The method of effective potentials in the quantum-statistical theory of plasmas

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Abstract
We provide a survey of the concept and several successful applications of
effective potentials. After introducing Kelbg's expression we discuss several
useful approximations and additional generalizations including non-diagonal
expressions. Finally, we present the recent results concerning non-diagonal
contributions and the relation to effective interactions arising from the dynamics
of Gaussian wave packets.

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1. Introduction

The Coulomb potential is a singular potential which gives rise to several divergences in
statistical thermodynamics. Taking quantum effects into account removes these singularities.
In fact two particles denoted by the indices i, j with masses m_i, m_j and thermal momentum
corresponding to temperature T do not 'see each other' as point particles but as charge clouds
with an effective diameter

$$\lambda_{ij} = \frac{\hbar}{\sqrt{2m_{ij}k_B T}}, \qquad \frac{1}{m_{ij}} = \frac{1}{m_i} + \frac{1}{m_j}. \tag{1}$$

The idea of effective potentials was first introduced in quantum chemistry by Hellman and
Gombas and in statistical physics by Morita. Since 1962 Kelbg and co-workers at Rostock
University have developed this method to a powerful tool in plasma physics [1]. The idea
of Günter Kelbg [1] was to replace the Coulomb potential by an effective potential which
is finite at zero distance due to quantum effects (figure 1). Kelbg's theory was originally
based on quantum perturbation theory for the diagonal matrix elements (Slater sums) of the
density matrix; he succeeded in obtaining exact expressions for the first order in e^2. His
theory was developed by a group at Rostock University (including Ahlbehrendt, Ebeling,
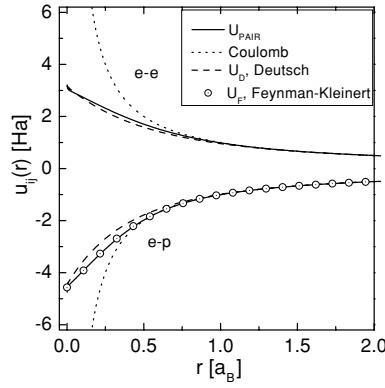
Figure 1. Effective pair potential for an electron–electron (e–e) and an electron–proton (e–p) pair at temperature $T = 10^6$ K in several approximations. Dotted lines: pure Coulomb interaction; solid lines: 'exact' pair potential U_{pair}; dashed lines: Deutsch potential, equation (4); open circles: U_F variational perturbative potential due to Feynman and Kleinert [12]. Distances are in $a_B = \hbar^2/m_e e^2$ and potentials are in Ha $= e^2/a_B$ units.

Hetzheim, Hoffmann, Kraeft, Kremp, Schmitz, Töwe, later joined by Röpke, Schlanges, Redmer, Bonitz and others). The Rostock School in Quantum Statistics formed by Günter Kelbg concentrated on analytical calculations of thermodynamic functions based on effective potentials [2–4]. Several authors calculated the two-particle density matrix from the known wave functions including numerical approaches [5–7]. Zelener, Zamalin, Norman and Filinov gave first applications within the Monte Carlo formalism [8, 9], Deutsch introduced useful approximations [10], Hansen, McDonald and Pollock [11] gave first applications to molecular dynamics, and Kleinert developed a variational approach [12].

2. The Kelbg potential, approximations and corrections

The effective interaction potential for two particles of species i, j derived by Kelbg reads:

$$u_{ij}(r) = \frac{e_i e_j}{r} \left[1 - \exp\left(-\frac{r^2}{\lambda_{ij}}\right) + \frac{\sqrt{\pi} r}{\gamma_{ij} \lambda_{ij}} \left(1 - \operatorname{erf}\left[\gamma_{ij} \frac{r}{\lambda_{ij}} \right] \right) \right], \qquad (2)$$

where λ_{ij} is the thermal wavelength given above, $\operatorname{erf}(x)$ is the standard error function and $\gamma_{ij} = 1$ in Kelbg's original formula. At zero distance the potential is finite, $u_{ij}(0) = (e_i e_j \sqrt{\pi})/\lambda_{ij}$. In addition, we may use the γ-parameter to modify the height at the origin; see below.

Since Kelbg's expression is quite complicated, several useful approximations have been proposed. One of the simplest approximations due to Zelener *et al* [8] uses the Coulomb potential for equal and opposite charges in the following form:

$$u_{+-} = -\frac{e^2}{r} \quad \text{if } r > r_0, \qquad u_{+-} = \epsilon \quad \text{if } r < r_0 = e^2/\epsilon. \qquad (3)$$

First MC simulations for dense plasmas were based on this simple effective potential [8]. Another simple expression has been proposed by Deutsch [10]:

$$u_{ij} = \frac{e_i e_j}{r} [1 - \exp(-\alpha r)], \qquad \alpha \simeq \frac{1}{\lambda_{ij}}. \qquad (4)$$

This potential has already been used in quantum chemistry by Kramers and Hellmann and in electrolyte theory by Glauberman and Juchnovskii. The MD simulations by Hansen *et al* [11] were based on this approximation.
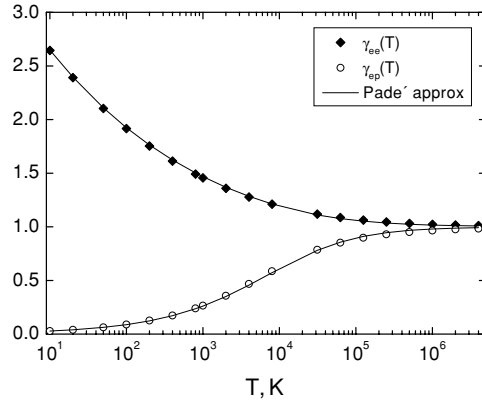
Figure 2. Heuristic parameter $\gamma_{ij}(T)$ which improves the Kelbg expression providing exact values for height and derivative at $r = 0$ obtained from exact solution of the two-particle problem [14].

We will discuss now heuristic corrections at small distances. As a result of Kelbg's approximations (first order in e^2) the effective potential is not exact at $r = 0$. It may differ from the expression obtained from the hydrogen wave functions, which is known and given in the form of tables [4, 6]. On the other hand, the first derivative of Kelbg's potential at $r = 0$ and the asymptotic $r \to \infty$ are correct, in agreement with quantum mechanics. This leads us to the idea to include the higher orders in e^2 by adapting the parameter γ_{ij} introduced formally into equation (2). By using in equation (2) the factor

$$\gamma_{ij} = u_{ij}^{\text{Kelbg}}(0) \big/ u_{ij}^{\text{exact}}(0) \tag{5}$$

and taking u_{ij}^{exact} from quantum mechanics we may improve Kelbg's expression substantially [13, 14]. This approximation will be called the improved diagonal Kelbg potential (IDKP). We represent in figure 2 the fit-parameter γ_{ij} as a function of temperature. We see that at $T < 10\,000$ K the deviations from an unchanged Kelbg potential become essential.

We propose here in addition a much simpler expression providing also exactness at the point $r = 0$, this formula might be useful for simulations.

$$u_{ij} = \frac{e_i e_j}{\lambda_{ij}} \left(\frac{\sqrt{\pi}}{\gamma_{ij}} - \frac{r}{\lambda_{ij}} \right) \quad \text{if } r < r_1, \qquad u_{ij} = \frac{e_i e_j}{r} \quad \text{if } r > r_1 \tag{6}$$

where r_1 follows from continuity. This approximation leads to very simple forces, which are constant at small distances and Coulombic for larger distances. We underline again that the height at $r = 0$ and the first derivative are exact by construction.

The parameters of effective potentials depend on the temperature; in non-equilibrium this concept is not well defined. Klimontovich *et al* have shown how effective potentials may be extended to non-equilibrium situations [15].

3. Off-diagonal effective potentials

The Kelbg potential describes the diagonal contributions to the binary density matrix. We proceed now to a calculation of the off-diagonal elements, defining the off-diagonal effective potential by means of the full binary density matrix

$$\rho_{ij}(\mathbf{r}_i, \mathbf{r}_j, \mathbf{r}_i', \mathbf{r}_j') = \rho_{ij}^{\text{ideal}} \exp[-\beta u_{ij}(\mathbf{r}_i, \mathbf{r}_j, \mathbf{r}_i', \mathbf{r}_j')]. \tag{7}$$
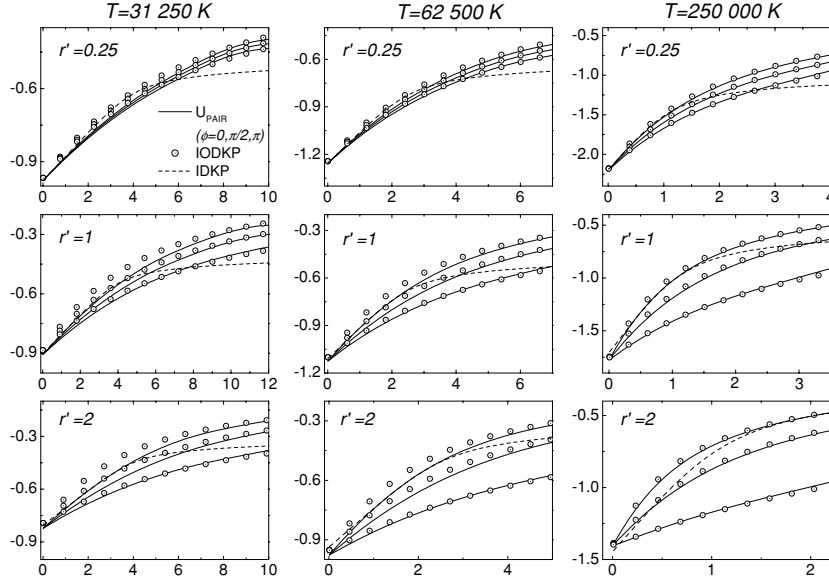
Figure 3. Off-diagonal potential of an electron–proton pair as a function of the distance r and three angles between the vectors $\mathbf{r}$ and $\mathbf{r}'$. In each panel the upper, middle and lower curves correspond to $\phi = 0, \pi/2$ and π, respectively. Distances are in units of electron Bohr radius, $a_B = \hbar^2/m_e e^2$ and the potential in electron Hartree, $Ha = e^2/a_B$.

Based on first-order perturbation theory we find [13, 14]

$$u_{ij}(\mathbf{r}_{ij}, \mathbf{r}'_{ij}) = e_i e_j \int_0^1 \frac{d\alpha}{d_{ij}(\alpha)} \, \mathrm{erf}\left(\frac{d_{ij}(\alpha)}{2\lambda_{ij}\sqrt{\alpha(1-\alpha)}}\right), \tag{8}$$

where $d_{ij}(\alpha) = |\alpha \mathbf{r}_{ij} + (1-\alpha)\mathbf{r}'_{ij}|$. In order to illustrate the dependence on the arguments we use the 'Mittelwertsatz'

$$u_{ij}(\mathbf{r}_{ij}, \mathbf{r}'_{ij}) = \frac{e_i e_j}{|\xi \mathbf{r}_{ij} + \xi' \mathbf{r}'_{ij}|} \, \mathrm{erf}\left(\frac{|\xi \mathbf{r}_{ij} + \xi' \mathbf{r}'_{ij}|}{2\lambda_{ij}\sqrt{\xi \xi'}}\right). \tag{9}$$

with two numbers satisfying $(\xi + \xi') = 1$. The diagonal elements of this expression are closely related to the effective potential used in wave packet dynamics [16]. We show in figure 3 the off-diagonal effective potential of an electron–proton pair for three different angles ϕ between the vectors $\mathbf{r}$ and $\mathbf{r}'$; the modulus of the second vector is fixed to $|\mathbf{r}'| = 0.25$, 1.0, 2.0. In each panel the upper curve corresponds to $\phi = 0$, the middle curve to $\phi = \pi/2$, and the lower curve to $\phi = \pi$. Solid lines show the 'exact' off-diagonal potential, $U_{\mathrm{pair}}(r)$, obtained using the matrix squaring technique [14]. The dotted line represents the diagonal approximation IDKP, $u_{ij}(\mathbf{r}_{ij}, \mathbf{r}'_{ij}) = \frac{1}{2}[u_{ij}(r_{ij}, r_{ij}) + u_{ij}(r'_{ij}, r'_{ij})]$. One can see that at distances $r' = 1.0, 2.0$ the diagonal approximation becomes very crude and does not capture the dependence on ϕ. Now it is interesting to compare this quantum mechanical result with the perturbation solution (8).

The off-diagonal potential (8) is exact only to first-order in e^2. In order to find an improved off-diagonal potential corresponding to equations (2) and (6) we use the splitting

$$\mathrm{erf}(x) = 1 - \exp(-x^2) + x e_1(x). \tag{10}$$

The function $e_1(x) = 1 + O(x)$ defined this way is well behaved. The wanted generalization correcting the behaviour at small distances is then

$$u_{ij}(\mathbf{r}_{ij}, \mathbf{r}'_{ij}) = \int_0^1 d\alpha \frac{e_i e_j}{d_{ij}(\alpha)} \left[1 - \exp \left(-\frac{d_{ij}^2}{4\lambda_{ij}^2 \alpha(1-\alpha)} \right) \right]$$
$$+ \frac{e_i e_j}{\gamma_{ij} \lambda_{ij}} \int_0^1 \frac{d\alpha}{2\sqrt{\alpha(1-\alpha)}} e_1 \left(\frac{d_{ij} \gamma_{ij}}{2\lambda_{ij}\sqrt{\alpha(1-\alpha)}} \right), \tag{11}$$

where $\gamma_{ij}(T)$ is the correction parameter defined in the previous section. Spin and symmetry effects may be included by certain combinations of the expressions given above [14]. The results for the improved off-diagonal Kelbg potential (11) (IODKP) are shown in figure 3 with the open circles. The splitting of the integral into two parts and correction of the second term by the temperature-dependent parameter $\gamma_{ij}(T)$ extends the applicability of the perturbation expression (8) to rather low temperatures, e.g. $T = 31\,250$ K, corresponding to the ground state of the hydrogen atom. As one can see from figure 3, even at this temperature the deviations from the exact result are quite small. At temperatures higher than $T = 250\,000$ K the agreement is excellent and all angular dependences of the off-diagonal potential are reproduced.

4. Applications of Kelbg-type effective potentials

Effective potentials found their main application in the field of equilibrium statistics [4]. The original idea due to Morita (1959) was to express the diagonal density matrix in the form of Boltzmann factors with two-particle, three-particle, etc, effective potentials. The advantage of this procedure is that the calculation of the partition function may be reduced to a purely classical problem including, however, many-particle interactions [4]. On the other hand, a well-known disadvantage of this method is that several many-particle effects, such as exchange and bound state effects, are not easily described. Most successful applications were given in the field of analytical thermodynamics. By means of cluster expansions exact virial expansions for the thermodynamic functions of quantum plasmas could be found up to the order $n^{5/2}$ in the density [2–4]. Since the convergence of this series is poor, the range of validity was extended by Padé methods. The available Padé formulae are widely used in applications in plasma and astrophysics. Recently good agreement of the Padé formulae with path integral Monte Carlo (PIMC) calculations has been shown [17, 18].

Let us discuss now the applications of effective potentials within the PIMC method, which is a new promising field of computational physics [17–19]. As is well known, PIMC calculations are based on the high-temperature approximations for the density-matrix and the Trotter–Feynman expansions of the exponential operator. This way we need for applications good expressions for the high-temperature density matrices, and in particular the off-diagonal elements. This is just the point where the formulae expressing the density matrix by effective potentials come into play. This procedure very much improves convergence and provides effective calculations.

Let us now discuss the applications of effective potentials to molecular dynamics simulations. We mentioned already the pioneering work of Hansen *et al* [11]. More recent MD simulations have shown that the use of Kelbg-type effective potentials provides good thermodynamic functions, correlation functions, microfield distributions and, to some extent, also non-equilibrium properties [20–26].

5. Time-dependent effective potentials

The basic idea of using effective potentials is to condense all quantum properties of the particles into some constant parameters, while their dynamics is traced according to classical equations of motion. Generally, the respective parameters depend on the macroscopic state of the system, such that every particle produces the same effective potential. While this concept is very successful in describing certain equilibrium aspects of strongly coupled plasmas, it is not well suited to study properties such as velocity distributions, velocity correlations, transport properties or non-equilibrium processes.

On the other hand, we have seen above that there is a strong analogy between the effective potentials and the resulting interactions between Gaussian wave packets (see equation (9)). In fact the time evolution of such wave packets (WPs) can be obtained from classical equations of motion by employing the variational formulation of the Schrödinger equation. This concept of a wave packet-molecular dynamics (WPMD), originally developed by Heller [27], has been successfully applied for a number of applications ranging from collision processes in nuclear physics [28] over atomic strong-field dynamics [29] to the description of dense plasmas [30]. Generally, one starts with a proper parametrization of the many-body wave function $\psi(\{\mathbf{r}_i\}, \{q_j\})$, where the dynamics of the parameters q_i is determined from the Dirac–Frenkel–McLachlan form of the Schrödinger equation [32]

$$\delta \int_{t_1}^{t_2} \langle \psi | \mathrm{i}\hbar \frac{\partial}{\partial t} - \hat{H} | \psi \rangle \, \mathrm{d}t = 0. \tag{12}$$

After some algebra evaluation of equation (12) leads to the following equations of motion for the parameters

$$\frac{\partial H}{\partial q_i} = \sum_j \mathcal{N}_{ij} \dot{q}_j, \qquad \mathcal{N}_{ij} = 2 \operatorname{Im} \left[\left\langle \frac{\partial \psi}{\partial j} \middle| \frac{\partial \psi}{\partial i} \right\rangle \right], \tag{13}$$

with $H = \langle \psi | \hat{H} | \psi \rangle$ being the expectation value of the Hamiltonian operator. We represent here the N-particle wave function by the following product state

$$\psi = \prod_{i=1}^{N} \phi_i,$$
$$\phi_i = \left(\frac{3}{2\pi \beta_i} \right)^{3/4} \exp\left(-\left(\frac{3}{4\beta} + \mathrm{i}p_\beta \right)(\mathbf{x}_i - \mathbf{r}_i)^2 + \mathrm{i}\frac{d}{\beta}(\mathbf{x}_i - \mathbf{r}_i)^4 - \mathrm{i}\mathbf{p}_i(\mathbf{x}_i - \mathbf{r}_i) \right) \tag{14}$$

of single particle WPs ϕ_i.[5] Here $\mathbf{r}_i$ and $\mathbf{p}_i$ parametrize the position and momentum of the WP centre, while β_i and p_{β_i} denote the WP width and its corresponding momentum. In difference to the standard ansatz [30] we included an additional constant phase shift $\mathrm{i}d(\mathbf{x}_i - \mathbf{r}_i)^4/\beta$, which will help us to treat several principal problems. The major benefit of the ansatz is that it results in Hamiltonian equations for the conjugated pairs $(\mathbf{r}_i, \mathbf{p}_i)$ and (β_i, p_{β_i}) with the effective Hamiltonian H.

The standard ansatz (equation (14) with $d = 0$) appears to provide a semiclassical description of the particle dynamics; however, the classical high-temperature limit, namely a strong narrowing of the individual WPs, cannot be recovered with such WPMD simulations. In fact, the divergence of the WP width not only leads to a divergent partition sum in parameter space but also causes technical problems in numerical plasma simulations even at finite temperatures. This is, in fact, not surprising as freely propagating WPs spread without bounds, while the transition to classical behaviour results from localization effects due to

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[5] Exchange effects may be taken into account by using a properly symmetrized wave function [30].
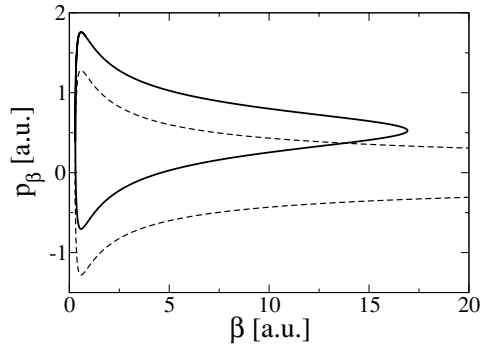
Figure 4. Phase-space trajectories of the WP width parameters, for $\alpha = 0$ (dashed line) and $\alpha = 1$ au (solid line). Atomic units are used.

decoherences caused by environmental influences. Despite the ongoing discussion about the way of extracting thermodynamic properties from time averages of quantum mechanical time evolution in a restricted trail space, WPMD simulations have been successfully applied to describe the statistical properties of strongly coupled plasmas [30, 33, 34], as long as the problem of a diverging WP width has been avoided. Thereby different ideas, such as fixing β at some value or assuming an adiabatic dynamics for the WP width, have been employed [29–31]. We may show that fixing the width by means of the thermal wavelength $\beta \propto \lambda^2$ leads us back to the previous approximation equation (9). Alternatively, we multiplied here (see equation (14)) the trail state by the additional phase factor $\exp[-\mathrm{i}d(\mathbf{x}_i - \mathbf{r}_i)^4/\beta]$ in order to model localization effects. It is important to note that the inclusion of this phase factor preserves the Hamiltonian character of the underlying equations of motion. However, the substitution of this ansatz results in a new effective Hamiltonian

$$H = \sum_i H_i + \sum_{i<j} V_{ij}, \qquad H_i = \frac{p_i^2}{2m} + \frac{\hbar^2}{m}\left(\frac{9}{8\beta_i} + 2\beta_i p_{\beta i}^2 + \frac{280}{9}d^2\beta_i - \frac{40}{3}d\beta_i P_{\beta_i}\right), \quad (15)$$

$$V_{ij} = \frac{e^2}{r_{ij}}\,\mathrm{erf}\left(\sqrt{\frac{3}{2(\beta_i + \beta_j)}}r_{ij}\right). \tag{16}$$

The effective interaction potential V_{ij} does not depend on the new phase factor α. Instead of fixing $\beta \propto \lambda^2$ which would lead us back to equation (9), we use here the full dynamics of $\beta(t)$. We note that our phase factor d is closely related to the procedure proposed in [30, 31].

As illustrated in figure 4, the additional phase factor causes the width to prescribe closed trajectories, even in the case of free particles. Therefore the resulting parameter-space partition sum of free particles is indeed finite

$$Z_p = \frac{\pi^2}{\alpha}\Lambda^{-5}\exp\left(-\frac{3\hbar^2\alpha}{mk_B T_p}\right), \tag{17}$$

where $\alpha = \sqrt{40}d/3$, $\Lambda = h/\sqrt{2\pi mk_B T_p}$ denotes the thermal wavelength and T_p is the temperature in the parameter space. Note that this temperature does not provide a unique measure of thermodynamic properties as it depends on the particular choice of the trail wave function ψ. However, from the correct quantum mechanical entropy one can find a relation

between T_p and the physical system temperature T, resulting in an average WP width of

$$\langle \beta \rangle = \frac{3}{4\alpha} \left(1 + \frac{mk_B T}{3\hbar^2 \alpha} \right). \tag{18}$$

From comparison of equation (16) with equation (9) one finds that $\langle \beta \rangle = 3\hbar^2/(mk_B T)$, which finally leads to the desired result

$$\alpha = \frac{(3 + \sqrt{89})}{40} \frac{mk_B T}{\hbar^2} \approx 0.31\lambda^{-2}, \tag{19}$$

ensuring the correct high-temperature limit of the system in thermodynamic equilibrium.

Finally, we would like to note that the problem of the diverging WP width can be directly overcome by starting from a density matrix description rather than propagating the individual wave function of the system and doing the averaging afterwards. As shown in [35], a Gaussian ansatz for the equilibrium density matrix together with the corresponding variational principle leads to promising results for equilibrium properties of strongly coupled plasmas and at the same time reproduces the known high temperature limit. An extension of this idea to dynamical processes, based on the time-dependent variational principle as presented in [27], may thus allow the study of more complex non-equilibrium situations without employing any additional constraints. This is however beyond the scope of the present paper and may be the subject of future work.

6. Conclusions

The method of effective potentials is nowadays a well-established tool in the theory of dense quantum plasmas; we extended the method here to non-diagonal contributions. In combination with quantum Monte Carlo methods this approach describes thermodynamic properties and spatial correlations in strongly coupled Coulomb systems quite well. In order to describe dynamical processes like transport phenomena, potentials with time-dependent parameters are required. We have discussed how these potentials may be introduced from wave packet methods and demonstrated how best agreement with the Kelbg-type potentials can be obtained.

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