Semiclassical model for the ionic self-diffusion coefficient in white dwarfs

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Under the extreme conditions of massive white dwarfs, which have ionic densities that exceed 10^{29} cm^{-3}, the ions can be both very strongly coupled and partially degenerate. We present a simple model for self-diffusion in such white dwarfs that utilizes the known one-component plasma diffusion coefficient and scalings derived from the short-time expansions of the velocity autocorrelation function and the memory function. Since the ions are weakly degenerate, we utilize a simple semiclassical correction to the classical dynamics. We find enhanced diffusion, relative to the purely classical calculation, which is more significant at smaller values of the Coulomb coupling parameter.

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I. INTRODUCTION

The end point of stellar evolution of more than 95% of stars is the white dwarf phase in which nuclear fuel no longer burns, residual energy radiates away, and the star slowly cools. Our knowledge of white dwarf evolution depends in part upon uncertainties in the microphysical processes that affect energy transport. Typical mass-radius relations [1] for white dwarf stars indicate that the ionic density n can become quite high; in particular, higher mass stars correspond to smaller radius stars, which implies very dense cores in massive white dwarfs. Particle densities and temperatures are in the $n \sim 10^{28}-10^{30}$ cm^{-3} and $T \sim 10^5-10^7$ K ranges, respectively, with older stars being cooler. These conditions place the stars in the strongly coupled Coulomb liquid phase in which the collisional mean free path can be less than the interparticle spacing and is, therefore, a meaningless concept; as the stars cool, crystallization occurs and processes such as diffusion eventually cease. Strong Coulomb coupling is defined in terms of the Coulomb coupling parameter $\Gamma = (Ze)^2/(aT)$, where Ze is the ionic charge and $a = (3/4\pi n)^{1/3}$ is the ion-sphere radius. Quantum corrections to ionic properties [3], such as the equation of state [4], can be non-negligible under such conditions because the ionic thermal deBroglie wavelength $\Lambda_{th} = \sqrt{2\pi\hbar^2/MT}$ (M is ionic mass) becomes comparable to the interionic spacing, which is of order the ion-sphere radius. The degeneracy can be characterized by $\Lambda_{th}/a = \sqrt{2\pi\Gamma/R_s}$, where the dimensionless quantum density parameter $R_s = a/a_{\mathrm{Bi}}$ is the ratio of the ion-sphere radius and the *ionic* Bohr radius $a_{\mathrm{Bi}} = \hbar^2/M(Ze)^2$. Typically, R_s is in the range $R_s \sim 10^3-10^4$, which reveals that $\Lambda_{th}/a \sim 0.05-0.5$ for typical conditions of a massive white dwarf with the largest values occurring for light elements (e.g., helium) and cooler temperatures. One such microphysical process is that of gravitational settling of impurities, which occurs at a rate determined by the diffusion coefficient [2]. Since white dwarf cooling is affected by energy transport processes, it is of interest to understand diffusion in the strong-coupled, mildly degenerate Coulomb liquid regime.

Bildsten and co-workers [2] have argued that some impurities settle towards the center of the star and thereby release gravitational energy that, in turn, affects the luminosity. Although there are many impurities, those that settle due to the internal electric field are those that have a neutron excess, and ^{22}Ne is the dominant species (mass fraction 0.02) with that property. As the ^{22}Ne drifts towards the center through the strongly coupled Coulomb liquid of mainly carbon and/or oxygen, the physical conditions vary from weakly coupled through crystallization, if the star is well evolved. In the weakly coupled regime, $\Gamma \ll 1$, diffusion can be described in terms of a sequence of independent binary collisions between Debye-screened particles [5]. At moderate couplings, $\Gamma \sim 1$, the collisions become strong and the simple Debye screening picture begins to lose its validity. Under conditions of strong coupling, $\Gamma \gtrsim 10$, the plasma shows liquidlike behavior in which particles experience rapid oscillations in a transient cage formed by its nearest neighbors [6] and the usual picture of a collision becomes inappropriate. As the coupling is further increased towards crystallization, collective modes play an important role and diffusion is dominated by many-body physics. White dwarfs, due to their diversity in size, composition, and evolutionary path, cover all regimes of diffusion.

A reduced model for impurity diffusion in white dwarfs has been constructed by Bildsten and co-workers [2]. In their model, the electrons form a uniform neutralizing background and the star's composition is taken to be described by a single species (carbon or oxygen) characterized by Γ. Their model allows the use of the *classical* one-component plasma (OCP) diffusion coefficient [7]

$$D = \omega_p a^2 \frac{2.95}{\Gamma^{1.34}}, \tag{1}$$

where $\omega_p = \sqrt{4\pi(Ze)^2 n/M}$ is the ion plasma frequency, and it is assumed that diffusion ceases ($D=0$) upon crystallization ($\Gamma > 173$). Our goal is to extend the classical result (1) into the quantal regime under the reasonable assumption that the extensions are small. This assumption allows us to use a simple, classical-looking model for the ions. Our model is described in the first section and its thermodynamic predictions are discussed. In the following section, a model for the diffusion coefficient is presented that employs properties of the velocity autocorrelation function and its memory func-

tion [8] that relate the known result (1) to the quantal result. Finally, simple fits and a discussion are given.

II. SEMICLASSICAL MODEL

White dwarf interiors consist of fully ionized, strongly coupled ions embedded in a homogeneous sea of very degenerate electrons. For this reason, white dwarfs are often considered to be the best realization of the OCP model. Because the quantal modifications are expected to be small ($\Lambda_{th} < a$), we use a semiclassical extension of the OCP model in which the classical ionic dynamics is modified via an effective pair interaction [9], viz.,

$$v(r) = \frac{(Ze)^2}{r}(1 - e^{-r/\Lambda}). \tag{2}$$

Here the parameter Λ is of order Λ_{th} and r is the ionic separation. Such a model accounts for the finite extent of the ionic wave function by smearing the usual Coulomb divergence at small r on the length scale of Λ_{th}. This semiclassical OCP model is obtained from a semiclassical electron-ion plasma in the limit of homogeneous electrons. Although it is not necessary to do so, we assume that the semiclassical OCP can be described by a single parameter, Λ, which we take to be an adjustable parameter that can be determined in a variety of ways, including by matching properties obtained from Eq. (2) to results from, e.g., $\hbar$ expansions [4] or path-integral Monte-Carlo calculations [11]. Often the specific form $\Lambda = \Lambda_{th}/\sqrt{2\pi^2}$ is used [9]. For a semiclassical system of N ions in volume Ω, the Hamiltonian can be written as

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2M} + V, \tag{3}$$

where the potential energy is

$$V = \frac{1}{2}\sum_{i=1}^{N}\sum_{j\neq i}^{N} v(r_{ij}) - n\sum_{i=1}^{N}\int_{\Omega} d^3r\, v(|\mathbf{r} - \mathbf{r}_i|) + V_0. \tag{4}$$

Here V_0 is the potential energy of the background. Given Eq. (3), we can estimate how quantum effects modify the transport properties in white dwarf interiors.

As a simple test of the validity of our model (3), we can compute the total energy density u and compare it with results obtained from different methods. For a system characterized by Γ and $\lambda \equiv \Lambda/a$, the (dimensionless) total energy density is

$$u(\lambda,\Gamma) = \frac{\langle H\rangle}{NT} = \frac{3}{2} + \frac{3\Gamma}{2}\int_0^{\infty} dR\, R^2 \tilde{v}(R)[g(R,\Gamma,\lambda) - 1], \tag{5}$$

where $g(R,\Gamma,\lambda)$ is the ionic pair distribution function, the brackets $\langle\cdots\rangle$ indicate ensemble averaging, $\tilde{v}(R) = 1/R(1 - e^{-R/\lambda})$, and $R = r/a$. The relation (5) is similar to the standard expression for u of neutral fluids, with the exception that the background contribution enters via the -1 term in the integral. In order to discuss the semiclassical correction to the OCP, Eq. (5) is decomposed as

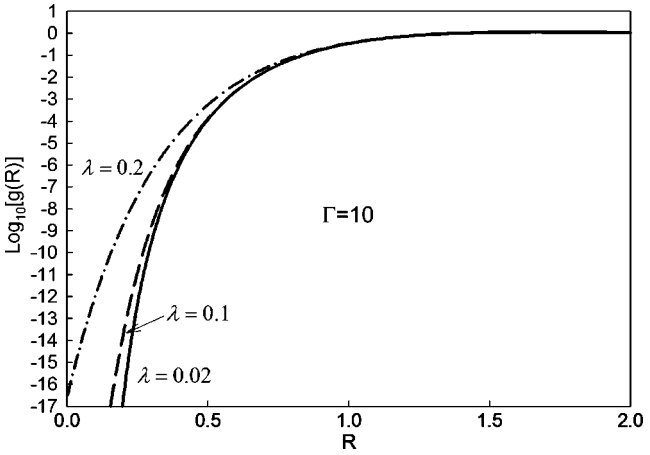

FIG. 1. The logarithm of the radial distribution function $g(R,\lambda)$ is shown for $\Gamma = 10$ and the three values $\lambda = 0.02, 0.1, 0.2$ as computed within the HNC approximation. Note that the ionic structure is modified only at small r and is nonzero at $r = 0$.

$$u(\lambda,\Gamma) = u_{\mathrm{OCP}}(\Gamma) + \delta u(\lambda,\Gamma), \tag{6}$$

where $u_{\mathrm{OCP}}(\Gamma) \equiv u(0,\Gamma)$ is the total energy density of the classical OCP [12]. To evaluate $\delta u(\lambda,\Gamma)$, the only unknown quantity is the pair distribution function $g(R,\Gamma,\lambda)$. For systems with long-range interactions it is known that this can be computed to high accuracy using the hypernetted chain (HNC) equations. Although greater accuracy could be achieved by including a bridge function, we note that the bridge function consistent with Eq. (2) is not known and the uncertainties in the models are likely to be larger than uncertainties created by the neglect of the bridge function. Of particular difficulty is the resolution of the scale λ, which tends to zero in the classical limit. As such, we employ a fast-Fourier transform in a standard HNC code with 16 384 bins within the range $R = 0-50$; this corresponds to a bin size of order $\delta R \sim 0.003$. A simple relaxation algorithm was also used that allows easy computation over the entire fluid regime [10]. In practice, quantities were computed from $\Gamma = 10-170$. Some typical HNC results are shown in Fig. 1 for $\Gamma = 10$ and $\lambda = 0.02, 0.1, 0.2$.

We have computed the semiclassical correction $\delta u(\lambda,\Gamma)$ over the range $\lambda = 0.02-0.3$ and fit the results to obtain

$$\delta u(\lambda,\Gamma) \approx \sqrt{2}\lambda^2\Gamma. \tag{7}$$

We can compare Eq. (7) with the exact result to order $\hbar^2$ [4] of $\Gamma^2/4R_s$. Here, if we make the common choice of $\Lambda = \Lambda_{th}/\sqrt{2\pi^2}$ [9], we obtain $\delta u(\lambda,\Gamma) = \sqrt{2}\Gamma^2/\pi R_s$. This result reveals that the scaling with Γ and λ is correct and that, numerically, there is agreement to within a factor of less than 2. This agreement suggests that the semiclassical model (2) might be reasonable for describing diffusion; however, higher-order $\hbar$ corrections [4] tend to spoil this agreement, suggesting that Eq. (2) is approximately valid to order $\hbar^2$. Figure 2 compares the total energy based on Eq. (2) with the $\hbar^4$ expansion of Hansen and Vieillefosse [4] and a path-integral Monte Carlo (PIMC) result of Jones and Ceperley [11]. This result indicates that our model (2) yields superior

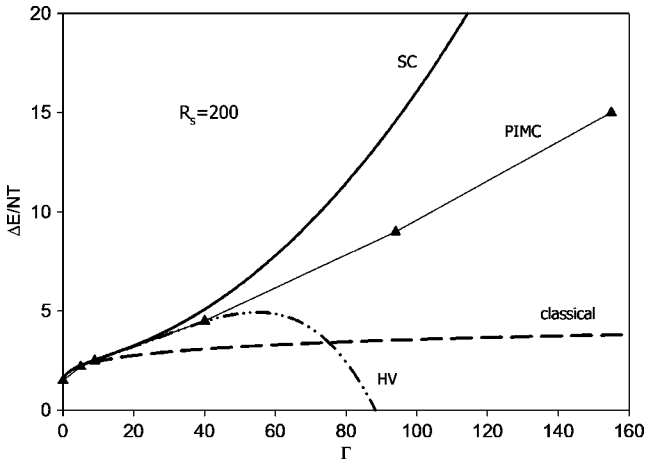

FIG. 2. The thermal excess energy $\Delta E/NT=(E-E^M_{\rm BCC})/NT$ of the OCP is shown based on Eq. (2) with $\Lambda=\Lambda_{th}/\sqrt{2\pi^2}$ (solid, "SC"), the Hansen-Vieillefosse $\hbar^4$ expansion (dot-dash, "HV"), and the Jones-Ceperley PIMC (triangles, "PIMC") result vs Γ for fixed $R_s=200$. The reference BCC Madelung energy is $E^M_{\rm BCC}/NT=-1.791\,85\,\Gamma/2$.

results to both the classical and the $\hbar^4$ expansion at large Γ. This result, however, fortuitously arises because of the poor convergence of the $\hbar^2$ expansion. The range of applicability of our model is clearly $R_s>200$, although Λ could be chosen to match the excess energy of the PIMC result for small R_s.

III. SELF-DIFFUSION COEFFICIENT

Plasma diffusion coefficients are typically obtained from a transport cross section that can be obtained either classically or quantum mechanically [13]. In the strongly coupled plasma regime, however, there are important structural and collective phenomena that are not accounted for in the simple binary collision picture. We therefore begin with the fact that diffusion is a measure of the mean-squared displacement of a single particle, which can be related to the velocity autocorrelation function (VACF) as

$$D=\lim_{t\to\infty}\frac{1}{6t}\langle|\mathbf{r}_i(t)-\mathbf{r}_i(0)|^2\rangle \tag{8}$$

$$=\frac{T}{M}\int_0^\infty dt\; Z(t), \tag{9}$$

where $Z(t)$ is the normalized VACF [14],

$$Z(t)=\langle\mathbf{v}_i(t)\cdot\mathbf{v}_i(0)\rangle/\langle\mathbf{v}_i^2(0)\rangle. \tag{10}$$

Here $\mathbf{r}_i(t)$ and $\mathbf{v}_i(t)$ are the position and velocity of any tagged particle in the system at time t. Despite the apparent simplicity of this formulation, the calculation of the diffusion coefficient is an example of the many-body problem. Many approaches, including the memory function formalism and kinetic theory, have been devised to model the VACF in simple liquids. The major difficulty arises from the fact that the diffusion coefficient depends on dynamical processes occurring over disparate time scales. In the case of the classical OCP [7], it is known that the VACF is strongly affected by both binary collisions and collective effects, and that simple approximations for the VACF, or its memory function, cannot accurately describe the diffusion coefficient (see below). In order to cope with this problem and keep the model simple, our approach proceeds as follows. Suppose that we have a model for $D(\lambda)\approx D_{model}(\lambda)$, where $D_{model}(\lambda)$ depends on quantities that we are able to calculate, like the pair distribution function. The ratio $\mathcal{R}(\lambda)=D_{model}(\lambda)/D_{model}(0)$ yields an approximation of the scaling between the semiclassical and the classical diffusion coefficient. Our approach is to assume that this scaling is exact, viz.,

$$D(\lambda)=\mathcal{R}(\lambda)D_C, \tag{11}$$

with $D_C=D(0)$ the classical OCP diffusion coefficient. A good estimate of D_C obtained with molecular-dynamics techniques is given by Eq. (1), which, when combined with a model for $\mathcal{R}(\lambda)$, allows one to evaluate the semiclassical diffusion coefficient $D(\lambda)$. Because of the emphasis placed upon the classical result, we improved Eq. (1) by combining the original data with that from Ranganathan *et al.* [15] and fitted the data to the form suggested by Robbins *et al.* [16] to obtain

$$D_C^*=0.0028+0.00525\left(\frac{173}{\Gamma}-1\right)^{1.154}. \tag{12}$$

This form, with three parameters, describes deviations from the simple, power-law fit used to obtain Eq. (1). The dimensionless diffusion coefficient is defined as $D^*=D/\omega_p a^2$. We have considered two models for $\mathcal{R}(\lambda)=D(\lambda)/D(0)$ that depend on spatial correlation functions. Since the models employ different correlation information, we will have an estimate of the sensitivity to a particular model.

The first model is obtained from the short-time expansion of $Z(t)$ in the following manner. The leading-order terms in such an expansion are

$$Z(t)=1-\omega_E^2\frac{t^2}{2}+\cdots, \tag{13}$$

where $\omega_E^2=(M/3T)\langle\dot{\mathbf{v}}_i^2\rangle$ is known as the Einstein frequency. Any function $f(t)$ satisfying Eq. (13) up to second-order in time and $I=\int_0^\infty f(t)dt<\infty$ is a possible approximation for $Z(t)$, exact up to the second-order in time; an example is given by the Gaussian approximation $Z(t)\approx e^{-\omega_E^2(t^2/2)}$. For the diffusion coefficient, one obtains

$$D(\lambda)\approx\frac{T}{M}I. \tag{14}$$

Note that in our model the *exact* value of the integral I does not matter as we consider the ratio $\mathcal{R}(\lambda)=D(\lambda)/D(0)$. The Einstein frequency can be written explicitly in terms of the ionic radial distribution function as

$$\omega_E^2(\lambda)=\frac{n}{3M}\int d^3r\nabla^2 v(r)[g(r,\Gamma,\lambda)-1]. \tag{15}$$

The many-body contributions to the diffusion of a single particle enter here through $g(r,\Gamma,\lambda)$. Following the proce-

dure described before, our approach yields the approximation

$$\mathcal{R}_1(\lambda) = \left(\lambda^{-2} \int_0^\infty dR\, Re^{-R/\lambda} [1 - g(R,\Gamma,\lambda)] \right)^{-1/2}, \quad (16)$$

which has the limit $D(\lambda) \to D_C$ as $\lambda \to 0$.

The second model is obtained by approximating of the memory function $\mathcal{M}(t)$ of the VACF. Recall that $\mathcal{M}(t)$ and $Z(t)$ are linked to each other by the generalized Langevin equation

$$\frac{d}{dt} Z(t) = - \int_0^t dt' \mathcal{M}(t') Z(t - t'), \quad (17)$$

and that the diffusion coefficient is exactly given by

$$D = \frac{T}{M} \left(\int_0^\infty \mathcal{M}(t) dt \right)^{-1}. \quad (18)$$

Approximations for $\mathcal{M}(t)$ can be constructed from the short-time expansion

$$\mathcal{M}(t) = \omega_E^2 \left(1 - \frac{t^2}{\tau^2} + \cdots \right), \quad (19)$$

with

$$\frac{\omega_E^2}{\tau^2} = - \frac{M}{3T} \langle \ddot{\mathbf{r}}_i^2 \rangle + \omega_E^4. \quad (20)$$

Any function $f(t)$ satisfying $f(t) = 1 - t^2 + \cdots$ and $I = \int_0^\infty f(t) dt < \infty$ defines an approximation of the memory function $\mathcal{M}(t) \approx \omega_E^2 f(t/\tau)$, exact up to the second-order in time; an example is given by $f(t) = \mathrm{sech}^2(t/\tau)$. For the diffusion coefficient, one obtains

$$D(\lambda) \approx \frac{T}{M \omega_E^2 \tau} \frac{1}{I}. \quad (21)$$

Such approximations have been widely used for neutral liquids and are referred to as the "binary-collision" approximation, as they essentially describe well the short-time dynamics of the memory function when binary collisions dominate. The time τ is interpreted as the duration of a binary collision. In our model, the exact value of the integral I does not matter as we consider the ratio $D(\lambda)/D(0)$. In order to use this model, we need to determine τ or equivalently the moment $\langle \ddot{\mathbf{r}}_i^2 \rangle$ [see Eq. (20)]. Introducing the triplet distribution function

$$n^2 g^{(3)}(\mathbf{r}, \mathbf{r}') = \frac{1}{N} \sum_{i,j \neq i, l \neq i,j}^{N} \langle \delta(\mathbf{r} - \mathbf{r}_{ij}) \delta(\mathbf{r} - \mathbf{r}_{il}) \rangle, \quad (22)$$

the moment $\langle \ddot{\mathbf{r}}_i^2 \rangle$ is explicitly

$$\langle \ddot{\mathbf{r}}_i^2 \rangle = \frac{2nT}{3m^3} \sum_{a,b} \int d^3 r \left(\frac{\partial^2 v(r)}{\partial r_a \partial r_b} \right)^2 g(r) + \frac{n^2 T}{3m^3} \sum_{a,b} \int d^3 r d^3 r' \left(\frac{\partial^2 v(r)}{\partial r_a \partial r_b} \right) \left(\frac{\partial^2 v(r')}{\partial r_a' \partial r_b'} \right) \times [g^{(3)}(\mathbf{r}, \mathbf{r}') + 1], \quad (23)$$

which differs from the expression for neutral liquids by the term +1 in the last integral. In the absence of detailed knowledge of $g^{(3)}$, we evaluate the second term on the right-hand side of Eq. (23) with the Kirkwood approximation

$$g^{(3)}(\mathbf{r}, \mathbf{r}') \approx g(r) g(r') g(|\mathbf{r} - \mathbf{r}'|) = g(r) g(r') \left\{ 1 + \frac{1}{8\pi^3 n} \int d^3 q [S(q) - 1] \times e^{-i\mathbf{q} \cdot (\mathbf{r} - \mathbf{r}')} \right\},$$

where $S(q)$ is the static structure factor. After some tedious manipulations, we obtain the approximation

$$\frac{\omega_E^2}{\tau^2} = \left(\frac{\omega_p^2}{3} \right)^2 \int_0^\infty dR\, R^2 g(R) \left[\tilde{v}''(R)^2 + 2 \left(\frac{\tilde{v}'(R)}{R} \right)^2 \right] - \frac{\omega_p^2}{3} \left(\omega_E^2 - \frac{\omega_p^2}{3} \right) + \frac{1}{9\pi} \left(\frac{\omega_p^2}{3} \right)^2 \int_0^\infty dQ Q^2 [S(Q) - 1] \times [\gamma_L^2(Q) + 2\gamma_T^2(Q)] \quad (24)$$

with

$$\gamma_L(Q) = \int_0^\infty dR\, R^2 g(R) \left[\{ j_0(QR) - 2 j_2(QR) \} \tilde{v}''(R) + 2 \{ j_0(QR) + j_2(QR) \} \frac{\tilde{v}'(R)}{R} \right], \quad (25)$$

$$\gamma_T(Q) = \int_0^\infty dR\, R^2 g(R) \left[\{ j_0(QR) + j_2(QR) \} \tilde{v}''(R) + \{ 2 j_0(QR) - j_2(QR) \} \frac{\tilde{v}'(R)}{R} \right], \quad (26)$$

where

$$j_0(x) = \frac{\sin(x)}{x}$$

and

$$j_2(x) = \frac{3}{x^2} \left[\frac{\sin(x)}{x} - \cos(x) \right] - \frac{\sin(x)}{x}$$

are the spherical Bessel functions of order 0 and 2, respectively, and $Q = aq$. Following the procedure described before, our approach yields the approximation

$$\mathcal{R}_2(\lambda) = \frac{\tau(0)}{\tau(\lambda)}, \quad (27)$$

with $\tau(\lambda)$ given by Eq. (24).

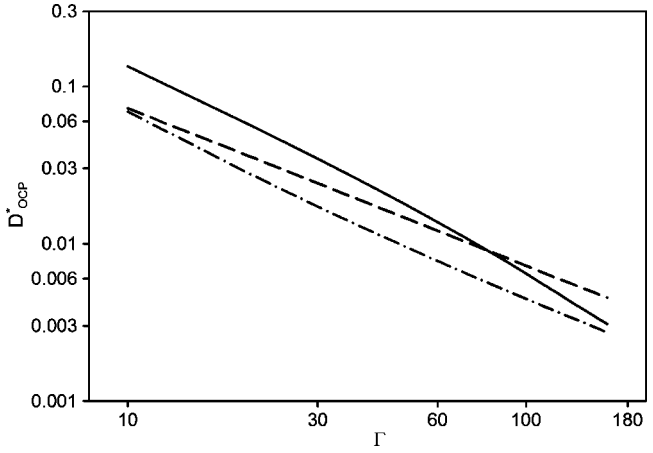

FIG. 3. The OCP diffusion coefficient is shown based on the fit (12) to molecular-dynamics data (solid), the Gaussian approximation for the VACF (dashed), and the hyperbolic secant approximation for the memory function (dot-dash). This result indicates the level of accuracy of the two theoretical models.

We compare in Fig. 3 the fit (12) to classical OCP predictions based on Eq. (14) with $I=\sqrt{(\pi/2)}(1/\omega_E)$ (Gaussian approximation) and Eq. (19) with $I=1$ (hyperbolic secant approximation) to assess the accuracy of the models. Note that both models are accurate to within a factor of about 2, which indicates that models for $Z(t)$ and $\mathcal{M}(t)$ can reasonably well predict diffusive behavior over the entire fluid regime. It is interesting that Eq. (19) underestimates Eq. (12) for the OCP, since results for neutral fluids suggest the reverse [8].

Next we have computed Eqs. (16) and (27) over the same range of parameters. The resulting data were fit to the form

$$D_Z^*(\lambda) = D_C^*\left[1 + 14.1\lambda^{4.9} + \frac{11\,238.7\lambda^{6.355}}{1 + 2341.7\lambda^{4.537}}\Gamma^{-1}\right],$$

$$D_{\mathcal{M}}^*(\lambda) = D_C^*[1 + 46.2\lambda^{4.72} - 0.007\,53\lambda^{3.20}\Gamma]. \quad (28)$$

Predictions from Eq. (28) are shown in Fig. 4 for $\lambda = 0.1, 0.2, 0.3$. These results illustrate that the quantal corrections are quite small when $\lambda < 0.1$ and that the correction is more important for small Γ.

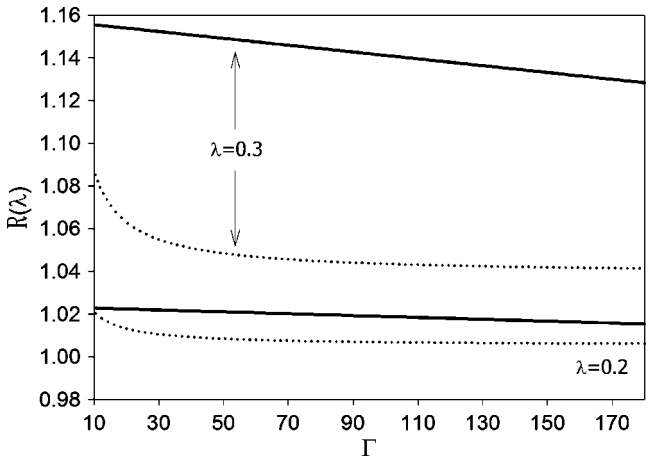

FIG. 4. The correction factor D_{SC}^*/D_C^* versus coupling parameter Γ for two values of λ: $\lambda = 0.2, 0.3$. Note that the correction is small for $\lambda < 0.2$ and decreases for increasing Γ.

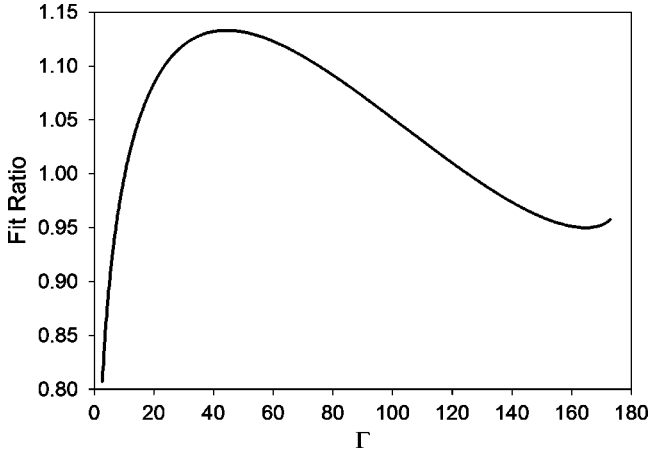

FIG. 5. The ratio of Eq. (12) to Eq. (1) is shown vs Γ. This indicates that the error of the fit is of the order of the semiclassical correction.

For very dense white dwarfs, we expect enhanced diffusion and therefore expedited sedimentation. Consider, for example, a pure carbon white dwarf with mass 1.2 M_O, radius $R=0.006R_O$, and temperature $T=10^7$ K. Such a star would have an ion number density of about $n=4\times10^{29}$ cm^{-3} or, equivalently, an ion-sphere radius of $a=8.5\times10^{-11}$ cm. These conditions correspond to $\Lambda_{th}/a \approx 0.17$ for which Eq. (28) predicts an $\sim$1% correction in the strongly coupled fluid regime. Typical choices for λ [9] will tend to have even smaller corrections. The quantal enhancement is expected to be larger than this example at higher densities, for lighter elements (e.g., helium), and at lower temperatures.

IV. DISCUSSION

To describe diffusive transport in massive white dwarf stars, we have constructed a model based on the effective semiclassical potential (2). Since this model can also predict thermodynamic quantities, we have compared the energy with two other approaches to evaluate the accuracy of such an approach. We found that Eq. (2) is accurate to order $\hbar^2$, but does not have the more unphysical behavior of the next $\hbar^4$ correction. Comparison with PIMC results indicates that our model becomes inaccurate for $R_s \lesssim 200$. This suggests that a detailed description of quantum dynamics will require a treatment beyond an $\hbar$ expansion.

Because the diffusion coefficient is difficult to calculate in the strongly coupled regime, we presented a model that employs the known diffusion coefficient of the classical OCP from molecular-dynamics simulation. We have given a slightly different fit (12) to the simulation results, due to the reliance on the classical limit. We should mention, however, that the original simulation results of Hansen, McDonald, and Pollock [7] were only accurate to about 20%, mainly due to the fit. In Fig. 5, we show the ratio of our fit (12) to the original fit (1), which indeed has an overall variation of

about 20%. Less is known about the systematic errors of the simulations themselves and sources of these errors merit further study.

To obtain the semiclassical diffusion coefficient from the classical result, we use, rather than a binary collision approach, properties of the VACF that incorporate ionic structural information through spatial correlation functions. Two approaches have been presented, one based on the short-time properties of the VACF itself and the other based on properties of its memory function, which gives us an estimate of the error of our model. We have compared predictions based on these models for the purely classical case and compared with Eq. (12) to show that the diffusion coefficient can indeed be predicted in the strongly coupled regime to within about a factor of 2. As mentioned above, we use the models in the form of the ratio (11) to ensure that the classical limit is exact. Our main result is shown in Fig. 4. We found, for typical white dwarf conditions, that the semiclassical correction is relatively small; in fact, the correction is smaller than the uncertainty in the classical result and its fit. The correction is larger for smaller values of Γ since ions can more effectively probe configurations with ionic distances of order Λ_{th}.

Our results reveal that better simulation results are needed for the classical OCP insofar as it is the basis for studies of impurity settling in white dwarfs. It would be straightforward to employ Eq. (2) in such simulations to extend the basic OCP result into the semiclassical regime. But, perhaps more importantly, there is a need for accurate simulations of the diffusion coefficient in strongly coupled mixtures with impurities [2].

ACKNOWLEDGMENTS

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[1] J. A. Panei, L. G. Althaus, and O. G. Benvenuto, Astron. Astrophys. **353**, 970 (2000).
[2] C. J. Deloye and L. Bildsten, Astrophys. J. **580**, 1077 (2002); L. Bildsten and D. M. Hall, Astrophys. J. Lett. **549**, L219 (2001).
[3] G. Chabrier, N. W. Ashcroft, and H. E. DeWitt, Nature (London) **360**, 48 (1992).
[4] J. P. Hansen and P. Vieillefosse, Phys. Lett. **53A**, 187 (1975).
[5] C. Paquette, C. Pelletier, G. Fontaine, and G. Michaud, Astrophys. J., Suppl. Ser. **61**, 177 (1986).
[6] Z. Donko, P. Hartmann, and G. J. Kalman, Phys. Plasmas **10**, 1563 (2003).
[7] J. P. Hansen, I. R. McDonald, and E. L. Pollock, Phys. Rev. A **11**, 1025 (1975).
[8] U. Balucani and M. Zoppi, *Dynamics of the Liquid State* (Oxford Science Publications, Oxford, 1994), p. 193.
[9] J. P. Hansen and I. R. McDonald, Phys. Rev. A **23**, 2041 (1981).
[10] K. C. Ng, J. Chem. Phys. **61**, 2680 (1974).
[11] M. D. Jones and D. M. Ceperley, Phys. Rev. Lett. **76**, 4572 (1996).
[12] S. Ichimaru, *Statistical Plasma Physics, Volume II: Condensed Plasmas* (Addison-Wesley Publishing Company, New York, 1994), p. 57.
[13] H.-S. Hahn, E. A. Mason, and F. J. Smith, Phys. Fluids **14**, 278 (1971).
[14] J. P. Boon and S. Yip, *Molecular Hydrodynamics* (Dover, Mineola, NY, 1991), p. 105.
[15] S. Ranganathan, R. E. Johnson, and C. E. Woodward, Phys. Chem. Liq. **14**, 123 (2003).
[16] M. O. Robbins, K. Kremer, and G. S. Grest, J. Chem. Phys. **88**, 3286 (1998); see also H. Ohta and S. Hamaguchi, Phys. Plasmas **7**, 4506 (2000).