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a = 72973525376 * 10 ^ -13; M = 510998910 / 1000; k = 1;

H[u_] := Simplify[M * {-(Z * a / r + 2) * u[[1]] - (k / r * u[[2]] + D[u[[2]], r]),
    -k / r * u[[1]] + D[u[[1]], r] + Z * a / r * u[[2]]}];

En[n_] := M * (1 - 1 / Sqrt[1 + (Z * a / (n - Abs[k] + Sqrt[k ^ 2 - (Z * a) ^ 2])) ^ 2]);
Table[N[En[i]], {i, 4}]

{13.6059, 3.40148, 1.51176, 0.850365}

Table[Z * a / (n - Abs[k] + Sqrt[k ^ 2 - (Z * a) ^ 2]), {n, 4}] // N

{0.00729755, 0.00364872, 0.00243247, 0.00182435}

Sqrt[k ^ 2 - (Z * a) ^ 2] // N

0.999973

ClearAll[e, g, f, h, p];
h := Exp[-729755 * 10 ^ -8 * r]; f := {1, 1} * h * r ^ 6;
n = 5; e = Table[0, {j, n + 1}, {k, n + 1}];

i = 1;
g[1] = f / Sqrt[Integrate[f.f, {r, 0, Infinity}]];
p = H[g[1]];
e[[1, 1]] = Integrate[p.g[1], {r, 0, Infinity}];
e[[2, 1]] = Sqrt[Integrate[p.p, {r, 0, Infinity}]] - e[[1, 1]] ^ 2;
g[2] = Simplify[(p - g[1] * e[[1, 1]]) / e[[2, 1]]];

While[i < n, i++;
    p = Simplify[H[g[2]] / h] * h;
    e[[i, i]] = Integrate[p.g[2], {r, 0, Infinity}]; p = Simplify[H[g[2]] / h] * h;
    e[[i, i]] = Integrate[Simplify[Collect[p.g[2] / h ^ 2, r]] * h ^ 2, {r, 0, Infinity}];
    e[[i + 1, i]] = Sqrt[Integrate[Simplify[Collect[p.p / h ^ 2, r]] * h ^ 2, {r, 0, Infinity}]] -
        e[[i, i]] ^ 2 - e[[i, i - 1]] ^ 2;
    g[3] = Simplify[Collect[(p - e[[i, i]] * g[2] - e[[i, i - 1]] * g[1]) / e[[i + 1, i]] / h,
        r]] * h;
    g[1] = g[2]; g[2] = g[3];]

e[[n + 1, n + 1]] = Integrate[Collect[H[g[3]].g[3] / h ^ 2, r] * h ^ 2, {r, 0, Infinity}];

e + Transpose[e] - DiagonalMatrix[Diagonal[e]] // MatrixForm // N

$$\begin{pmatrix} -511620. & 511005. & 0. & 0. & 0. & 0. \\ 511005. & -510377. & 5.1339 & 0. & 0. & 0. \\ 0. & 5.1339 & -462299. & 508687. & 0. & 0. \\ 0. & 0. & 508687. & -559699. & 25.3547 & 0. \\ 0. & 0. & 0. & 25.3547 & -433478. & 505139.7807304210 \\ 0. & 0. & 0. & 0. & 505139.7807304210 & -588520. \end{pmatrix}$$


Eigenvalues[%]

{-1.02201 × 106, -1.022 × 106, -1.022 × 106, 17.3164, 5.65015, 2.9763}

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**Eigenvalues [%]**

$\{-1.02206 \times 10^6, -1.02201 \times 10^6, -1.022 \times 10^6, 58.0108, 11.7053, 5.29056\}$