Comparison of second-order impact line shifts

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The second-order impact shifts in hydrogen obtained from the Baranger formalism are compared with those from a kinetic theory approach. The resulting $\Delta n=0$ contributions to the shift from the two theories are shown to be identical, except for the neglect of electron-electron correlations in the Baranger formalism. It is also shown that some care is required in taking the classical limit for the perturbing electrons, or else the shift from $\Delta n=0$ interactions vanishes.

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I. INTRODUCTION

The possibility that a plasma may cause a shift in spectral lines has been a long-standing topic of interest. The line shift is of fundamental importance since it involves many-body aspects of the line-shape theory due to interactions between the radiator and the plasma. According to semiclassical estimates [1–3], the major contribution to the small shifts of hydrogen and singly ionized helium lines is from collisional interactions with plasma electrons. However, these estimates were based on a second-order, semiclassical, impact-parameter method [4], and such calculations are very dependent on the strong-collision cutoff procedure [3,5]. Consequently, the semiclassical estimates are subject to theoretical uncertainties.

Recently, shift calculations with a quantum-mechanical-impact approximation including higher-order terms have been reported [6–8]. These calculations utilized the formalism developed by Baranger [9], and essentially confirm, for temperatures of interest, the most recent semiclassical results [3]. However, there is some question concerning the physical meaning and significance of the agreement. In particular, it is not clear whether contributions to the shift involving $\Delta n=0$ interactions (i.e., interactions not accompanied by changes in the principal quantum number) are correctly accounted for in the various calculations.

For example, using a kinetic theory approach [10], it was shown that the $\Delta n=0$ contribution to the net shift in hydrogen is comparable to the $\Delta n\neq 0$ contribution [3]. However, earlier calculations [1,2] did not include this term since the perturber ensemble average exactly vanishes for a classical electron gas [4,10]. Furthermore, the Baranger formalism factorizes the density operator, while the kinetic theory approach formally retains correlations between the radiator and plasma.

The purpose of the present Brief Report is to examine the connection between the shifts in the Baranger formalism and the kinetic theory. Only shifts from the $\Delta n=0$ terms in hydrogen are considered and then only to second order in the atom-electron interaction in the impact approximation. Furthermore, the lower state broadening and level splitting due to the ion microfields are neglected.

II. THEORY

Consider Baranger's expression for the shift caused by electron impacts for an upper atomic state $|\mu\rangle$ (in units with $\hbar=1$) [9],

$$d_\mu=-\frac{2\pi N}{m}\mathrm{Re}[f_\mu(0)]_{\mathrm{avg}} . \tag{1}$$

Here, N is the perturbing electron density, $f_\mu(0)$ is the elastic forward-scattering amplitude for an electron and hydrogen atom in state $|\mu\rangle$, and $[\ ]_{\mathrm{avg}}$ denotes an ensemble average over the perturbing electron gas. That is,

$$[\ ]_{\mathrm{avg}}=\frac{1}{(2\pi)^3}\int \mathbf{dp}\phi(\mathbf{p})(\ ) , \tag{2}$$

where $\phi(\mathbf{p})$ is the one-electron momentum distribution normalized to unity. Expansion of Eq. (1) to second order in the atom-electron interaction leads to

$$d_\mu^{(2)}=\mathrm{Re}[N\langle\mu|V(\mathbf{k}=0)|\mu\rangle] -N\frac{1}{(2\pi)^3}\int \mathbf{dk}\, D_{\mu\mu}(\mathbf{k}) \times\frac{1}{(2\pi)^3}\int \mathbf{dp}\, P\left[\frac{\phi(\mathbf{p})}{E(\mathbf{p}+\mathbf{k})-E(\mathbf{p})}\right] , \tag{3}$$

where P denotes the principal part, and $E(\mathbf{p})$ is the energy of the perturbing electron in a plane-wave state of momentum $\mathbf{p}$. The matrix element $D_{\mu\mu}(\mathbf{k})$ is defined by

$$D_{\mu\mu'}(\mathbf{k})=\sum_{\mu''}\langle\mu|V(\mathbf{k})|\mu''\rangle\langle\mu''|V(-\mathbf{k})|\mu'\rangle , \tag{4}$$

where the atomic states are restricted to having the same principal quantum number, and $V(\mathbf{k})$ is the atom-

electron interaction in Fourier-transform space with $\mathbf{k}$ the electron momentum transfer variable. Note that the first term in Eq. (3) is identical to Eq. (2.12) of Ref. [10] (with no lower state broadening) and vanishes for neutral radiators.

The ensemble average (integral over $\mathbf{p}$) in Eq. (3) may be rewritten using the isotropy of $\phi(\mathbf{p})$ and $E(\mathbf{p})$ and the relation

$$\phi(\mathbf{p})-\phi(\mathbf{p}+\mathbf{k}) = \phi(\mathbf{p})(1-\exp\{-\beta[E(\mathbf{p}+\mathbf{k})-E(\mathbf{p})]\}) \quad (5)$$

(valid for both the quantum and classical electron gas) to obtain

$$\frac{1}{(2\pi)^3}\int d\mathbf{p}\, P\left[\frac{\phi(\mathbf{p})}{E(\mathbf{p}+\mathbf{k})-E(\mathbf{p})}\right]=\frac{1}{2}\frac{1}{(2\pi)^3}\int d\mathbf{p}\,\phi(\mathbf{p})\left[\frac{1-\exp\{-\beta[E(\mathbf{p}+\mathbf{k})-E(\mathbf{p})]\}}{E(\mathbf{p}+\mathbf{k})-E(\mathbf{p})}\right]\approx\frac{\beta}{2}\ , \quad (6)$$

where β^{-1} is the temperature, which, for cases of interest, is large compared to the electron-energy difference, thus allowing the expansion of the exponential. Substitution of Eq. (6) into Eq. (3) yields

$$d_\mu^{(2)}=-\frac{N\beta}{2}\frac{1}{(2\pi)^3}\int d\mathbf{k}\, D_{\mu\mu}(\mathbf{k})\ . \quad (7)$$

The result in Eq. (7) does not vanish and is identical to Eq. (2.25) of Ref. [10] if electron-electron correlations in the latter are neglected [set $S(k)=1$]. Recall that electron-electron correlations are not included in Eq. (1) above [9].

III. COMMENTS

The discussion above presents an explicit comparison of the second-order, impact-approximation shifts from the Baranger formalism to those from a kinetic theory approach. It was shown that for the $\Delta n=0$ interactions both approaches yield identical results (neglecting electron-electron correlations).

It is important to note that the asymmetry of the electron ensemble average in Eq. (6) due to detailed balance must be retained in order to obtain a nonzero result. For example, if the classical limit is taken prematurely in Eq. (6), then [10]

$$d_\mu^{(2)}\to 0\ , \quad (8)$$

which erroneously neglects a significant contribution to the shift [3]. The asymmetry has a simple interpretation. In a collision the perturbing electron may give or receive energy from the radiator. However, for the colliding electron to give energy, it must possess it, thus introducing the Boltzmann factor involving the energy difference in Eq. (6). While the discussion here has been limited to second order, the same physics should still be present in an all-order calculation. That is, the perturber ensemble average must satisfy the detailed balance condition.

Finally, the results above show that a calculation of the Baranger expression for the impact shift does not require any corrections due to factorizing the density matrix, at least to second order in the radiator-perturber interaction. The agreement is due to the impact limit, since only for these infinite times does the system lose memory of the initial conditions. Interestingly, Blaha and Davis [6] examined the $\Delta n=0$ contribution to the shift in He^+ and found their answer to be only about 30% smaller than the semiclassical result [3]. Similar comparisons using the strong-coupling method [7,8] should prove interesting.

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[1] H. R. Griem, Phys. Rev. A **27**, 2566 (1983).
[2] H. R. Griem, Phys. Rev. A **28**, 1596 (1983).
[3] H. R. Griem, Phys. Rev. A **38**, 2943 (1988).
[4] H. R. Griem, *Spectral Line Broadening by Plasmas* (Academic, New York, 1974).
[5] C. A. Iglesias, D. B. Boercker, and R. W. Lee, Phys. Rev. A **32**, 1906 (1985).
[6] M. Blaha and J. Davis, Phys. Rev. A **41**, 6928 (1990).
[7] K. Unnikrishnan, J. Callaway, and D. H. Oza, Phys. Rev. A **42**, 6602 (1990).
[8] K. Unnikrishnan and J. Callaway, Phys. Rev. A **43**, 3619 (1991).
[9] M. Baranger, Phys. Rev. **112**, 855 (1958).
[10] D. B. Boercker and C. A. Iglesias, Phys. Rev. A **30**, 2771 (1984).