Temperature-modified Coulomb potential for the electron–proton system

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Abstract. The finite-temperature Schrödinger equation, derived recently from the Bethe-Salpeter equation for the bound states of an electron and a proton interacting via the instantaneous Coulomb interaction, is studied in the coordinate space. An expression for the temperature-modified Coulomb potential is obtained and briefly discussed.

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The Bethe-Salpeter equation for the Wick-Cutkosky model (Wick 1954; Cutkosky 1954) in the instantaneous approximation was recently generalized to arbitrary temperatures, and was shown to possess temperature-dependent discrete spectra in the large-temperature limit (Malik and Pande 1988). This motivated us to carry out a similar investigation for the electron–proton bound state system interacting via the instantaneous Coulomb interaction. The finite temperature Bethe-Salpeter equation (FTBSE) so obtained is, however, very difficult to handle, but can be reduced, in a non-relativistic approximation, to a finite temperature Schrödinger equation (FTSE). Using momentum space methods, we have shown that the latter equation possesses solutions which seem to be of great relevance to X-ray astronomy (Malik et al 1988—MPVI hereafter). The purpose of this note is to study the same FTSE in coordinate space and obtain an expression for the temperature-modified Coulomb potential which governs its spectra.

The FTBSE for the electron–proton bound state system is (MPVI):

\[ S_{ij}(p) = \frac{e^2}{4\pi^2} \Lambda_j^a(p) \Lambda_i^b(p) \int \frac{d^3q}{(q-p)^2} \sum_{k,l} S_{kl}(q) \times \frac{(\tanh A_k + \tanh B_j)}{[E - E^*_j(q) - E_i^*(q)]}, \]

where \( i, j, k \) and \( l \) take on values + or − and \( \Lambda_\pm \) are the usual positive and negative energy projection operators given by

\[ \Lambda_\pm^a(p) = [E^{a,b}(p) \pm H^{a,b}(p)]/2E^{a,b}(p), \]
with
\[ \pm E^{a,b}(p) = E_\pm^{a,b}(p) = \pm\left(p^2 + m^2_{a,b}\right)^{1/2}, \]
\[ H^{a,b}(p) = (m_{a,b} \alpha^{a,b} \pm p \alpha^{a,b}), \]
where \( \alpha \) and \( \beta \) are the standard Dirac matrices, associated with the electron if they carry the superscript \( a \) and with the proton if they carry the superscript \( b \). The positive sign in (4) goes with \( a \) and the negative sign with \( b \). \( m_a \) and \( m_b \) are, respectively, the masses of the electron and the proton and \( p \) is their relative three-momentum. \( E \) represents the energy eigenvalue of (1). The functions \( A_\pm \) and \( B_\pm \) are given by
\[ A_\pm = (1/2)\beta[\mu_a E - E_\pm^a(p)], \]
\[ B_\pm = (1/2)\beta[\mu_b E - E_\pm^b(p)], \]
with
\[ \mu_{a,b} = m_{a,b} / (m_a + m_b) \]
and
\[ \beta = 1/kT, \]
where \( T \) is temperature and \( k \) the Boltzmann constant; \( \hbar = c = 1 \).

If we now neglect spin and negative energy components, only an approximated version, say \( S_+^0 \), of the function \( S_+ \) will survive in (1). In terms of a function \( S(p) \) defined by
\[ S(p) = \tanh A_+ + \tanh B_+ \]
\[ \frac{e^2}{4\pi^2} \cdot Q_\beta(W, p^2) \frac{d^3p}{(q - p)^2} S(q), \]
the equation can then be written as
\[ \left( W - \frac{p^2}{2\mu} \right) S(p) = \frac{e^2}{4\pi^2} \cdot Q_\beta(W, p^2) \frac{d^3p}{(q - p)^2} S(q). \]

Note that simultaneous with the neglect of spin etc., we have introduced the appropriate non-relativistic kinematics:
\[ E - E^a(p) - E^b(p) \simeq W - (p^2/2\mu), \]
\[ W \equiv -|W| = E - m_a - m_b, \]
where
\[ \mu = m_a m_b / (m_a + m_b) \]
and
\[ \tanh A_+ + \tanh B_+ \]
\[ \simeq \tanh\left( \frac{1}{2}\beta\mu_a W - \frac{\beta p^2}{4m_a} \right) + \tanh\left( \frac{1}{2}\beta\mu_b W - \frac{\beta p^2}{4m_b} \right) \]
\[ = Q_\beta(W, p^2). \]

For zero temperature, \( Q_\beta(W, p^2) = -2 \). Equation (10) then reduces to the normal
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Schrödinger equation. We now write

\[ Q_\beta(W, p^2) = \frac{\tanh\left(\frac{\beta \mu_a W}{2}\right) - \tanh\left(\frac{p^2 \beta}{4m_a}\right)}{1 - \tanh\left(\frac{\beta \mu_a W}{2}\right) \tanh\left(\frac{\beta p^2}{4m_a}\right)} \]

+ \frac{\tanh\left(\frac{\beta \mu_b W}{2}\right) - \tanh\left(\frac{p^2 \beta}{4m_b}\right)}{1 - \tanh\left(\frac{\beta \mu_b W}{2}\right) \tanh\left(\frac{p^2 \beta}{4m_b}\right)} \quad (15) \]

and make the approximation

\[ \tanh\left(\frac{\beta p^2}{4m_{a,b}}\right) \approx \frac{p^2 \beta}{4m_{a,b}}; \quad (16) \]

such an approximation is in keeping with the spirit of (10). We thus get

\[ Q_\beta(W, p^2) \equiv \frac{(d_1 - d_2 p^2)/(1 - d_3 p^2)}{1 - d_3 p^2}, \quad (17) \]

where

\[ d_1 = a + b; \quad d_2 = \frac{\beta}{4 \mu}(1 + ab); \quad d_3 = \frac{\beta}{4}\left(\frac{a}{m_a} + \frac{b}{m_b}\right) \]

and

\[ a = \tanh\left(\frac{1}{2}(\beta \mu_a W)\right); \quad b = \tanh\left(\frac{1}{2}(\beta \mu_b W)\right). \quad (18) \]

We now write

\[ \tilde{Q}(W, p^2) = D_1 + \frac{D_2 D_3}{D_2 + p^2}; \quad (19) \]

where

\[ D_1 = d_2/d_3; \quad D_2 = -1/d_3; \quad D_3 = [d_1 - (d_2/d_3)] \quad (20) \]

and consider (10) with \( Q_\beta(W, p^2) \) replaced by \( \tilde{Q}_\beta(W, p^2) \) as given in (19). We obtain

\[ \left( W - \frac{p^2}{2\mu} \right) \psi(p) = \frac{e^2}{4\pi^2} D_1 \int \frac{d^3q \psi(q)}{(q - p)^2} \]

\[ + \frac{e^2 D_2 D_3}{4\pi^2} \int \frac{d^3q \psi(q)}{(q - p)^2 (q^2 + D_2)} \quad (21) \]

\[ \equiv T_1 + T_2, \]

where \( \psi(p) \) is related to \( S(p) \) through

\[ \psi(p) = [\tilde{Q}_\beta(W, p^2)]^{-1} S(p). \quad (22) \]

To investigate (21) in coordinate space, let \( u(r) \) be the fourier transform (FT) of \( \psi(p) \),
i.e.,
\[ u(r) = \frac{1}{(2\pi)^{3/2}} \int d^3 p \exp(-ip \cdot r)\psi(p) \]  
(23)
and
\[ \psi(p) = \frac{1}{(2\pi)^{3/2}} \int d^3 r \exp(ip \cdot r)u(r). \]  
(24)

We now take the FT of (21). The FT of the term on the left hand side is trivial to calculate. To calculate the FT on the right hand side, we note that the functions \( \exp(-mr^2) \) and \( (4\pi)(2\pi)^{-3/2}(p^2 + m^2)^{-1} \) form a FT pair, where \( r = |r| \). For the case of the Coulomb potential, we simply put \( m = 0 \). Thus,

\[ T_1 \to e^{2D_1} \frac{1}{4\pi^2} \frac{1}{(2\pi)^{3/2}} \int d^3 q \psi(q) \cdot \frac{\exp(-ip \cdot r) d^3 p}{(q - p)^2} \]
\[ = e^{2D_1} \frac{1}{4\pi^2} \frac{1}{(2\pi)^{3/2}} \int d^3 q \exp(iq \cdot r)\psi(q) \cdot \int \frac{\exp(-ip \cdot r) d^3 p'}{p'^2} \]
\[ = e^{2D_1} \frac{2\pi^2}{4\pi^2} \frac{1}{r} \frac{1}{(2\pi)^{3/2}} \int d^3 q \exp(-iq \cdot r)\psi(q) \]
\[ = e^{2D_1} \frac{2\pi^2}{2r} u(r); \]

\[ T_2 \to e^{2D_2D_3} \frac{1}{4\pi^2} \frac{1}{(2\pi)^{3/2}} \int d^3 q \psi(q) \cdot \int \frac{\exp(-ip \cdot r) d^3 p}{(q^2 + D_2)} \]
\[ = e^{2D_2D_3} \frac{2\pi^2}{4\pi^2} \frac{1}{r} \frac{1}{(2\pi)^{3/2}} \int d^3 q \exp(-iq \cdot r)\psi(q) \cdot \frac{1}{(q^2 + D_2)} \]
\[ = e^{2D_2D_3} \frac{2\pi^2}{2r} \frac{1}{4\pi^2} \cdot \int d^3 r' u(r - r')\exp(-\sqrt{D_2}r')/r', \]

where in the last step we have used the convolution theorem for FTs. In coordinate space, (21) may therefore be written as

\[ \left( W + \frac{1}{2\mu} \nabla^2 \right) u(r) = \frac{e^{2D_1}}{2r} u(r) + \frac{e^{2D_2D_3}}{8\pi r} \]
\[ \times \int d^3 r' [\exp(-\sqrt{D_2}r')/r'] u(r - r'). \]  
(25)

Equation (25) shows how, for the bound state problem, the Coulomb potential gets modified by temperature. In addition to an attractive Coulomb term whose coupling is \( (e^{2D_1}/2) \)—note that \( D_1 \) is always negative, we now have another \( (1/r) \)-type term. The latter term involves an integration of a Yukawa-like term over the space of the wavefunction. The characteristic energy of the associated Yukawa particle, a phonon, is given by \( (D_2)^{1/2} \). It may be noted that the \( T \to 0 \) limit of (25) yields the equation for the normal hydrogen; this is either fortuitous (because the equation was obtained after the approximation in (16) had been made), or it tells us that \( p^2 \to 0 \) faster than \( T \to 0 \).
Further insight into the structure of (25) can be obtained by directly solving it. This will not be attempted here. An alternative method consists of using the information obtained from the solutions of the corresponding equation in momentum space. The details of such solutions have been reported in MPVI. We note here that:

(i) The sign of \( D_2D_3 \) as well as the overall sign of the second term on the right side of (25) is always positive. This term therefore causes repulsion.

(ii) The system has an infinite number of energy levels for each value of the angular momentum, \( l \). Let these levels be labelled as \( E_{nl} \). It is seen that—refer to table 1, which corresponds to \( T = 1.6 \times 10^6 \) K and is reproduced from MPVI—the energy levels become degenerate for large \( n \) and/or large \( l \). We then have the constraint \( n \geq l \) and essentially a \( l/n^2 \)-pattern for the eigenvalues. For such a situation, (25) may be written as

\[
\left( W - \frac{p^2}{2\mu} \right) u(r) = \left( -\frac{e_{\text{eff}}^2}{r} \right) u(r),
\]

where

\[
-\frac{e_{\text{eff}}^2}{r} = e^2 \left( \frac{1}{2}D_1 + \frac{1}{2}D_2D_3X \right),
\]

which follows by writing the integral on the right side of (25) as

\[
\int d^3r' \left[ \exp \left( -D_2r'/r' \right) \right] u(r - r') \approx 4\pi X u(r).
\]

The energy levels \( E_{nl} \equiv E_n \) of (26) are given by

\[
E_n = -\frac{1}{\mu} \left( e_{\text{eff}}^2/n^2 \right).
\]

For \( E_{15,0} = 13.893 \),

\[
e_{\text{eff}}^2 \approx 0.1106396.
\]

\[e_{\text{eff}}^2\]

\[E_n = -\frac{1}{2\mu} \left( e_{\text{eff}}^2/n^2 \right).
\]

\begin{table}[h]
\centering
\begin{tabular}{cccc}
\hline
\textbf{n} & \textbf{E_{n0}(eV)} & \textbf{E_{n1}} & \textbf{E_{n2}} & \textbf{E_{n3}} \\
\hline
1 & 4333.555 & & & \\
2 & 1178.483 & 1244.684 & & \\
3 & 432.737 & 438.005 & 439.645 & \\
4 & 211.778 & 212.143 & 212.240 & 212.282 \\
5 & 129.295 & 129.341 & 129.352 & 129.357 \\
6 & 88.233 & 88.242 & 88.244 & 88.245 \\
7 & 64.336 & 64.338 & 64.339 & 64.339 \\
8 & 49.076 & 49.077 & 49.077 & 49.077 \\
9 & 38.700 & 38.700 & 38.701 & 38.701 \\
10 & 31.312 & 31.312 & 31.312 & 31.312 \\
14 & 15.950 & 15.950 & 15.950 & 15.950 \\
\hline
\end{tabular}
\caption{Energy eigenvalues, \( E_{n0} \), of equation (10) at \( 1.6 \times 10^6 \) K (for details, MPVI).
\centering
\end{table}
For any degenerate eigenvalue of table 1, we may now calculate the quantity $X$ occurring in (27). Our results are given in table 2. We also give, in this table, the values of the terms $D_1$ and $D_2D_3X$. These values show that both the terms on the right side of (25) are equally important.

Unfortunately, at this stage, we are not able to give an estimate of the integral in (25) for energy levels which do not follow an effective Coulomb pattern. This aspect and the other ramifications of temperature-dependent approach to explain the discrete spectra of hot plasmas are currently under investigation.

**References**

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