Charge Particle Diffusion and the Effective Interactions in the Liquid Phase: Based on Positron Diffusion Studies

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Abstract. Based on the theoretical formula, which explains an anomalous diffusion mechanism of positrons in the liquid phase, we propose an origin of the attractive interactions between like charged ions in the liquid phase. It is suggested that the attractive interactions are attributed to exchange interactions of the massive gauge fields between changed ions.

1. Introduction

The interionic interactions in fluids can be described by pairwise additive solvent-mediated potentials. Further, one can describe the long range ion-ion interparticle correlations at infinite dilution via a dielectric continuum description, employing bulk solvent properties. It is possible to study the short ranged solvent-ion and ion-ion correlations in the context of a correction to the continuum picture. The calculation [1], by the use of Ornstein-Zernike-like integral equation, has predicted the attractive interaction between an anionic ions, $\text{Cl}^-\text{Cl}^-$, in water near contact with respect to infinite separation. The origin of the attractive interaction between like changed ions has not been confirmed so far.

Since fluctuation from the equilibrium medium is preferable in liquid phases, localization of charged particles like positrons is highly probable [2, 3]. Free energy density functional theories [4, 5] provide self-trapping as a solution of the charged particle in a given host liquid. The sensitivity of positrons to changes induced by melting has already been reported by angular correlation [6, 7, 8] and lifetime [9, 10] studies of liquids. Gramsh et al. [11, 12] have observed very different behavior of the diffusion length $L_+$ of positrons in liquid and solid metals. That is, on melting, $L_+$ decreases remarkably, and in the liquid phase, $L_+$ increases with temperature. Kanazawa and coworkers [13-17] proposed a qualitative explanation for the increase with temperature of the positron diffusion length in the liquid phase, by using the theoretical formula, which is based on the gauge-invariant effective Lagrangian with spontaneously broken density (the hedgehog-like a fluctuation) and the massive internal gauge fields. In this study, extending that theoretical formula, we shall propose an origin of the attractive interaction between like charged ions in the liquid phase.
2. The spontaneously broken density with internal Yang-Mills fields and the effective interaction

The connection on gauge field describes how the orientation of the fiber changes as one goes along a path in base space, or how the path in the base space is lifted into a path in the fiber bundle. We introduce a field-theoretical model to treat the problem of a charged particle in a fluid host in three spatial dimensions. It has been proposed that the parameter \( \rho(t, r, u) = \rho(t, x, y, z, u) \) in three dimensional liquids is specified by the rotation, which is related to the gauge fields \( A^a_\mu \) of SO(4) symmetry of \( S^3 \). The curvature can be represented by using a component, \( u \), in the other-axis direction, if the three spatial dimensional axes are \( x, y, \) and \( z \). It is preferable that we think of the anomalous fluctuation around the charged particle in the three dimensional liquid as the hedgehog-like fluctuation (soliton), taking into account the curvature. We adopt the parameter \( \rho(\rho, u) = \rho^a(a = 1, 2, 3, 4) \), which is similar to that in the Sachdev and Nelson model [18]. The SO(4) quadruplet fields, \( A^a_\mu \), are spontaneously broken through the Higgs mechanism similar to the way in which the fluid host is broken around a charge particle. When the hedgehog-like fluctuation (soliton) around a charged particle is created, we set the symmetry breaking as follows, \( \langle 0 | \rho | 0 \rangle \), equal to \( (0, 0, 0, \nu_4) \). Now, we can introduce the approximate Lagrangian as follows,

\[
L = \psi^+ (i \partial_0 - g_2 T^a A^a_0) \psi - \frac{1}{2m} \psi^+ (i \nabla - g_2 T^a A^a_{\mu \neq 0})^2 \psi \\
- \frac{1}{4} (\partial_\mu A^a_\mu - \partial_\mu A^a_\mu + g_1 e_{abc} A^b_\mu A^c_\mu)^2 \\
+ \frac{1}{2} (\partial_\mu \rho^a - g e_{\beta \alpha \gamma} A^a_\mu \rho^\gamma)^2 + e^2 \rho^a \rho^a - \lambda_3 (\rho^a \rho^a)
\]

Then, we set the symmetry breaking as follows,

\[
\rho^a \to (0, 0, 0, \nu_4) + (\rho^1, \rho^2, \rho^3, \rho^4).
\]

Thus, we can introduce the effective Lagrange density,

\[
L = \psi^+ (i \partial_0 - g_2 T^a A^a_0) \psi - \frac{1}{2m} \psi^+ (i \nabla - g_2 T^a A^a_{\mu \neq 0})^2 \psi \\
- \frac{1}{4} (\partial_\mu A^a_\mu - \partial_\mu A^a_\mu + g_1 e_{abc} A^b_\mu A^c_\mu)^2 \\
+ \frac{1}{2} (\partial_\mu \rho^a - e_{\beta \alpha \gamma} A^a_\mu \rho^\gamma)^2 + m_1^2 [(A^a_\mu)^2 + (A^a_\mu)^2] \\
+ m_1 (A^1_\mu \partial_\mu \rho^1 - A^2_\mu \partial_\mu \rho^1) + m_1 (A^2_\mu \partial_\mu \rho^2 - A^3_\mu \partial_\mu \rho^2) + m_1 (A^3_\mu \partial_\mu \rho^1 - A^1_\mu \partial_\mu \rho^3) \\
+ g_1 m_1 (\rho^1 (A^a_\mu)^2 + (A^a_\mu)^2 + (A^a_\mu)^2 - A^a_\mu (\rho^1 A^a_\mu + \rho^2 A^a_\mu + \rho^3 A^a_\mu)) \\
- \frac{m_2^2}{2} (\rho^1)^2 - \frac{m_2 g^2}{2m_1} (\rho^1)^2 - \frac{m_2 g^2}{8m_1^3} (\rho^1 \rho^1)^2.
\]

where \( m_1 = \nu_4 g \) and \( m_2 = 2 \sqrt{2} \lambda_3 \nu_4 \). The effective Lagrange density, \( L_{\text{eff}} \), represents three massive vector fields \( A^{1 \mu}, A^{2 \mu}, A^{3 \mu} \), and one mass less vector field \( A^{4 \mu} \). Based on the effective Lagrangian in eq.(2), Kanazawa and coworkers [13-17] has proposed the explanation for the increase of the positron diffusion length with temperature in liquid metals. That is, as the temperature increases, the effective mass of the positron decreases due to the restoration of the
spontaneously broken density around the positrons in the liquid phase. The generation function \( Z[J] \) for Green’s functions is shown as follows;

\[
Z[J] = \int \mathcal{D}A D\bar{D} Dc D\bar{c} D\psi D\bar{\psi} \cdot \exp i \int d^4x \left( \mathcal{L}_{eff} + \mathcal{L}_{GF+FP} + J \cdot \Phi \right),
\]

(3)

where \( B^a \) and \( \epsilon^a \) are the Nakanishi-Lautrup (NL) fields and Faddeev-Popov fictitious fields, respectively.

\[
\mathcal{L}_{DF+FP} = B^a \partial^\mu A_\mu^a + \frac{1}{2} \alpha B^a B^a + i \bar{\epsilon}^a \partial^\mu D_\mu \epsilon^a,
\]

(4)

BRS-quartet \([19, 20]\) in the present theoretical formula are \((\phi_1, B^1, C^1, \bar{C}^1), (\phi_2, B^2, C^2, \bar{C}^2), (\phi_3, B^3, C^3, \bar{C}^3), (A^4_{L,\mu}, B^4, C^4, \bar{C}^4)\) where \( A^4_{L,\mu} \) is the longitudinal component of \( A^4_\mu \). So we need these fields are unobservable and fictitious ones. Since these masses are created through the Higgs mechanism by introducing a charged particle in the fluid host, the massive gauge fields \( A^1_\mu, A^2_\mu, A^3_\mu \) are localized around the charged particle. Now, extending that theoretical formula, we shall discuss an origin of the attractive interaction between like charged ions in the liquid phase.

Integral equation methods have been used by Petti and Rossky \([1]\) to study solvent-averaged forces and the effective interactions or the potentials of mean force for the alkali halides in water at infinite dilution. Integral equations revealed that the potential of mean force of unlike charged ions in water display clear minima in the ion-contact and solvent-separated region. The presence of such minima and maxima is not predicated by continuum solvent theory. Especially it is of significance that the \( \text{Cl}^- - \text{Cl}^- \) pair indicates the possibility of a substantial minimum at the ion-contact pair distance \([1]\). Furthermore, these studies \([1, 21]\) suggest strongly the attractive interaction in the distance between \( \text{Cl}^- - \text{Cl}^- \) ions from \(~3.5\) to \(~5.0\) Å.

Here, if inverse of the mass, \( m_1 \), of the massive gauge fields \( A^1_\mu, A^2_\mu, A^3_\mu \) in eq.(2) is \(~5.0\) Å, the attractive potential, \(-\frac{e^2}{4\pi}\frac{1}{r}e^{-mr}\), in the distance (below \(~5.0\) Å) between negative two ions is derived from massive gauge fields \( A^1_\mu, A^2_\mu, A^3_\mu \) exchange interactions. This attractive potential might correspond to one in the distance between \( \text{Cl}^- - \text{Cl}^- \) ions from \(~3.5\) to \(~5.0\) Å.

3. Conclusion

Based on the gauge-invariant effective Lagrangian with the spontaneously broken density and internal Yang-Mills gauge fields, we have discussed the origin of attractive interactions between like charged ions in the liquid phase. It is shown that the attractive interactions might be attributed to exchange interactions of the massive gauge fields between changed ions.
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