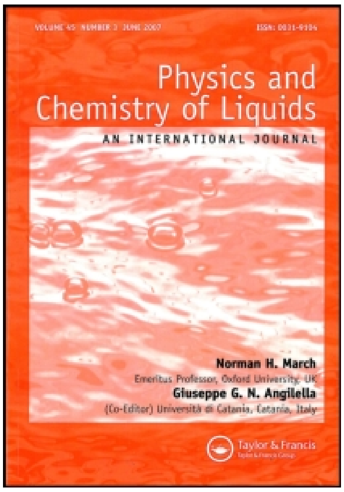

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Asymptotic Behaviour of the Pauli Potential for a Perfectly Screened Charge embedded in an Almost Degenerate Dense Plasma

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LETTER

Asymptotic Behaviour of the Pauli Potential for a Perfectly Screened Charge embedded in an Almost Degenerate Dense Plasma

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The asymptotic behaviour of the Pauli potential is established at zero and elevated temperatures for a perfectly screened charge embedded in jellium.

KEY WORDS: Electron liquid, occupation numbers, Pauli potential.

There are several ways to tackle the many-electron problem, the density functional theory providing one of the most compact of these. By virtue of the Slater–Kohn–Sham approach to density functional theory, the many-electron problem can be reduced to a set of one-electron Schrödinger equations. It has turned out that a further simplification can be achieved, at least in principle, namely the square root of the electron density $\rho(\mathbf{r})$, referred to below as the density amplitude, satisfies a Schrodinger equation having a "correction" term called the Pauli potential in addition to the Slater–Kohn–Sham one-body potential $V(\mathbf{r})$. Knowledge of the Pauli potential, in addition to $V(\mathbf{r})$, would allow the many-electron problem to be reduced to the solution of a single equation for the density amplitude $\rho(\mathbf{r})^{1/2}$. Consequently, studies to clarify the behaviour of the Pauli potential are of obvious importance. The exact form of this potential seems presently to be known only for two- and three- level atoms and ions. In addition, several exact properties of the Pauli potential have been derived. Here the asymptotic behaviour of the Pauli potential is studied for a perfectly screened charge embedded in the simplest electron liquid, namely jellium.

From the work of Blandin *et al.*[1], and the independent later studies of March and Murray[2] it is known that the charge $\Delta\rho(\mathbf{r})$ displaced around such a perfectly screened charge embedded in jellium of mean density ρ_0 has the form, with k_f the Fermi wave number:

$$\Delta\rho(\mathbf{r}) = \rho(\mathbf{r}) - \rho_0 = A\,\frac{\cos(2k_f r + \phi)}{r^3}: \rho_0 = \frac{k_f^3}{3\pi^2}. \tag{1}$$

We have recently studied the Pauli potential[3] for Be, C and other first row atomic ions in free space[4]. Here, our aim is to calculate the asumptotic form of the Pauli potential for an atom or ion which is perfectly screened as in Eq. (1) in jellium.

In Ref. 3, the Pauli potential was defined through

$$\Delta\psi + \frac{2m}{\hbar^2}[\varepsilon - V - V_{\text{Pauli}}]\psi = 0: \psi = \rho^{1/2} \tag{2}$$

where V is the customary one-body potential of density functional theory introduced above. Here, our object is to point out that the form (1) yields an explicit asymptotic expression for the total potential $\mathscr{V}(\mathbf{r}) = V + V_{\text{Pauli}}$ in Eq. (2).

From Eq. (1), the asymptotic form of the density amplitude $\psi = \rho^{1/2}$ is readily written as

$$\psi = \rho_0^{1/2} + \frac{1}{2}\frac{A}{\rho_0^{1/2}}\frac{\cos(2k_f r + \phi)}{r^3} + \cdots \tag{3}$$

From Eq. (2) in the form (with $\mathscr{V}(\mathbf{r})$ written for $V(\mathbf{r}) + V_{\text{Pauli}}(\mathbf{r})$)

$$\mathscr{V}(\mathbf{r}) - \varepsilon = \frac{1}{\psi}\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d\psi}{dr}\right) \tag{4}$$

one obtains the asymptotic large r result

$$\mathscr{V}(\mathbf{r}) - \varepsilon \sim \frac{-\hbar^2 k_f^2}{m\rho_0}\Delta\rho(\mathbf{r}) = -2E_f\frac{\Delta\rho(\mathbf{r})}{\rho_0} \tag{5}$$

with E_f denoting the Fermi energy.

The final comment to be made on this ground-state calculation, beyond the fact that $\mathscr{V}(\mathbf{r}) - \varepsilon$ "follows" the displaced charge $\Delta\rho(\mathbf{r})$ at sufficiently large r is that, for a given one-body potential $V(r)$ which is analytic at the Fermi sphere diameter $2k_f$, the amplitude A and the phase ϕ in Eq. (1) are determined[1,5,6] solely by the phase shifts η_1 of the partial waves at the Fermi surface caused by scattering off $V(r)$. The expressions are:

$$A = \left(\frac{1}{2\pi^2}\right)\left(\left\{\sum_l (2l+1)[-\sin\eta_l\cos(\eta_l - l\pi)]\right\}^2 + \left\{\sum_l (2l+1)[-\sin\eta_l\sin(\eta_l - l\pi]\right\}^2\right)^{1/2} \tag{6}$$

and

$$\phi = \tan^{-1}\frac{\sum_l (2l+1)\sin\eta_l\cos(\eta_l - l\pi)}{\sum_l (2l+1)\sin\eta_l\sin(\eta_l - l\pi)}. \tag{7}$$

For given $V(r)$, standard methods can, of course, be used to calculate the phase shifts η_l at the Fermi level in Eqs (6) and (7) and hence $\Delta\rho(\mathbf{r})$ at large r from Eq. (1). Subtraction of $V(r)$ from $\mathscr{V}(\mathbf{r})$ in Eq. (5) evidently suffices to determine the Pauli potential asymptotically at large r.

Let us turn now to discuss the same problem at elevated temperatures. Following earlier work especially on the non-degenerate limit[7] appropriate to the screening of ionized impurities in semiconductors[8,9], Flynn and Odle[10] have shown that at large distances and moderate temperatures the density decay contains a factor

$$(\pi k_f k_B T/2E_f)\ \mathrm{csch}\ [(\pi k_B T/E_f)k_f r] \tag{8}$$

and reduces at zero temperature to the asymptotic form (1).

Using a generalization to arbitrary occupation numbers similar to that in our earlier work on first row isolated atoms and ions[4], the corresponding form of the Pauli Potential is readily found to be

$$-\frac{k_f}{\pi\rho_0} k_B T A(k_f)\ \mathrm{csch}\left\{\left(\frac{\pi k_B T}{E_f}\right)k_f r\right\} \frac{\cos(2k_f r + \phi)}{r^2} = -2E_f \frac{\Delta\rho(\mathbf{r})}{\rho_0} \tag{9}$$

which is to be compared with Eq. (5) valid at $T = 0$.

Equation (5), when combined with Eqs (1), (6) and (7) at $T = 0$, and Eq. (9) at elevated temperatures, constitute the main results of the present work for the asymptotic properties of the Pauli potential.

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