Dislocation-Mediated Melting:  
The One-Component Plasma Limit

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Abstract

The melting parameter $\Gamma_m$ of a classical one-component plasma is estimated using a relation between melting temperature, density, shear modulus, and crystal coordination number that follows from our model of dislocation-mediated melting. We obtain $\Gamma_m = 172 \pm 35$, in good agreement with the results of numerous Monte-Carlo calculations.

Key words: melting, dislocation, one-component plasma, Monte-Carlo simulations  
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1 Introduction

The classical one-component plasma (OCP) is an idealized system of mobile ions of charge $Ze$, number density $n$, and temperature $T$, immersed in a neutralizing background of uniform charge density $-Zne$. The OCP is realized in nature only at the enormous densities occurring in white dwarfs and neutron stars. The thermodynamics of the classical OCP is completely described in terms of the dimensionless coupling parameter [1]

$$\Gamma = \frac{(Ze)^2}{ak_B T},$$  \hfill (1)

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where \( a = (3/4\pi n)^{1/3} \) is the Wigner-Seitz radius. In the quantum regime, one more parameter, \( a \) or \( T \), is needed to characterize the system. Melting of a classical OCP occurs at a fixed value, \( \Gamma_m \), of the plasma coupling parameter. When \( \Gamma > \Gamma_m \), a OCP is either a glass \([2]\), or it has a bcc crystal structure provided that it is subject to only hydrostatic stress. The evaluation of \( \Gamma_m \) for melting from the bcc structure has been the subject of extensive Monte Carlo (MC) calculations \([3-16]\) employing the Ewald potential, which yields data pertinent to an infinite system from simulations using only a finite number of particles confined to a cubic computational cell with periodic boundary conditions. By fitting simple functional forms, guided by theory, to the measured excess potential energy per particle for both liquid and solid phases of the OCP, it is possible to obtain the Helmholtz free energy as a function of \( \Gamma \). The intersection of the liquid and solid free-energy curves gives the value of the melting parameter \( \Gamma_m \). In their pioneering study \([3]\), Brush, Sahlin and Teller observed melting in a 32-particle system at \( \Gamma_m \approx 125 \). Subsequently Hansen \([4]\) and Pollock and Hansen \([5]\) followed with an improved calculation and found \( \Gamma_m = 155 \pm 10 \). Van Horn \([6]\) used the empirical Lindemann melting criterion to obtain \( \Gamma_m = 170 \pm 10 \). Other MC studies resulted in the following values of \( \Gamma_m \): 144 \([7]\), 168 \( \pm 4 \) \([8]\), 178 \( \pm 1 \) \([9]\), 180 \( \pm 1 \) \([10]\), 172 \([11]\), and 173 \([12]\). Values of very similar magnitude have been obtained in MC simulations of a strongly-coupled screened-Coulomb (Yukawa) system in the limit of zero screening: 171 \([14]\) and 171.8 \([15]\). Recent path-integral MC simulations of the OCP \([16]\) give \( \Gamma_m = 175 \). Hence, numerous MC studies suggest that \( \Gamma_m \approx 170 – 180 \) for the classical bcc OCP.

In this paper we calculate \( \Gamma_m \) using a melting relation obtained from our model of dislocation-mediated melting \([17, 18]\). Before proceeding with the calculation of \( \Gamma_m \), we briefly recapitulate the main ideas and assumptions of our melting model. As first proposed by Mott \([19]\), dislocations are assumed to be the basic degrees of freedom underlying the melting transition. Dislocation interactions beyond a distance of order the mean dislocation separation are assumed negligible because of screening, and steric interactions are ignored. Accordingly, dislocations are taken to be non-interacting and therefore uncorrelated, and are modeled as lines lying along the nearest-neighbor links of the lattice. The links coincide with the shortest perfect-dislocation Burgers vectors, which have magnitude \( b \). The dislocation configurations (Brownian, self-avoiding, open, closed, etc.) are parametrized by a single parameter \( q > 1 \), in terms of which the mean dislocation length is given by \( \langle L \rangle = 4qb/(q – 1) \). In addition to \( q \), the partition function depends on the temperature-dependent effective dislocation line tension, that is, the energy cost to create unit length of dislocation at temperature \( T \). The effective line tension vanishes at the critical temperature \( k_B T_{cr} = \sigma b/\ln(z – 1) \). Here \( z \) is the coordination number of the lattice and \( \sigma \), which we discuss in more detail below, is the \( \rho \)-dependent self-energy per unit length, \( \rho \) being the dislocation density. Dislocations proliferate as \( T_{cr} \) is approached from below, while at temperatures just above \( T_{cr} \) the partition function diverges, an indication that a new phase appears. So \( T_{cr} \) corresponds to a phase transition, namely melting, and we identify \( T_{cr} \) with the melting temperature, \( T_m \). A full defect theory of melting, a version of which is presently available \([20]\), would have to include the effects of both dislocations and disclinations. In our model we ignore the effects of disclinations under the assumption that they will produce only small changes of the order of 10% to the
melting temperature.

Under the assumption that dislocation strain fields are screened away at distances beyond the mean interdislocation spacing, the self-energy per unit length is given by

\[ \sigma = \frac{1 - \nu/2}{1 - \nu} \frac{Gb^2}{4\pi} \ln \left( \frac{\alpha R}{b} \right) = \frac{1 - \nu/2}{1 - \nu} \frac{Gb^2}{8\pi} \ln \left( \frac{\alpha^2}{4b^2 \rho} \right), \]

(2)

where \( 2R \approx 1/\sqrt{\rho} \) is the mean distance between dislocations, \( \nu \) is the Poisson ratio, \( G \) is the shear modulus and \( \alpha \) accounts for non-linear effects in the dislocation core. Many authors have successfully used this \( \ln(1/\rho) \) form for \( \sigma \), so we chose it as well, even though it has not been thoroughly investigated theoretically. Careful derivations have been carried out only for nearly parallel dislocations. However, the \( \ln(1/\rho) \) form is expected to hold in a three-dimensional ensemble of non-directed dislocations provided the mean dislocation length is much larger than the mean distance between dislocations, that is, \( \langle L \rangle \sqrt{\rho} \gg 1 \).

In our model the \( \ln(1/\rho) \) self-energy leads to a dislocation free energy

\[ F = -a_1 \rho \ln \rho - a_2 \rho - a_3 \rho^4, \]

and the \( \rho \ln \rho \) term results in a first-order melting transition.

We obtain the following melting relation:

\[ k_B T_m = \frac{1 - \nu/2}{1 - \nu} \frac{\lambda G(T_m)v_{WS}(T_m)}{8\pi \ln(z - 1)} \ln \left( \frac{\alpha^2}{4b^2 \rho(T_m)} \right). \]

(3)

Here \( v_{WS} \) is the Wigner-Seitz volume, \( \lambda \equiv b^3/v_{WS} \) is a geometric factor characterizing the lattice, and \( \rho(T_m) \) is the dislocation density at melt. Note that the factor \( \ln(z - 1) \) explicitly accounts for the influence of crystal structure on melting. This melting relation plus experimental data on over half the elements in the periodic table gives \( b^2 \rho(T_m) = 0.61 \pm 0.20 \).

In ref. we applied Eq. (3) to the zero-pressure elemental data for more than half of the periodic table and found that it is accurate to 17%. Here we investigate the validity of this relation in the OCP limit by using it to calculate the value of \( \Gamma_m \), which is then compared to the available MC data.

Calculation of \( \Gamma_m \) from Eq. (3) requires that we make the reasonable assumption that \( \alpha^2/b^2 \rho(T_m) \) is a pressure-independent constant. Then we can estimate this quantity for the OCP from zero-pressure data on the alkali metals. It is well known that the deviations of alkali-metal Fermi surfaces from perfect spheres are of order 1% or less, clear evidence that the valence electrons are very nearly free. In addition, the ratio of ionic radius to half the interatomic distance increases from 0.4 in Li to only 0.7 in Cs, hence the overlap between alkali ions is small, and so to a good approximation the ions are effectively point charges. With respect to many of its physical properties (third-order elastic constants are one exception), an alkali metal can be regarded as a bcc lattice of point positive ions in a uniform background of free electrons, i.e., a one-component plasma.

2 Analysis of alkali metal data

Let us first discuss the temperature dependencies of \( G \) and \( v_{WS} \), since their values to be used in Eq. (3) should be those at \( T = T_m \), not the measured values at room temperature.
### 3 OCP melting parameter $\Gamma_m$

We first consider the Poisson ratio in the OCP limit. In terms of $G$ and the bulk modulus, $B$, the Poisson ratio is given by [28]

$$\nu = \frac{3B - 2G}{2(3B + G)}. \quad (7)$$

We approximate $B^{\text{OCP}}$ by the bulk modulus of the electron gas since the negative electrostatic (Madelung) contribution never exceeds 10% of the bulk modulus of the gas. The variation of $B^{\text{OCP}}$ with density changes from a $n^{5/3}$ dependence in the non-relativistic case
to a $n^{4/3}$ dependence in the extreme relativistic limit, whereas the OCP shear modulus always varies as $n^{4/3}$. Hence, in a non-relativistic gas, $B/G \sim n^{1/3} \gg 1$, so $\nu \to 1/2$, as seen from Eq. (7). Although $B$ and $G$ both vary as $n^{4/3}$ in the extreme relativistic limit, we find $B/G \approx 1000 Z^{-2/3}$, so again $B/G \gg 1$ and $\nu \approx 1/2$.

Hence, as follows from Eqs. (1),(3) and (6) with $\nu = 1/2$, the OCP melting parameter is given by
\[ \Gamma_m = (0.385 \pm 0.052) 8\pi \ln 7 \frac{2}{3} \frac{(2\pi/3)^{1/3}(Ze)^2 n^{4/3}}{G_{\text{OCP}}(\Gamma_m)}, \]  
where we have used $v_{WS} = 1/n$.

The bcc OCP elastic constants were recently obtained by Ogata and Ichimaru, using MC simulations [29], as functions of $\Gamma$. However, the formula for the effective shear modulus used in ref. [29],
\[ G_{\text{eff}} = \frac{c_{11} - c_{12} + 3c_{44}}{5}, \]  
is in fact the Voigt (upper) bound [30] on the shear modulus, and therefore does not give the correct value of $G$, which is known to always lie between the Voigt and the Reuss (lower) [31] bounds.

An analysis by Kröner [32] shows that successively narrower bounds can be placed on the shear modulus as the degree of disorder in grain orientation increases. In the limit of perfect disorder, the shear modulus can be obtained as a root of a cubic equation with coefficients that depend on the single-crystal elastic constants. In the case of the OCP, where the shear modulus is down by a factor of $n^{1/3}$ from the bulk modulus, the cubic equation reduces to a quadratic with only one positive real root:
\[ G = \frac{1}{6} \left[ c_{44} + \sqrt{c_{44}^2 + 12(c_{11} - c_{12})c_{44}} \right]. \]  
In Table I we present the values of the elastic constants from ref. [29] and the correct values of $G_{\text{OCP}}$ as calculated from Eq. (10).

| $\Gamma$ | $(c_{11} - c_{12})/2$ | $c_{44}$ | $G_{\text{OCP}}$ |
|----------|-------------------|------|----------|
| $\infty$ | 0.02454           | 0.1827 | 0.0930   |
| 800      | 0.024(2)          | 0.174(1) | 0.089(12) |
| 400      | 0.025(2)          | 0.167(1) | 0.087(11) |
| 300      | 0.025(3)          | 0.157(4) | 0.084(19) |
| 200      | 0.019(3)          | 0.12(1)  | 0.064(28) |

Table I. The elastic constants and shear modulus, in units of $(4\pi/3)^{1/3}(Ze)^2 n^{4/3}$.

Let us again assume a linear temperature dependence of $G_{\text{OCP}}$ on $T \propto 1/\Gamma$:
\[ G_{\text{OCP}}(\Gamma) = G_{\text{OCP}}(\infty) \left( 1 - \frac{\eta}{\Gamma} \right). \]  

Fitting the values in Table I to this linear formula, and taking into account their uncertainties, we obtain

$$\eta = 36.7 \pm 30.4.$$  \hspace{1cm} (12)

Finally, we evaluate the OCP melting parameter $\Gamma_m$ in the framework of melting as a dislocation-mediated phase transition. As follows from Eqs. (8), and (11),(12) with the value of $G^{OCP}(\infty)$ from Table I,

$$\Gamma_m = 172 \pm 35.$$  \hspace{1cm} (13)

This value is in good agreement with the available data from MC simulations, albeit with 20% uncertainty. We note that most ($\approx 2/3$) of this uncertainty comes from the uncertainty in the value of $\eta$.

The OCP value of the parameter $\gamma$ defined in Eq. (4) is simply related to $\eta$ and $\Gamma_m$:

$$\eta \equiv \gamma^{OCP} \Gamma_m.$$  \hspace{1cm} (14)

From Eqs. (12) and (13) we get $\gamma^{OCP} = 0.21 \pm 0.18$, which is consistent with the value of $\gamma$ at $p \sim 0$, namely 0.23 [26].

## 4 Concluding remarks

Our central value for $\Gamma_m$, that is 172, agrees well with the more recent MC results. Two-thirds of the 20% uncertainty in this value is attributable to the error in the MC-calculated temperature dependence of the OCP single-crystal elastic constants.

Our previous study of the melting curves of 18 elements [34] revealed that the melting relation (3) is in good agreement with data up to pressures $\sim 100–200$ GPa. Here we have demonstrated that Eq. (3) also holds in a classical OCP. These successful comparisons of Eq. (3) with experimental data and MC calculations suggest, but of course do not by themselves prove, that melting is a dislocation-mediated phase transition.

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