{\vec{R}} + H_{\vec{u}} \quad (3)$$

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 $\vec{u}$:

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

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

$$(- \nabla^2_{\vec{u}} + \frac{1}{4} ku^2 + 1/u)\phi_0(\vec{u}) = \epsilon \phi_0(\vec{u}),$$

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 $k$. 

1
To obtain an analytic solution, expand \( \phi_0(\mathbf{u}) \) as a power series in \( u \) times the gaussian decay due to the oscillator potential:

\[
\phi_0(\mathbf{u}) = Y_{lm}(\Omega_u) \sum_{j=1}^{N} c_j u^j \exp(-u^2/2u_o^2),
\]

where \( u_o = \sqrt{2/\omega} \) is the length scale of the oscillator in the absence of the Coulomb repulsion, and \( \Omega_u \) denotes the direction of \( \mathbf{u} \). 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],

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

This ‘Hooke’s law atom’ has been used to study the Coulomb cusp condition on the ground state two electron wavefunction at \( \mathbf{r}_1 = \mathbf{r}_2 \) [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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